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

**Sponsors**
ASMS gratefully acknowledges the support of these companies.

**Waters**
THE SCIENCE OF WHAT’S POSSIBLE.”
Mobile App and WiFi

**Sciex**
Opening Reception

**Agilent Technologies**
Webcasting

**Shimadzu**
Excellence in Science
Closing Event

**Bruker**
Conference Sponsor

**Contributors**
Advanced Energy
ETP Electron Multipliers
Fluid Management Systems
IDEX Health & Science
Microliter Analytical Supplies
(A WHEATON Company)
New Objective
Pall Laboratory
Thermo Fisher Scientific
Zef Scientific

**Table of Contents**

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Information</td>
<td>2</td>
</tr>
<tr>
<td>Hotels</td>
<td>5</td>
</tr>
<tr>
<td>ASMS Board of Directors</td>
<td>6</td>
</tr>
<tr>
<td>Interest Groups and Committees</td>
<td>7</td>
</tr>
<tr>
<td>Awards</td>
<td>8</td>
</tr>
<tr>
<td>Convention Center Floor Plans</td>
<td>11</td>
</tr>
<tr>
<td>Corporate Hospitality Suites</td>
<td>13</td>
</tr>
<tr>
<td>ASMS Corporate Members</td>
<td>14</td>
</tr>
<tr>
<td>Program Acknowledgements</td>
<td>19</td>
</tr>
<tr>
<td>Program Overview</td>
<td>20</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Day</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sunday</td>
<td>25</td>
</tr>
<tr>
<td>Monday Oral Sessions</td>
<td>25</td>
</tr>
<tr>
<td>Monday Workshops</td>
<td>32</td>
</tr>
<tr>
<td>Tuesday Oral Sessions</td>
<td>34</td>
</tr>
<tr>
<td>Tuesday Workshops</td>
<td>40</td>
</tr>
<tr>
<td>Wednesday Oral Sessions</td>
<td>42</td>
</tr>
<tr>
<td>Wednesday Workshops</td>
<td>48</td>
</tr>
<tr>
<td>Thursday Oral Sessions</td>
<td>50</td>
</tr>
<tr>
<td>Poster Overview</td>
<td>57</td>
</tr>
<tr>
<td>Monday Posters</td>
<td>59</td>
</tr>
<tr>
<td>Tuesday Posters</td>
<td>93</td>
</tr>
<tr>
<td>Wednesday Posters</td>
<td>129</td>
</tr>
<tr>
<td>Thursday Posters</td>
<td>162</td>
</tr>
<tr>
<td>Index of Authors</td>
<td>195</td>
</tr>
</tbody>
</table>
**GENERAL INFORMATION**

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

**ATTENTION UNDERGRADUATE STUDENTS AND FIRST TIME (AT ASMS) GRADUATE STUDENTS**
4:00 - 5:00 pm, Sunday, Stars Ballroom 1, level 3
Plan Your Strategy: What to See and Do at ASMS

**SUNDAY TUTORIAL SESSION, 5:00 - 6:30 PM**
Hall 1, level 1
5:00 - 5:45 pm
Forensic Mass Spectrometry
#TellMeSomethingIDontKnow

Facundo Fernandez
Georgia Institute of Technology

Glen Jackson
West Virginia University

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

Lars Konermann
University of Western Ontario

**SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM**
Hall 1, level 1

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

A Molecular Arsenal Against Ebola Virus
Erica Ollmann Saphire
The Scripps Institute-La Jolla

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

**PLENARY SESSIONS**

**MONDAY AWARD LECTURE, 4:45 - 5:30 PM**
Hall 1, level 1

Award for a Distinguished Contribution in Mass Spectrometry
Scott A. McLuckey
Purdue University

**TUESDAY AWARD LECTURE, 4:45 - 5:30 PM**
Hall 1, level 1

Biemann Medal
Kristina Häkansson
University of Michigan

**THURSDAY PLENARY LECTURE, 4:45 - 5:30 PM**
Hall 1, level 1

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

**DON'T MISS**

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

• **CLOSING EVENT, THURSDAY, 6:30 - 9:00 PM**
Briscoe Western Art Museum
Let's celebrate! Stroll to the Briscoe for a western barbecue under the live oak trees of the terrace overlooking the San Antonio Riverwalk. View the exhibits which preserve and interpret the art, history, and culture of the American West. The evening continues with music, dancing and karaoke. Ticket is required, $30.
Oral Sessions are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

Level 1
Session A (MOA, TOA, WOA, ThOA) ..................... Hall 1

Level 2
Session B (MOB, TOB, WOB, ThOB) ..................... Room 221

Level 3
Session C (MOC, TOC, WOC, ThOC) ..................... Stars 1
Session D (MOD, TOD, WOD, ThOD) ..................... Stars 2-3
Session E (MOE, TOE, WOE, ThOE) ..................... Stars 4
Session F (MOF, TOF, WOF, ThOF) ..................... Hemisfair 3
Session G (MOG, TOG, WOG, ThOG) ..................... Hemisfair 2
Session H (MOH, TOH, WOH, ThOH) ..................... Hemisfair 1

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

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

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

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

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

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

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

Poster Authors must be present at posters on scheduled days at these times:
- 10:30 am - 1:00 pm, Odd-numbered posters
- 12:00 - 2:30 pm, Even-numbered posters

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

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

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

Exhibitors must staff exhibit booths as follows:
- Sunday Reception 7:45 pm - 9:00 pm
- Monday - Thursday 10:30 am - 2:30 pm

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

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

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

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

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

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

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

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

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

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

Single Use/Family Restrooms are available on each level.

Mother’s Room is Room 215 (for mothers only). From the Ballroom Level proceed to the Hemisfair Ballroom foyer and take escalators down. Room 215 is on the right side of the foyer space.
**Corporate Breakfast Seminars** are located in the convention center and at the Grand Hyatt. Reservations are required and may be made at company exhibit booths.

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

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

**Conference Regulations**

- **Name badge is required** for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- **No smoking** is permitted in the convention center.
- **All devices** must be silenced and screens darkened in oral sessions.
- **No photography** or recording is allowed in oral sessions or in the poster/exhibit Hall.
- **Parents**. Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices for child transport are prohibited in the Poster/Exhibit Hall and hospitality suites.
- **Material presented or displayed** at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without express written authority of the author.
- **The placement of advertising** in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.
- **Hardware, accessories or any items for sale** may be displayed only in corporate exhibit booths and hospitality suites.
- **Designated publisher tables** in the conference registration area are for the display of books and journals and must be reserved in advance.
- **There are tables in the registration area for authors** who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.
- **No organized activities (even off-site)** other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- **Corporate hospitality suites** may be used during the daytime hours of 8:00 am – 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.
- **Corporate or institutional logos** on slides or posters may appear only one time in the presentation.
<table>
<thead>
<tr>
<th>Hotel</th>
<th>Telephone</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Convention Center</td>
<td>(210) 207-8500</td>
</tr>
<tr>
<td>2. Crockett Hotel</td>
<td>(210) 225-6500</td>
</tr>
<tr>
<td>3. Drury Inn &amp; Suites Riverwalk</td>
<td>(210) 212-5200</td>
</tr>
<tr>
<td>4. Emily Morgan</td>
<td>(210) 225-5100</td>
</tr>
<tr>
<td>5. Fairfield Inn &amp; Suites</td>
<td>(210) 212-6262</td>
</tr>
<tr>
<td>6. Grand Hyatt San Antonio</td>
<td>(210) 224-1234</td>
</tr>
<tr>
<td>7. Hilton Palacio del Rio</td>
<td>(210) 222-1400</td>
</tr>
<tr>
<td>8. Homewood Suites by Hilton</td>
<td>(210) 222-1515</td>
</tr>
<tr>
<td>9. La Quinta Inn &amp; Suites</td>
<td>(210) 222-9181</td>
</tr>
<tr>
<td>10. Menger Hotel</td>
<td>(210) 223-4361</td>
</tr>
<tr>
<td>11. Marriott Rivercenter</td>
<td>(210) 223-1000</td>
</tr>
<tr>
<td>12. Marriott Riverwalk</td>
<td>(210) 224-4555</td>
</tr>
<tr>
<td>13. Springhill Suites San Antonio</td>
<td>(210) 222-2121</td>
</tr>
<tr>
<td>14. Westin Riverwalk</td>
<td>(210) 224-6500</td>
</tr>
</tbody>
</table>
President
Jenny Brodbelt
University of Texas
Austin, TX

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University of Texas Health Science Center
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Member at Large for Publications
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Georgia Institute of Technology
Atlanta, GA

Member at Large for Digital Communications
Brian Searle
University of Washington
Seattle, WA

ConGRaTulaTIons
to these members who were elected to the ASMS Board

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Gainesville, FL

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LaJolla, CA

Staff
Judith A. Sjoberg, Executive Director
Jennifer Watson
Cindi Pettit, Lola Priest, Miquela Sena
Marin Walker, Brent Watson
### Interest Group Coordinators

<table>
<thead>
<tr>
<th>Interest Group</th>
<th>Coordinator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical Laboratory Managers</td>
<td>Brett Phinney, Aliss Chien</td>
</tr>
<tr>
<td>Bioinformatics for MS</td>
<td>Sangtae Kim, Meena Choi</td>
</tr>
<tr>
<td>Biotherapeutics</td>
<td>Damian Houde, Ashley Ruth</td>
</tr>
<tr>
<td>Clinical Chemistry</td>
<td>Tim Garrett, Brian Rappold</td>
</tr>
<tr>
<td>Data Independent Acquisition</td>
<td>Ludovic Gillet, Jarrett Egerton</td>
</tr>
<tr>
<td>Drug Metabolism &amp; Pharmacokinetics</td>
<td>Kevin Bateman, Philip Tiller</td>
</tr>
<tr>
<td>Energy, Petroleum &amp; Biofuels</td>
<td>Mark Barrow, Lateefah Stanford</td>
</tr>
<tr>
<td>Environmental Applications</td>
<td>Marc Engel, Chris Gill</td>
</tr>
<tr>
<td>Exposomics</td>
<td>David Balshaw, Anthony Macherone</td>
</tr>
<tr>
<td>Flavor, Fragrance and Foodstuff</td>
<td>Walter Hammock, David Schroeder</td>
</tr>
<tr>
<td>Forensics &amp; Homeland Security</td>
<td>Adam Hall, Guido Verbeck</td>
</tr>
<tr>
<td>FTMS</td>
<td>David Kilgour, Don Smith</td>
</tr>
<tr>
<td>Fundamentals</td>
<td>Alessandra Ferzoco, Michael Van Stipdonk</td>
</tr>
<tr>
<td>H/D Exchange, Covalent Labeling &amp; Cross Linking</td>
<td>Joshua Sharp, David Weis</td>
</tr>
<tr>
<td>Imaging MS</td>
<td>Vilmos Kertesz, Raf Van de Plas</td>
</tr>
<tr>
<td>Ion Mobility MS</td>
<td>Erin Baker, Stephen Valentine</td>
</tr>
<tr>
<td>Ion Trap MS</td>
<td>Daniel E. Austin, Zheng Ouyang</td>
</tr>
<tr>
<td>Lipids &amp; Lipodomics</td>
<td>Christer Esjing, Todd Mitchell</td>
</tr>
<tr>
<td>LC/MS Related Topics</td>
<td>Michael Bereman, Brent Dixon</td>
</tr>
<tr>
<td>Metabolomics</td>
<td>Andrew Patterson, Tim Garrett</td>
</tr>
<tr>
<td>Metal Ion Coordination Chemistry</td>
<td>Cheng Lin, Alex Shvartsburg</td>
</tr>
<tr>
<td>Oligonucleotides &amp; Nucleic Acids</td>
<td>Patrick Limbach, Laixin Wang</td>
</tr>
<tr>
<td>Pharmaceuticals</td>
<td>Christine Gu, Matthew Schenauer</td>
</tr>
<tr>
<td>Photoionization MS</td>
<td>Jack Syage, Ralf Zimmerman</td>
</tr>
<tr>
<td>Polymeric Materials</td>
<td>Stephen Rumbelow, Gyorgy Vas</td>
</tr>
<tr>
<td>Regulated Bioanalysis</td>
<td>Jian Wang</td>
</tr>
<tr>
<td>Undergraduate Research in MS</td>
<td>Elaine Marzluff, Megan Gessel</td>
</tr>
<tr>
<td>Young Mass Spectrometrists</td>
<td>Violet Lee, Kristin Wildsmith</td>
</tr>
</tbody>
</table>

### Committees

<table>
<thead>
<tr>
<th>Committee</th>
<th>Chair</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asilomar Conference (ACMS)</td>
<td>Sharon Pitteri, Matt Bush, Lingjun Li, Susan Weintraub</td>
</tr>
<tr>
<td>Corporate Liaison</td>
<td>Jack Henion, Susan Weintraub</td>
</tr>
<tr>
<td>Digital Communications</td>
<td>Brian Searle, Ashley Ruth, Bruce Pascal, Brett Phinney</td>
</tr>
<tr>
<td>Education</td>
<td>Igor Kaltashov, Allessandra Ferzoco, Damian Houde, Dasi Surendra, Susan Van Riper, Elizabeth Stenler</td>
</tr>
<tr>
<td>Nominating</td>
<td>Gary Glish, Ben Garcia, Michael Easterling, Ljiliana Pasa-Tolic, David Tabb</td>
</tr>
<tr>
<td>Publications</td>
<td>Facundo Fernandez, Lorna De Leoz, Leslie Hicks, Richard Perry, Will Thompson, Joseph Loo (ex officio)</td>
</tr>
<tr>
<td>Sanibel Conference</td>
<td>Erin Baker, Fanyu Meng, Victor Ryzhov, Patrick Griffin</td>
</tr>
</tbody>
</table>
AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2016 RECIPIENT: SCOTT A. MCLUCKEY

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

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

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

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

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

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

RON A. HITES AWARD

OUTSTANDING RESEARCH PUBLICATION IN JASMS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3

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


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

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

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

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

2016 POSTDOCTORAL AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3

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

John Cahill
Oak Ridge National Laboratory
Andrew DeBlase
Purdue University
Catherine Going
Stanford University
Pengyuan Liu
The Wistar Institute

2016 STUDENT AWARDS

AWARD PRESENTATION: ASMS MEETING, 4:45 PM WEDNESDAY, STARS BALLROOM 1, LEVEL 3

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

GRADUATE STUDENT AWARDS

Xibei Dang, Florida State University
Zachery Gregorich, University of Wisconsin-Madison
Nathan Hendricks, University of California, Riverside
Johanna Hofman, Max Planck Society
Ramsunder Iyer, University of Tennessee
Brent Kuenzi, University of South Florida
Anumita Saha-Shah, Indiana University
Stephen Sciuto, The University of Toronto
Candice Ulmer, University of Florida
Yeijing Weng, Chinese Academy of Sciences

UNDERGRADUATE STUDENT AWARDS

Willem Duckworth, Clarkson University
Carlo Eikani, Saint Mary's College of California
Matthew Kazaleh, University of Florida
Yekaterina Kori, University of Massachusetts Amherst
Rebecca Marin, Florida International University
Rachel Martini, University of Michigan
Evan Perez, Duquesne University
LEVEL 3 - BALLROOM LEVEL

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

Workshops, Breakfast Seminars
(Rooms 301 - 305)

LEVEL 2 - MEETING LEVEL

Sessions B (Room 221)

Workshops, Breakfast Seminars
(Rooms 220 - 225)

Speaker Room (Room 222)

LEVEL 1 - STREET LEVEL

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

Session A, Plenary
Sessions (Hall 1)

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

PROGRAM COMMITTEE

<table>
<thead>
<tr>
<th>Jon Amster</th>
<th>Asiri Galhena</th>
<th>Liljana Pasa-Tolic</th>
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<tbody>
<tr>
<td>Matthew Bernier</td>
<td>David Gaul</td>
<td>Dennis R. Phillips</td>
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<td>Sebastian Boecker</td>
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<td>Jessica Prenni</td>
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<td>Amanda Hummon</td>
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<td>Franklin E. Leach III</td>
<td>David Smalley</td>
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<td>Prabha Dwivedi</td>
<td>Ron Orlando</td>
<td>Kasi V. Somayajula</td>
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<td>David Fischler</td>
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<td>Molly Soper</td>
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<tr>
<td>Jay Fosythe</td>
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<td>Jeff Spraggins</td>
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PROGRAM ACKNOWLEDGEMENTS

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

SESSION CHAIRS

<table>
<thead>
<tr>
<th>Theodore Alexandrov</th>
<th>Livia D. Eberlin</th>
<th>Franklin E. Leach III</th>
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<tr>
<td>Daniel Amador-Noguez</td>
<td>Jim Edwards</td>
<td>Young Jin Lee</td>
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<td>Alison E. Ashcroft</td>
<td>Marc E. Engel</td>
<td>Jennifer Liu</td>
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<td>Silvia Balbo</td>
<td>Katherine L. Fiedler</td>
<td>Xiaowen Liu</td>
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<td>David M. Balshaw</td>
<td>John Froehlich</td>
<td>Ginger Milne</td>
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<td>Candice Bridge</td>
<td>Juan F. Garcia-Reyes</td>
<td>Catherine Minogue</td>
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<td>Corey D. Broeckling</td>
<td>Wendell P. Griffith</td>
<td>Nina Morgner</td>
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<td>Nicholas Brunelli</td>
<td>Patrick G. Hatcher</td>
<td>Amber L. Mosley</td>
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<td>Michael L. Heien</td>
<td>Christopher C. Mulligan</td>
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<td>Natalie Castellana</td>
<td>Shawna Hengel</td>
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<td>Matthew M. Champion</td>
<td>Martin F. Jarrod</td>
<td>Andrew K. Ottens</td>
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<td>Hilika Kenttamaa</td>
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<td>Paul Kowalski</td>
<td>Nichole Reisdorph</td>
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<td>W. Alexander Donald</td>
<td>Heather C. Kuiper</td>
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<tr>
<td>Ashok R. Dongre</td>
<td>Cris Lapthorn</td>
<td>Jinhua Ren</td>
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WORKSHOP ORGANIZERS

<table>
<thead>
<tr>
<th>Daniel Austin</th>
<th>Hongying Gao</th>
<th>Pat Limbach</th>
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<tr>
<td>Erin Baker</td>
<td>Fabio Garofolo</td>
<td>Elaine Marzluff</td>
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<td>Mark Barrow</td>
<td>Tim Garrett</td>
<td>Yehia Mechefre</td>
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<td>Megan Gessel</td>
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<td>Ludovic Gillet</td>
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<td>Michael MacCoss</td>
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<td>Mehdi Moini</td>
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<td>Valerie Gabelica</td>
<td>Violet Lee</td>
<td>Bindesh Shrestha</td>
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Workshop Organizers

<table>
<thead>
<tr>
<th>Alexandre A. Shvartsburg</th>
<th>Pat Limbach</th>
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<tr>
<td>Vincent Sica</td>
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<td>Bindesh Shrestha</td>
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### Saturday

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<tr>
<td>9:00 AM - 3:30 PM</td>
<td>Short Courses</td>
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<tr>
<td>1:00 - 5:00 PM</td>
<td>Registration</td>
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### Sunday

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

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

### Tuesday

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

#### WEDNESDAY

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

**Thursday**

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

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

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

5:00 – 5:45 pm
Forensic Mass Spectrometry
#TellMeSomethingIDontKnow
Facundo Fernandez
Georgia Institute of Technology

Glen Jackson
West Virginia University

5:45 – 6:30 pm
An Analyte’s Journey from Solution into the Gas Phase
Lars Konermann
University of Western Ontario

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

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

A Molecular Arsenal Against Ebola Virus
Erica Ollmann Saphire
The Scripps Institute-La Jolla

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

MONDAY MORNING ORAL SESSIONS

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

MOA am 08:30
Mechanistic Studies of Hafnocene Catalyzed Olefin Polymerization; Anthony Paul Gies1; Roger Kuhlman2; Cristiano Zuccaccia3; Alceo Machioni2; Dow Chemical Company; Freeport, TX; Univation Technologies, Freeport, TX; Dipartimento di Chimica, Biologia e Biotecnologie and CIRCC, University of Perugia, Perugia, Italy

MOA am 08:50
Analytical Characterization of PEG and PEG conjugates by Mass Spectrometry; Guanghui Han1; Wilson Phung1; Whitney Shatz2; Julie Q. Hang3; Justin Scheer4; Paul Schnier4; Wendy Sandov1; Genentech Inc, South San Francisco, CA

MOA am 09:10
The Use of Iodo-functionalized Polydisperse Polymers as Mass-defect Tuned Calibrants; Joseph A. Giesen1; Jennifer L. Marple1; Scott M. Grayson1; Tulane University, New Orleans, LA

MOA am 09:30
Sequence and Conformational Analysis of Recombinant Polypeptide-Polymer Conjugates; Sahar Sallam1; Bradford A Paik2; Xinqiao Jia2; Chrys Wesdemiotis1; The University of Akron, Akron, OH; University of Delaware, Newark, DE

MOA am 09:50
Using MS/MS to Design Information-Encoded Synthetic Copolymers; Laurence Charles1; Jean-François Lutz2; Aix-Marseille University, Marseille

Cedex 20, PACA; 1Institut Charles Sadron, Strasbourg, France

Peptoid Fragmentation -The Bias toward Y-Ion Formation; Jianhua Ren1; Yuan Tian2; Ekram Hossain3; Michael Connolly4; Ronald Zuckermann4; University of the Pacific, Stockton, CA; University of the Pacific, Stockton, CA; Lawrence Berkeley National Laboratory, Berkeley, CA

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

MOB am 08:30
Preparation of a Dianion with the Highest Known Proton Affinity: Ortho-Diethynyl Benzene; Berwyck Poad1; Nicholas Reed2; Christopher Hansen3; Adam Trevitt3; Stephen J. Blanksby4; Emily Mackay5; Michael Sherburn5; Bun Chant6; Leo Radom7; Queensland University of Technology, Brisbane, Australia; University of Wollongong, Wollongong, Australia; Australian National University, Canberra, Australia; The University of Sydney, Sydney, Australia

MOB am 08:50
Evaluating Gas-Phase Folding of Protein Ions Using Cation to Anion Proton Transfer; Kenneth J. Laslo4; Eleanor B. Munger4; Stephanie C. Heard5; Matthew F Bush6; University of Washington, Seattle, WA; Kalamazoo College, Kalamazoo, MI
8:30-10:30 am MONDAY

INSTRUMENTATION: FTMS
Hilikka Kenttamaa (Purdue University)
Stars Ballroom 2-3, level 3

MOD am 08:30
New Gated Approach for Coupling Trapped Ion Mobility Spectrometry to Fourier Transform Ion Cyclotron Mass Spectrometry; Mark Ridgeway¹; William Danielson²; Jeremy Wolf³; Melvin Park⁴
¹Bruker Daltonic, Billerica, MA; ²Danielson Software Consulting, Richland, WA

MOD am 08:50
Multi-CRAFTI: Simultaneous Measurement of Relative Collision Cross Sections for Multiple Ions Measured using Fourier Transform Ion Cyclotron Resonance Linewidths; David V. Dearden¹; Anupriya Anupriya¹; ¹Brigham Young University, Provo, UT

MOD am 09:10
21 Tesla FT-ICR Mass Spectrometer for Ultrahigh Resolution Analysis of Complex Mixtures; Donald F. Smith¹; David C. Podgorski²; Yuri E. Corio¹; Christopher L. Hendrickson¹; ¹National Magnetic Field Laboratory, Tallahassee, FL; ²Future Fuels Institute, FSU Tallahassee, FL

MOD am 09:30
Surface Induced Dissociation (SID) of Protein Complexes in a Hybrid FT-ICR; Jing Yan¹; Mowei Zhou²; Gilbert Joshua¹; Jeremy J. Wolff³; Randall E. Pedder⁴; Arpad Somogyi⁵; Royston S. Quintyn⁶; Lindsay Morrison⁷; Michael L. Easterling⁵; Ljiljana Pasa-Tolick³; Vicki H. Wysocki¹; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ³Bruker Corporation, Billerica, MA; ⁴Antara Technologies L.P., Ardana, PA; ⁵OSU Mass Spectrometry & Proteomics Facility, The Ohio State University, Columbus, OH

Construction of a Dual-Detector Fourier Transform Electrostatic Linear Ion Trap Utilizing In-Trap Potential Lift; Eric Dziekonski¹; Robert Santini²; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN

Amino Acid Separation using Different Drift Gases in an RF-Confining Drift Cell; Kimberly Davidson¹; Matthew F Bush¹; ¹University of Washington, Seattle, WA

8:30-10:30 am MONDAY

DIAGNOSTIC CLINICAL CHEMISTRY
Heather C. Kuiper (CDC)
Stars Ballroom 4, level 3

MOE am 07:50
Intraoperative Diagnosis of Gliomas using Desorption Electrospray Ionization Mass Spectrometry: A Review of Clinical Cases; Valentina Pirro¹; Alan K. Jarmsch¹; Zane R. Baird²; Clint Alfaro³; Eyas Hattab⁴; Aaron Cohen-Gadol⁵; Graham R Cooks³; ¹Purdue University, West Lafayette, Indiana; ²Purdue University, West Lafayette, IN; ³Indiana University School of Medicine, Indianapolis, IN

MOE am 08:50
DESI-MSI-based Diagnostics of Cirrhotic Liver Diseases; Anna Mroz¹; Francesca Rosini¹; Alex Pechilivian¹; Luisa Doria¹; Evaggelia Liaskou¹; Gideon Hirschfeld²; Simon Taylor-Robinson³; David Jones⁴; Robert Goldin⁵; Elaine Holmes⁶; Zoltan Takats³; ¹Imperial College London, London, United Kingdom; ²Deutsches Krebsforschungszentrum, Heidelberg, Germany; ³University of Manchester, Manchester, UK; ⁴University of Manchester, Manchester, Manchester;
⁵University of Wisconsin-Madison, Madison, WI; ⁶Michigan State University, East Lansing, MI

MOE am 08:30
Influence of Ion Clouds Micromotion on FTICR Mass-Spectrometer Performances in Ultrahigh Resolution Mode of Operation; Eugene Nikolaev¹; Gleb Vladimirov¹; Goekhan Baykut³; Roland Jertz³; ¹Institute for Energy Problems of Chemical Physics, Moscow, Russia; ²Skolkovo Institute of Technology, Moscow, Russia; ³Bruker Daltonic GmbH, Bremen, Germany

1University of Manchester, Manchester; 2University of Washington, Madison, WI; 3University of State, Richland, WA

MOD am 08:50
High-Throughput Screening Strategy for Tracking Synthetic Biology Variants Libraries using Robotic Platforms and Colormetric Assays Combined with Fast LC-IM MS; Gunda-Young¹; Martin Williams¹; Daniel F. McManus¹; ¹University of Michigan, Ann Arbor, MI

MOD am 08:50
Surface Induced Dissociation (SID) of Protein Complexes in a Hybrid FT-ICR; Bing Yan¹; Mowei Zhou²; Gilbert Joshua¹; Jeremy J. Wolff³; Randall E. Pedder⁴; Arpad Somogyi⁵; Royston S. Quintyn⁶; Lindsay Morrison⁷; Michael L. Easterling⁵; Ljiljana Pasa-Tolick³; Vicki H. Wysocki¹; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; ³Bruker Corporation, Billerica, MA; ⁴Antara Technologies L.P., Ardana, PA; ⁵OSU Mass Spectrometry & Proteomics Facility, The Ohio State University, Columbus, OH
8:30-10:30 am MONDAY

INFORMATICS: DISCOVERY PROTEOMICS

Xiaowen Liu (Indiana University)

Hemisfair Ballroom 3, level 3

MOF am 08:30

Enabling Massive Blind Database Search using Multiple Enzyme Proteomics: Laurence E. Bernstein1; Seungjin Na1; Nuno Bandeira2,3,4; 1University of California San Diego, San Diego, CA; 2Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; 3Computer Science and Engineering, University of California San Diego, La Jolla, CA; 4Skaggs School of Pharmacy, UC San Diego, La Jolla, CA

Embracing Complexity and Diversity: Discovery Metaproteomics of Multiple Microbiomes using the Galaxy Framework: Pratik Jagtap1; Brian Sandri1; Somaiah Afiuni-Zadeh1; Kevin Viken1; Kristin Boylan1; Jim Johnson1; Thomas F McGowan1; Maneesh Bhargava2; Chris Wendt1; Amy Skubitz1; Joel Rudney1; Tim Griffin1; 1Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN; 2University of Minnesota, Minneapolis, MN; 3University of Minnesota Supercomputing Institute, Minneapolis, MN

Maximizing Shotgun Proteomics Isobaric Tagging Data Output using MS/MS Multi-Objective Optimization Algorithm: John Corthesy1; Kostantinos Theofiliatos2; Seferina Mavroudis3,4; Ornella Cominetti1; Mona Remlawi1; Francesco Ferraro1; Antonio Núñez Galindo1; Ivan Montoliu1; Martin Kussmann1; Spiros Likothanassis5,6; Loïc Dayon1; 1Molecular Biomarkers Core, Nestlé Institute of Health Sciences, Lausanne, Switzerland; 2InSybio Ltd., London, United Kingdom; 3Department of Social Work, School of Sciences of Health and Care, Technological Educational Institute of Patras, Patras, Greece; 4Bio System Informatics, Nestlé Institute of Health Sciences, Lausanne, Switzerland; 5Department of Computer Engineering and Informatics of the University of Patras, Patras, Greece

MOG am 08:30

Automated Solid Phase Extractions Coupled with Ion Mobility-Mass Spectrometry Analyses Allow Rapid Metabolomic Screening of Complex Plasma and Urine Samples: Erin S. Baker1; Xing Zhang1; Xueyun Zheng1; Kristin E. Burnum-Johnson1; Jennifer E. Kyle1; Young-Mo Kim1; Erika M. Zink1; Matthew E. Monroe1; Yehia M. Ibrahim1; Daniel J. Orton1; Justin G. Teeguarden1; Thomas O. Yates III1; 1The Scripps Research Institute, La Jolla, CA; 2UCSD, La Jolla, CA; 3The Salk Institute, La Jolla, CA

Untargeted Profiling with Single-cell MS Uncovers Small-Molecule Cell Heterogeneity along the Left-Right Body Axis in the Frog Embryo: Rosemary Masu Onjiko1; Sydney E. Morris1; Sally A. Moody1; Peter Nemes1; 1Department of Chemistry, The George Washington University, Washington, DC; 2Department of Anatomy & Regenerative Biology, The George Washington University, Washington, DC

MOG am 08:50

Untargeted Profiling of FS-FTICR-MS Spectra of Culture Supernatants to Identify Known and Novel Natural Products and Their Biosynthetic Gene Clusters using a Metabologenomics Approach: Anthony Goering1; Ryan A. McClure2; James R. Doroghazi3; Kou-San Ju4; Jessica C. Albright1; Nicole A. Haverland1; 1Thermo Fisher Scientific, San Jose, CA; 2Battelle Memorial Institute, Columbus, OH; 3Center for Proteomics and Metabolomics, LUMC, Leiden, NL; 4Department of Medical Statistics, LUMC, Leiden, NL

8:30-10:30 am MONDAY

METABOLOMICS: UNTARGETED PROFILING

Corey D. Broeckling (Colorado State University)

Hemisfair Ballroom 2, level 3

MOG am 08:30

Real-Time Informatics: A Database Search Increases Depth and Accuracy of Isobaric Label Quantitation in Discovery Proteomics: Christopher Michael Rose1; Derek J. Bailey2; Joao Paulo3; Jeremy D O’Connel1; David P. Nusinov1; Joel M. Chick1; Steven P. Gygi1; 1Harvard Medical School, Boston, MA; 2Thermo Fisher Scientific, San Jose, CA

MOG am 08:50

An Informatic Framework for Defining Multi-Proteoform Complexes (MPCs) by Native Top-Down Mass Spectrometry: Nicole A. Haverland1; Owen S. Skinner1; Pierre C. Havugimana1; Luca Fornelli1; Bryan F. Early1; Joseph B. Greer1; Ryan T. Feilers1; Kenneth R. Durbin2; Luis H. F. Do Vale2; Rafael D. Melani1; Henriëtte S. Seckler1; Micah Nelp1; Richard D. LeDuc1; Vahe Bandarian3; Philip D. Compton1; Neil L. Kelleher1; 1Northwestern University, Evanston, IL; 2University of Brasilia, Brasilia, Brazil; 3University of Arizona, Tucson, Arizona

MOG am 09:00

TargetSeeker-MS: A Bayesian Inference Approach for Drug Target Discovery using Protein Fractionation Coupled to Mass Spectrometry: Mathieu Lavallée-Adam1; Alexander Pelleter2; 1Université de Montréal, Montreal, QC, Canada; 2Johnson & Johnson, New Brunswick, NJ

MOG am 09:10

MetaProteomics Increases Depth and Accuracy of Isobaric Label Quantitation in Discovery Proteomics: Christopher Michael Rose1; Derek J. Bailey2; Joao Paulo3; Jeremy D O’Connel1; David P. Nusinov1; Joel M. Chick1; Steven P. Gygi1; 1Harvard Medical School, Boston, MA; 2Thermo Fisher Scientific, San Jose, CA

MOG am 09:20

Metabolomics: Elemental Composition from Ultrahigh Resolution FT-ICR MS: Structure from Motion and Informatics of the University of Patras, Patras, Greece; 2University of Minnesota, Minneapolis, MN; 3The Salk Institute, La Jolla, CA

MOG am 09:30

High-Throughput Discovery of New Natural Products and Their Biosynthetic Gene Clusters using a Metabologenomics Approach: Anthony Goering1; Ryan A. McClure2; James R. Doroghazi3; Kou-San Ju4; Jessica C. Albright1; Nicole A. Haverland1; Yongbo Zhang2; Regan J. Thomson2; William W. Metcalf2; Neil L. Kelleher1; 1Northwestern University, Evanston, IL; 2University of Colorado, Denver, CO; 3The Scripps Research Institute, La Jolla, CA; 4Ohio State University, Columbus, OH
MONDAY MORNING ORAL SESSIONS

Chicago, IL; 1Northwestern University, Evanston, IL; 2University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

MOG am 09:50 Untargeted Stable-isotope Tracing of Folate-mediated 1-C Trafficking in Cancer Cells and an in vitro 3D model of Neural Tube Closure; Qiuying Chen1; Amanda K Vaughn2; John W Steel2; Robert M Cabrera2; Richard H Finnell1; Steven Gross1; 1Weill Medical College of Cornell, New York, NY; 2University of Texas at Austin, Austin, TX

MOG am 10:10 Integration of Personal Metabolome and other Omics: Application to the Onset of Type 2 Diabetes; Kevin Contrepois1; Michael Snyder2; 1Stanford University, Stanford, California; 2Stanford University School of Medicine, Palo Alto CA

8:30-10:30 am MONDAY
MEMBRANE PROTEIN MS

Nina Morgner (Johann Wolfgang Goethe-University)
Hemisfair Ballroom 1, level 3

MOH am 08:30 Ion Mobility-Mass Spectrometry Reveals the Stoichiometry and Structures of Lipid Bound Amyloidogenic Peptide Complexes within Nanodiscs; Richard A Kerr1; Jukyung Kang1; Anna Schwendeman1; Brandon T Ruotolo1; 1University of Michigan, Ann Arbor, MI

MOH am 08:50 Surface Induced Dissociation Provides Insight into Membrane Protein-Lipid Interactions; Sophie Harvey1, 2; Yang Liu1; Wen Liu2; Vicki Wysocki1; Arthur Laganowsky2; 1The Ohio State University, Columbus, Ohio; 2University of Manchester, Manchester, United Kingdom

MOH am 09:10 Identification and Characterization of Small Membrane Protein Complex Subunits Presenting Challenges for Routine Mass Spectrometric Analysis; Julian Langer1; Anja Resemann2; Martin Kohlstaedt1; Detlev Suckau1; Hartmut Michel1; 1MPI for Biophysics, Frankfurt Am Main, Germany; 2Bruker Daltonic GmbH, Bremen, Germany

MOH am 09:30 XL-FASP: A New Integrated Cross-Linking Workflow to Study Extra Large Membrane Protein Complexes; Martial Rey1; Eric Durand1; 1Institut Pasteur, Paris, France; 2Institut de Microbiologie de la Méditerranée, CNRS, Marseille, France; 3CNRS, Paris, France

MOH am 09:50 Top-down and Middle-down High-Resolution Mass Spectrometry of Lipidated Proteins; Julian Whitelegge1; Joseph Capri1; Whitaker Cohn1; Don Pupccione1; Pasqual Liaux2; Frederic Halgand2; 1University of California, Los Angeles Los Angeles, CA; 2Ruhr University Bochum, Bochum, Germany; 3University Paris Sud, Orsay, France

MOH am 10:10 Monitoring the Dynamic N-linked Cell Surface Glycoproteome by Quantitative Proteomics; Christian Eberl1; Mathias Kalkdorf1; Stephan Gade1; Marcus Bantscheff1; 1Cellzome GmbH a GSK company, Heidelberg, Germany

10:30 AM – 2:30 PM, MONDAY
MONDAY POSTER SESSION

Poster/Exhibit Hall
Lunch Concessions are open 11:00 am - 2:00 pm
Odd-number posters present 10:30 am - 1:00 pm
Even-number posters present 12:00 - 2:30 pm

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

2:30-4:30 pm MONDAY

FOOD SAFETY AND CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS
Katherine L. Friedler (U.S. FDA)
Hall 1, level 1

MOA pm 02:30 Analyses of Human Milk Oligosaccharides
Discover Factors that Enhance and Diminish Infant Growth; Jasmine C. C. Davis1; Sarah Totten1; Lauren D. Wu1; Sridevi Krishnan1; Mark R. Charbonneau1; Michael J. Barratt1; Jeffrey I. Gordon1; Angela M. Zivkovic1; Carlito B Lebrilla1
1University of California, Davis, Davis, CA; 2Stanford University School of Medicine, Palo Alto CA; 3Washington University in St. Louis, St. Louis, MO

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

MOA pm 03:30 Chemical Changes in a Gamma Ray-irradiated Rodent Diet Revealed by nanoLC-MS/MS; Jeevan K Prasain1; Landon Wilson1; Clinton J Grubbs1; Stephen Barnes2; 1University of California, Davis, Davis, CA; 2University of Washington School of Medicine, Traverse City, MI

MOA pm 04:10 Forensic Analysis of a Mass Poisoning in Mozambique Associated with a Homebrewed Beverage using LC-HRAM MS and DART-MS; Sara Kern1; Travis M. Falconer2; Jennifer L Brzezinski1; Brian L Boyd1; James A Turner1; Jonathan J Litza2; 1US FDA, Cincinnati, OH; 2Ultraspec LLC, Columbia, MD

2:30-4:30 pm MONDAY

FUNDAMENTALS: ION SPECTROSCOPY
Thomas Rizzo (École Polytechnique Fédérale de Lausanne (EPFL))
Room 221, level 2

MOB pm 02:30 Structural Transitions in Gas Phase Proteins Investigated via IR Spectroscopy: from Native to Helical to Unzipped; Isabel Gonzalez1; Eike Mucha1; Jongcheol Seo1; Waldemar Hoffmann2; Stephan Warnke3; Kevin Pagel4; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2University of California, Riverside, Riverside, CA; 3University of California, Riverside Riverside, CA

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

MOB pm 03:10 Conformation-specific IR-UV Double-resonance Spectroscopy and Structural Analysis of Sodiated Leucine Enkephalin; Nicola Burke1; Christopher Harrilal1; Andrew DeBlase1; Timothy Zwier2; Scott A McLuckey1; 1Purdue University, West Lafayette, IN

MOB pm 03:30 Action-Excitation Energy Transfer for the Structural Characterization of Proteins; Nathan Hendricks1; Ryan R Julian2; 1University of California, Riverside, Riverside, CA; 2University of California, Riverside Riverside, CA

MOB pm 03:50 Gas-phase VUV Photoionization and Photofragmentation of Geometrically Well-Defined Coinage Metal Nanocluster Cations; Richard A. J. O'Hair1; Steven Daly2; Athanasios Zavras3; Laurent Nahon4; Jaye Li5; Alexandre Giuliani6; Rodolphe Antoine5; Philippe Dugourd6; 1University of Melbourne, Victoria, Australia; 2University of Lyon, Lyon, France; 3University of Melbourne, Melbourne, Australia; 4SOLEIL, l’Orme des Merisiers, St Aubin, Gin sur Yvette Cedex, France; 5University of Melbourne, Victoria, Australia; 6CRNS, Lyon, France

2:30-4:30 pm MONDAY

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

MOC pm 02:30 Measuring Masses of Single Bacterial Whole Cells with Laser Induced Acoustic Desorption Plasma Charge Detection Quadrupole Ion Trap Mass Spectrometer; Shao-Yu Liang1; Chou-Hsun Han1; Dineshkumar Yograj Turkar2; Avinash Adhikrao Patil3; Szu-Wei Chou1; 1National Dong Hwa University, Shoufeng Hualien, Taiwan; 2University of Washington, Seattle, WA; 3University of Texas, Houston, TX

MOC pm 02:50 Near Field Ablation High Lateral Resolution Sampling for Mass Spectrometry; Pan Cao1; Fabrizio Donnarumma1; Kermit K Murray2; 1Louisiana State University, Baton Rouge, LA

MOC pm 03:10 Ultra-Soft Picosecond Laser Extraction of Biological Compounds from Water and Tissue for Mass Spectrometry; Wesley Robertson1; Yinfei Lu1; Cornelius L Pieterse2; Frederik Busse3; R.J.Dwayne Miller4; 1Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

MOC pm 03:30 Automated High Throughput Identification of Microorganisms using Rapid Evaporative Ionisation Time of Flight Mass Spectrometry (REIMS-ToF-MS); Zsolt Bodai1; Daniel Simon2; Schaffer Richard3; Frankie Bolt4; Tamas Karancsi5; Julia Balog6; Simon Cameron7; Kate Hardiman8; Monica Reboc9; Zsolt Takats10; 1Imperial College, London, United Kingdom; 2Waters Research Center, Budapest, Hungary

MOC pm 05:00 A Robotic Trapping Column Exchanger for Increasing Clinical Assay Throughput by Capillary Liquid Chromatography-Mass Spectrometry; Sandra E. Spencer1; Huilin Shi2; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2University of Washington, Seattle, WA

MOC pm 04:10 Open Probe Fast GC-MS – Combining Ambient Sampling, Ultra-Fast Separation and In-Vacuum Ionization for Real Time Forensic Analysis; Uri Keshet1; Aviv Amirav2; Alexander B Fialkov1; Tal Alon1; 1Tel Aviv University, Tel Aviv, Israel; 2Tel-Aviv University, Tel-Aviv, Israel
2:30-4:30 pm MONDAY
ANTIBODIES AND ANTIBODY DRUG CONJUGATES
Shawna Hengel (Seattle Genetics, Inc.)
Stars Ballroom 2-3, level 3

MOD pm 02:30
Leveraging Antibody Structure Analysis via Data Multiplexing in Top-Down Targeted Protein analysis; Kristina Szretscić1; Konstantin Nagornov2; Anton N Kozhinov2; Yury O Tsybin1; 'Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; 2Spectroswiss Sàrl, Lausanne, Switzerland

MOD pm 02:50
Extending the Middle-Down HDX-MS Method for Residue-Level Structural Characterization of Antibody-Antigen Complexes; Jingxi Pan1; Suping Zhang2; Christoph H. Borchers1,3; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2MRM Proteomics, Inc., Victoria, BC, Canada; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

MOD pm 03:10
A Modular and Adaptive Mass Spectrometry-Based Platform for Support of Bioprocess Development toward Optimal Host Cell Protein clearance; Feng Yang1; Donald E. Walker2; Joseph Carver1; David A. Michaels3; Christopher Yu4; 1Genentech Inc, South San Francisco, CA

MOD pm 03:30
Where Did the Linker-Payload Go? A Quantitative Investigation on the Destination of Released Linker-Payload from Antibody-Drug-Conjugate with Maleimide-Linker in Plasma; Cong Wei1; Guodong Zhang2; Tracey Clark1; Frank Barletta1; Nathan Tumey1; Brian Rago1; Steven Hansel1; Xiaogang Han1; 1Pfizer, Groton, CT; 2Shire, North America

MOD pm 03:50
Profiling Multiple Post-translational Modifications of Therapeutic Antibodies Circulating in Human Patients; Yinyin Li1, Michael Monine1; Yu Huang1; Patrick Swann2; Yelena Lyubarskaya3; 'Biogen Inc., South San Francisco, CA

MOD pm 04:10
Model-Based Algorithms for Intact Mass Analysis of Biotherapeutics; Marshall W. Berg1; Yong J Ki1; Eric Carlson1; Doron Kletter1; Wilfred Tang1; Christopher Becker1; 1Protein Metrics, Palo Alto, CA; 2Protein Metrics, San Carlos, CA

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

MOE pm 02:30
LC-SWATH-MS/MS Data Acquisition with Deconvolution of High-Resolution MS Data in Metabolomics; Tomas Caika1; Oliver Fiehn1; 1UC Davis Genome Center, Davis, CA

MOE pm 02:50
A Promising Alternative to SWATH-MS1-based Strategy (IonStar) Enables In-Depth and Reproducible Proteomics Quantification in Large Cohorts with High Accuracy and Extremely-Low-Level-Missing-Data; Xiaomeng Shen1,2; Jun LP3; Shichen Shen1,2; Qiang Hu1; Xin Miao1; Chengjian Tu1,2; Lei Nie1; Xue WANG1; Jianmin Wang1; William J Jusko1; Benjamím C Orsborn1; Jun QIU1,2; 1Dept. of Biochemistry at SUNY at Buffalo, Buffalo, NY; 2Center of Excellence in Bioinformatics & Life Sci., Buffalo, NY; 3Dept. of Pharmaceutical Sci. at SUNY at Buffalo, Buffalo, NY; 4Roosewell Park Cancer Institute, Buffalo, NY; 5Shandong University, Jinan, Shandong; 6Thermo Fisher Scientific, San Jose, CA

MOE pm 03:10
Qualitative and Quantitative Characterization of a Novel DIA Method for Omics Analysis and its Application to Biomedical Analyses; Arthur Moseley1; Chris Hughes2; Erik J. Soderblom3; Keith Richardson1; Will Thompson4; Jason Wildgoose5; James Langridge2; 1Duke University School of Medicine, Durham, NC; 2Waters, Waltham, United Kingdom; 3Duke University School of Medicine, Durham, NC; 4Duke University School of Medicine, Durham, NC

MOE pm 03:30
Bidimensional FT-ICR MS: a fully Data Independent Acquisition; Fabrice Bray1; Lionel Chiron1; Matthiae Wiltz2; Marc-André Delsuc3; Christian Rolando3; 1Univ. de Lille 1, Sciences et Technologies, Villeneuve d’Ascq, France; 2CASC4DE, Strasbourg, France; 3Bruker Daltonic GmbH, Bremen, Germany; 4Université de Strasbourg, Strasbourg, France; 5Univ. de Lille 1, Sciences et Technologies, Villeneuve d’Ascq

MOE pm 03:50
Data Independent Acquisition for the Rapid Screening of de novo Protein Designs; Jason Michael Gilmore1; Jorge Fallas1; David Baker2; 1University of Washington, Seattle, WA

MOE pm 04:10
High Content Discovery Proteomics of a Breast Tumor Tissue Microarray using Data Independent Acquisition; Bin Fang1; Douglas C Marchion1; Amol Prakash2; Scott M Peterman3; Michelle Fournier1; Zena Sayegh1; Joseph J Johnson1; Agnieszka Kasprzak1; Daryoush Saeedi-Khara1; Roohi Ismail-Khan1; Steven A Eschrich1; Anthony M Magliocco2; John Koomen1; 1Moffitt Cancer Center, Tampa, FL; 2Optsys Tech Corporation, Philadelphia, PA; 3Thermo Fisher, San Jose, CA; 4H. Lee Moffitt Cancer Center, Tampa, FL

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

MOF pm 02:30
Collaborative Human Computing: The Next Generation Paradigm in Metabolomics; Mingxun Wang1; 2FDR-controlled Metabolite Annotation for High-Resolution Imaging Mass Spectrometry; Andrew Palmer1; Michael Becker2; Ilya Chernyavsky3; 1European Molecular Biology Laboratory, Heidelberg, Germany; 2Bruker Daltonic GmbH, Bremen, Germany; 3University of Bremen, Bremen, Germany; 4Skaggs School of Pharmacy, UC San Diego La Jolla, CA; 5SCILS GmbH, Bremen, Germany

MOF pm 02:50
FDR-controlled Metabolite Annotation for High-Resolution Imaging Mass Spectrometry; Andrew Palmer1; Michael Becker2; Ilya Chernyavsky3; Dominik Fay1; Artem Tarasov1; Vitaly Kovaliev4; Jens Fuchsner5; Sergey Nikoleno1; Theodore Alexandrov1,2,3,4,5; 1European Molecular Biology Laboratory, Heidelberg, Germany; 2Bruker Daltonic GmbH, Bremen, Germany; 3University of Bremen, Bremen, Germany; 4Skaggs School of Pharmacy, UC San Diego La Jolla, CA; 5SCILS GmbH, Bremen, Germany

MOF pm 03:10
Tandem Mass Spectral Libraries of Recurrent Unidentified Spectra for Urine and Plasma: A New Kind of Library for Metabolomics Applications; Yami Simon1; Ramesh Marupakakad2; Xinjing Yan2; Yuri Mirokhin3; Kelly H. Telu1; William E Wallace1; Stephen E Stein1; 1NIST, Gaithersburg, MD; 2NIST, Gaithersburg MD

MOF pm 03:30
Hydrogen Rearrangement Rules for Computational MS/MS Fragmentation; Hiroshi Tsugawa1; Wataru Tanaka1; Ryo Nakabayashi1; 1Biogen Inc., Cambridge, MA
COVALENT LABELING AND CHEMICAL CROSSLINKING

Juri Rappsilber (University of Edinburgh and TU Berlin)

Crosslink-assisted Structure Determination of the Human Spliceosomal Subcomplex, U4/U6.U5 tri-snRNP. Oleksandr Dybko\(^1\); Romina V. Hofele\(^1,2\); Dmitry E. Agafonov\(^1\); Berthold Kastner\(^1\); Wen-Ti Liu\(^1\); Holger Stark\(^1,3\); Reinhard Luehrmann\(^1\); Henning Urlaub\(^1,2\); "Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; "University Medical Center (UMG), Goettingen, Germany; "Georg-August-Universitaet Goettingen, Goettingen, Germany

MOH pm 02:50

Developing a New Quantitative Cross-linking Mass Spectrometry (XL-MS) Strategy to Define in vivo Structural Dynamics of Protein Complexes. Clinton Yu\(^1\); Xiaorong Wang\(^1\); Rosa I Viner\(^1\); Alex Huszagh\(^1\); Eric Novitsky\(^1\); Tonya Second\(^1\); Scott Rychnovsky\(^1\); "University of California, Irvine, Irvine, CA; "Thermo Fisher Scientific, San Jose, CA

MOH pm 03:10

Solving the Tertiary Structure of SallBII Protein by Chemical Cross-Linking/Mass Spectrometry and Molecular Modeling. Allan Jhonathan Ramos Ferrar\(^1\); Hugo Cesar de Jesus\(^1\); Marcio Vinicius Bertacine Dias\(^2\); Luciana Gonzalez de Oliveira\(^3\); Peter Leadlay\(^1\); Fabio Cesar Gozzo\(^1\); "University of Campinas, Campinas, Brazil; "University of São Paulo, São Paulo, SP; "University of Cambridge, Cambridge, UK

MOH pm 03:30

Combining Zero-Length Cross-Linking and Label-free Proteomics to Identify Functional Binding Residues in an Ordered-Disordered Heterodimeric Protein Complex. Michele Dubuke\(^1\); Stephanie Maniatis\(^1\); Mary Munson\(^1\); Scott A. Shaffer\(^1\); "UMass Medical School Department of Biochemistry and Molecular Pharmacology, Worcester, MA

MOH pm 03:50

Charting the Cellular Interactome by Proteome-Wide Cross-Linking Mass Spectrometry. Pan Liu\(^1\); Philip Lossi\(^1\); Richard Scheltema\(^1\); Rosa Viner\(^1\); Albert Heck\(^1\); "Utrecht University, Utrecht, The Netherlands; "Thermo Fisher Scientific, San Jose, CA

MOH pm 04:10

Global XL-MS: Proteome-scale Interactomes Unifying Cross-Linked Datasets. Devin Schweppe\(^1\); Chunxiang Zheng\(^1\); Juan Chavez\(^1\); Arti Navare\(^1\); Xia Wu\(^1\); Jimmy K Eng\(^1\); James Bruce\(^1\); "University of Washington, Seattle, WA

Award for a Distinguished Contribution in Mass Spectrometry

Scott A. McLuckey

Purdue University
Patients with advanced ovarian cancer are at increased risk of developing secondary cancers. The incidence of these secondary cancers is higher than in the general population, and the mortality rate is also higher. This workshop will begin with short introductory presentations by researchers who have recently conducted large-scale proteogenomics studies, and be followed by audience driven discussions.

It will begin with short introductory presentations by researchers who will discuss bioinformatics challenges and opportunities in proteogenomics. Traditionally, it was mainly used to improve genome annotation of newly or partially sequenced organisms, but now it is also increasingly applied in cancer studies. In this workshop, we will provide an update from the Consortium for Top Down Proteomics, discussing new community-wide pilot projects. We will also review and discuss common roadblocks to successful top down proteomics experiments from sample preparation to data acquisition to data analysis in a panel format. A limited number of 5 minute ‘lightning talks’ will be available for researchers to provide rapid-fire updates on recent achievements and accomplishments of note. Contact workshop chairs if you are interested in presenting.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

This workshop will begin with a brief discussion of the most exciting technological advances in the field of metabolomics over the past year. The moderators will highlight 2-3 noteworthy metabolomic publications that they feel are particularly impressive achievements and survey the audience for their opinions. Three-four invited scientists with expertise in the technologies highlighted will serve as panelists and answer questions posed by the moderators and attendees. The workshop will close with a discussion among the panelists on their perspectives of emerging trends and the role that these technologies are playing in future development. Advances intended to be highlighted are: (i) advances in chromatographic separation of metabolites and its influence on metabolomics data, (ii) innovative experimental designs, and (iii) new tools for metabolite identification.
**09 Polymer MS Technology: Advancements and Discussion**  
*Young Mass Spectroscopists Interest Group*  
Stephen Rumblow and Gyorgy Vas presiding  
Room 302A, level 3  
This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques for both characterization and quantitation of oligomeric species. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, and different type of products such as packaging and medical devices.

**10 MS Analysis of Antibody-Drug Conjugates**  
*Pharmaceuticals Interest Group*  
Christine Gu and Matthew Schenauer presiding  
Room 302BC, level 3  
Due to the success of pharmaceutical interest group workshops since 2013, and continued interest in MS analysis of antibody drug-conjugates (ADCs), we propose a similar workshop for 2016. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis in the industry for the discovery and development. Potential areas of discussion may include the large range of characterization required for ADCs from initial MAb assessment to bioanalytical assay development, with the focus on Mass Spec method development and optimization. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

**11 Protocol Repositories for Proteomics and Metabolomics**  
*Analytical Lab Managers Interest Group*  
Allis Chien and Brett Phinney presiding  
Room 303A, level 3  
Protocols and SOP’s are the lifeblood of any analytical core facility. Although finding detailed protocols has gotten easier over the years (Nature Protocols for example), finding protocols that have been validated, via successful use by numerous people, is still challenging and fraught with failure. Often even following a detailed published protocol can fail and the user is left wondering: What happened? In this workshop we will discuss options for finding and using protocol repositories for mass spectrometry-based analytical core facilities (Proteomics and Metabolomics). Specifically, we will discuss the new protocol repository set up by the Association of Biomolecular Resource Facilities (ABRF) along with several other freely available options.

**12 Miniaturization of Ion Traps and Related Devices**  
*Ion Trap Interest Group*  
Daniel Austin and Zheng Ouyang presiding  
Room 303BC, level 3  
Ion traps constitute a major portion of the effort to produce miniaturized mass spectrometers. In addition, the wealth of new ionization techniques have led to many new devices for introduction, transmission, and detection of ions in the context of portable devices. The workshop will start with short (4-minute) snippets from several groups working in this area. Next, a panel-led discussion will address opportunities, applications, and challenges of portable mass spectrometry.

**13 MS Career Options: How to Kick-Start your Career**  
*Young Mass Spectroscopists Interest Group*  
Kristin Wildsmith and Violet Lee presiding  
Room 304, level 3  
The workshop features an interactive panel discussion on professional development (Bring your questions). Topics will be centered around career planning and management, fundamental training, industrial internship, and diversity of career options within the MS field. A panel of representatives from government, industrial (domestic and foreign) and academic organizations, will share their knowledge, experience, and practices on career prospects.

**14 System Performance: Tracking through Statistical QC**  
*Monitoring (LC/MS & Related Topics Interest Group)*  
Michael Bereman and Brent Dixon presiding  
Room 305, level 3  
Liquid chromatography mass spectrometry systems are recognized as highly sensitive and specific tools for metabolomic and proteomic analyses. Ensuring the integrity of data through a system of controls referred to as quality control standards enables a higher level of confidence in the obtained results. Providing intra-laboratory personnel with quality control charts allows for correction when standards exceed acceptance limits. Control charts may be used in an inter-laboratory manner to compare results across labs. By monitoring performance standards, a higher level of commutability of experimental results may be achieved.

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

Integrating quality control and performance standards in the experimental design is not a new concept. However, the intention to monitor these standards over time and across experiments presents an opportunity. A major limitation in the broader analysis of experimental control performance has been aggregation and visualization. Precious samples may be better utilized by identifying a trend and performing a preventive action to avoid a failed assay. The overall aim is to shift to a prospective action driven review rather than a retrospective control review approach.
TOB am 08:30

**TOB am 08:30** Molecular Composition of Petroleum Interfacially Active Species: Implications in Emulsion Science; Ryan P. Rodgers; Amy C. Clingenpeel; Winston K. Robbins; Steven Rowland; Yui E. Corilo; David C. Podgorski; Natl’l High Magnetic Field Lab, Tallahassee, FL; "FSU Department of Chemistry and Biochemistry, Tallahassee, FL; "National High Magnetic Field Laboratory, Tallahassee, FL; "Future Fuels Institute, FSU Tallahassee, FL"

TOA am 09:10

**TOA am 09:10** Gas-phase Hydride Transfer between Carbocations and Analyte Alkanes Provides a Gentle and Controllable Ionization Method with Minimal Fragmentation; Mingzhe Li; Chunfen Jin; Hanyu Zhu; Mark Romanczyk; Yury Kostyukevich; Alexey S Kononikhin; "University of Science and Technology of China/University of Utah, Salt Lake City, UT; 2FSU Department of Chemistry and Biochemistry, Framingham, MA; 3Max-Planck Inst für Energie Problems of Chemical Physics, Moscow, Russia; 4Emanuel Institute of Biochemical Physics, Moscow, Russia; 5Moscow Institute of Physics and Technology, Moscow, Russia; 6Institute of Energy Problems of Chemical Physics, Moscow, Russia; 7Energetics Institute of the Russian Academy of Sciences, Moscow, Russia; 8Institute of Energy Problems of Chemical Physics, Moscow, Russia; 9University of Science and Technology of China; 10Russian Academy of Sciences, Moscow, Russia; 11Moscow Institute of Physics and Technology, Moscow, Russia; 12State Higher School of Economics, Moscow, Russia; 13Waters Corporation, Wilmslow, UK; 14Waters Corporation, Milford, MA; 15Sanofi Genzyme, Framingham, MA; 16Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 17Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; 18Laboratory of Catalysis, University of Liege, Belgium"

TOA am 09:50

**TOA am 09:50** Gel Permeation Chromatography (GPC) Inductively Coupled Plasma High Resolution Mass Spectrometry (ICP HR MS) Parameters Study in Petroleum Product Analysis; Sara Gutierrez Sama; Alain Desprez; Gabriel Krier; "Buckinghamshire New University, High Wycombe, UK; 2Sanofi Genzyme, Framingham, MA; 3Merck, Darmstadt, Germany; 4Emanuel Institute of Biochemical Physics, Moscow, Russia; 5Institute for Energy Problems of Chemical Physics, Moscow, Russia; 6Institute of Energy Problems of Chemical Physics, Moscow, Russia; 7Energetics Institute of the Russian Academy of Sciences, Moscow, Russia; 8Institute of Energy Problems of Chemical Physics, Moscow, Russia; 9University of Science and Technology of China; 10Russian Academy of Sciences, Moscow, Russia; 11Moscow Institute of Physics and Technology, Moscow, Russia; 12State Higher School of Economics, Moscow, Russia; 13Waters Corporation, Wilmslow, UK; 14Waters Corporation, Milford, MA; 15Sanofi Genzyme, Framingham, MA; 16Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 17Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; 18Laboratory of Catalysis, University of Liege, Belgium"

TOA am 10:10

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

**8:30-10:30 am TUESDAY**

**ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND METHOD DEVELOPMENT**

**TOB am 08:50** Supermetalization of Peptides and Proteins; Yury Kostyukevich; Alexey S Kononikhin; Maria Indeykina; Evgeny Kukaev; Igor A Popov; Eugene Nikonov; Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; "Moscow Institute of Physics and Technology, Moscow, Russia; 2Institute for Energy Problems of Chemical Physics, Moscow, Russia; 3Emanuel Institute of Biochemical Physics, Moscow, Russia; 4Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; 5Institute of Energy Problems of Chemical Physics, Moscow, Russia; 6Institute of Energy Problems of Chemical Physics, Moscow, Russia; 7Energetics Institute of the Russian Academy of Sciences, Moscow, Russia; 8Institute of Energy Problems of Chemical Physics, Moscow, Russia; 9University of Science and Technology of China; 10Russian Academy of Sciences, Moscow, Russia; 11Moscow Institute of Physics and Technology, Moscow, Russia; 12State Higher School of Economics, Moscow, Russia; 13Waters Corporation, Wilmslow, UK; 14Waters Corporation, Milford, MA; 15Sanofi Genzyme, Framingham, MA; 16Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 17Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; 18Laboratory of Catalysis, University of Liege, Belgium"

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

**TOB am 09:30** Capture of Reactive Monophosphine Ligated Palladium(0) Intermediates by Mass Spectrometry; Qiuiling Zheng; Yong Liu; Qinghao Chen; Melong Hui; Roy Herlihy; Edward Sherer; Christopher Welch; "Ohio University, Athens, OH; 2Merck, Darmstadt, Germany"

**TOB am 09:30** Revisiting Organometallic Chemistry by Ion Mobility; Izabela Czerwinska; Sophie Rappé; Carlos Larrriba-Andaluz; Nicolas Smargiasso; Christopher Kune; Albert Demonceau; Johann Far; Lionel Delaude; "Edwin A De Pauw; Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 2Department of Mechanical Engineering, Indiana University-Purdue University, Indiana; 3Laboratory of Catalysis, University of Liege, Belgium"

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

**TOB am 08:30** Analysis of Host Cell Proteins throughout Biopharmaceutical Purification; Martha Stapels; Michelle Busch; Samantha Cooper; Veena Wanikoo; Kate Zhang; "Sanofi Genzyme, Framingham, MA"

**TOB am 08:50** Exploring the Use of HRMS for Circumventing Complex and Lengthy Sample Pre-Treatment for Absolute Quantification of mAbs in Plasma/ Serum Samples; Ulik Hvid Mistaar; Tam T. T. N. Nguyen; Amaury Herbet; Narciso Costa; Didier Boquet; Christophe Junot; Francois Becher; Kasper Dyberg Rand; "Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; 2CEA Saclay, DSV/Bi Tec-SL LEMM, Gil sur Yvette, France"

**TOC am 08:00** Evaluation of Ion Mobility and Targeted QToF Acquisition Modes for the Quantitative Analysis of Peptides; Jayne Kirk; Mark Wrona; Kelly Doering; Russell Mortishire-Smith; Lisa A Vasicek; Kevin P Bateman; "Waters Corporation, Wilmslow, UK; 2Waters Corporation, Milford, MA; 3Merck & Co., West Point, PA"

**TOB am 09:10** Bioanalysis and in vivo Stability Evaluation of a PEyGylated Protein Drug by UHPLC-HRMS using a Disulfide-Containing Surrogate Peptide; Naiyu Zheng; Juming Zeng; Amy Manney; ""
TOE am 08:50

High-throughput MALDI TOF Mass Spectrometry for Drug Discovery in the Ubiquitin Pathway; Virginia De Cesare1; Axel Knebel1; Matthias Tröst1; 1MRC PPU, University of Dundee, Dundee, United Kingdom

TOC am 09:10

Simultaneous Quantitation and Metabolite Profiling of RG-125, a GalNAc-conjugated Oligonucleotide, and Its Five Metabolites using HRAM LC/MS; Brandon Wilcock1; Kai Liu2; Daniel J. Mauchley3; Min Meng2; Troy Voelker3; Brian P. Schultz2; Tate Owen2; John Grundy3; Covance, Salt Lake City, UT; 2Regulus Therapeutics Inc., San Diego, CA

TOE am 09:50

TOF am 08:50

TOE am 10:10

TOF am 09:10

TOE am 10:30

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TOF am 08:30

TOF am 08:50

TOF am 08:50

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TOE am 08:30

TOE am 08:50
TOF am 09:30  System Architecture for Charge-independent Mass Spectrometry using Nanomechanical Resonators; Shawn Fostner; Sergio Dominguez Medina1, Marc Sansa Perna1,2, Thomas Alava1,2, Ann-Kathrin Stark1,4, Ariel Brenac5,6, Henri Blanc1,2, Marc Gely1,2, Sébastien Hentz1,2, Christophe Masselon1,4, Université Grenoble Alpes, Grenoble, France; 2CEA LETI, Grenoble, France; 3CEA BIG-BGEGrenoble, France; 4INSEERM U1039, Grenoble, France; Université Grenoble Alpes, INAC-SP2M, Grenoble, France; 5CEA, INAC-SP2M, Grenoble, France.

TOF am 09:50  Dual-Polarity Ion Trap Mass Spectrometry: Dynamic Control and Monitoring of Gas-phase Ion-Ion Reactions; Muyi He, Dan Guo; You Jiang2; Xiong Xingchuang2; Zijian Huang2; Xiang Fang2; Wei Xu1; Beijing Institute of Technology, Beijing, China; National Institute of Metrology, Beijing, China.

TOF am 10:10  Quadrupole Wideband Isolation Directed by Ion Mobility Drift Separation for Analyzing Complex Protein Digests; Bruce Wang1; Ruwan T Kurulugama1; George Stafford1; John Fieldsted1; Joseph Roark1; Frank Kuhmann1; Gregor Overney1; Agilent Technologies, Santa Clara, CA.

LIDIPS AND PROFILING

Ginger Milne (Vanderbilt University) Hemisfair Ballroom 2, level 3

TOG am 08:30  Enhanced Discrimination of Healthy Human Brain Tissue and Glioma using Positive and Negative Polarity Desorption Electrospray Ionization with Data Fusion; Clint Miles Alfaro1; Alan K Jarmusch2; Valentina Pirro2; Eyas M Hattab3; Sheher Mohsin1; Gene S Hall2; Joe Hedrick3; University of Pittsburgh, Pittsburgh, PA.

TOG am 08:50  A Novel Post-column Derivatization Method for Profiling “Diolome” using LC/MS/MS; Jun Yang1; Chang Wang1; Bruce D Hammock1; University of California, Davis, Davis, CA.

TOG am 09:10  Separation and Characterisation of Human Meibum Lipids by Differential Ion Mobility Mass Spectrometry; Sarah E Hancock1; Peta Snikeris1; Almog Chotiner2; Michal Sharon2; Weizmann Institute of Science, Rehovot, Israel; 2National Institute of Metrology, Utrecht, The Netherlands.

TOG am 09:30  Nitrate Fatty Acids: Biomarkers of Inflammation and Regulators of Redox Homeostasis; Stacy Gelhaus Wendell1; Bruce A Freeman1; Franca Golin-Bisello1; Gregory Buchanan1; Sonia Salvatore1; Soma Jobbagy1; Kara Hughan1; Mark Gladwin1; University of Pittsburgh, Pittsburgh, PA.

TOG am 09:50  Structure Elucidation of Omega-3 Fatty Acid Fish Oil Glycerolipid Dietary Supplements by Supercritical Fluid Chromatography Q-TOF-MS; Sherer Mohsin1; Gene S Hall1; Joe Hedrick2; Agilent Technologies, Schaumburg, IL; Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, Piscataway, NJ; Agilent Technologies, Wilmington, DE.

TOG am 10:10  Characterizing the Natural History of Acute Radiation Syndrome of the Gastrointestinal Tract: Combining High Mass and Spatial Resolution using MALDI-FTICR-MSI; Claire Louisa Carter1; Jace W Jones1; Kim Hankey2; Ann M Fares2; Thomas J MacVittie2; Maureen A Kane1; University of Maryland, School of Pharmacy, Baltimore, MD; 2University of Maryland School of Medicine, Baltimore, MD; 3University of Maryland, Baltimore, USA.

8:30-10:30 am tUESDAY

NATIVE MS IN STRUCTURAL BIOLOGY

Alison E. Ashcroft (University of Leeds) Hemisfair Ballroom 1, level 3

TOH am 08:30  Accurate Determination of the Carbohydrate Content of Highly Heterogeneous Glycoproteins by Native Mass Spectrometry; Guanbo Wang1,2; Albert J. R. Heck1,2; Biomolecular Mass Spectrometry and Proteomics, Utrecht University, Utrecht, The Netherlands; 2Netherlands Proteomics Center, Utrecht, The Netherlands.

TOH am 08:50  High-Confidence Models of Multiprotein Complexes from Ion Mobility-Mass Spectrometry Datasets: Frontiers in Model Generation and Assessment; Joseph D Erschweiler1; Aaron T. Frank1; Brandon T Ruotolo1; University of Michigan, Ann Arbor, MI.

TOH am 09:10  Structural Characterization of Missense Mutations using High Resolution Mass Spectrometry: The Parkinson’s Related Protein DJ-1 Case Study; Gili Ben-Nissan1; Almog Chotiner1; 2Michal Sharon1; Weizmann Institute of Science, Rehovot, Israel; 2Weizmann Institute of Science, Rehovot, Israel.

TOH am 09:30  Characterization of a Nitrogenase Complex from Azotobacter Vinelandii in Gas Phase using Native Mass Spectrometry And Ion Mobility; Monika Tokmina-Lukaszewska1; Natasha Pence1; Rhesa Ledbetter2; Stephen Keable1; Sudipta Shaw1; Zhiyong Yang1; John Peters1; Lance Seefeldt1; Brian Bothner1; MUS, Bozeman, MT, Bozeman, MT; Utah State University, Logan, UT.

TOH am 09:50  Top Down Proteomics and Native Ion Mobility-MS Reveals Phosphorylation-Mediated Effects on NF-kB Conformation and Interactions; Matthias Vonderach1; Manohar Dange1; Claire Evers1; University of Liverpool, Liverpool, United Kingdom.

TOH am 10:10  Charge Detection Mass Spectrometry Monitors Virus Assembly from Single Subunit to Complete Capsid; Corinne Lutomski1; Kevin Zhao2; Adam Zlotnick2; Martin F Jarrold3; Indiana University, Bloomington, IN; 3Indiana University, Bloomington, IN.

10:30 AM – 2:30 PM, TUESDAY TUESDAY POSTER SESSION Poster/Exhibit Hall Lunch concessions are open 11:00 am – 2:00 pm Odd-number posters present 10:30 am - 1:00 pm Even-number posters present 12:00 – 2:30 pm
2:30:4:30 pm TUESDAY
ENVIRONMENTAL: NEW INSTRUMENTATION AND APPROACHES

Alla Zelenyuk (Pacific Northwest National Laboratory)
Hall 1, level 1

TOA pm 02:30
Comparison of Soft Ionisation Techniques for the High Resolution Mass Spectrometry Analysis of Environmental Samples with Complex Matrices: Ivan Kourtchev1; Pak Yiu Paddy Szeto1; Duncan Scott1; Ian P O Connor1; Oleakan Popoola1; Arthur Zielinski1; John C Wengert2; Markus Kalberer1; 1University of Cambridge, Cambridge, UK; 2University College Cork, Cork, Ireland

TOA pm 02:50
Laser Diode Thermal Desorption (LDTD)-MS and Machine Learning: a novel Approach for Ultra Fast Environmental Analysis; Pier-Luc Plante1; 2; Prudencio Tossou1; Alexandre Drouin1; Francis Brochu1; François Laviolette1; Mario Marchand1; Jacques Corbeil1; 2Université Laval, Québec, Canada; 2Centre de recherche du CHU de Québec, Québec, QC

TOA pm 03:10
Measurement of Protonated Ions as Sensitive Indicator for Neutral Polycyclic Aromatic Hydrocarbon Chemistry in Combustion by Time-of-Flight Mass Spectrometry; Yasin Karakaya1; Thomas Bierkandt1; Tina Kasper1; 1Thermodynamics, University of Duisburg-Essen, Duisburg, Germany

TOA pm 03:30
Ultrafast Quantitative Analysis of Pesticides in Food and Environmental Matrices by SPME-Transmission Matrix and Direct Analysis in Real Time; Emanuela Gionfriddo1; German Augusto Gomez-Rios1; Justen Poole1; Janusz Pawliszyn1; 1University of Waterloo, Waterloo ON, Canada

TOA pm 03:50
Multivariate Statistics Applied to MALDI-TOF MS Data of Pollen Samples; Franziska Lauer1; 2; Stephan Seifert1; 2; Janina Knipp1; 2; Steffen M. Weidner1; 2; Federal Institute f. Material Research and Testing, Berlin, Germany; 2Humboldt University, Berlin, Germany; 3Fed.Inst.f.Mat.Research, Berlin, Berlin

TOA pm 04:10
On the Application of Electrochemistry-Mass Spectrometry to Study the Biotransformation of UV Blockers in the Environment; Pedro A. Segura1; Delphine Canion1; Emmanuel Eysyseric1; 1Université de Sherbrooke, Sherbrooke, QC

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

TOB pm 02:30
The Dynamics of Superconducting Tunnel Junction Cryodetector Energy Response as it Relates to Ion Structure, Surface Area and Density; Logan D. Plath1; David M Sipe2; Jonathan Feldman1; Chenjie Zeng1; Yuxiang Chen1; Rongchao Jin1; 1Mark E. Bier1; 2Carnegie Mellon University, Pittsburgh, PA

TOB pm 02:50
A Novel Charge Detection Rectilinear Ion Trap Mass Spectrometer (C-RIT MS) for Detection of High Mass Proteins; Avinash Adhikara Patil1; 2; Szu-Wei Chou1; Chen-Wei Lee1; Wen-Ping Peng1; 1National Dong Hwa University, Shoufeng Hualien, Taiwan

TOB pm 03:10
Neutralization Charge Detection Method Facilitating Fast and Sensitive Hetero-Phase Ion Detection; Ko-Keng Chang1; 2; Yi-Hong Cai1; Yi-Sheng Wang1; 1Genomics Research Center, Academia Sinica Taipei, Taiwan; 2Chemistry Department, National Taiwan University, Taipei, Taiwan

TOB pm 03:30
Maximising Ion Detection Efficiency using Cycloidal Transport Of Secondary Electrons In Crossed Electric and Magnetic Fields; Dick Stresau1; Scott Morgan1; Toby Shanley1; 1ETP Ion Detect, Clyde, Australia

TOB pm 03:50
A Novel Wide Dynamic Range oa-ToF Detection System Based on Dual 10-bit ADCs and FPGA Processing; Martin Green1; Garry Scott1; Stephen Platt1; Peter Spreadbury1; Darrell Williams1; Frank Buckley1; Witold Nikolowski1; Stephen Hinde1; Martin Palmer1; John Chipperfield1; 1Waters, Wilmslow, United Kingdom

TOB pm 04:10
Multiple Frequency Resonance Methods in Quadrupole Ion Trap Mass Spectrometry: Expanding Capabilities and Improving Performance; Dalton Snyder1; Christopher Pulliam1; Joshua S Wiley2; Jason Duncan1; R Graham Cooks1; 1Purdue University-Department of Chemistry, West Lafayette, IN; 2California Institute of Technology, Pasadena, CA

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

TOC pm 02:30
The Potential of Micro Sampling in Regulated Bioanalysis using LC-MSMS; Martin Hilhorst1; Roderik Prins2; Frank Schalken3; PRA Health Sciences, Assen, Drenthe; 2PRA Health Sciences, Assen, The Netherlands

TOC pm 02:50
Universal LBA/LCMS Workflow for Protein Biotherapeutics PK Analysis in Preclinical Assay; Bruce Aungst1; Caroline Becker1; Xun Wang1; Lei Xiong1; Witold Woroniecki1; Yihan Li1; Suma Ramagiri2; Hua-fen Liu2; Zamas Lam1; 1QPS, Newark, DE; 2SCiEX, Redwood City, CA

TOC pm 03:10
A Trapping micro-LCMS for Ultra-sensitive, Robust and High-Throughput Quantification of Biotherapeutics and Biomarkers in Complex Matrices; Bo An1; Ming Zhang1; Yang Qu1; Jun Qu1; 1SUNY at Buffalo, Buffalo, NY

TOC pm 03:30
Measuring Drug-Target Engagement in Tissue Biopsies Using Affinity Extraction LC-MS/ MS; Eugene F. Ciccimaro1; Yongxin Zhu2; Dmitry Ostanian1; Suzanne Suchard1; James MacGuire1; Qing Xiao1; Ashok R Dongre1; Petia A Shipkova1; Timothy Olah1; 1Bristol-Myers Squibb, Princeton, NJ; 2Phytronix Technologies, Newark, DE; 3Acuity Brands Lighting Inc, Lafayette, IN

TOC pm 03:50
A Label-free, Mass Spectrometry-based High Throughput Candidate Drug Screening Assay: Application to Smith-Lemli-Opitz Syndrome; Jaqueline A Picache1; Stephanie M Cologna2; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb, Princeton, NJ

TOC pm 04:10
Cleavable Antibody Drug Conjugate (ADC) Assay Support Enables ADC ADME and Discovery Programs; Brian Raq1; Fengping Li1; Cong Wei1; Xiaogang Han1; Tracey Clark1; Lindsay King1; Nathan Turme1; Frank Barletta1; Mauricio Leal1; Steven Hansel1; 1Pfizer, Groton, CT
2:30-4:30 pm TUESDAY

ION MOBILITY, FAIMS & DMS: NEW DEVELOPMENTS & APPLICATIONS

George Stafford (Agilent Technologies)
Stars Ballroom 2-3, level 3

TOE pm 02:30
Integration of High-field Asymmetric Waveform Ion Mobility and Ambient Ionization Mass Spectrometry for Biological Tissue Imaging; Clara Feider1; Livia S. Eberlin2; 1University of Texas at Austin, Austin, Texas; 2University of Texas at Austin, Austin, TX

TOE pm 03:00
A Theoretical and Empirical Approach to Separating Isomer Classes in Uniform Field Ion Mobility; James Dods1; Jody C May1; John A McLean1; 1Vanderbilt University, Nashville, TN

TOE pm 03:30
Separation and Identification of Isomeric Lipids using a Combination of Differential Mobility Spectrometry and Ozone-induced Dissociation; Stephen J Blanksby1; Berwyn L. J. Poa1; Alan T. Maccarone1; Todd W Mitchell1; 1Queensland University of Technology, Brisbane, QLD; 2Queensland University of Technology, Brisbane, Australia; 3University of Wollongong, Wollongong, Australia

TOE pm 04:00
Gas Phase Epitope Mapping - A Mass Spectrometric Method for Accurate, Facile, and Rapid Identification of Specific Antibody-Peptide Reactivities; Yelena Vefremova1; Frimpong-Manso Kwabena Opuni1; Hans-Juergen Thiesen1; Michael O Glocker1; 1Proteome Center Rostock, Rostock, Germany; 2Bioanalytical Sciences and Bioinformatics, Bayreuth, Germany; 3Oxford University, Oxford, United Kingdom

2:30-4:30 pm TUESDAY

QUALITATIVE AND QUANTITATIVE ANALYSIS OF POST-TRANSLATIONAL MODIFICATIONS

Amber L. Mosley (Indiana University School of Medicine)
Stars Ballroom 4, level 3

TOE pm 02:30
Disease-specific Post-translational Modifications in Cystic Fibrosis; Sandra Pankow1; Casimir Bamberger1; John Yates1; 1The Scripps Research Institute, La Jolla, CA

TOE pm 02:50
PTM‘omics: What Do We Learn from Surveying Many Modifications Simultaneously in Non-Enriched Proteomes? A Study of Lysine Acylations; Hong Nguyen1; Michael Mckerney1; Robert Gunalsalus1; Joseph A Loo1; Rachel Ogorzalek Loo1; 1UCLA, Los Angeles, CA; 2University of Oklahoma, Norman, OK

TOE pm 03:10
Redox Proteomics to Study Cysteine Status in Alzheimer’s Disease; Rená A. S. Robinson1; Liqing Gu1; 1University of Pittsburgh, Pittsburgh, PA

TOE pm 03:30
The Phosphoproteome of the NCI-60 Cell Line Panel Reveals Markers of Drug Sensitivity; Benjamin Ruprecht1; Chen Meng1; Martin Frejno1; Alexander Hogrebe1; Dominic Helm2; Bernhard Kuster1; 1TU Muenchen, Freising, Germany; 2University of Pennsylvania, Philadelphia, PA

TOE pm 03:50
Identification of Histone ADP-Ribosylation Sites using High Resolution Mass Spectrometry; Kelly Karch1; Benjaimin A. Garcia1; Ben E. Black1; 1University of Pennsylvania, Philadelphia, PA

2:30-4:30 pm TUESDAY

IMAGING: COMPUTATIONAL METHODS AND ANALYSIS

Theodore Alexandrov (EMBL / UCSD / SCiLS)
Hemisfair Ballroom 3, level 3

TOF pm 02:30
Absorption Mode Processing of MALDI-FT-ICR Imaging Data Improves Mapping of Gram-Negative Bacterial Virulence Factors on-Tissue; Alison Scott1; David P A Kilgour2; Robert K Ernst1; David R Goodlett1; 1University of Maryland, Baltimore, MD; 2Nottingham Trent University, Nottingham, UK

TOF pm 02:50
Deep Autoencoders for Dimensionality Reduction of 3D Mass Spectrometry Imaging Data-sets for Tumour Classification and Novel Subtypes Identification; Paolo Indege1; James McKenzie1; Anna Mróz1; James Kinross1; Elaine Holmes1; Zoltan Takats1; Jeremy K Nicholson1; Robert C Glende1; 1University College London, South Kensingtont Campus London, United Kingdom; 2University of Cambridge, Cambridge, UK

TOF pm 03:10
Dimensionality Reduction of MALDI Imaging Datasets using Non-Linear Redundant Wavelet Transform-based Representations; Luis Mancera1; Lorna Sellar1; Jamie Culliffe1; Luis Gonzalez1; Omar Belgacem1; 1Clover Bioanalytical Software, Granada, SPAIN; 2Shimadzu, Kratos Manchester, United Kingdom

TOF pm 03:30
Current Status and Applications of the Open Data Format imzML; Nicolas Desbonet1; Amol Fatangare1; Andreas Roempp2; 1Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany; 2Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

TOF pm 03:50
Generation of Realistic Synthetic Mass Spectrometry Imaging (MSI) Data for the Validation of Multivariate Analysis Methods; Alexander Dexter1; 2; Alan Race1; Iain B Styles1; Helen J Cooper1; Josephine Bunch1; 1University of Birmingham, Birmingham, UK; 2National Physical Laboratory, Teddington, United Kingdom; 3University of Nottingham, Nottingham, UK

TOF pm 04:10
Characterisation of Molecular Signatures in the Xenograft Microenvironment using Novel Tools to Combine Histopathology and Mass Spectrometry Imaging Data; Jo Connell1; Gert B Eijkel1; Martha Ingola1; Richard J A Goodwin2; Peter Webborn2; Ron M A Heeren1; 1M4I Institute - Maastricht University, Maastricht, The Netherlands; 2Nottingham Trent University, Nottingham, UK
TOG pm 02:30  
**SYMBIOTIC INTERACTION BETWEEN LEGUMES AND RHIZobia EXPLORED BY LASER ABLATION ELECTROSpraY IONIZATION MASS SPECTROMETRY WITH Ion MOBILITY SEPARATION**; **SYLVIA S T enrollment**; **BEVERLY AGTUC**; **CHRISTOPHER ANDERTON**; **DAVID W KOPPENAAL**; **LJILJANA PASA-TOLIC**; **GARY STACEY**; **AKos VERTE**; **GEORGE WASHINGTON UNIVERSITY, WASHINGTON, DC, USA**; **UNIVERSITY OF MISSOURI, COLUMBIA, MO, USA**; **PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA, USA**

**METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS**  
**JOHN S. KLASSEN** (University of Alberta); **CARL FRIEDEN**; **MICHAEL L. GROSS**; **BRENT BENTON**; **VICKI H. WSOCZK**; **LJILJANA PASA-TOLIC**; **GEORGE WASHINGTON UNIVERSITY, WASHINGTON, DC, USA**; **PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA, USA**

TOG pm 03:30  
**TEMPORAL ANALYSIS OF LIVING HUMAN BRONCHIAL EPITHELIAL CELL SIGNALING AND DRUG TRANSPORTATION USING nano-DESI MS**; **INGELA LANEKOFF**; **ERIK LUNDIN**; **JAN-CHRISTER ULLINGE**; **MARK NICHOLAS**; **UPPSALA UNIVERSITY, UPPSALA, SWEDEN**; **ASTRAZENECA R&D, GOTHENBURG, SWEDEN**

TOG pm 03:50  
**SOLID PHASE MICROEXTRACTION AS A SAMPLE PREPARATION TOOL FOR UNTARGETED ANALYSIS OF BRAIN TISSUE**; **NATHALY REVES-GERC**; **EZEL BOYACI**; **GERMAN AUGUSTO GOMEZ-RIOS**; **BARBARA BOJKO**; **JANUSZ PAWLSZYN**; **UNIVERSITY OF WATERLOO, WATERLOO, ON, CANADA**

**AN INTEGRATED PLATFORM FOR QUANTITATIVE FULL-SCAN POLAR LC/MS METABOLIC REVEALS STRUCTURED ENVIRONMENTAL STRESS RESPONSE IN THE YEAST SACCHAROMYCES CEREVISIAE**; **AMY ANNE CAUDY**; **JONATHAN HOPPER**; **OLGA ZASLAYER**; **SOUMAYA ZITINI**; **ADAM ROSEBROCK**; **UNIVERSITY OF TORONTO, TORONTO, ON, CANADA**

**HIGHER-THROUGHPUT TARGETED METABOLOMICS OF CoA METABOLITES FOR MODULATION OF ANTIBIOTIC INFLUX AND EFFLUX IN GRAM NEGATIVE BACTERIA**; **CHRISTOPHER M. RATH**; **BRET BENTON**; **JAVIER DE VICENTE**; **CINDY LI**; **BOB MOREAU**; **XIAOYU SHEN**; **LISHA WANG**; **BRIAN FENG**; **NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, EMERYVILLE, CA, USA**; **DENAHL THERAPEUTICS, SOUTH SAN FRANCISCO, CA, USA**

**HIGHER-THROUGHPUT ANNOTATION OF PLANT METABOLITES USING SPECTRAL MATCHING, COMPUTATIONAL IDENTIFICATION TOOLS AND EMPIRICAL UPLC-MS-SPE-NMR**; **LOYD W. SUMNER**; **FENG QIU**; **DENNIS FINE**; **DANIEL WHERRITT**; **ZHENTIAN LEI**; **AIKO BARSCH**; **UNIVERSITY OF MICHIGAN, ANN ARBOR, MI, USA**; **DUKE UNIVERSITY, DURHAM, NC, USA**; **BRUKER DALTONICS, BREMEN, GERMANY**

**TETRAMERIC BANLEC NEUTRALISES HIV THROUGH BIDENTATE BINDING TO SPECIFIC VIRAL GLYCAN STRUCTURES**; **JONATHAN HOPPER**; **OLIVER GRANT**; **STEPHEN AMBROSE**; **STEFANIE KRUNM**; **TIMOTHY ALLISON**; **MARK TULLY**; **LAURA PRITCHARD**; **GABRIEL OZROWSKI**; **ANDREW WARD**; **MAX CRISPIN**; **KATIE DOORES**; **ROBERT J WOODS**; **JUSTIN BENECH**; **CAROL V ROBINSON**; **WESTON STRUWE**; **UNIVERSITY OF OXFORD, OXFORD, UK**; **UNIVERSITY OF GEORGIA, ATHENS, GA**; **KING’S COLLEGE LONDON, LONDON, UK**; **DIAMOND LIGHT SOURCE, DIDCOT, UK**; **THE SCRIPPS RESEARCH INST., LA JOLLA, CA**

**TARGETED MS-BASED APPROACH FOR PROTEIN LIGAND BINDING ANALYSIS IN COMPLEX BIOLOGICAL MIXTURES USING A PHENACYLBROMIDE MODIFICATION STRATEGY**; **LORRAINE JAN**; **CAROL H BALL**; **MICHAEL C FITZGERALD**; **DUKE UNIVERSITY, DURHAM, NC, USA**; **AGILENT TECHNOLOGIES, SANTA CLARA, CA**

**UNVEILING THE HETEROGENEITY OF AN UNCHARACTERIZED MANGANESE OXIDIZING MULTICOPPER OXIDASE USING HIGH RESOLUTION NATIVE MASS SPECTROMETRY AND SURFACE INDUCED DISSOCIATION**; **MOWEI ZHOU**; **JING YAN**; **CHRISTINE ROMANO**; **YANG SONG**; **JEREMY J WOLFF**; **JOSHUA GILBERT**; **RANDALL E PEDDER**; **BRADLEY TEBO**; **VICKI H. WSOCZK**; **LJILJANA PASA-TOLIC**; **PACIFIC NORTHWEST NATIONAL LABORATORY - PNNL, RICHLAND, WA, USA**; **OHIO STATE UNIVERSITY, COLUMBUS, OH**; **OREGON HEALTH & SCIENCE UNIVERSITY, PORTLAND, OR**; **BRUKER DALTONICS, BILICERIA, MA**; **ARDARA TECHNOLOGIES L.P., ARDARA, PA**

**PROBING KIX-PEPTIDE ALLOSTERIC INTERACTIONS BY Ion Mobility-Mass Spectrometry**; **JESSICA RABUCK-GIBBONS**; **JEAN M LODGE**; **ANNA K MAPP**; **BRANDON T RUOTOTO**; **UNIVERSITY OF MICHIGAN, ANN ARBOR, MI, USA**

**TETRAMERIC BANLEC NEUTRALISES HIV THROUGH BIDENTATE BINDING TO SPECIFIC VIRAL GLYCAN STRUCTURES**; **JONATHAN HOPPER**; **OLIVER GRANT**; **STEPHEN AMBROSE**; **STEFANIE KRUNM**; **TIMOTHY ALLISON**; **MARK TULLY**; **LAURA PRITCHARD**; **GABRIEL OZROWSKI**; **ANDREW WARD**; **MAX CRISPIN**; **KATIE DOORES**; **ROBERT J WOODS**; **JUSTIN BENECH**; **CAROL V ROBINSON**; **WESTON STRUWE**; **UNIVERSITY OF OXFORD, OXFORD, UK**; **UNIVERSITY OF GEORGIA, ATHENS, GA**; **KING’S COLLEGE LONDON, LONDON, UK**; **DIAMOND LIGHT SOURCE, DIDCOT, UK**; **THE SCRIPPS RESEARCH INST., LA JOLLA, CA**

**PRESENTATION OF THE 2016 RESEARCH AWARDS**

4:15 PM, TUESDAY AFTERNOON AWARD LECTURE  
**JENNY BRODBELT** (University of Texas, Austin) presiding

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

**BIEMANN MEDAL**

**KRISTINA “KICKI” HÅKANSSON**

United States of America
There are light refreshments in common areas.

01 Glycoproteomics: Site Specific Glycan Analysis
Ron Orlando presiding
Room 220, level 2
Modulating the activities and functions of proteins is a significant role of post-translational modifications (PTMs), with glycosylation being an excellent example. Glycan moieties of glycoproteins affect protein folding, stability, and localization and thus play a role in numerous biological functions, including cell signaling, adhesion, and communication. The analysis of released glycans has been a primary focus of glyco-analytical development over the past several years. However, these glycan centric analyses do not provide information on the glycans present at each glycosylation sites. Often the site occupancy is critical for biological activity. This behavior is clearly shown with therapeutic antibodies, where glycans located in the variable domain influence the serum clearance rate while glycans in constant domain affect the activity. The comprehensive characterization of protein glycosylation microheterogeneity entails the identification and quantitation of isomeric glycan occupancy of potentially all glycosylation sites on a protein, which is a significantly more difficult challenge than glycomic profiling. This workshop critical evaluation of state-of-the-art methods currently employed for enrichment and analysis at a glycoproteomic level.

02 Ion Mobility: How to Interpret the Data
(Ion Mobility MS Interest Group)
Erin Baker, Valerie Gabelica, and Stephen Valentine presiding
Room 221, level 2
Over the past decade, MS instrumentation featuring various forms of mobility-based separations have proliferated. One hurdle to intra- and inter-instrumental data comparison is, however, the lack of common interpretation schemes and practical tools. In part this results from gaps in knowledge related to correct data interpretation. This workshop will discuss the tools currently available for ion mobility data analyses, and participants will be invited to show tricky cases where data analysis can lead to ambiguous or erroneous interpretations. The workshop discussion will help make progress toward finding common ground and sound fundamental principles for the correct interpretation of ion mobility data.

03 H/D Exchange, Covalent Labeling & Cross-Linking
(H/D Exchange, Covalent Labeling & Cross-Linking Interest Group)
Joshua Sharp and David Weis presiding
Room 225A, level 2
This workshop will provide a forum for discussing hydrogen exchange, covalent labeling, and cross-linking approaches for protein analysis (structure, function, folding, dynamics). There will be a several brief presentations introducing late-breaking advances in MS-based methods, experiments, data analysis, and applications to the attendees. The goal of these abbreviated presentations will be to stimulate discussion. There will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

04 Food Safety & Security: HRMS Applications
(Flavor, Fragrance & Foodstuff Interest Group)
Walter Hammack and David Schroeder presiding
Room 225B, level 2
A continued discussion of applications and developments in the use of High Resolution Mass Spectrometry (HRMS) in food safety and food security. A focus on new developments and applications in pesticide residue analysis, non-target screening, and natural product authenticity.

05 Microcontrollers and Microcomputers:
Emerging Technologies
Vincent Sica and Bindesh Shrestha presiding
Room 225C, level 2
Smaller is becoming better - computers as smart phones, nanotechnology, miniature mass spectrometers, even tiny homes! The latest trend in “do-it-yourself” (DIY) electronics is microcontrollers (i.e. Arduino) and microcomputers (i.e. Raspberry Pi). These small, yet powerful devices have put electronic innovation right into our hands. Sensors, displays, and detectors can all be added at a whim without requiring the knowledge of advanced computer circuitry.

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

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

06 DNA/RNA Adducts: Assay Development in
Detection and Quantification
(Oligonucleotides and Nucleic Acids Interest Group)
Patrick Limbach and Laixin Wang presiding
Room 225D, level 2
Recent mass spectrometry developments now enable high sensitivity detection of DNA or RNA adducts (or modifications). This workshop will focus on the practical issues involved in developing MS-friendly assays to measure these adducts. Selected presentations will illustrate assay development with a focus on sample prep, HPLC conditions, and data analysis. An emphasis in these informal discussions will be on pitfalls and “what did not work” to freely share strengths and weaknesses of assay development. The remaining time will be spent discussing challenges facing MS assays, especially given the advantages now being presented by high-throughput genome-based technologies.

07 Petroleum and Biofuels: Handling the Data
(Energy, Petroleum & Biofuels Interest Group)
Mark Barrow and Lateefah Stanford presiding
Room 301A, level 3
Petroleum-related mass spectra, often acquired using ultrahigh resolution instruments, are well-known for their complexity. With coupling of ion mobility and chromatography becoming more widespread, the level of complexity will be expected to significantly increase. Accompanying this, issues such as data size, data analysis, usage of chemometrics, software development, and comparisons of results from different analytical techniques will become progressively important. The workshop will highlight some of the existing approaches and will focus upon an active discussion of the current and emerging challenges.

08 Metabolism of Biotherapeutics: When, Why and How?
(DMPK Interest Group)
Kevin Bateman and Philip Tiller presiding
Room 301BC, level 3
Biotherapeutics are a steadily growing proportion of the pharmaceutical research and development landscape. Molecules are evolving beyond traditional monoclonal antibodies and antibody-drug conjugates

5:45 - 7:00 PM TUESDAY WORKSHOPS
to include bispecifics, truncated mAbs, nanobodies, cyclic and stapled peptides, Ig fragments, Non-Ig based scaffolds and so on. Understanding the metabolism of these new modalities is an expanding opportunity for mass spectrometry and requires that traditional small molecule scientists adapt to these new large(r) molecules. The goal of this workshop is to stimulate a discussion on the when, why and how for the metabolism of biotherapeutics in the discovery, pre-clinical and clinical arena. A panel will offer opening comments on the current state and provide thoughts on where the field is going. Questions from the audience will be strongly encouraged to stimulate robust discussion.

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

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

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

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

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

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

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

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

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

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

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

This workshop will focus on initiating a discussion between the instrument users, regulators and the instrument vendors, to discuss issues relating to regulatory compliance. More rigorous regulatory expectations are requiring higher instrument qualification standards and more involved calibration processes. This workshop is intended to discuss best practice approaches and potential qualification issues.
8:30-10:30 am WEDNESDAY ENERGY, PETROLEUM AND BIOFUELS: STRUCTURE, QUANTIFICATION, AND DATA ANALYSIS
Patrick G. Hatcher (Old Dominion University)
Hall 1, level 1

WOA am 08:30
In ESI-source H/D Exchange Facilitated a Structural Characterization of Individual Compound in Complex Mixtures by FTICR MS; Alexey S Kononikhin1,2; Yury Kostyukevich1,2; Alexander Zherebkov1; Igor A Popov1; Oleg N Kharytin2; Evgeny Kukueva2; Andrey Konstantinov2; Irina V Perminova2; Eugene Nikolaev1,2,3,5,6,7; 1Moscow Institute of Physics and Technology, Moscow, Russia; 2Institute for Energy Problems of Chemical Physics, Moscow, Russia; 3Skolkovo Institute of Science and Technology, Skolkovo, Russia; 4Lomonosov Moscow State University, Moscow, Russia; 5Emanuel Institute of Biochemical Physics, Moscow, Russia; 6Institute of Biomedical Problems RAS, Moscow, Russia; 7Skolkovo Institute of Technology, Moscow, Russia

WOB am 08:50
Mechanistic Study of Gas Phase In-source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-ESI/Tandem Mass Spectrometry; Huaming Sheng1; Rong-Sheng Yang1; Katrina M Lox1; Edward Sherer1; Li-Kang Zhang1; Bangping Kong1; Roy Helmy1; 1Merck, Darmstadt, Germany

WOB am 09:30
Mechanistic Study of Gas Phase In-source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-ESI/Tandem Mass Spectrometry; Huaming Sheng1; Rong-Sheng Yang1; Katrina M Lox1; Edward Sherer1; Li-Kang Zhang1; Bangping Kong1; Roy Helmy1; 1Merck, Darmstadt, Germany

WOB am 09:50
Probing the Effect of Charge on the Energetics and Reactivity of Distonic Peroxy Radical Ions in the Gas Phase; Peggy Williams1; Nadia Skeljo1; David Marshall1; Benjamin Kirk2; Berwyck Poad3; 2National High Magnetic Field Laboratory, Tallahassee, FL

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

WOB am 08:30
Mechanistic Study of Gas Phase In-source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-ESI/Tandem Mass Spectrometry; Huaming Sheng1; Rong-Sheng Yang1; Katrina M Lox1; Edward Sherer1; Li-Kang Zhang1; Bangping Kong1; Roy Helmy1; 1Merck, Darmstadt, Germany

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

WOC am 08:30
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 08:50
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:00
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:10
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:20
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:30
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:40
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA

WOC am 09:50
C60-SIMS Imaging of Pharmaceutical Compounds within Mammalian Cells; Anna N Bloom1; Hua Tian1; Nicholas Winograd2; 1Pennsylvania State University, University Park, PA
INSTRUMENTATION: MINIATURIZATION OF MS
Christopher C. Mulligan (Illinois State University)
Stars Ballroom 2-3, level 3

Development of a Point-of-Care (POC) Miniature Mass Spectrometry System: Xiaowang Wang1; Yue Ren1; Li Linfan1; Xinwei Liu2; Zheng Quyang1,3; Purdue University, West Lafayette, IN; 3Massachusetts Institute of Technology, Cambridge, MA; 4Department of Chemistry and Chemical Engineering, Northeastern University, Boston, MA; 5Department of Radiation Oncology, Mayo Clinic, Rochester, MN

Linear Ion Trap Mass Spectrometer for Space Flight Applications: Andrei Grubisic1,2; William B Brinckerhoff; Friso Van Amerom3; Ryan Danell; Veronica T Pinnick; Ricardo Arevalo; Xiang Li; Stephanie Getty; Daniel Glavin; Lars Hovmand; Phil Chu; Kris Zacyn; Steve Rogacki; Timothy J Cornish; Paul Mahaffy; University of Maryland, College Park, MD; NASA GSFC, Greenbelt, MD; 3Mini-Mass Consulting, Inc., Hyattsville, MD; 4Danell Consulting, Inc., Winterville, NC; 5University of Maryland, Baltimore County Greenbelt, MD; 6Linear Labs LLC, Washington DC, DC; 7Honeywell Robotics, Pasadena, CA; 8University of Michigan, Ann Arbor, MI; 9C&E Research, Inc. Columbus, OH

Reverse Gas Stack Model for Localization of Chemical Interests Utilizing Mobile Mass Spectrometry: Phillip Mach1; Kenneth C Wright2; Guido F Verbeck3; University of North Texas, Denton, TX; 4Inficon, Syracuse, NY

miniSPLAT-A Miniaturized Aircraft-Compatible Single Particle Mass Spectrometer for in-situ Quantitative Multidimensional Single Particle Characterization: Alla Zelenyuk1; Dan Imre2; Jacqueline Wilson; David Bell3; Pacific Northwest National Laboratory, Richland, WA; 4Imre Consulting, Richland, WA

Biomarkers: Qualitative Analysis
Jennifer Van Eyk (Cedars-Sinai Medical Center)
Stars Ballroom 4, level 3

Organismal Level Dynamic Molecular Map of Mouse Proteome: Bingyun Sun1; Shizhen Qin1; Cynthia Lorang2; Gray Li3; Zhiyuan Hu4; Ken Liu5; Leory Hood6; 7Simon Fraser University, Burnaby, BC; 8University of North Carolina Chapel Hill, Chapel Hill, NC

Intact Metabolome Analysis of Mice Biological Tissues by Probe Electrospary Ionization-Tandem Mass Spectrometry and Its Preliminary Application to Real-Time Analysis: Kei Zaitsev1; Yumi Hayashi2; Tsukuru Murata3; Hiroki Nakajima4; Tetsuya Ishikawa5; Maiko Kusano6; Hitoshi Tsuchihashi7; Akira Ishii8; Nagoya University Graduate School of Medicine, Nagoya, Japan; 2Global Application Development Center, Shimadzu Corporation, Kyoto, Japan

Profiling of Intact Proteins in the CSF of Alzheimer’s Disease Patients using Top Down Proteomics: Revealing Specific Isoform Biomarker Candidates: Jerome Vialaret1; Schmit Pierre-Olivier; Audrey Gabelle; Christophe Hirtz1; Sylvain Lehmann1; LBPC-IRB, CHU de Montpellier Montpellier, France; 2Bruker Daltonique S.A., Wissembourg, Bas-Rhin; 3Centre Mémorie Ressources Recherche, Montpellier, France

A Mass Spectrometry Approach to Discover Naturally-occurring Oxidation-specific Malondialdehyde Adducts: Juliane Weiller1; Christoph J Binder2; Keiryn L Bennett; CeMM Research Center for Molecular Medicine, Vienna, Austria; 2Medical University of Vienna, Vienna, Austria
**8:30-10:30 am WEDNESDAY**
**INFORMATICS: MULTIMICS INTEGRATION AND APPLICATION**

**WOF am 08:40**

Integrating and Mining Spatial Omics through Imaging Mass Spectrometry and Anatomical Atlases; **Nico Verbeek**; Jeffrey Spraggins; Junhui Yang; Étienne Waelkens; Richard M. Caprioli; Raf Van de Plas; Delft University of Technology, Delft, The Netherlands; 2Vanderbilt University, Nashville, TN; 3KU Leuven, Leuven, Belgium; 4Sybioma, Leuven, Belgium

**WOF am 08:50**

Mitochondrial Protein Functions Revealed by Global Mass Spectrometry Profiling; Jonathan A Stefely; Nicholas W Kwiecien; Alexander S Hsbert; Alicia L Richards; Elyse C Freiberger; Jyoti Choudhary; Michael S Westphall; David J Pagliarini; Joshua J Bender; Alvis Brazma; Jennifer Harrow; Christine Swaminathan; Peder J Lund; Caleb C Marceau; Stepping Away from the Streetlamp, Madison, Wisconsin; 2Morgridge Institute for Research, Madison, Wisconsin; 3KU Leuven, Leuven, Belgium; 4European Bioinformatics and Annotation Team, Wellcome Trust Sanger Institute, Cambridge, UK; 5Department of Human Genetics, The Netherlands; 2Netherlands Proteomics Center, Utrecht, The Netherlands; 3University of Wisconsin Madison, Madison, Wisconsin; 4Sybioma, Leuven, Belgium

**WOF am 09:10**

Incorporating Multiple Information Layers to Understand Viral Antigen Presentation: Stepping Away from the Streetlamp; Kayva Swaminathan; Peder J Lund; Caleb D Marceau; Nicolas E Olsson; Mark M Davis; Jan Carette; Joshua E Elias; Stanford University, Stanford, CA

**WOF am 09:30**

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

**WOF am 09:50**

Integrated Analysis of Human Tissues with a Multi-Omics Approach; Hannah Hahne; Dongxue Wang; Björn Hallström; Lihua Li; Anna Asplund; Mathias Wilhelm; Harald Marx; Frederik Ponten; Mathias Uhlen; Bernhard Küster; "OmicScouts GmbH, Freising, Germany; 2Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 3KTH Royal Institute of Technology, Stockholm, Sweden; 4Uppsala University, Uppsala, Sweden; 5University Wisconsin-Madison, Madison Sweden

**WOF am 10:10**

Integration of Multiple 'Omics' Data Sets via Application of OnPLS Methodology; Johan Trygg; Izabella Surowiec; "Computational Life Science Cluster (CLiC), Umeå University, Umeå, Sweden

**8:30-10:30 am WEDNESDAY**
**MS IN THE QC LAB**

**WOF am 08:30**

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

**WOF am 08:50**

Monitoring Product Attributes in Biopharmaceutical Development and QC with LC/HRMS; Scott Berger; Liuxi Chen; Min Du; Henry Y Shion; Ying-Qing Yu; Waters Corporation, Milford, MA

**WOF am 09:10**

Extending the Capabilities of a MS Based Multi Attribute Characterization Method to Promote Quality by Design In Biotherapeutic Drugs; Michael Blank; Jonathan L Josephs; Richard Rogers; "Thermo Fisher Scientific, San Jose, CA; 2Just Biotherapeutics, Seattle, WA

**WOF am 09:30**

Development of QC-Friendly Mass Spectrometry Assays for Monitoring Antioxidant Oxidation; Izabela Sokolowska; Jingjie Mo; Jia Dong; Michael J Lewis; Ping Hu; "Janssen Research & Development, Malvern, PA

**WOF am 09:50**

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

**WOF am 10:10**

Practical Applications of Mass Spectrometry in a Quality Control Laboratory; Patrick Bulau; Roche Diagnostics GmbH, Penzberg, Germany

**8:30-10:30 am WEDNESDAY**
**MACROMOLECULAR COMPLEXES**

**Mowei Zhou** (Pacific Northwest National Laboratory)

**WOH am 08:30**

A Native Proteomics Platform for Untargeted Identification and Characterization of Protein Complexes; Owen Skinner; Rafael Melani; Luca Carnevali; Nicole Haverland; Luis Henrique Ferrer Do Vale; Henrique Seckler; Peter Dubleday; Luis Schachner; Neil L Kelleher; Compton Philip; 1Northwestern University, Evanston, IL

**WOH am 08:50**

Towards Routine Native Mass Spectrometric Analysis of Affinity-Isolated Endogenous Protein Complexes; Paul Dominic B. Olnares; Amelia D Dunn; Julio C Padovan; Javier Fernandez-Martinez; Michael P Rout; Brian T Chait; "The Rockefeller University, New York, NY

**WOH am 09:10**

Integrating Native MS, Crosslinking-MS and HDX-MS with High-Resolution Cryo-Electron Microscopy Reveals the Molecular Architecture of the Sub-Megadalton Circadian Oscillator KaiCBA; Philip Lööhl; Joost Sijbers; 2,3 Jan Michael Schuller; Anika Wiegard; Ilka MAxmann; Jürgen M Plitzko; Friedrich Förster; Albert J R Heck; "Utrecht University, Utrecht, The Netherlands; 2Netherlands Proteomics Center, Utrecht, The Netherlands; 3University of Washington, Seattle, WA; 4Max Plank Institute for Biochemistry, Martinsried, Germany; 5Heinrich Heine University, Düsseldorf, Germany

**WOH am 09:30**

Mobile-Proton MD Simulations for Modeling Biological Relevance; Wael Hamouda; Hyo Chung; "Janssen Research & Development, Malvern, PA

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**WOF am 08:30**

A Native Proteomics Platform for Untargeted Identification and Characterization of Protein Complexes; Owen Skinner; Rafael Melani; Luca Carnevali; Nicole Haverland; Luis Henrique Ferrer Do Vale; Henrique Seckler; Peter Dubleday; Luis Schachner; Neil L Kelleher; Compton Philip; 1Northwestern University, Evanston, IL

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**WOH am 09:30**

Mobile-Proton MD Simulations for Modeling the Dissociation of Electrosprayed Protein Complexes; Vlad Popp; Danielle Trecroce; Robert G McAllister; Lars Konermann; "University of Western Ontario, London, Canada
Confirmation of Subunit-Subunit Connectivity and Topology of Computationally Designed Protein Complexes using Surface Induced Dissociation/Ion Mobility; Anirudha Sahasrabuddhe; Yang Hsia; Florian Busch; David Baker; Vicki Wysocki; The Ohio State University; Columbus, OH; University of Washington; Seattle, WA

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

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

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

Hall 1, level 1

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

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

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

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

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

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

WOB pm 03:30 Molecular Dynamics/Kinetic Theory Algorithm for Numerical Determination of Electrical Mobility; Carlos Larriba Andaluz; Indiana University-Purdue University Indianapolis, Indianapolis, IN

WOB pm 03:50 Multi-scale Simulations Coupled with Ion Mobility Experiments Reveal the Fate of Nucleic Acids in the Gas Phase; Massimiliano Porrini; Clémence Rabini; Josephine Abi-Ghanem; Frédéric Rosu; Valerie Gabelica; INSERM-U1212, ARNA laboratory, Bordeaux, France; CNRS-UMR5320, ARNA laboratory, Bordeaux, France; Université de Bordeaux, IECB, ARNA laboratory, Pessac, France; CNRS UMS 3033, IECB, University of Bordeaux, Pessac, France

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

WOC pm 02:30 Hydraulic Fracturing Impacts on Drinking Water: High Resolution-MS Uncovers New Chemical By-Products; Jennifer Richardson; Hannah K. Liberator; Jeanne M. VanBriesen; Plewja Michael; Leslie H. Cizmas; University of South Carolina, Department of Chemistry and Biochemistry, Columbia, SC; University of South Carolina, Columbia, SC; Carnegie Mellon University, Pittsburgh, PA; University of Illinois, Urbana, IL; Texas A&M, College Station, TX

WOC pm 02:50 Heterogeneous Atmospheric Reactions: Identification of the Oxidation Products of Polycyclic Aromatic Hydrocarbons; Richard E. Cochran; Shokouh Haddadi; Rebeka Fisseha
Derese1; Alena Kubatova1; 1University of North Dakota, Grand Forks, ND; 2University of California San Diego, San Diego, CA; 3SUNY Oswego, Oswego, NY

WOC pm 03:10 Data-independent Mass Spectrometry for Development of Occupational Nanomaterial Exposure Biomarkers; Andrew K. Ottens2; Pretal P. Muldoon1; Aleksandar Vucetic1; Demetris R. Carter1; Stefan Tenzer2; Matthew J. Campen3; Aaron D. Eredly4; Dept. Anatomy and Neurobiology, Virginia Commonwealth University, Richmond, VA; 3Institute of Immunology, University of Mainz, Mainz, Germany; 4Dept. Pharmaceutical Sciences, University of New Mexico, Albuquerque, NM; 1National Institute for Occupational Safety and Health, Centers for Disease Control and Prevention, Morgantown, WV

WOC pm 03:30 Tracing Gadolinium-based Contrast Agents from Surface Water to Drinking Water by means of Speciation Analysis; Uwe Karst1; Marvin Birka2; Oliver Hachmöller1; Michael Sperling1; Christoph Alexander Wehe1; 1University of Münster, Münster, DE

WOC pm 03:50 Determination of Unknown Dichlorophenols from the Oxidation of Tricosanol Using Hydrogen Peroxide; Matthew Reichert1; Paul M Chiarelli1; 1Loyola University, Chicago, IL

WOC pm 04:10 Identification of Emerging Contaminants from a Waste Water Influenced Water Body Using High Resolution Accurate Mass LC/MS and Statistical Analysis; Jerry Zweigenbaum1; Tarun Anumol1; Linda Kennedy1; 1Agilent Technologies, Wilmington, DE; 2Mansfield University of Pennsylvania, Mansfield, PA

2:30-4:30 pm WEDNESDAY IMAGING: BIOMEDICAL APPLICATIONS Bindesh Shrestha (Waters Corporation)

Stars Ballroom 2-3, level 3

WOD pm 02:30 Guided DESI-MS Imaging Allows Accelerated Mapping of Heterogeneity in Breast Cancer; Alessandra Tata1; Michael Woolman1; Milan Ganguly1; Manuela Ventura1; Nicholas Bernards1; Adam Gribble2; Alex Vitkin2; Howard Ginsberg3; 1University of Health Network, Toronto, Canada; 2University of California, Los Angeles, CA; 3Northwestern University, Evanston, IL

WOD pm 02:50 Three-dimensional MALDI Imaging to Understand Metastasis in Pediatric Medulloblastomas; Martin R L Paine1; Jingbo Liu1; Danning Huang1; Shane R Ellis1; Ron M A Heeren1; 1St. Michael Hospital, Toronto, Canada

WOD pm 03:10 Formalin-Fixed Paraffin Embedded Tissue Analysis by DESI-MSI and its Potential Use in Diagnostics; Renata Soares1; James McKenzie1; Anna Mróz1; Francesca Rosini1; James L Alexander1; Robert Goldin1; Zoltan Takata1; 1Imperial College London, London, United Kingdom

WOD pm 03:30 Redefining the Pathogen-host Interaction: Imaging Mass Spectrometry Reveals Staphylococcus Aureus Proteins within Host Tissues; Jessica Moore1; Neal D. Hammer1; Kristie M Lindsey Rose1; Jeffrey M Spraggin1; James Cassal1; Eric P Skaar2; Richard M Caprioli1; 1, 2Vanderbilt University MSRC, Nashville, TN; 3Michigan State University, East Lansing, MI
2:30-4:30 pm WEDNESDAY

MS IN THE REGULATORY ENVIRONMENT

Jennifer Liu (Amgen)

Hemisfair Ballroom 3, level 3

WOF pm 02:30

The Use of Mass Spectrometry in FDA Applications for Biotherapeutics: A Retrospective Review; Sarah Rogstad1; Anneleise Faustino1; David Keire2; Michael T Boyne2; Jun Park3; 1FDA, Silver Spring, MD; 2Food and Drug Administration, St. Louis, MO; 3Biotechlogic, Chicago, IL

WOF pm 02:50

The Roles and Opportunities for Mass Spectrometry in Regulatory CMC Submissions; Heidi Zhang; Genentech, SSF, CA

WOF pm 03:10

Quantitative Analysis of Influenza Vaccine Antigens: How Does the H3 Method Compare to Methods Requiring Labeled Isotopes?; Daryl G S Smith1; Lisa Walrond1; Marybeth Creskey1; Genevieve Gingras1; Yves Aubin1; Caroline Gravel1; Sean Li1; 1Terry D Cyr1; 2Nathalie Mechin2; Richard B. Cole1; 3Biotechlogic, Faustino1; David Keire2; Michael T Boyne3; Jun Park4; 1FDA, Silver Spring, MD; 2Food and Drug Administration, St. Louis, MO; 3Biotechlogic, Chicago, IL

WOF pm 03:30

Development of a LC-SRM Method Based on Anion Attachment Mass Spectrometry for Improved Detection of Neutral Anabolic Androgenic Steroids; Quentin Dumont1; Marianna Barcenas1; Isabelle Bailloux1; Corinne Buisson1; Nathalie Mechin1; Richard B. Cole1; 1Terry D Cyr1; 2Nathalie Mechin2; Richard B. Cole1; 3Biotechlogic, Faustino1; David Keire2; Michael T Boyne3; Jun Park4; 1FDA, Silver Spring, MD; 2Food and Drug Administration, St. Louis, MO; 3Biotechlogic, Chicago, IL

WOF pm 03:50

NISmAb Reference Material 8671: A Tool for Advancing Biopharmaceutical Mass Spectrometry; John Schiel1; Trina Formolo2; Abigail Turner2; Katharina Yandroski2; 1NIST, Gaithersburg, MD; 2NIST, Rockville, MD

WOF pm 04:10

The Challenges in Quantifying Tree Nut Residues of Phosphonic Acid and its Salts with LC-MSMS and CESI-MSMS; Simeon V Dovinci1; Yehia M Ibrahim2; Ian K Webb3; Ahmed M Hamid1; Liuliu Deng1; Erin S Baker1; Xueyun Zheng4; Richard D Smith5; 1Pacific Northwest National Laboratory, Richland, WA; 2DFA of California, Fresno, CA - California; 3University of Zagreb, Zagreb, Croatia; 4Institute of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 5Department of Pathology, Medical School Zagreb, University of Zagreb, Zagreb, Croatia

2:30-4:30 pm WEDNESDAY

NEW SEPARATIONS APPROACHES COUPLED TO MS

Michael L. Heien (University of Arizona)

Hemisfair Ballroom 1, level 3

WOH pm 02:30

Fundamentals of Ion Dynamics in Structures for Lossless Ion Manipulations (SLIM); Sandiya V R Garmella1; Yehia M Ibrahim2; Ian K Webb3; Ahmed M Hamid1; Liuliu Deng1; Erin S Baker1; Xueyun Zheng4; Richard D Smith5; 1Pacific Northwest National Laboratory, Richland, WA; 2DFA of California, Fresno, CA - California; 3University of Zagreb, Zagreb, Croatia; 4Institute of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 5Department of Pathology, Medical School Zagreb, University of Zagreb, Zagreb, Croatia

WOH pm 03:10

A Novel Sensitive Sheathless CE-MS Device for Peptide and Protein Analysis; Tam T T N. Nguyen1; Nickolaj J. Petersen2; Kasper D. Rand1; 1University of Copenhagen, Copenhagen, Denmark; 2Department of Haematology, Mater Misericordiae University Hospital, Dublin, Ireland; 3Faculty of Science University Zagreb, University of Zagreb, Zagreb, Croatia; 4Institute for Pathology and Cytology, University Hospital Merkur, Zagreb, Croatia; 5Department of Pathology, Medical School Zagreb, University of Zagreb, Zagreb, Croatia

WOH pm 03:30

Developing an Ultra UltraHigh Pressure Liquid Chromatography (UHPLC) system for LC-MS Based Metabolomics; Beixi Wang1; Jeremy Felton1; Paige Malec1; Stephanie Moore2; James Treadway2; Dan Lunn3; James Jorgenson2; Robert Kennedy1; 1University of Michigan, Ann Arbor, MI; 2University of North Carolina at Chapel Hill, Chapel Hill, NC; 3Department of Chemistry, University of Wisconsin - Madison, Madison, WI; 4Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 5Molecular and Biological Sciences, University of Wisconsin-Madison, Madison, WI

WOH pm 03:50

Characterization of the Sarcomeric Proteome by Multidimensional Liquid Chromatography Fractionation and Top-down High-Resolution Mass Spectrometry; Trisha Tucholski1; Wenxuan Cai1,2; Andrew J Alpert1,2; Bifan Chen1; Yuting He1; Ying Ge1,2; 1Department of Chemistry, University of Wisconsin - Madison, Madison, WI; 2Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; 3Department of Pathology, Medical School Zagreb, University of Zagreb, Zagreb, Croatia
There are light refreshments in common areas.

01 Bioanalysis: Current Status of Strategy and Practice of a Tiered Approach (Regulated Bioanalysis Interest Group)
Fabio Garofolo and Jian Wang presiding
Room 220, level 2
The workshop will review the recent development and current status of strategy and practice of tiered approach in bioanalysis. The recommendations from various bioanalytical societies and organizations such as Global Bioanalytical Consortium (GBC) and European Bioanalytical Forum (EBF) and from Crystal City Conferences will be discussed. A pre-workshop survey will be conducted among ASMS members on the tiered approach in bioanalysis. The workshop will provide an opportunity for attendees to exchange opinions, experiences, and practices with the ultimate goal of having a better understanding of how to apply a tiered approach as part of the bioanalytical strategy.

02 Large-Scale Analysis of MS Big Data: From Data to Knowledge and Back
Nuno Bandeira presiding
Room 221, level 2
Advances in mass spectrometry instrumentation, integration with genomics/transcriptomics data and the public availability of hundreds of Terabytes of mass spectrometry data have created significant challenges for the analysis of proteomics and metabolomics data. This workshop will focus on publicly available algorithms and resources illustrating how distributed computing and mass spectrometry data repositories can be used to assist with the analysis of newly acquired data. Furthermore, we will also discuss ways to productively engage the mass spectrometry community in aggregating their contributions into a community-wide knowledge base reusable for both experimental design and continuous reanalysis towards complete annotation of public mass spectrometry data.

03 FTMS: Day-to-Day Concerns for High Resolution Mass Analysis (FTMS Interest Group)
David Kilgour and Don Smith presiding
Room 225A, level 2
This year’s workshop will be a round-table discussion focusing on day-to-day considerations for optimum FTMS operation and data collection. A poll will be taken prior to the workshop to determine the most popular discussion points. In addition, there will be an open discussion on any other points of interest. What are the most important opportunities to make the next generation of FTMS instruments better than the current ones? What are the most common day-to-day struggles that FTMS users encounter? Worried about mass calibration or mass errors? Bad or variable sensitivity? Instrument maintenance? Data processing and confidence in results? There are many more besides these. But, which are the most important to us as a community and can we use this information to shape our own future? Our aim will be to identify those key priority areas which might inform future programs for improving the capabilities offered by FTMS instrumentation.

04 Novel Mass Spectrometry Instrumentation: Moving into the Hands of Practitioners (Forensics & Homeland Security Interest Group)
Guido Verbeck presiding
Room 225B, level 2
Researchers are pushing the limits on trace forensic analysis and novel sampling techniques. They are also making mass spectrometry (MS) portable and durable for direct field applications; not just gas inlet, but liquid and solid sampling also. Recent developments in portable mass spectrometry present several interesting questions for workshop attendees to discuss. Questions for discussion include: Is it possible to create a reliable analytical tool that is “red light - green light”? Can portable MS become a tool that first responders can use without the need for extensive training? Will portable MS be considered a screening or a confirmatory method of analysis (e.g. by SWGDRUG) or will the error rates be measured (e.g. to meet Daubert requirements). How readily will portable MS be admissible in court? Could on-site measurements influence the way the criminal justice system operates and thereby save money?
Here we will explore these issues, and have a series of presentations that include portable MS developers and representatives from the practitioner/law enforcement perspectives. We will explore the courtroom, and what burden-of-proof is laid at the feet of the tool developer. A discussion will be moderated about moving portable MS forward as the presumptive test, as well as the prosecutorial final test.

05 Photoionization: New Developments (Photoionization MS Interest Group)
Jack Syage and Ralf Zimmermann presiding
Room 225C, level 2
This will be the fourth year for a Photoionization (PI) workshop. Previous ones were very successful with strong turnout and varied and vigorous discussions. There are two flavors of photoionization currently being practiced today: (1) atmospheric pressure photoionization (APPI) is a commercial technology and practiced mostly on LC/MS instrumentation though there are vibrant growing new applications in direct ambient analysis, GC/MS and direct vapor (or vaporized) sample analysis. (2) Vacuum photoionization more commonly referred to as single-photon ionization (SPI) involves VUV light sources including lasers that ionize sample inside the vacuum chamber and is more of a research tool for studying spectroscopic properties of molecules, but also finding powerful applications in air monitoring particularly pollutant monitoring such as vehicle or flue exhaust.
In this fourth year we will focus on new applications. APPI and PI are finding unique uses in high volume applications, most specifically explosives detection in security environments for its unique benefits that are not provided by competing ionization methods.
06 The NIH Review and Funding Process
Charles Edmonds, Salvatore Sechi, and Douglas Sheeley presiding
Room 225D, level 2
A major source of financial support for many ASMS members and participants is the National Institutes of Health. During this workshop the general funding and review process of grant proposals will be presented. Issues like identifying the best NIH contact, writing an effective application, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. A "mock" NIH study section presentation will provide additional insight into the review process and opportunity for discussion with NIH staff. Substantial time will be allotted for discussion and questions.

07 Entrepreneurship: Creating a Job in Mass Spectrometry
Alexandre Shvartsburg presiding
Room 301A, level 3
Much of the employment growth and technological advance in North America has lately come from start-ups. While spectacular successes of young companies in the IT and new media arena are widely covered and acclaimed, the entrepreneurial opportunities in other hi-tech areas are much less known. In mass spectrometry, start-ups have hugely contributed to the maturation of novel instrumentation and methods that define the frontline of our field and provided exciting and gainful employment for many analytical chemists including recent graduates.

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

08 Protein Quantitation (Absolute) by LC-MS: Biomarker and Biotherapeutic
Dawn Dufield and Nalini Sadagopan presiding
Room 301BC, level 3
With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

09 Isomeric Glycans: Characterization & Quantitation
Yehia Mechref presiding
Room 302A, level 3
Glycosylation of proteins is one of the most common protein posttranslational modifications (PTM). A correlation between changes in the glycan moieties of glycoproteins and many mammalian diseases, including hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been suggested. The diverse biological roles of glycans and their implications in diseases have created a demand for reliable glycomic strategies, permitting sensitive monitoring of isomeric glycans in biological systems. These strategies are needed to better understand the roles and attributes of glycan in biological systems. In this workshop, the use of different MS/MS and LC-MS/MS strategies for the compressive characterization of glycan isomers will be critically described and discussed. These strategies employ several separation and mass spectrometric techniques, including liquid chromatography (different modes), matrix-assisted laser desorption ionization-mass spectrometry (MALDI-MS), and electrospray ionization-mass spectrometry (ESI-MS).

10 Protein Therapeutics: Characterization using MS (Biotherapeutics Interest Group)
Damian Houde and Ashley Ruth presiding
Room 302BC, level 3
This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will begin with a discussion of hot topics identified at this year’s Sanibel Conference on Protein Therapeutic Characterization. This may include a variety of topics, ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.

11 The Exposome: MS-based Metabolomic Workflows to Characterize the Exposome (Exposomics Interest Group)
Anthony Macherone presiding
Room 303A, level 3
The exposome compliments the genome and integrates genetic information with non-genetic exposures and the associated biological response pathways in the search for causative factors of chronic human disease. Within the exposome paradigm, the internal environment is composed of all bio-active chemicals circulating in the body regardless of their origin e.g. genetically derived or exposure derived. Examples include dietary chemicals, drugs, persistent organic pollutants, bio-transformation products (metabolites), foreign DNA, reactive electrophiles adducted to human serum albumin and other sources of exposure (e.g., noise pollution, place of residence, lifestyle choices, etc.) that stimulate biochemical responses.

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

12 Biomarker Translation: Quality Control & Quality Assurance (Clinical Chemistry Interest Group)
Timothy Garrett and Brian Rappold presiding
Room 303BC, level 3
Quality control and quality assurance (QC/QA) procedures for translating discovery assays to clinical use are poorly, if at all, defined. This workshop will offer brief topic introductions regarding the expectations of QC/QA in clinical diagnostics for multimarker assays, including algorithm based assessments. A similar dearth of QC/QA procedures is found in technologies which are highly naive to the industry, such as high resolution MS and tissue/ imaging. As such, speakers from the field will introduce concepts related to QC/QA in such methodologies to enable discussion amongst the group. Hopefully, such discussion will introduce new approaches to ensuring quality in translational workflows for all attendees.
It is increasingly common for Imaging MS to make up part of multimodal imaging studies in which a set of different image types are brought to bear on the same or related samples. Analytical approaches that characterize a sample using different principles, measuring for example functional, chemical, as well as biological information within a single experiment, can often provide insights not available from a single modality alone. While multimodal imaging that includes a mass spectral modality has greatly advanced, different research groups have gone about such studies with widely-varying workflows and approaches. In this workshop, we want to discuss how challenges can be tackled at the sample preparation, at the instrumental, as well as at the computational level. Furthermore, we want to see whether an overall direction for the field and a set of best practices can be distilled, complemented by a list of major challenges that yet need to be tackled. The central topic of the workshop will therefore be “Imaging by Mass Spectrometry as part of Multimodal Imaging Studies”.

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

1. Experimental design - How to design a good multimodal imaging MS experiment? (e.g., What modalities to acquire? How to make the collected image types synergistic and not just a simple combination?)
2. Measurement - How to acquire the different image types? (e.g., How do you properly prepare the sample for multimodal measurements? Is it better to integrate mass spectrometry and other image type measurements into a single device? Or are we better off keeping separate instruments?)
3. Data analysis - How can multimodal data be brought together, and what are the advantages and disadvantages of the different approaches? (e.g., What are the different strategies to handle/visualize multimodal data sets?)

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

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

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

The workshop will be led by both developers and users well-versed in others. An overview of the current state of software available in Galaxy for proteomics and multi-omics applications will also be provided.

Attendees are encouraged to bring a laptop computer to participate.
NEW DEVELOPMENTS IN IONIZATION AND SAMPLING FOR DMPK

Naidong Weng (Johnson & Johnson)
Stars Ballroom 1, level 3

Coated Blade Spray-Mass Spectrometry (CBS-MS) as a Versatile Approach for Quantitative Analysis in Small and Large Sample Volumes of Biofluids: German Augusto Gomez-Brosi; Nathaly Reyes-Garcés; Ezel Boyacı; Justen Poole; Janusz Pawliszyn

Functionalized Sampling Probe for Direct Mass Spectrometry Analysis of Lipids in Blood Samples: Wenpeng Zhang; Zheng Ouyang

Microfluidic Electrochemical Cell for Studying the Adduct Formation of Reactive Metabolites by ESI-MS: Tina Wigger; Floris T.G. van den Brink; Mathieu Ödijk; Wouter Oltius; Albert van den Berg; Uwe Karst

Effective Coupling of CE with nanoESI MS via a True Sheathless Metal-coated Emitter Interface for Robust and Sensitive Sample Quantification: Keqi Tan; Xuejiang Guo; Thomas Fillmore; Yuqian Gao

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

Development of a Novel Rapid Evaporative Ionisation Mass Spectrometry (REIMS) Platform ‘Endoscope’ for in vivo Chemical Histology during Colonoscopy: James Alexander; Louise Gildes; Julia Balog; Abigail Speller; Anna Mroz; Alasdair Scott; James McKenzie; Kirill Veselkov; Robert Goldin; James Kinross; Jonathan Hoare; Julian P Teare; Zoltan Takats; Imperial College London, United Kingdom; Waters, Manchester, United Kingdom

Rapid Identification of Carbapenem-resistant Klebsiella Pneumoniae using High-Resolution Tandem Mass Spectrometry: Raja Sekhar Nirujogi; Sreelakshmi K Sreenivasamurthy; Santosh Renuse; Pranita J Tamma; Patricia J Simner; Akhilesh Pandey; Nathaly Reina; Robert-Jan Hassing; Wil Goessens; Lona Waldron; Jeffrey D. Steimle; Nicholas C. Gomez; Stanley Velileka; Robert Goldin; James Kinross; Jonathan Hoare; Julian P Teare; Zoltan Takats; Imperial College London, United Kingdom; Waters, Manchester, United Kingdom

Ultrafast Detection of Amino Acid Substitutions in DNA Gyrase A Related to Fluoroquinolone-Resistant Typhoidal Salmonella Isolates using PRM: Robert-Jan Hassing; Wil Goessens; Lona Zeneyedpour; Sadaf Sultan; Jeroen van Kampen; Annelies Verbon; Perry van Gendehren; John Hayes; Theo Luijder; Fernard Dekker; Erasmus Medical Center, Rotterdam, Netherlands; Havenziekenhuis, Rotterdam, The Netherlands

A Physical and Genetic Interaction between the Cardiac Transcription Factor Tbx5 and Chromatin Remodeling Complexes is Essential for Cardiac Septation: Todd M. Greco; Lauren Waldron; Jeffrey D. Steimle; Nicholas C. Gomez; Marilyn Stearns; Junghun Kweon; Brenda Temple; Xinan Holly Yang; Caralynn M. Wilczewski; Ian J. Davis; Ivan P. Moskwitcz; Frank L. Conlon; Ileana M. Cristea; Princeton University, Princeton, NJ.
8:30-10:30 am THURSDAY
GLYCOPROTEINS AND GLYCOPROTEINS
Franklin E. Leach III (Photochemical Technologies)

Hemisfair Ballroom 4, level 3

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

ThOE am 08:50
Comprehensive Glycoproteomics of Glioblastoma Biospecimens: Chun Shao1; Joshua Klein1; Joanna Phillips2; Joseph Zaia3; "Department of Biochemistry, School of Medicine, Boston University, Boston, MA; "Department of Neurological Surgery and Pathology, University of California, San Francisco, San Francisco, CA

ThOE am 09:10
Quantification of Human Cell Surface N-Glycoprotein Dynamics: Haopeng Xiao1; Ronghu Wu1; "Georgia Institute of Technology, Atlanta, USA

ThOE am 09:30
Isomeric Separation of Glycopeptides using Aporous Graphitic Carbon (PGC) LC-MS Platform: Rui Zhu1; Jingfu Zhao1; Aying Yu1; Yehia Mechref1; "Texas Tech University, Lubbock, Texas

ThOE am 09:50
Advanced Workflows and Concepts for the Analysis of High Throughput Targeted Proteomics Experiments of Large Heterogeneous Datasets: Isabell Bludau1; George Rosenberger2; Ben Collins1; Uwe Schmidt1; Patrick Pedrioli1; Ruedi Aebersold2; "ETH Zurich, Zurich, CH; "ID Scientific IT Services, ETH Zurich, Zurich, CH

ThOE am 10:10
Detection and Quantification of Proteins in SWATH-MS Analysis without using Spectral Libraries: Stephen A. Tate1; jamie Sherman1; Pradeep Narayanaswamy1; "SCEIX, Concord, ON; "University of Michigan, Ann Arbor, MI; "EMBL-EBI, Hinxton, UK

8:30-10:30 am THURSDAY
APPLICATION OF STABLE ISOTOPE LABELING IN MS
Jim Edwards (Saint Louis University)

Hemisfair Ballroom 2, level 3

ThOG am 08:30
Quantity: An Isobaric Tag for Quantitative Glycomics: Shuwei Wang1; Chen Sun2; Xiaoshi Wang1; Zuo-Fei Yuan1; Jing Fan1; Kelly R. Karch1; Lauren E. Ball1; John M. Denu1; Benjamin A. Garcia1; "University of Pennsylvania School Of Medicine, Philadelphia, PA; "University of Wisconsin Madison, Madison, WI

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

Hemisfair Ballroom 3, level 3

ThOF am 08:50
A Novel Framework for Spectral Assay Library Construction and Targeted Quantitative Data Extraction in Metabolomics with Data Independent Acquisition: Genobo Chen1; Scott Walmsley2; Lei Zhou3; Liyan Chen4; Ching-Yu Cheng5; Roger W. Beumer1; Tien-Yin Wong1; Gemmy C.M. Cheung6; Hyungwon Choi7; "National University of Singapore, Singapore, Singapore; "University of Colorado Denver-Anschutz In Aurora, CO, Denver, USA; "Singapore Eye Research Institute, Singapore, Singapore; "Duke-NUS Graduate Medical School, Singapore, Singapore

Targeted Analysis of MS1 Data for Quantitative Studies: Roland M. Bruderer1; Yue Xuan1; Ian Lienert1; Oliver M. Bernhardt1; Tejas Gandhi1; Lukas Reiter1; "Biognoys AG, Schlieren, Switzerland; "Thermo Fisher Scientific, Bremen, DE

ThOF am 09:10
Benchmarking SWATH by LQGBench: a Multi-Centered Study Evaluates and Improves Data-Independent-Acquisition-Based Label Free Quantitative Tools: Pedro Navarro1; Joerg Küharev2; Ludovic C. Gillet1; Oliver M. Bernhardt1; Brendan MacLean1; Stephen Tate1; Chih-Chiang Tsou2; Lukas Reiter1; George Rosenberger2; "University of Colorado Denver-Anschutz In Aurora, CO, Denver, USA; "Singapore Eye Research Institute, Singapore, Singapore; "Duke-NUS Graduate Medical School, Singapore, Singapore
High-Performance Chemical Isotope Labeling LC-MS for Tracking Disease Progression: Metabolomic Study of Alzheimer’s Disease in a Mouse Model; Liao Li; Wei Han; Kevin Hooton; Dorothea Mung; Keding Cheng; Sharon Simon; David Knox; University of Alberta, Edmonton, Canada; Public Health Agency of Canada, Winnipeg, Canada

An Integrated Workflow for Qualitative Fluix Analysis by Accurate Mass LC/MS; Stephen Madden; Alex Apfel; Xinning Jiang; Ed Darland; Yinghang Yang; Xiangdong Li; Crystal Cody; Norton Kitagawa; Agilent Technologies, Inc., Santa Clara, CA; Agilent Technologies, Santa Clara, CA

8:30-10:30 am THURSDAY ION MOBILITY: STRUCTURE Hemisfair Ballroom 1, level 3

An Ion Mobility, Molecular Dynamics, Top-Down and H/DX Study of Monoclonal Antibody Structural Collapse in the Gas-phase: Iain D.G. Campuzano; Morgan Lawrence; Carlos Larriba-Andaluza; Huilin Li; Ulrik H Mistarz; Kasper Rand; Joseph Loo; Amgen, Inc., Thousand Oaks, CA; Indiana University-Purdue University, Indianapolis, IN; UCLA, Los Angeles, CA; University of Copenhagen, Copenhagen, Denmark

Analysis of Protein Structural Changes with High Resolution Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-Mass Spectrometry; Ian K. Webb; Liulin Deng; Ahmed M Hamid; Gordon A Anderson; Randolph V Norheim; Spencer A Prost; Sandiya V. B. Garimella; Erin S Baker; Yehia M Ibrahim; Jeffrey Agar; Northeastern University, Boston, MA; Bruker Daltonic, Billerica, MA

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

Combining Ion Mobility with Cryogenic Ion Spectroscopy for Filtering Peptide Structure on the Way from Solution to the Gas Phase: Liludmila Voronina; Antoine Masson; Michael Kamrath; David E Clemmer; Carsten Baldauf; Thomas R Rizzo; Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; UC Berkeley, Berkeley, CA

Insights from TIMS-MS, IR Spectroscopy and Molecular Dynamics on Nicotinamide Adenine Dinucleotide Structural Dynamics: NAD+ vs NADH; Juan Camilo Molano; Walter Gonzalez; Jaroslava Mikosovska; Philippe Maître; Francisco Fernandez Lima; Florida International University, Miami, FL; Laboratoire de Chimie Physique, Orsay, Orsay, France

Polymers as Model Systems to Understand Ion Mobility Mass Spectrometry Structures in Gas Phase; Jean R. N. Haler; Denis Morsa; Johann Far; Christline Jérome; Edwin De Pauw; Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; CERM, University of Liege, Liege, Belgium
ThOA pm 03:50  Instantaneous Determination of Cocoa Content and Cocoa Bean origin of Commercial Products with Rapid Evaporative Ionization Mass Spectrometry; Julia Balog¹ ²; Richard Schäffler¹; Tamas Juhász¹; Tamas Karancsi¹; Steven D Pringle²; Zoltan Takats²; ¹Waters Research Centre, Budapest, Hungary; ²Imperial College London, London, United Kingdom; ³Waters, Milwaukwe, United Kingdom

ThOA pm 04:10  Classification of Olive Oils using Direct Analysis Atmospheric Pressure Chemical Ionization-Mass Spectrometry; Pablo Perez-Hurtado¹; Amy Giles¹; Mark Allen¹; Lourdes Arce³; Matthew Turner¹; Jim Reynolds¹; ¹Loughborough University, Loughborough, United Kingdom; ²Advice UK Ltd, Essex, United Kingdom; ³Universidad de Cordoba, Cordoba, SPAIN; 4Loughborough University, Loughborough, Leicestershire

2:30-4:30 pm THURSDAY FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION

Arpad Somogyi (The Ohio State University) Room 221, level 2

ThOB pm 02:30  Charge Transfer Dissociation (CTD): High Energy Radical Fragmentation of Glycans, Peptides and Lipids; Glen Paul Jackson¹; Iris Kret¹; Pengfei Li¹; David Ropartz¹; Hélène Rogniaux¹; ¹West Virginia University, Morgantown, WV; ²INIRA, UR1268 Biopolymers Interactions Assemblies Nantes, France

ThOB pm 02:50  Improvement of Hydrogen Attachment/Abstraction Dissociation (HAD) Efficiency for Low-Charged Peptides using Supplemental Activation; Hidori Nakashima¹; Sadanori Sekiya¹; Takashi Nishikaze¹; Shosei Yamauchi¹; Shinichi Iwamoto¹; Motoki Wada¹; Koichi Tanaka¹; ¹Shimadzu Corporation, Kyoto, Japan; ²Doshisha University, Kyotanabe, Japan

ThOB pm 03:10  Conformational Effects on the Dissociation Kinetics of Proton-Bound Heterodimer Ions; Applications to Gas-Phase Acidities of Alkanols; Kent M. Ervin¹; Jerry G Lanorio¹; Surja B Ghale¹; Alex A Nickels¹; ¹University of Nevada, Reno, Reno, NV; ²Univeristy of Nevada, Reno Reno, NV

ThOB pm 03:30  Mobile C-H Protons in a Proton Deficient Peptide; Damodor Koirala¹; Paul G Wenthold¹; ¹Purdue University, West Lafayette, IN; ²Purdue University, West Lafayette, IN

ThOB pm 03:50  Tandem MS of Synthetic Nanoparticles through Analysis of Metastable Fragments using MALDI-TOF MS with Superconducting Tunnel Junction Cryodetection; Logan D Plath¹; Chenjie Zeng¹; Yuxiang Chen¹; Rongchao Jin¹; Mark E Bier¹; ¹XenoBiotic Laboratories, Inc. WuXi AppTec Inc Plainsboro, NJ; ²Cerno Bioscience, Yardley, PA; ³Cerno Bioscience, Norwalk, CT

ThOC pm 02:50  Understanding the Metabolism of Protein and Peptide Therapeutics by Developing a Top-Down Protein Metabolite Identification Platform; Xiang Yu¹; Arthur Fridman¹; Kristen A Kwasnik¹; Ping Lu¹; Zhiling Li¹; Sherrie Xu¹; Ansu Bagchi¹; Mark T Cancilla¹; ¹Merck & Co., West Point, PA

ThOC pm 03:10  Utilizing Tandem Mass Spectrometry for the Identification of Primary and Secondary Sulfonamide Functionalities in Protonated Analytes via Ion/Molecule Reactions; John Kong¹; Ravikiran Yerabolu¹; Huaming Sheng¹; Weijuan Tang¹; Raghavendhar Kotha¹; Chungang Gu¹; Hilika Kenttämaa¹; ²Purdue University, West Lafayette, IN; ³AstraZeneca, Boston, MA

ThOC pm 03:30  Software Aided Integrated Workflow for Identification of Metabolic "Soft-spots" of Macromolecular Peptides in Drug Discovery; Aoko Ranaasangko¹; Serhiy Hnatyshyn¹; Eugene Cicimaro¹; Celia D'Arienzo¹; Timothy Olay¹; ¹XenoBiotic Laboratories, Inc WuXi Asoka Ranasinghe¹; Serhiy Hnatyshyn¹; Eugene Cicimaro¹; Celia D'Arienzo¹; Timothy Olay¹; ¹XenoBiotic Laboratories, Inc. WuXi AstraZeneca, Boston, MA

2:30-4:30 pm THURSDAY AMBIENT IONIZATION: INSTRUMENTATION & APPLICATIONS

Nicholas Brunelli (The Ohio State University) Stars Ballroom 2-3, level 3

ThOD pm 02:30  Coupling Electrochemistry with Probe Electrospray Ionization Mass Spectrometry (PESI-MS); Yi Cai¹; Hao Chen¹; ¹Ohio University, Athens, OH

ThOD pm 02:50  Fundamental Studies of Inlet Ionization with Sample Introduction at Atmospheric Pressure; Sarah Trimpin¹; Stephan Rauschenbach¹; I-Chung Lu¹; Casey Foley¹; ¹Wayne State University, Detroit, MI; ²Max-Planck-Institute for Solid State Research, Stuttgart, Germany; ³Wayne State University, Detroit, MI

ThOD pm 03:10  Successful Direct SPME-DBDI Coupling for Rapid, Ultrasensitive and Non-Chromatographic Analysis of Pesticides and Illicit Drugs in Complex Matrices; Mario Francesco Mirabelli¹; Emanuela Gionfriddo¹; Janusz Pawliszyn²; Renato Zenobi¹; ¹ETH Zurich, Zürich, Switzerland; ²University of Waterloo, Waterloo ON, Canada

ThOD pm 03:30  Direct Biofluid Analysis using Hydrophobic Paper Spray Mass Spectrometry; Deidre Damon¹; Abraham Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH; ²The Ohio State University, Columbus, Ohio
THURSDAY AFTERNOON ORAL SESSIONS

2:30-4:30 pm THURSDAY

INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION
Natalie Castellana (Digital Proteomics LLC)
Hemisfair Ballroom 3, level 3

ThOF pm 02:30
A Graph-based Method for Proteoform Identification and Quantification by Top-down Multiplexed Tandem Mass Spectra; Zhu Kaiyuan1; Xiaowen Lü2; 1Indiana University, Bloomington, IN; 2Indiana, IN

ThOF pm 02:50
High Quality Estimation of False Discovery Rate for Proteoform Identification with Top Down Proteomics; Richard Leduc1; Daniel Shams2, 3; Ryan T Fellers1; Bryan Early1; Joseph Greer1; David Schwab2; Neil L Kelleher1, 4, 5, 6; 1Proteomics Center of Excellence, Northwestern University, Evanston, IL; 2Department of Physics and Astronomy, Northwestern University, Evanston, IL; 3Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; 4Department of Chemistry, Northwestern University, Evanston, IL; 5Department of Molecular Biosciences, Northwestern University, Evanston, IL

2:30-4:30 pm THURSDAY

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

ThOG pm 02:30
A Quantitative Positive/Negative Ion Switching Method for Shotgun Lipidomics via High Resolution LC-MS/MS from any Biological Source; Min Yuan1; Ying Xu1; Susanne Breitkopf1; Stephane Ricoult2; John M Asara1; 1National Physical Laboratory, Teddington, United Kingdom; 2ION-TOF GmbH, Munster, Germany; 3Thermo Fisher Scientific, Bremen, DE; 4GlaxoSmithKline, Stevenage, UK; 5University of Nottingham, Nottingham, UK

ThOG pm 02:50
Lipidomic Imaging with a New Hybrid 3D SIMS Molecular Imaging Instrument; Melissa K. Passarelli1; Alexander Pirk2; Rudolf Moellers2; Ewald Niehuis2; Alexander A Makarov2; Henrik Arlinghaus2; Rasmus Havelund2; Paulina Rakowska1; Alina Majonis2; Rasmus Havelund2; Melissa K. Passarelli1

2:30-4:30 pm THURSDAY

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

ThOE pm 02:30
Disrupted Stoichiometric Relationships as Biomarkers of Altered Cellular States; Marisia Bulian1; Tiannan Guo1; Qing Zhong1; Ulrich Wagner2; Li Li2; Andreas Beyer2; Peter Wild2; Ruedi Aebersold1; 1Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; 2Institute of Surgery, University Hospital Zurich, Zurich, Switzerland; 3University of Cologne, Cologne, Germany

ThOE pm 02:50
Understanding Biological Heterogeneity through Mass Cytometry; Jennifer Frahm1; Christina Loh2; Tad George2; Mark Konrad1; Olga Ovastsky1; Daniel Majonis1; Andrei Terekidi1; Gary Impey1; 1Fluidigm Corporation, South San Francisco, CA USA; 2Fluidigm Canada Inc., Markham, CANADA

ThOE pm 03:10
Antibody-Independent, Deep-Dive Targeted Quantification of Proteins at Ten Picogram per Milliliter Levels in Non-Depleted Human Serum/Plasma; Song Nie1; Tujin Shi1; Thomas Fillmore1; Yuguian Gao1; Athena A Shepmoes1; Heather Brewer1; Wei-juan Qian1; Karin D Rodland1; Richard D Smith1; Tao Lu1; 1Biological Sciences Division and Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

ThOE pm 03:30
Mass Spectrometry Based Identification and Quantitation of Maturation Stage Specific Surface Markers of Human Stem Cell Derived Cardiomyocytes; Matthew Waas1; Erin Kropp1; Alyssa Nyvz1; Chelsea Fujinaka1; Rebekah Gundry1; 1Medical College of Wisconsin, Milwaukee, WI

ThOE pm 03:50
Discovery and Quantitative Metabolomics to Characterize Metabolites of Bacterial Origin as Biomarkers for Cystic Fibrosis; Jace W Jones1; Angela Nguyen1; Bennett Giardina1; Luke Brewer1; Angela Wilks1; Amanda Oegsby-Sherrouse1; Matthew M Champion1; 1University of Oklahoma, Dept. of Chem & Biochem Norman, OK

ThOE pm 04:10
Quantifying Concentrations of Molecules in Live Single Cells using the Single-probe MS Technique; Ning Pan1; Wei Rao1; Haiqing Yu1; Naga Rama Kothapalli1; Mei Sun1; Anthony Burgett1; Zhibo Yang1; 1University of Oklahoma, Bloomington, IN; 2Indiana University, Bloomington, IN; 3University of Michigan, Ann Arbor, MI

2:30-4:30 pm THURSDAY

INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION
Natalie Castellana (Digital Proteomics LLC)
Hemisfair Ballroom 3, level 3

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2:30-4:30 pm THURSDAY

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

ThOG pm 02:30
A Quantitative Positive/Negative Ion Switching Method for Shotgun Lipidomics via High Resolution LC-MS/MS from any Biological Source; Min Yuan1; Ying Xu1; Susanne Breitkopf1; Stephane Ricoult2; John M Asara1; 1National Physical Laboratory, Teddington, United Kingdom; 2ION-TOF GmbH, Munster, Germany; 3Thermo Fisher Scientific, Bremen, DE; 4GlaxoSmithKline, Stevenage, UK; 5University of Nottingham, Nottingham, UK
GENERAL INFORMATION

PAGE 56      64TH ASMS CONFERENCE ON MASS SPECTROMETRY

THURSDAY AFTERNOON ORAL SESSIONS

ThOG pm 03:10
Electron-induced Dissociation (EID) of Lipids: Diagnostic Product Ions for Confident Identification of Isomers; Jace W. Jones1; Claire Louise Carter1; Maureen A Kane1; 1University of Maryland, School of Pharmacy Baltimore, MD

ThOG pm 03:30
Broad Characterization of Isomeric Lipids by High-Resolution Differential Ion Mobility Separations with Tandem Mass Spectrometry; Rinat R Abzalimov1; Andrew Bowman2; Alexandre A Shvartsburg3; 1City University of New York - Advanced Science Research Center, New York City, NY; 2City University of New York - Advanced Science Research Center, New York City, NY; 3Wichita State University, Wichita, KS

ThOG pm 03:50
Nano-DESI Imaging of Lipids and Metabolites in Developing Lung; Son N. Nguyen1; Ryan L Sontag1; Richard A Corley2; Charles K Ansong3; Mathew Thomas4; James Carson5; Julia Laskin1; 1Pacific Northwest National Laboratory, Richland, WA; 2University of Texas at Austin, Austin, TX

ThOH pm 04:10
In depth Sphingomyelin and Triacylglycerol Structure Identification using Electron Impact Excitation of Ions from Organics (EIEIO) and Mass Spectrometry; Takashi Baba1; Larry J Campbell1; Yves J C LeBlanc1; Paul RS Baker2; 1SCIEX, Concord ON, Canada; 2SCIEX, Redwood City, CA

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

ThOH pm 02:30
HX-MS Epitope Mapping of a Ricin Toxin Chain A Double Mutant (RTA*); Ronald Toth1; Siva Krishna Angalakurthi1; John Hickey1; Sangeeta Joshi1; Charles Russell Middaugh2; Greta Van Slyke3; Nicholas Mantis1; David Volkin4; David Weis5; 1Department of Pharmaceutical Chemistry and Macromolecule and Vaccine Stabilization Center; University of Kansas, Lawrence, KS; 2Division of Infectious Disease, Wadsworth Center, New York State Department of Health, Albany, NY; 3Department of Biomedical Sciences, University at Albany School of Public Health, Albany, NY; 4Department of Chemistry and R. N. Adams Institute for Bioanalytical Chemistry; University of Kansas, Lawrence, KS

ThOH pm 02:50
The Role of Conformational Dynamics in Differing Activity and Substrate Specificity amongst Isozymes; Andrew Fairman1; Peter Sidhu2; David Joseph3; Derek Wilson4; 1York University, Toronto, Canada; 2University of Guelph, Guelph, Canada

ThOH pm 03:10
Structural basis for the formation and function of the complement effector protein iC3b; Malvina Papanastasiou1; Sophia Koutsogiannaki2; Yiannis Sarigiannis3; Daniel Ricklin4; John D. Lambris1; 1Dept. Pathology & Lab. Medicine, Perelman School of Medicine, UPENN, Philadelphia, PA

ThOH pm 03:30
A New Automation Platform Provides Significant Improvements in Both the Capacity and Flexibility of the HDX-MS Experiment; Ruben Haro1; Alfonso Espada1; Manuel Molina-Martin1; Jesus Castanon1; Bruce D Pascal2; Pat Griffin3; Jeffrey A Dodge4; Michael Chalmers5; 1Eli Lilly and Company, Alcobendas, SPAIN; 2The Scripps Research Institute, Jupiter, Fl; 3Eli Lilly and Company, Indianapolis, IN

ThOH pm 03:50
Intramolecular Interactions in Heme Oxygenase 2 in the Presence and Absence of Lipid Membranes; Brent A Kuchert1; Angela S Fleischacker1; Stephen W Ragsdale2; John R Engen3; 1Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; 2Department of Chemistry, University of Michigan, Ann Arbor, MI

ThOH pm 04:10
The Analytical Potential of HDXMS in Providing Localized Structural Dynamics Insight to Each Subunit of an Asymmetric Non-Crystallizable Protein Homodimer; Morten Beck Trelle1; Alice Østergaard2; Jeppe Buur Madsen1; Shona Pedersen1; Sørøe Risom Kristensen2; Thomas J.D. Jørgensen1; 1University of Southern Denmark, Odense, Denmark; 2Department of Clinical Medicine, Aalborg University Hospital, Aalborg, Denmark, Ålborg, Denmark

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

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

William Bialek
Princeton University

6:30 – 9:00 PM, THURSDAY CLOSING EVENT BRISCOE WESTERN ART MUSEUM
Ticket is required.
ODD-NUMBERED POSTERS PRESENT 10:30 AM - 1:00 PM. EVEN-NUMBERED POSTERS PRESENT 12:00 - 2:30 PM.

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

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

Antibodies & Antibody Drug Conjugates (Separations)..........................001 - 028
Biomarkers: Quantitative Analysis (Part 1)...........................................029 - 054
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling (Cross-Linking).................................055 - 075
Data Independent Acquisition (SWATH).............................................076 - 095
Drug Discovery/DMPK/ADME (Applications)..........................................113 - 129
Drug Metabolism: Qualitative and High Throughput Analysis..................130 - 144
Energy: Hydrocarbon & Petrochemical (Hi Res and Nominal)....................145 - 163
Environmental Analysis: General (Part 2)............................................164 - 188
FAIMS and DMS..................................................................................189 - 209
Food Safety (Pesticides in Food).........................................................210 - 235
Foodomics’ MS Characterization of Food and Nutritional Supplements (Part 1)...........236 - 250
Forensics (Part 1)...............................................................................251 - 278
Glycoproteins....................................................................................279 - 296
High Mass Accuracy/High Performance MS Methods and Developments ..........297 - 312
Imaging MS: Disease Markers ............................................................313 - 344
Imaging MS: Pharmaceutical Applications ............................................345 - 363
Immunomics: Peptide ID and Quantification ........................................364 - 391
Instrumentation: General..................................................................392 - 416
Instrumentation: New Developments in Mass Analyzers..........................417 - 442
Ion Mobility: Applications (Proteins & Peptides)......................................443 - 470
Ion Mobility: New Developments in Mass Analyzers..............................471 - 498
LC-MS: Chromatography and Software (Part 1).....................................499 - 518
Metabolomics: Sample Preparation.....................................................519 - 529
Microorganisms: Identification and Characterization..................................530 - 557
Microorganisms: Untargeted Metabolite Profiling (Cells/Plants)..................558 - 582
Nucleic Acids.....................................................................................583 - 605
Peptides: PTM Identification..................................................................584 - 605
Phosphopeptides: Quantitative Analysis................................................606 - 623
Proteins: Complexes/Non-covalent Interactions........................................624 - 659
Proteomics: Clinical Applications (Development toward Clinical Application)........660 - 681
Proteomics: Infectious Diseases .............................................................682 - 702
Proteomics: Quantitative (Application Biological Research).......................703 - 727
Small Molecules: Quantitative Analysis (Animal, Plant/Insect, and Methodology)........728 - 762
Top Down Protein Analysis (Applications)..............................................TP 728 - 762
Top Down Protein Analysis (Methodology).............................................TP 763 - 775

Antibodies & Antibody Drug Conjugates (Intact and Characterization)..........................001 - 020
Biomolecular Structure Analysis: Covalent Labeling and Related Software..........................021 - 039
Carbohydrates....................................................................................040 - 055
Data Independent Acquisition.............................................................056 - 070
Diagnostic Clinical Chemistry (Applications)..........................................071 - 094
Drug and Metabolite Analysis: Novel Approaches for Dried Biological Samples........095 - 103
Energy: Hydrocarbon and Petrochemical (Ultra Hi Res)..........................104 - 122
Environmental Analysis: General (Part 1)............................................123 - 147
Environmental Analysis: Pharmaceuticals and Pesticides..........................148 - 176
Epigenetic Modifications.....................................................................177 - 194
High Mass Accuracy/High Performance MS Applications..........................195 - 210
Imaging MS: Instrumentation...............................................................211 - 231
Imaging MS: Sample Preparation..........................................................232 - 243
Imaging MS: Software.........................................................................244 - 249
Informatics: Metabolomics.................................................................250 - 264
Informatics: Multiomics Integration......................................................265 - 280
Instrumentation: New Concepts............................................................281 - 302
Intact Proteins....................................................................................303 - 319
Ion Activation/Dissociation.................................................................320 - 340
Ion Mobility: Applications (Other/Instrumentation)..................................341 - 373
Ion Mobility: Applications (Other/Instrumentation)..................................341 - 373
Ion Molecule, Ion/Ion, Ion/Electron Interactions.......................................374 - 398
Ion Spectroscopy................................................................................399 - 411
LC-MS: Chromatography and Software (Part 1).....................................412 - 440
Lipids: General....................................................................................441 - 456
Metabolomics: General.......................................................................457 - 495
Microorganisms: Definition and Characterization......................................496 - 517
Phosphopeptides: Enrichment Methods................................................518 - 529
Polymers..............................................................................................530 - 548
Proteins: General and Membrane........................................................549 - 571
Proteins: PTMs (Part 1).................................................................572 - 596
Proteomics: Clinical Applications (Applied Proteomics)..........................597 - 621
Proteomics: Quantitative Analysis........................................................622 - 650
Small Molecules: Qualitative Analysis...................................................651 - 680
Systems Biology (Multiomics and Other)................................................681 - 707
Top Down Protein Analysis (Applications)..............................................708 - 727

64TH ASMS CONFERENCE ON MASS SPECTROMETRY PAGE 57
POSTER OVERVIEW

WEDNESDAY POSTERS

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

THURSDAY POSTERS

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

Ambient Ionization: Fundamentals and Instrumentation
(Probes, Paper Spray, DESI/ESI, Tissue/Tools)...........001 - 029
Antibodies & Antibody Drug Conjugates (Sequencing,
Modifications & Hi Res) .........................................030 - 061
Biomarkers: Discovery (Part 1).................................062 - 088
Biomarkers: Quantitative Analysis (Part 2) ..............089 - 116
Carbohydrates (Glycans) ........................................117 - 138
Carbohydrates (Glycans) ........................................117 - 138
Disease Biomarkers .................................................139 - 153
Drug Discovery/DMRP/ADME (General) ..............154 - 177
Energy: Biofuels and Algae .......................................178 - 189
Environmental Analysis: Water Quality .................190 - 206
Food Safety: Other Contaminants (Part 1) ..............207 - 235
Foodomics’ MS Characterization of Food and
Nutritional Supplements (Part 2) .........................236 - 252
Forensics (Part 2) ..................................................253 - 278
GCMS: Instrumentation and Applications
(Instrumentation-New Developments) ..................279 - 293
Glycoproteins (Tandem MS, Separations, and
Automation/Software) ...........................................294 - 313
H/D Exchange: Hardware, Software and Methodology ...314 - 327
H/D Exchange: Protein Structure/Function (Part 1) ...328 - 336
ICP and Isotope Ratio MS: Elemental .......................337 - 341
Imaging MS: Method Development (DESI/SIMS/Misc) ..342 - 364
Informatics: Algorithms and Statistical Advances ........365 - 389
Informatics: Workflow and Data Management ..........390 - 405
Instrumentation: Mini/Portable/Fieldable MS ..........406 - 425
Instrumentation: New Developments in Ionization
and Sampling (Sampling) ........................................426 - 438
Ion Mobility: Fundamentals .....................................439 - 463
Ion Structure/Energetics ..........................................464 - 482
LC-MS: Sample Preparation (Part 1) .......................483 - 504
Lipids: Profile Analysis ...........................................505 - 536
Metabolomics: Clinical Applications ......................537 - 549
Metabolomics: Untargeted Metabolite Profiling
(Animal/Human/Other) .......................................550 - 574
Nanoscale and Microfluidic Separations and MS .......575 - 586
Plant ‘omics’ ......................................................587 - 613
Protein Therapeutics: Quantitative Analysis .............614 - 650
Proteomics: New Approaches (Global) ...................651 - 674
Proteomics: Quantitative (Labeling/Tagging/MS/
Quantitation) ......................................................675 - 704
Small Molecules: Quantitative Analysis (Part 1) ......705 - 728

Ambient Ionization: Fundamentals and Instrumentation
(Dart/Plasma, Laser, SAWN) ...................................001 - 030
Biomarkers: Discovery (Part 2) ...............................031 - 058
Biomarkers: Quantitative Analysis (Small Molecules &
Metabolites) .....................................................059 - 089
Drug Metabolism: Quantitative Analysis ..................090 - 107
Food Safety: Other Contaminants (Part 2) ..............108 - 141
GCMS: Instrumentation and Applications (Applications) ...142 - 171
H/D Exchange: Protein Structure/Function (Part 2) ....172 - 195
Imaging MS: Method Development (MALDI) ...........196 - 215
Imaging MS: Small Molecules .................................216 - 247
Informatics: General, SRM, and DIA ......................248 - 269
Informatics: Protein ID and Quantification ...............270 - 281
Instrumentation: New Developments in Ionization
and Sampling (Ionization) .....................................282 - 308
Ionization Mechanisms ..........................................309 - 323
LC-MS: Sample Preparation (Part 2) .......................324 - 345
Lipids: Quantitative Analysis ...................................346 - 375
MALDI: Sample Preparation ....................................376 - 401
Metabolomics: Identification of Unknown Metabolites ....402 - 425
Metabolomics: Quantitative Analysis .....................426 - 446
Natural and Nanomaterials .....................................447 - 455
Peptides: Fragmentation Mechanisms ........................456 - 470
Peptides: Quantitative Analysis ..............................471 - 504
Peptides: Sequence Analysis .................................505 - 518
Peptidomics ........................................................519 - 530
Protein Therapeutics: Structural Characterization .......531 - 566
Proteins: Conformation Analysis and Structural Biology ....567 - 585
Proteins: PTMs (Part 2) ..........................................586 - 605
Proteomics: New Approaches (Other) ....................606 - 625
Proteomics: Quantitative (Pre-MS and Platforms/
Informatics/MultiOmics/Dynamics) .......................626 - 649
Proteomics: Tissue ...............................................650 - 675
Small Molecules: Quantitative Analysis (Part 2) .........676 - 698
Systems Biology (Protein Modifications and Cells) .......699 - 719
Toxicology ..........................................................720 - 748
**MONDAY POSTERS**

**Set up all Monday posters** .............................................7:30 – 8:00 am

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**Energy: Hydrocarbon and Petrochemical (Ultra Hi Res) ......104 - 122**

**Environmental Analysis: General (Part 1) .........................123 - 147**

**Environmental Analysis: Pharmaceuticals and Pesticides ....148 - 176**

**Epigenetic Modifications ..................................................177 - 194**

**High Mass Accuracy/High Performance MS Applications ...195 - 210**

**Imaging MS: Instrumentation .........................................211 - 231**

**Imaging MS: Sample Preparation ....................................232 - 243**

**Imaging MS: Software ....................................................244 - 249**

**Informatics: Metabolomics .............................................250 - 264**

**Informatics: Multimomics Integration ..............................265 - 280**

**Instrumentation: New Concepts .......................................281 - 302**

**Intact Proteins .................................................................303 - 319**

**Ion Activation/Dissociation .............................................320 - 340**

**Ion Mobility: Applications (Other/Instrumentation) ..........341 - 373**

**Ion Molecule, Ion/Ion, Ion/Electron Interactions ................374 - 398**

**Ion Spectroscopy ..............................................................399 - 411**

**LC-MS: Chromatography and Software (Part 1) ...............412 - 440**

**Lipids: General ...............................................................441 - 456**

**Metabolomics: General ....................................................457 - 495**

**Microorganisms: Identification and Characterization ........496 - 517**

**Phosphopeptides: Enrichment Methods ........................518 - 529**

**Polyoxymers .................................................................530 - 548**

**Proteins: General and Membrane ................................549 - 571**

**Proteins: PTMs (Part 1) ....................................................572 - 596**

**Proteomics: Clinical Applications (Applied Proteomics) ....597 - 621**

**Proteomics: Quantitative ................................................622 - 650**

**Small Molecules: Qualitative Analysis ............................651 - 680**

**Systems Biology (Multimomics and Other) .......................681 - 707**

**Top Down Protein Analysis (Applications) .........................708 - 727**

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

**MP 006 Developability Assessment of Multispecific Biopharmaceuticals: Kadir Iker Sen; Eric Ball; Hirsh Nanda; Andrew Mahan; Darryl Davis; Janssen Research and Development, Spring House, PA**

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

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

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

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

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

**MP 012 A Comprehensive Mass Spectrometry Workflow for Characterizing Therapeutic Antibodies: Alicia Biek; Paula Mangrelli; Beth McLeod; Colleen McClung; Beth Paschal; Cristian I Ruse; Xiaofeng Shi; Ellen Guthrie; New England Biolabs, Ipswich, MA**

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

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

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

**MP 016 Strategy to Rapidly and Comprehensively Characterize Innovator Biologics and their Biosimilars via Stress Testing Studies: Esthelle Hoedt; St John Skilton; Yong J Kii; Eric Carlsson; Chris Becker; Beatrice M Ueberheide; NYU School of Medicine, New York City, NY; Protein Metrics, Hopkinton, MA; Protein Metrics, San Carlos, CA; Protein Metrics Inc., San Carlos, CA**
MONDAY POSTERS

MP 017  Method Development for the Detection and Quantitation of Monomethyl Auristatin F (MMAF) in Cell Culture Media; Maria Christina Malina1; Melissa M. Williams1; Cody Warhurst1; Julien Dugal-Tessier1; Josh T. Snyder1; Brian Mendelsohn1; Hui Zhao1; Sara Guessserian1; Hosein Kouros-Mehr1; Kendall Morrison1; "Agensys, Inc. Santa Monica, CA

MP 018  In-Depth Characterization of Monoclonal Antibodies with a Single Experiment and Fully Automated Data Analysis; Paul Taylor1; Johnathan Kneger1; Qixin Liu2; Mingjie Xie1; Lian Yang2, 3; Bin Ma3; "Complex Carbohydrate Research Center UGA, Athens, GA; 2University of Mississippi, University, MS; 3School of Pharmacy, University of Mississippi, Oxford, MS

MP 019  Antibody Variable Domains as Intramolecular Luciferase Inhibitors for the Generation of Proteinolysis-Activated Biosensors; Lining Zhu1; Teresa Hong1; Nicola McNiven1; Markus Kalkum1; "City of Hope, Duarte, CA

MP 020  Novel Strategy Based on Dual Enrichment and Double Lists for Characterization of Host Cell Proteins; Zheng-Xiang Zhang1; Jimmy Chan1; Shuai Zuo1; Tao Bo1; Rong An1; "Agilent Technologies (China) Limited, Beijing, China

MP 021  Using High Resolution Structural Analysis to Determine if FPOP Modification Perturbs Native Protein Structure; Emily Hart1; Lisa M Jones1; "IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN

MP 022  Extension of the FPOP Method for Oxidative Modification in Live Tissue; Jessica Arlett Espino1; Anthony J Baucum1; Lisa M Jones1; "Indiana University-Purdue University Indianapolis, Indianapolis, IN; "Indiana University Purdue University Indianapolis, Indianapolis, IN

MP 023  Epitope Map of Malarial Antigen PvDBP revealed by Fast Photochemical Oxidation of Proteins (FPOP); Manolo David Plasencia1; Yining Huang1; Henry W Rohrs1; Edwin Chen1; Nichole D. Salinas1; Nairaj H. Tolia1; "University of Georgia, Athens, GA; 2Department of Biochemistry and Cell Biology, Stony Brook University, Stony Brook, NY

MP 024  The Application of “Droplet-Like” Methods to FPOP; Don L. Rempel1; Supratik Dutta1; Ben Niu1; Yining Huang1; Manolo Plasencia1; Michael Gross1; "Center for Biomedical and Bioorganic Mass Spectrometry, Washington University in St. Louis, St. Louis, MO; "Washington University School of Medicine, St. Louis, MO

MP 025  Normalization of High Resolution Hydroxyl Radical Protein Footprinting Data to Protein Structural Properties; Boer Xie1; Amika Sood1; Robert J Woods1; Joshua S. Sharp1; "University of Georgia, Athens, GA; 2University of Mississippi, University, MS

MP 026  Automated Hydroxyl Radical Protein Footprinting for the Determination of Biopharmaceutical Protein Conformation; Ming Cheng1; Supratik Dutta1; Ben Niu1; Yining Huang1; Manolo Plasencia1; Michael Gross1; "Complex Carbohydrate Research Center UGA, Athens, GA; 2School of Pharmacy, University of Mississippi, Oxford, MS

MP 027  Develop Isotope-encoded Photoaffinity Footprinting Reagent for Structural Mass Spectrometry Studies; Ming Cheng1; Michael L Gross1; "Washington University in St. Louis, St. Louis, MO

MP 028  Exploring the Peroxidase Activation and Deactivation of Cytochrome C by Heme-Catalyzed Oxidative Labeling and ESI-MS; Victor Yin1; Lars Konermann1; "Western University, London, Canada

MP 029  Comprehensive Measurement of Protein Dynamics in Complex Environments Using Footprinting Mass Spectrometry with Inexpensive MS2 Quantification of Labeled Cysteines; Jenna Gray Caldwell1; Pehr A. B. Harbury1; "Stanford University School of Medicine, Palo Alto CA

MP 030  Using Covalent Labeling and Mass Spectrometry to Study b-2-Microglobulin-Inhibitor Binding Sites; Tianying Liu1; Richard W Vachet1; "University of Massachusetts Amherst, Amherst, MA

MP 031  Towards an Improved Understanding of Diazirine Labeling for Structural Mass Spectrometry Applications; Daniel Ziemiansockz1; Chris Etienne2; David Schriemer1; "University of Calgary, Calgary, Canada; "Thermo Fisher Scientific, Rockford, IL

MP 032  Characterisation Proteolytic Process by Protein N-Terminal Derivatisation in - Gel Using MS-Based Approach in Drosophila; Nina Guilmoulot1; Florian Veillard1; Jean-Marc Reichhart1; Alain Van dorsselaer1; Christine Schaeffer-Reiss1; "Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, Université de Strasbourg, CNRS, UMR1718, Strasbourg, Strasbourg, France; "Institut de Biologie Moléculaire et Cellulaire, IBMC, Université de Strasbourg, CNRS UPR 9022, Strasbourg, Strasbourg, France

MP 033  Covalent Labeling Denaturation Mass Spectrometry for Sensitive Localized Higher Order Structure Comparisons; James A. Madsen1; Yan Yin1; Jing Qiao1; Vanessa Gill1; Kutrulathanan Renganathan1; Wing-Yee Fu1; Stephen Smith1; James Anderson1; "Momenta Pharmaceuticals, Cambridge, MA

MP 034  Xilmass: A New Approach Towards the Identification of Cross-Linked Peptides; Sule Yilmaz1, 2, 3; Friedel Drexper4; Maša Černić5; Kris Gevaert1, 2, 3; Anastassios Economou6; Bettina Warscheid1; Lennart Martens1, 7, 10; Eilen Vandermaelrië1, 7, 10; "Department of Biochemistry, Ghent University, Ghent, BELGIUM; "Laboratory of Molecular Bacteriology, Rega Institute for Medical Research, Department of Microbiology and Immunology, KULeuven, Leuven, BELGIUM; "Institute of Molecular Biology and Biotechnology-FoRTH, Department of Biology – University of Crete, Iraklio, Crete, Greece; "Bioinformatics Institute Ghent, Ghent University, Ghent, BELGIUM

MP 035  Crosslinkers with Isotope-Coding and Cleavable Spacers Improve Peptide Crosslink Identification by a Semi-Supervised Machine Learning Algorithm; Karl A T Makepeace1; Evgeniy V Petrochtko1; Christoph H. Borchers1, 2; "University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; "University of Victoria - Genome BC Proteomics Centre, Victoria, BC; "Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

MP 036  A Simple Approach for Creating Protein Structural Models Based on Cross-Linking Data; Zsusanna Orban-Nemeth1; Evelyn Ramlperf1; Thomas Stranzl2; David Maria Hollenstein1; Otto Hudec2; Peter Schloegelhofer1; Karl Mechtler1, 3; "Institute of Molecular Pathology, Vienna, Austria; "Department of Biochemistry and Cell Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria; "Institute of Molecular Biotechnology, Austrian Academy of Sciences, Vienna, Austria; "Department
CARBOHYDRATES

**DATA INDEPENDENT ACQUISITION**

**MP 040** Quantifying Cycloexetrin-Drug Interactions by ESI-MS; Emma-Dune Lerche1; Ping Zhang2; Aixia Wang3; Yuyu Yao4; Chang-Chun Ling2; Elena N Kitova1; John S Klaseen1; 1University of Alberta, Edmonton, Canada; 2University of Calgary, Calgary, Canada

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

**MP 042** Development of Negative Mode Free Radical Activated Glycan Structure Elucidation Reagents; Jinshan Gao1; Nikunj Desai1; Jungeun Lee2; 1Montclair State University, Montclair, NJ

**MP 043** Carbohydrate Analysis using Gas Chromatography Vacuum Ultraviolet Spectroscopy in Comparison with Gas Chromatography Mass Spectrometry; Jamie Schenk1; Xiaojian Mao2; Jonathan Smuts2; Gabe Nagy3; Nicola L. B. Pohl1; Phillip Walsh1; Peter Kroll1; Kevin A Schug1; 1University of Texas at Arlington, Arlington, TX; 2UUV Analytics, Inc., Cedar Park, TX; 3Indiana University, Bloomington, IN

**MP 044** Understanding the Reaction Products of Methanalysis and Butanolation of Heparan Sulfate; Marten F Snel1; Paul J Trim2; John H Hopwood3; Qi Qi He4; Vito Ferro5; 1South Australian Health and Medical Research Institute, Adelaide, South Australia; 2LRU, Nutrition and Metabolism Theme, South Australian Health and Medical Research Institute, Adelaide, Australia; 3School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Australia

**MP 045** LC-MS Analysis of the Complete Molecular Weight Distribution of Low Molecular Weight Heparins; Yuewei Sheng1; Chun Shao2; Kishlij Khatri1; Joseph Zaia3; 1Boston University School of Medicine, Boston, MA; 2Boston University, Boston, MA

**MP 046** Size-Selective Controlled Heparin Depolymerization to Obtain Heparin Oligosaccharides; Sandeep K Misra1; Joshua S Sharp1; 1Dept of Biomolecular Sciences, University of Mississippi, Oxford, MS

**MP 047** Oxidation of Glucose at Gold Nanoparticles and Mass Spectrometric Product Analysis; Marilyn Wooten1; Wendell P. Griffith2; 1University of Texas at San Antonio, San Antonio, TX

**MP 048** Study of Rearrangement Products in Collision-Induced Dissociation and Surface-Induced Dissociation of Oligosaccharides and Glycoconjugates; Forouzan Aboufazeli1; Eric D Dodds1; 1University of Nebraska-Lincoln, Lincoln, NE

**MP 049** Single Stage Tandem Mass Spectrometry Assignment of the C-5 Uronic Acid Stereochemistry in Heparan Sulfate Tetrasaccharides using Electron Detachment Dissociation; Isaac Agyekum1; Chengi Zong2; 1Chonnam National University, South Korea; 2University of Queensland, Brisbane, Australia

**MP 050** Mass Spectrometric Quantification of Cell Wall Composition Differences in Enterococcus Using Stable Isotope Labeling by Amino Acids; James Chang1; Ashley Wallace2; Erin Foster3; Alex Guinn4; Sung Joon Kim5; 1Baylor University, Waco, TX

**MP 051** High Resolution CESI-MS Analysis of N-Glycans of Biopharmaceutical Interest; Fonslow Bryan; Marton Szigi1; Andreas Guttmann1; 1University of Debrecen, Debrecen, Hungary; 2AB Sciex, San Diego, CA

**MP 052** Probing Carbohydrate Isomerism through Transition Metal Ion Adduction, Gas-Phase Ion Chemistry, and Collision-Induced Dissociation; Katherine Schumacher1; Yuting Huang1; Lauren Petrosh2; Eric D Dodds3; 1University of Nebraska - Lincoln, Lincoln, NE

**MP 053** ESI-TOF-MS Study of Carbohydrate Interaction with Metal Complexes with Carboxylate-Rich Ligand; Fangzhi Yan1; Christopher D. Stewart1; Stephan B. H. Bach2; Wendell P Griffith3; Ghezai T. Musie1; 1University of Texas at San Antonio, San Antonio, TX

**MP 054** Fragmentation of Derivatized and Non-Derivatized Metal-Adducted Oligosaccharides; Ranelle Schaller-Duke; 1The University of Alabama, Tuscaloosa, AL

**MP 055** A Novel Method for High-Throughput Analysis of Bioactive Oligosaccharides; Randall Robinson1; Daniela Barile1; 1University of California, Davis, Davis, CA

**MP 056** Advances in Targeted Omics Quantitation Using a Novel Scanning Quadrupole DIA Method; Chris Hughes1; Keith Richardson1; Jason Wildgoose2; Martin R Green3; Richard Chapman4; Arkadiusz Grzyb5; Praveen Harapanahalli1; Kirsten Craven1; 1Waters, Wilmslow, United Kingdom

**MP 057** Optimisation of Data Independent Acquisition (DIA) Data Extraction for Proteome Quantification; Gauthier Husson1; Alvaro Sebastian Vaca Jacome1; Maxime Eveque1; Christine Carapito1; 1Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO), IPHC, Strasbourg University, CNRS, UMR7178, Strasbourg, France

**MP 058** Improved Multiplexed Data Independent Acquisition: Sensitivity, Dynamic Range, and Full-Spectrum Demultiplexing; Jarrett Ebertson1; Ying Siaing Ting2; Philip M Remes3; Romain Huguet4; Derek Bailey5; Michael Senko6; Vlad Zabrouskov5; Michael J MacCoss6; 1Univ of Washington, Seattle, WA; 2Thermo Fisher Scientific, San Jose, CA

**MP 059** Analytical Validation of a Data-Independent Acquisition Mass Spectrometry Workflow for Quantification and Identification of Myofilament Proteoforms in Cardiac Biopsies; Irene van den Broek1; Irina Tchernyshyov2; Vidya Venkataraman1; Giulio Agnetti2; Amol Prakash2; Scott Peteman3; Jennifer E Van Eyk4; 1Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; 2Division of Cardiology, Johns Hopkins University School of Medicine, Baltimore, MD; 3Department of Biomedical and Neuromotor Sciences, University of Bologna, Bologna, Italy; 4Optys Tech Corporation, Brighton, MA; 5Thermo Fisher Scientific, Cambridge, MA
MP 060 Computational Workflows to Improve DIA Data Analysis Without Reference Libraries for Quantitative Proteomics and PTM Analysis; Jesse Gerard Meyer1; Birgit Schilling1; Samir Sofic2; C. Ronald Kahn2; Bradford W Gibson1; 1Buck Institute for Research on Aging, Novato, CA; 2Justin Diabetes Center and Harvard Medical School, Boston, MA

MP 061 Evaluation of the Efficacy of Data-Independent Acquisition Using Hyper Reaction Monitoring in Quantitative Proteome Profiling of Diverse Species; Jing Wang1; Jeong-Jin Park1; David R Gang1; 1Washington State University, Pullman, WA

MP 062 Data Independent Infrared Multiphoton Dissociation for Selective Identification of Cysteine Oxidized Peptides; Nicholas Borotti1; Phillip McClory1; Jaimeen Majmudar1; Brent Martin1; Kristina Hakansson1; 1University of Michigan, Ann Arbor, MI

MP 063 Effect of Peptide Assay Library Size and Composition in Targeted Data Independent Acquisition-Mass Spectrometry Analyses; Vidya Venkatraman1; Sarah Parker1; Jennifer E Van Eyk1; 1Advanced Clinical Biosystems Research Institute, Los Angeles, CA

MP 064 Spectral Library with High Confident PTM Site Localization for Phosphoproteome DIA Analysis; Wei Zhang1; Yue Zhou1; Jing Li1; 1Thermo Fisher Scientific (China), Shanghai, China

MP 065 Triple Quad Two-Dimensional Scanning: A Novel Scan Approach to Highlight Relationships and Couplings between Unknowns in Complex Mixtures; Cassandra L. Smith1; Vincent S. Pagnotti2; PPG Industries, Allison Park, PA; 2PPG Industries, Allison Park, PA

MP 066 A Case for Generating Organized and Comprehensive Digital Chromatogram Archives of Every Peptide Quantified in Large-Scale DIA Proteomics; Michael R Heaven1; Archie L Cobbs1; Harsha P Gunawardena2; Adam J Funk1; Michael J Ford1; Scott A Shaffer1; Jeremy L Norris1; 1Vulcan Analytical, Birmingham, USA; 2University of North Carolina, Chapel Hill, NC; 3University of Cincinnati, Cincinnati, Ohio; 4MS Bioworks, LLC Ann Arbor, MI

MP 067 Unraveling the Proteome of Differentiating Human Embryonic Stem Cells Using HMDSEMDIA MS; Elisabeth Govaert1; Katleen Van Steendam1; Maarten Dhaenens1; Liesbeth Vossaert1; Dieter Deforce1; 1Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium

MP 068 Analysis of Phosphorylation Site and Occupancy Using Data Independent Acquisition with Electron Transfer Dissociation Mass Spectrometry; Chein-Hung Chen1; Ya-Ping Lin1; Chia-Lin Wu1; Jung-Lee Lin2; Chung-Hsuan Chen2; 1Academia Sinica, Taipei, Taiwan; 2Genomics Research Center, Academia Sinica Taipei, Taiwan

MP 069 Using 2-Dimensional Mass Spectrometry (2DMS) for Proteomics; Peter B. O’Connor1; Maria van Aghoven1; Pui Yiu Lam2; Federico Floris3; Alice Lynch4; Marc-André Delsuc5; 1Warwick University, Coventry, West Midlands; 2University of Warwick, Coventry, UK; 3University of Strasbourg, Strasbourg, France

MP 070 Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA; Andreas Huemer1; Ignacio Ortega1; Michael Blank1; Daniel Lopez-Ferrer1; Romain Huguet1; David Horn1; 1Thermo Fisher Scientific, San Jose, CA; 2IMBIC, Cordoba, Spain

DIAGNOSTIC CLINICAL CHEMISTRY (APPLICATIONS) 071 - 094

MP 071 Mass Spectrometric Identification and Clarification of the in Vesica Formation of the Diuretic Chlorazanil in Sports Drug Testing Samples; Mario Thewi1; Hans Geyer2; Andreas Thomas2; Laura Tretzel2; Isabelle Bailloux3; Corrine Buissuin4; Markus Kellmann4; Catharina Cron4; Thomas Moehring5; Wilhelm Schänzer5; 1German Sport University, Cologne, NRW; 2German Sport University, Cologne, DE; 3Agence Française de lutte contre le Dopage, Chatenay-Malabry, France; 4Thermo Fisher Scientific, Bremen, DE

MP 072 Development of a Sensitive and Specific LC-MS/ MS Method for Rapid Diagnosis of Niemann-Pick C Disease; Rohini Sidhu1; Xuntian Jiang2; Sarah Gale3; David Scherrer2; Jean Schaffer2; Daniel Orly3; 1Washington University in Saint Louis, Saint Louis, MO; 2Washington University in Saint Louis, Saint Louis, MO; 3Washington University in Saint Louis, Saint Louis, MO

MP 073 A UHPLC-MS/MS Method for the Simultaneous Quantification of 10 Antihypertensive Drugs in Human Plasma; Amedeo De Nicolò1; Marco Simiele1; Gabriele Bonifacio1; Valeria Avataneo1; Paolo Mulatero1; Franco Rabbia1; Franco Veglio1; Giovanni Di Perri1; Antonio D’Avolio1; 1Laboratory of Clinical Pharmacology and Pharmacogenetic, University of Turin, Department of Medical Sciences, Amedeo di Savoia Hospital, Turin, Italy; 2Unit of Internal Medicine, University of Turin, Department of Medical Sciences, “Città della Salute e della Scienza”, Turin, Italy

MP 074 Multiplexed Enzymatic Assay for New-Born Screening of Mucopolysaccharidoses (type II, IIIB, IVA, VI, VII) and Neuronal Cereoid Lipofuscinosis II; Yang Liu1; Zdenek Spacil1; Hsuan-Chieh Liao1; Martin Sadilek1; Michael Glei2; Ronald Scott3; Frantisek Turecek1; 1University of Washington, Seattle, WA; 2Masaryk University, Research Centre for Toxic Compounds in the Environment, Brno, Czech Republic; 3University of Washington, Department of Pediatrics, Seattle, WA

MP 075 Early release of 1-pyrroline by Pseudomonas aeruginosa Cultures Discovered Using Ambient Corona Discharge Ionization Mass Spectrometry; Juchao Liang1; Konstatin Chinning1; Longhua Hu2; Yaping Hang2; Huanwen Chen3; 1East China Institute of Technology, Nanchang, China; 2The Second Affiliated Hospital of Nanchang University, Nanchang, China; 3East China University of Technology, Nanchang, Mainland

MP 076 Skin Transplant Quality Assessment by Multiplexed 2D MRM Mass Spectrometry – A Step Forward to Improve Clinical Success Rates; Jingzi Yang1; Juncong Yang1; Andrew Percy1; Uwe vonFitschen1; Juliane C. Finke1; Christoph H. Borchers1; 2Michael O. Glöcker2; 3Proteome Center Rostock, Rostock, Germany; 4University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 5HELIOS Clinic Emil von Behring, Berlin, Germany; 6Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; 7Proteome Center Rostock, Rostock, Germany

MP 077 Quantitative Clinical Chemistry Proteomics Applied to Apolipoproteins A-I / B / C-I / C-II / C-III / E in Serum; Yuri EM van der Burg1; Renee Ruhaak2; Nico PM Smit2; Fred PHTM Romijn1; Arnoud van der Laarse1; Christa M Cobbaert1; 1Leiden University Medical Center (LUMC), Leiden, The Netherlands

MP 078 Characterizing Traumatic Brain Injury with New Astroglial Injury Biomarkers Measured by Targeted Mass Spectrometry; Shen Sean1; Julia Halford1; Ina-Beate Wanner1; Joseph A. Loo1; 1UCLA, Los Angeles, CA
MP 080 High-Sensitivity, High-Throughput Quantification of Catecholamines and Metanephrine in Plasma by Automated WCX-SPE Coupled to LC/MS/MS for Clinical Research; Ichiro Hirano1; Atsushi Toyama1; Kumie Satou2; Yuki Nakamura2; Jun Watanebe3; Shimadzu Corporation, Kyoto, Japan; LSI Medience Corporation, Tokyo, Japan

MP 081 LC/MS/MS Determination of Plasma Catecholamine Metabolites Without Requiring Solid-Phase Extraction or Sample Dry-Up for Clinical Research; Yusuke Inohana1; Atsushi Toyama1; Ichiro Hirano1; Shimadzu Corporation, Kyoto, Japan

MP 082 Discovery and Targeted Proteomics on Cutaneous Biopsies Infected by Borrelia for the Diagnosis of Lyme Disease; Benoit Westermann1; Antoine Grillot2; Gilles Schnell3; Benoit Jaulhac2; Nathalie Boulanger2; Laurence Ehret4; Sabatier5; Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), CNRS-Université de Strasbourg, Strasbourg, France; EA7290, Virulence bactérienne précoce, groupe Borréliose, Université de Strasbourg, Strasbourg, France

MP 083 Increased Levels of Serum Protein Complexes are Associated with Type 2 Diabetes; Yujie Liu1; Bingchao Chen2; Yanmin Wang3; Mo Zhang1; Zhili Li4; Institute of Basic Medical Sciences, CAMS &PUMC, Beijing, CN; Heze Municipal Hospital, Heze, CN; IIBMS, CAMS&PUMC, Beijing CN

MP 084 A Quantitative Assay for Serum Albumin and Creatinine in Urine Based on MALDI-TOF MS; Stephen J. Hattan1; Marvin Vestal2; Kenneth C Parker2; Mark Duncan4; Jane Yang5; David Herold6; Virgin Instruments/SIMULTOF, Marlborough, MA; Virgin Instruments/SIMULTOF, Marlborough, MA; University of Colorado, Boulder, Colorado; University of Colorado School of Medicine, Aurora, CO; University of California San Diego, La Jolla, CA; University of California. San Diego La Jolla, CA

MP 085 Microorganism Identification/Classification by High Resolution Tandem Mass Spectrometry with Accurate Statistical Significance; Gelo Alves1; Guanghuai Wang2; Aleksey Ogurtsov3; Steven Drake1; Marjan Guczek4; Anthony Saffredini5; David Sacks6; YI-KUO YU7; National Center for Biotechnology Information, NLM, NIH, Bethesda, MD; Proteomics Core, NHLBI, NIH, Bethesda, MD; Critical Care Medicine Department, Clinical Center, NIH, Bethesda, MD; Department of Laboratory Medicine, Clinical Center, NIH, Bethesda, MD

MP 086 Urinalysis of Opiates Using a Small Benchtop Instrument Combining Microfluidic Capillary Electrophoresis-ESI with High Pressure Mass Spectrometry; Michael P Goodwin1; Scott Mellors2; Christopher D Brown1; 1908 Devices Inc., Boston, MA

MP 087 Rapid, Simultaneous Analysis of Urinary Monoamine Neurotransmitters and their Metabolites by UPLC-MS/MS; Zhengzhi Xie1; Sanjay Srivastava2; Pawel Lorkiewicz2; 1Heze Municipal Hospital, Heze, CN; IIBMS, CAMS&PUMC, Beijing CN; 2Institute of Microbiology, Prague, Czech Republic; 3IBMS, CAMS &PUMC, Beijing China

MP 088 Screening and Quantitation of Pain and Antidepressant Drugs in Human Urine by Liquid Chromatography-High Resolution Mass Spectrometry; Ana Celia Grenier1; Lawrence Joseph Andrade1; 1Dominion Diagnostics, North Kingstown, RI

MP 089 LC-MS Method for Quantitation of HbA1c in the Presence of the Most Common Hemoglobin Variants (S, C, D, and E); Shawn Connolly1; Kuanshy Kabytave; Curt Rohlfing1; Randie Little1; 1Department of Pathology &Anatomical Sciences University of Missouri Columbia, Columbia, MO

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

MP 091 Functionalized Surfaces for Direct Immuno-Affinity Mass Spectrometry - Detection of Haptoglobin Phenotypes; Petr Pompach1,2; Jana Novakova1; Daniel Kavan1,2; Oldrich Benada; Viktor Ruzicka5; Michael Volny7; Petr Novak2,3,7; 1Institute of Microbiology, Prague, Czech Republic; 2Faculty of Science, Charles University in Prague, Prague, Czech Republic; 7AffiPro, Mratin, Czech Republic

MP 092 Identifying Vitamin D2 and D3, Their 25-OH Metabolites, and 3′ Epimers in a Single LCMS Run; Ken Tseng; Toshi Ono2; Tsunehisa Hirose1; Nacalai USA Inc., San Diego, CA; Nacalai USA Inc., San Diego, CA; 2Nacalai Tesque Inc., Kyoto, Japan

MP 093 A Simple and Effective LC/MS/MS Method Development for the Determination of Underivatized Vitamin B1 and B6 in Human Whole Blood; Xianrong (Jenny) Wei1; Sean Oto2; Robert Slusher3; Nacalai Tesque Inc., Kyoto, Japan; 2Laboratory of Clinical Pharmacology, University of California, San Diego La Jolla, CA; 3IBMS, CAMS &PUMC, Beijing China

MP 094 Speciation of Fatty Acids in Human Serum by Gas Chromatography/Mass Spectrometry; Bruce A. Benner1; Benjamin J Place1; Jacolin A Murray1; 1NIST, Gaithersburg, MD

MP 095 Insights on Microsampling Implementation in Drug Discovery: Sample Collection, Matrix Effect, Recovery, Aging and Automation’s Assessment for an Emerging Technology; Grazziella Bovi1; Silvana Olivieri1; Giuseppe Santo1; Mariangela Corradin1; James Rudge2; Fabio Garofolo2; Serena Tongiani1; 1Angelini Research Center, Pomezia (Rome), Italy; 2Neoteryx, Torrance, CA

MP 096 A New Microsampling Hematocrit- Compatible Dried Plasma Card for Fully Automated Online DBSA-SPE-LCMS/MS Bioanalysis of Opioids in Blood; Imelda Ryona1; Jack Henion1; 1Q2 Solutions, Ithaca, NY

MP 097 Bioanalytical (ACU-4429) in Whole Blood Collected with Volumetric Absorbent Microsampling by LC-MS/MS; Zhixin Miao1; James G Farnham1; Glenn Hanson1; Terry Podoll2; Michael J. Reid3; 2Covance, Madison, WI; 3Acucela, Bothell, WA

MP 098 Improving Transplant Patient’s Welfare; Standardising and Advancing the Therapeutic Drug Monitoring of the Immunosuppressant Drug Tacrolimus; Dima AlMekdad1; Mark Christian Parkin2; Chris Mussell2; 1King’s College London, London, UK; 2LGC, Teddington, UK; 3King’s College London, London, United Kingdom

MP 099 Development and Validation of an UHPLC-MS/MS Method to Quantify Imatinib, Desmethylimatinib, Dasatinib,Nilotinib and Ponatinib in Dried Plasma Spots; Alessandra Ariuado1; Simiele Marco1; Fabio Favata1; Luca Paglietti1; Silvia De Francia1; Giovanni Di Perri1; Antonio D’Avolio1; 1Laboratory of Clinical Pharmacology and Pharmacogenetics. Department of Medical Sciences, University of Turin, Amedeo di Savoia Hospital, Turin, Italy; 2Laboratory of Clinical Pharmacology, Department of Clinical and Biological Sciences, University of Turin, San Luigi Hospital, Orbassano (Turin), Italy; 3Laboratory of Clinical Pharmacology, Orbassano, Italy

MP 100 Evaluation of Blood Fractionation Membranes for the Analysis of Dried Plasma Spots from Whole Blood Using Paper Spray Mass Spectrometry; Brandon Bills1; Nicholas E Manicke1; 1IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN

MP 093 A Simple and Effective LC/MS/MS Method Development for the Determination of Underivatized Vitamin B1 and B6 in Human Whole Blood; Xianrong (Jenny) Wei1; Sean Oto2; Robert Slusher3; Nacalai Tesque Inc., Kyoto, Japan; 2Laboratory of Clinical Pharmacology, University of California, San Diego La Jolla, CA; 3IBMS, CAMS &PUMC, Beijing China

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MP 099 Development and Validation of an UHPLC-MS/MS Method to Quantify Imatinib, Desmethylimatinib, Dasatinib,Nilotinib and Ponatinib in Dried Plasma Spots; Alessandra Ariuado1; Simiele Marco1; Fabio Favata1; Luca Paglietti1; Silvia De Francia1; Giovanni Di Perri1; Antonio D’Avolio1; 1Laboratory of Clinical Pharmacology and Pharmacogenetics. Department of Medical Sciences, University of Turin, Amedeo di Savoia Hospital, Turin, Italy; 2Laboratory of Clinical Pharmacology, Department of Clinical and Biological Sciences, University of Turin, San Luigi Hospital, Orbassano (Turin), Italy; 3Laboratory of Clinical Pharmacology, Orbassano, Italy

MP 100 Evaluation of Blood Fractionation Membranes for the Analysis of Dried Plasma Spots from Whole Blood Using Paper Spray Mass Spectrometry; Brandon Bills1; Nicholas E Manicke1; 1IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN
MP 101 Method Development Considerations for Paper-Spray Mass Spectrometry - Direct Ionization Technique for Physiological Fluid Analysis; Maria C. Prieto CONAWAY1; Jeff Patrick2; Joseph Kennedy3; Kristine Van Natta4; Marta Kozak5; 1Thermo Fisher Scientific, San Jose, CA; 2Prosolia, Inc. Indianapolis, IN; 3Thermo Fisher Scientific, San Jose, CA

MP 102 Ambient Mass Spectrometric Analysis of Herbal Medicines with Flowing Atmospheric-Pressure Afterglow; Xinyue Liang1; Xiaoxia Gong2; Songyue Shi4; Mohammad Choudhury3; Gerardo Gamez1; Texas Tech University, Lubbock, TX

MP 103 Evaluation of Protein Stability in Dried Plasma Spots Using Targeted and Untargeted Mass Spectrometry Techniques; Victoria David1; Kristine Tsatslalis1; Matthew Rosenow1; Marissa Saltzman1; Lizzi Neylon2; David Carpentieri2; Konstantinos Petrits3; Patrick Pirrotle1; 1Translational Genomics Research Institute, Phoenix, AZ; 2Phoenix Children’s Hospital, Phoenix, AZ

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

MP 104 Understanding the Oxygenation Mechanism of Hydrocarbons in the Ocean Utilizing SA-TIMS-FT-ICR MS; Paolo Benigni1; Rebecca Marin1; Kathia Sandoval1; Christopher J Thompson2; Mark E Ridgway2; Melvin Park2; Piero Gardinali2; Francisco Fernandez-Lima2; 1Florida International University, Miami, FL; 2Brunner Daltonic, Billerica, MA

MP 105 Unsupervised Chemical Structure Assignment Based on SA-TIMS-FTICR MS Mass and Mobility Measurements for Oxygenation Products of Hydrocarbons in the Ocean; Rebecca Marin1; Paolo Benigni1; Francisco Fernandez-Lima2; Christopher Thompson2; Mark E Ridgway2; Melvin Park2; 1Florida International University, Miami, FL; 2Brunner Daltonic, Billerica, MA

MP 106 Ionization of Paraffin Samples With/Without Solvents and Analysis Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Izaak Tyson-Hirst1; Mark P. Barrow1; 1University of Warwick, Coventry, United Kingdom

MP 107 Structural Elucidation of N-Containing Compounds in Crude Oil Using Positive Ion ESI FT-ICR MS/MS; Ammar Nasli1; Christianne Wicking2; Mike Hodges3; John Couves3; Lillian Valdares Tose4; 1University, Saarbrücken, Germany; 2Purdue University, West Lafayette, IN; 3Chevron Research, Richmond, CA; 4Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany

MP 108 Asphaltene Generateds from Low-temperature Cracking of Type II Kerogen: Molecular Characterization by Negative ESI-FT-ICR-MS and Kinetic Parameters; Albert Kamga1; Patrick G Hatcher2; Francois Behar4; Francois Baudin1; 1ODU Research Foundation, Norfolk, VA; 2Old Dominion University, Norfolk, VA; 3TOTAL Refining and Chemicals, Gonfreville l’Orcher, France; 4Univesite Paris Descartes, Sorbonne Paris Cite Paris, France

MP 109 Structural Determination of Nitrogen-Containing Compounds in Petroleum Using Collision Cross Section Calculations (CCS) and Collision-Induced Dissociation (CID); Hossein Maleki1; Sadeh Faramarzi Ganjabad1; Samaneh Ghassabi Kondalaji2; Stephen James Vetere1; 1West Virginia University, Morgantown, WV; 2IFPEn, Solaize, France

MP 110 Petroleomic Analysis of Tyre Pyrolysis Oils by Using High-Resolution ESI/APPI FT-ICR Mass Spectrometry; Janne Janis1; University of Eastern Finland, Joensuu, NA

MP 111 Two-Dimensional Matrix Plots for Mapping Genealogical Links in Complex Mixtures of Lignin Degradation Products; Yulin Qi1; Dietrich A Volmer2; 1Saarland University, Saarbrücken, Saarland; 2Saarland University, Saarbrücken, Germany

MP 112 Adaptation of SARA Fractionation with Emphasis on Resins and Asphaltenes Characterization in Crude Oils with Different API Gravity Using FT-ICRMS; Jandyson M Santos1, 2; Alberto Wisniewski Jr3; Marcos N Eberlin1; 1Universidade Federal de Santa Catarina, Florianópolis, SC; 2Universidade Federal Fluminense, Niterói, RJ; 3Universidade de São Paulo, São Paulo, SP

MP 113 Extrography and Column Chromatography Fractionation as Tools for Increasing Compositional Space Accessibility in HRMS Analysis of Crude Oils; Deisy Giraldo-Davila1; Martha L. Chacon2; Marianny Y Combariza1; Cristian Blanco-Tirado1; Andrea Gomez-Escudero2; Jorge A Orrego-Ruiz2; 1Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; 2Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; 3Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia

MP 114 HRMS Analysis of Naphthenic Acids Isolated from Heavy Crude Oils Using Ion Exchange and Solid Phase Extractions; Jeferson A. Valencia-Dávila1; Martha L. Chacón-Patiño2; Jorge A. Orrego-Ruiz2; Cristian Blanco-Tirado1; Marianny Y. Combariza1; 1Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; 2Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia

MP 115 New Approaches in Petroleomics: Extending the Characterization of Nitrogen in Vacuum Residue via SPE Fractionation and Analysis by ESI FT-ICR MS; Gessica Vasconcelos1; Veronica Vale Carvalho1; Carla Santos Freitas1; Lilian Valdares Tose2; 1Federal University of Goiás, Goiânia, GO; 2Federal University of Espírito Santo, Vitória, Brazil; 3Petrobras, Rio de Janeiro, RJ

MP 116 Nitrogen Speciation in Petroleum Distillates Fractionated by SPE Using a Complementary and Powerful Approach by GCxGC-NCD and FT-ICR/MS; Florian Albreieux1; Lodovic Chahen2; Lyès Assam3; Fabien Chainet1; Vincent Souchon3; 1IFFPEN, Solaize, 69360; 2IFFPEN, Solaize, France

MP 117 Asphaltenes Adsorption, Aggregation and Occlusion from a High-Resolution Mass Spectrometry Point of View; Martha Liliana Chacon-Patiño1; Marianny Yajaira Combariza1; Cristian Blanco-Tirado1; Andrea Gomez-Escudero2; Jorge A. Orrego-Ruiz2; 1Universidad Industrial de Santander, Bucaramanga, Santander, Colombia; 2Ecopetrol, Instituto Colombiano del Petróleo, Piedecuesta, Colombia

MP 118 Petroleum Aromatic Compounds by APPI, FI, and GCEI; a Sensitivity Study; Michael T Cheng1; Matthew Hurt1; 1Chevron Research, Richmond, CA

MP 119 Coupling of APCl / CS2 with Collisionally Activated Dissociation of Model Compounds for Structural Determination of Asphaltenes in Crude Oil; Mark Romanczyk1; Xueming Dong2; Hilika Kenttämaa2; 1Purdue University, West Lafayette, IN; 2Purdue University, West Lafayette, IN

MP 120 High-field FT Orbitrap MS as a Competitive Alternative for the Analysis of Complex Mixtures; Alessandro Vetere1; Wolfgang Schrader2; 1Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; 2Bruker Daltonics, Billerica, MA
**ENVIRONMENTAL ANALYSIS: GENERAL (PART 1)**

**MP 123** Determination of Nitro Polycyclic Aromatic Hydrocarbons in PM2.5 Using GC-MS/MS. Sun Qian; Fan Jun; Deng XiaoLi; Li Yueqi; Yang Guixiang; Huang Taohong; Yuki Hashi; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Shanghai, China; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Beijing, China; Shimadzu (China) Co., Ltd., Beijing, China.

**MP 124** Detection of Picogram or Sub-Picogram Semi-Volatile Compounds by Full Scan GCMS Using a High Efficiency Source – A Game Changer? Dale Walker; Harry Prest; Agilent Technologies, Little Falls, DE; Agilent Technologies, Santa Clara, CA.

**MP 125** Lewisite and VX Degradation By-Product Method Development for Environmental Remediation by Liquid Chromatography/Tandem Mass Spectrometry. Stuart Willson; Carolyn Koester; Deon Anex; Romy Campisano; Eugene Arrey; Thomas McKellar; Stuart Harrad; Ian B. McEwan; Thomas I. McKellar; The University of North Dakota, Grand Forks, North Dakota; Lawrence Livermore National Laboratory, Livermore, CA; AERL, Burlington, VT; 2Lawrence Livermore National Laboratory, Livermore, CA; 3University of North Dakota, Grand Forks, North Dakota; 4University of North Dakota, Grand Forks, North Dakota.

**MP 126** Atmospheric Contaminant Source Identification Using Chemometric Approaches with Mobile Membrane Introduction Mass Spectrometry (MMISs). Larissa C. Richards; Nicholas G. Davey; Erik T. Krogh; Christopher G. Gill; Appl. Env. Res. Labs. (AERL), Nainamo, BC, Canada; University of Victoria, Victoria, BC, Canada; University of Victoria, Victoria, BC, Canada; University of Victoria, Victoria, BC, Canada; University of Victoria, Victoria, BC, Canada; University of Victoria, Victoria, BC, Canada; University of Victoria, Victoria, BC, Canada.

**MP 127** In vivo Real-time Monitoring of Aphrodisiac Phenomenon Release of Small White Cabbage Butterflies (Pieris rapae). Yue Li; Robert A. Mathews; The University of Maryland, College Park, MD; Department of Entomology, Smithsonian Institution, National Museum of Natural History, Washington, DC.

**MP 128** Molecular Identification of Natural Organic Matter Interactions with Mercury by Ultrahigh Resolution Mass Spectrometry. Hongmei Chen; Benjamin F. Mann; Rosalie K Chu; Nikolai Tolic; Baohua Gu; Oak Ridge National Laboratory, Oak Ridge, TN; Environmental Molecular Sciences Laboratory, PNNL, Richland, WA.

**MP 129** Quantification of 1-Hydroxyxyprene in Undiluted Human Urine Samples Using Magnetic Solid-Phase Extraction Coupled with Internal Extractive Electrospray Ionization Mass Spectrometry. Hua Zhang; Haiyan Lu; Xiaowei Fang; Bi-Feng Yuan; Yu-Qi Feng; Huanwen Chen; Key Laboratory of Analytical Chemistry for Biology and Medicine (Ministry of Education), Department of Chemistry, Wuhan University, Wuhan, China; East China University of Technology, Nanchang, China.

**MP 130** High Throughput Detection and Identification of Chemical Excursions via GC-MS. Parminder Kaur; Corey Sedwell; Daniel DeBord; 1st Detect Corporation, Webster, TX.

**MP 131** That’s the Law : Tracking Down Trace Levels of HBCD Isomers in Recycled Polystyrene; Claude-Paul LaFrance; Maxim Maheux; TransBioTech, Lewis, QC; TransBioTech, Lewis, Canada.

**MP 132** Quantification of Twelve Polychlorinated Biphenyls in Human Urine. Kayoko Kata; Janice Ma; Antonia M. Calafat; Xiaoyun Ye; CDC, Atlanta, GA.

**MP 133** Quantification of Triazole Biocides in Treated Wood Using Solid-Phase Extraction Coupled with Liquid Chromatography – Electrospray High Resolution Mass Spectrometry. Kija Ondrusova; Brianna Gysbers; Alena Kubatova; University of North Dakota, Department of Chemistry, Grand Forks.

**MP 134** Tandem GC/MS Analysis of sub-pg/μL Quantities of PBDEs, Including BDE-209 Using the Novel High Efficiency EI Source. Stephen Baumann; Agilent Technologies, Inc., Alpharetta, GA.

**MP 135** Accurate Mass Analysis of Naphthenic Acids by Ammonia NCI. Matthew Curtis; Stephen Baumann; Mark Hewitt; Richard Frank; Dayue Shang; Marcus Kim; Agilent Technologies, Santa Clara, CA; Environment Canada, Burlington, Canada; Environment Canada, North Vancouver, BC.

**MP 136** Method optimization for Rapid Analysis of Brominated Flame Retardants in Polymers: with DART-Orbitrap HRAM. Antonella Guzzonato; Olaf Schiebner; Tabiwang Arrey; Thomas Moehring; Stuart Harrad; University of Birmingham, Bremen, Bremen, Germany; Thermo Fisher Scientific, Dreieich, Germany; Thermo Fisher Scientific, Bremen, DE; University of Birmingham, Birmingham, United Kingdom.

**MP 137** SIFT-MS: A Complete Real-Time Solution for Analysis of Ambient Air. Daniel B Milligan; David Hera; Thomas Hughes; Nic Lamont; Vaughan S. Langford; Murray J. McEwan; Thomas I. McKellar; Syft Technologies Ltd, Christchurch, New Zealand; University of Canterbury, Christchurch, New Zealand; University of Canterbury, Christchurch, Canterbury.

**MP 138** Determination of Trace Concentrations of Carboxylic Acids and Aldehydes in Wood Smoke Particulate Matter. Jana Rejsova; University of North Dakota, Grand Forks, North Dakota.

**MP 139** Chlorinated Dioxins, Furans and Biphenyls Analysis in Complex Matrices Using Automated Extraction and Reduced Solvent Volume Column Chromatography. Rudolf Addink; Philip Bassignani; Toxic Report, Watertown, MA.

**MP 140** Automated Pressurized Liquid Extraction and Sample Clean Up of River Sediment in POPs Analysis. Sudan Pellenjjan; Rudolf Addink; Toxic Report, Watertown, MA.

**MP 141** Characterization of Trihalomethanes in Meat Processing Plant Effluent. Tiffany Lidien; Doug D. Carlton; Kevin A. Schug; University of Texas at Arlington, Arlington, TX - Texas; University of Texas at Arlington, Arlington, TX.

**MP 142** Method Development for the Identification of Novel Brominated Flame Retardants Using a Q Exactive HRAM Mass Spectrometer. Aristide P. Gandi; Tabiwang N. Arrey; Thomas Moehring; Stuart Harrad; University of Birmingham, Birmingham, United Kingdom; Thermo Fisher Scientific (GmbH), Bremen, Germany.

**MP 143** Population Assessment of Perfluoroalkyl Acids (PFAs) in the Plasma of Wild American Alligators at Kennedy Space Center, FL. Jacqueline T. Bangma; John A. Bowden; Jessica Reiner; Russell H. Lowers; Matthew P. Guillette; Louis J. Guillette Jr.; Medical University of South Carolina, Charleston, SC; NIST, Charleston, SC; Integrated Mission Support Service, Titusville, FL.
**ENVIRONMENTAL ANALYSIS: PHARMACEUTICALS AND PESTICIDES**

**MP 144** Reducing and Normalizing Matrix Effects for the Quantification of BTEX in Contaminated Soils using Ionic Liquids in HS-GC/MS; Emmanuel Varona-Torre1; Michelle Reyes1; Doug D Carlson Jr.1,2; Kevin A Schug1,2; 1University of Texas at Arlington, Arlington, TX; 2Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX

**MP 145** Ultra Low-Level Detection of Perfluoroalkyl Substances (PFASs) using LC MS/MS; Sarah Dowd1; Lauren Mullin2; Jennifer A Burgess2; Waters Corporation, Beverly, MA; 1Water’s Conservation, Milford, MA

**MP 146** Creation of Accurate Mass Library with GC/MS Quadrupole Data and Its Application to Higher Confidence Unknown Identification; Ming Gu1; Yongdong Wang1; Cerno Bioscience, Norwalk, CT

**MP 147** GC-MS/MS Determination of Synthetic Musks in Human Serum; Ivanova Kosarac1; Carlton Kubwabo1; Guru Prasad Katur1; Exposure and Biomonitoring Div, Health Canada, Ottawa, ON

**MP 148** Mass Spectrometric Evidence of the Carbanion Reaction Intermediate in Chlordecone Environmental Decomposition; Andrei Starostine1; L Lomheim2; S. Gaspard3; E. Edwards4; 1University of Toronto, Toronto, ON; 2University of Toronto, Toronto, Canada; 3Universite des Antilles et de la Guyane, Pointe-a-Pitire, Guadeloupe, French West Indies

**MP 149** Analysis of Halogenated Environmental Contaminants in Food Products by Plasma-Assisted Reaction Chemical Ionization (PARCI); Paolo Lecchi1; Yao Lu1; Kunyu Zheng1; Peter Hafner1; Kaveh Jarobachi1; DSM Nutritional Products, Columbia, MD; 2Dept of Chemistry, Georgetown University, Washington, DC

**MP 150** UHPLC-Liquid-El/MS/MS Interface: A New Frontier of Multiclass Environmental Risk Factors Assessment in Sudden Infant Death Syndromes; Veronica Termopoli1; Giorgio Famigli1; Pierangelina Palma1; Achille Cappiello1; 1University of Urbino, Urbino, Italy

**MP 151** Fast and Robust 210 Multi-Residue Pesticide Screening of Five Washed and Unwashed Non-Organic Berries by LC-MS/MS with Simple QuEChERS Preparation; Joshua Ye1; Frank Kero2; Craig Young2; Sharanya Reddy2; 1Cerno Bioscience, Norwalk, CT; 2PerkinElmer, Shelton, CT

**MP 152** A Highly Specific and Robust Multi-residue Analysis of Pesticides in Water Using Time of Flight in All Ion Acquisition Mode.; Padma Marwah1; Ashok Marwah2; Sue D’antonio3; Paul Zimba1; 1Texas A&M University, Corpus Christi, TX; 2Self, Corpus Christi, TX; 3Agilent technologies Inc, Cedar Creek, TX

**MP 153** Multiplexed Analysis of 215 Pesticides Using Scout-MRM; Romain Carriere1; Blandine Rougemont1; Christelle Margoun2; Mathieu Le Dréau3; David Cox4; Yves J C LeBlanc5; Jerome Lemoine6; 1Institut des Sciences Analytiques, UMR 5280 CNRS, Université de Lyon, Villeurbanne, France; 2IRSTEa, Villeurbanne, France; 3Sciex, Concord, ON

**MP 154** Automated Multi Residue Pesticides Analysis Using Pressurized Liquid Extraction and Gel Permeation Chromatography; Philip Bassignan1; Ruud Addink1; 1Fluid Management Systems, Watertown, MA

**MP 155** Target and Not-target Screening of Pesticides and Metabolites in Paddy Water; Eleonora Mazzuco1; Fabio Goseiti1; Bianca Bolfi1; Marcello Manfredi1; Arianna Facchi1; Marco Romani2; Simone Silvestri3; Elisa Robotti3; Emilio Maneiro3; 1università Del Piemonte Orientale, Alessandria, Alessandria; 2University of Piemonte Orientale, Alessandria, Italy; 3SALUT-DISIT, University of Piemonte Orientale, Alessandria, Italy; Dipartimento di Scienze Agrarie e Ambientali, Università degli Studi di Milano, Milano, Italy; 4Ente Nazionale Risi, Pavia, IT

**MP 156** Rapid and Easy Comparison of Quechers Sample Preparation Methods for the Analysis of Pesticide Residues in Peas Using LC-ESI-QQQ; Victor Manuel Mondragon Olguin1; Jose Luis Freire2; 1Agilent technologies Inc, Mexico, DF

**MP 157** Comprehensive, Sensitive, and Quantitative Screening of Pesticides in Selected Swiss Headwater Catchments by an Online-SPE-LC-Orbitrap Method; Heinz Singer1; Rahel Comte2; Simon Mangold3; Christoph Mosche4; Christian Stamm5; Tobias Doppler6; Irene Wittmer6; 1Eawag, Dübendorf, CH; 2Eawag, Dübendorf, Switzerland

**MP 158** LC-MS/MS Method Development and Validation for the Quantification of LB-100 and Endothall Metabolite in Biological Matrices; Changyu Quang1; Jennifer L. Simko2; William C Nether1; Elizabeth A Grober1; John S Kovach1; 1WIL Research, Ashland, OH; 2L-lite Biotechnology Holdings, Inc., East setauket, NY

**MP 159** Ultra-Sensitive and Rapid Assay of Neonicotinoids, Fipronil and Some Metabolites in Honey by UHPLC-MS/MS; Mikhail Lev1; Aurore Jaffuel1; Stephane Moreau1; 1shimadzu France, Noisiel, France; 2Shimadzu Europe GmbH, Duisburg, Germany

**MP 160** Parts-per-trillion (ppt) Level High-Throughput Quantitation of Glyphosate, Aminomethylphosphonic Acid (AMPA) and Glufosinate in Water Samples by LC-MS/MS; Javier Lopez1; Miguel Angel Perez2; Carsten Baessmann1; Louis Maljers3; 1Bruker Esponola, S.A., Madrid, Spain; 2Bruker Daltonik GmbH, Bremen, -; 3Bruker, Fremont, CA; 4Bruker Ltd., Milton, Canada

**MP 161** Direct Analysis of Formulated Pesticide Product Matrices by Paper Spray Mass Spectrometry; Khang To1; Steven L Reeber2; Gary Glisch2; 1University of North Carolina Chapel Hill, Chapel Hill, NC

**MP 162** Human Biomonitoring for Pesticide Exposure and Effects on Metabolism using Convergence Chromatography-Mass Spectrometry; Zdenek Spacil1; Garry Codling1; Petra Booij2; Jana Klanova2; 1Masaryk University, Brno, Czech Republic

**MP 163** Multiresidue Determination of non-HPLC-ESI-MS-Amenable Organochlorine Pesticides with Liquid Chromatography Dielectric Barrier Discharge Ionization Mass Spectrometry (LC-DBDI-TOFMS); Jose Robles-Molina1; Felipe J Lara-Ortega1; Bienvenida Gilbert-Lopez2; Antonio Molina-Diaz3; Juan F. Garcia-Reyes1; Alexander Schutz4; Sebastian Brandt4; Joachim Franke4; 1University of Jaen, JAEN, ES; 2CSIC-CIAL, Madrid, ES; 3University Of Jaen, Jaen, Andalucia; 4Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany

**MP 164** An Unknown Screening Approach to Analyze Micropolutants Degradation by Different Disinfection Processes; Julia Quilitzki1; Patricia van Baar1; Uwe Dünnbier1; 1Berliner Wasserbetriebe, Berlin, Germany; 2Thermo Fisher Scientific, Bremen, Germany

**MP 165** Removal and Transformation of Persistent Emerging Contaminants via Advanced Oxidation Techniques; Julia Quilitzki1; Patricia van Baar1; Uwe Dünnbier1; 1Berliner Wasserbetriebe, Berlin, Germany; 2Thermo Fisher Scientific, Bremen, Germany

**MP 166** Micropolutants Degradation by Different Disinfection Processes; Julia Quilitzki1; Patricia van Baar1; Uwe Dünnbier1; 1Berliner Wasserbetriebe, Berlin, Germany; 2Thermo Fisher Scientific, Bremen, Germany
EPIGENETIC MODIFICATIONS
177 - 194

MP 166
Quantitation and Identification of Legal and Illicit Drugs in Water: A Case Study Using Volatile Liquid Chromatography and High-Resolution Quadrupole Mass Spectrometry

MP 167
Sensitive Screen of Pharmaceuticals and Personal Care Products (PPCPs) in Water Using Agilent 6545 LC/Q-TOF High Resolution Mass Spectrometer: Increased Throughput in the Determination of PPCPs in Environmental Water

MP 168
Non-Target Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) – Identification of Unknown Environmental Pollutants

MP 169
LCMS-MS Method for Quantification of PPCPs in Environmental Water: Validation and Implementation

MP 170
LC–TOF-MS and GC–MS Analysis of Pharmaceuticals and Personal Care Products in Wastewaters of Eastern North Carolina: Characterization of HistonE Pre-translation Modification

MP 171
Analysis of Potential Genotoxic Impurities (PGI) in Active Pharmaceutical Ingredients (API) by GCMS/MS: Monitoring the Safety of Drug Products

MP 172
Combining Commercial and Open-Source Accurate Mass MS/MS Library Information for Suspect and Non-Target Screening Workflows: Combining Commercial and Open-Source Accurate Mass MS/MS Library Information for Suspect and Non-Target Screening Workflows

MP 173
Increased Throughput in the Determination of PPCPs in Water Using Optimized MS Cycle Times in a High Sensitivity UHPLC-QQQ System: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MP 174
Development of a New Method for the Quantitative Determination of PPCPs in Water Using Optimized MS Cycle Times in a High Sensitivity UHPLC-QQQ System: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MP 175
Extraction of Organochlorine Pesticides with In-line Florisol Cleanup using an Acid-Base-Neutral Solid Phase Extraction System: Using High Resolution MS: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MP 176
One Step Extraction, Cleanup and Concentration of Chlorinated Pesticides in Raw Coffee Beans: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MP 177
Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MP 178
Quantitative Histone Mass Spectrometry Identifies Elevated Histone H3 Lysine 27 Methylation in Melanoma: Improving Quantitative Analysis of Modified DNA Nucleosides by Liquid Chromatography-Triple-Quadrupole Mass Spectrometry

MONDAY POSTERS
MP 186  
Turnover Profiles of Histone Post-Translational Modifications in a Myogenic Model Using SILAC Labeling, Enzyme Networks and Trend Clustering Analysis; Natrajhan Bhanu1; Simone Sidoli1; Benjamin A Garcia1;  
1University of Pennsylvania, Philadelphia, PA  

MP 187  
Middle-Down Characterization of Histone H4 Combinatorial Post-Translational Modification Codes for Breast Cancer Invasion; Tingting Jiang1; Yu Chen1; Michael E Hoover2; Christopher L Hendrickson1;  
1Michael A Freitas3; Alan G Marshall4; Nicolas L Young2;  
2Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL;  
3The Roy J. Carver Biotechnology Center University of Illinois at Urbana-Champaign, Urbana, IL;  
4Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH;  
5Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL;  
6Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX

MP 188  
LC-MS/MS for the Sensitive Quantification of 5-Methylcytidine in RNA; Gwendolyn Gonzalez1; Lijuan Zhao2; Patrick Trojer2; Lesley Murray1; Marie Classon1;  
1Genentech Inc, South San Francisco, CA;  
2University of California - Riverside, CA;  
3Japan Atomic Energy Agency, Takasaki, Japan;  
4JEOL USA Inc., Peabody, MA  

MP 189  
Less is More: Single-Neuron Epitranscriptomics using a Tandem Mass Spectrometric Approach; Maria Basanta-Sanchez1; Andrea B. Kohn2; Lenka Halamkova3;  
1The RNA Institute, Albany, NY;  
2High School of Protestant College, Debrecen, Hungary;  
3University of Debrecen, Debrecen, Hungary  

MP 190  
Contributions of Quantitative Histone PTM Analysis to Target Discovery, Compound Triage, and in vivo Experiments into Epigenetic Drug Tolerance; Tommy K. Cheung1; Tobias Maier1; Erin McNamara1; Feng Zhao1; Patrick Trojer2; Lesley Murray1; Marie Classon1;  
1Department of Molecular Virology, Immunology and Medical Genetics, The Ohio State University, Columbus, OH;  
2The RNA Institute, University at Albany, Albany, NY;  
3Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL;  
4Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX  

MP 191  
Quantitation of Post-Translational Modifications in the Nucleus: Effects of Histone Modifying Enzymes on their Histone and Non-Histone Substrates; Anastasia Lindahl1; Michael Smalegani1; Josue Baeza1; James Dowell1; Kimberly A Krautkramer1; John M Denu2;  
1UW-Madison, Madison;  
2University of Wisconsin Madison, Madison, Wisconsin;  
3Univ of Wisconsin, Madison, WI

MP 192  
in vitro Characterization of Histone Acyl-Posttranslational Modifications Using LC-MS; Johavra Simithy1; Simone Sidoli1; Zuo-Fei Yuan1; Benjamin A Garcia1;  
1University of Pennsylvania, Philadelphia, PA  

MP 193  
Probing the UV-Induced Effects on RNA and DNA-Modifications by LC-MS; Congliang Sun1; Zafra Abdel-Malek1; Kazumasa Wakamatsu2; Limbach A Patrick3;  
1Agilent Technologies India Pvt. Ltd, Bangalore, India;  
2University of Texas at San Antonio, San Antonio, TX;  
3University of California - San Diego, La Jolla, CA  

MP 194  
Parallel Reaction Monitoring Mass Spectrometry for Histone H3 Modification Analysis of Differentiating MEL cells; Michael Sweredoski1; Annie Moradian1; Matthias Raedele1; Sonja Hess1;  
1California Institute of Technology, Pasadena, CA;  
2Hochschule Weienstephan-Triesdorf, Weihenstephan-Triesdorf, Germany;  
3Caltech, Pasadena, CA  

MP 195  
HRAM LC/MS Screen for Prostaglandins found in Consumer Products; Bethany Hanson1; Toomey Valerie1;  
1FDA/Forensic Chemistry Center, Cincinnati, OH  

MP 196  
Quantitation of Potential Genotoxic Impurities in Active Pharmaceutical Ingredients, Drug Products, and Process Intermediates by High Resolution LC-MS; Robert Mengel1;  
2James Winter1; Alwyn Forbes1; Andy Lo1;  
2Feng Wang; Shannon Higgins-Gruber1; Ed Bishop1; Naijun Wu; Colgene, Summit, NJ  

MP 197  
Determination of Chemical Components of KABA Meteoreite by LDI and ESI Ionization Methods Using a 1ST FT-ICR Instrument; Arpad Somogyi1; Mihaly M. Nagy2; Jozsef Posta1;  
2Ohio State University, Columbus, OH;  
3High School of Protestant College, Debrecen, Hungary;  
4University of Debrecen, Debrecen, Hungary

MP 198  
Origin Discrimination of Red Pepper Powder Using UHPLC-Q-Orbitrap HRMS with Multivariate Analysis; Dong-Jin Kang1; Ji-Young Moon1; Seong-Hun Lee1;  
1Experimental Research Institute, NAQS Gimcheon-si, Korea  

MP 199  
Orbitrap Fusion Tribid Mass Spectrometer for Pharmaceutical Impurity Analysis; Kate Comstock1; Caroline Ding2;  
1Thermo Fisher Scientific, San Jose, CA;  
2Thermo Fisher Scientific, San Jose, CA

MP 200  
MALDI-spiral-TOFMS and Kendrick Mass Defect Analysis of Mycotic Acids from Bacteria which Accelerate the Formation of Antibiotics; Kanae Teramochi1; Shumpei Asamizu1; Taro Ozaki1; Katsuya Satoh1; Hiroyasu Onaka1; Robert Cody1;  
1JEOL Ltd., Akishima, Tokyo;  
2The University of Tokyo, Bunkyo, Tokyo, Japan;  
3Japan Atomic Energy Agency, Takasaki, Japan;  
4JEOL USA Inc., Peabody, MA  

MP 201  
Top-down analysis of Calmodulin and Lysozyme Using MS/2DMS on an FT-ICR MS; Federico Floris1;  
1Maria van Aghoven1; Lionel Chiron1; Mark P Barrow2;  
2Marc-André Delsuc1, 3; Peter B O’Connor1;  
3University of Warwick, Coventry, United Kingdom;  
4C4SC4DE, Illkirch-Graffenstaden, France;  
5IGBMC, Illkirch-Graffenstaden, France

MP 202  
Characterization of Impurities of HIV NNRTI Doravirine by High Resolution UPLC-MS and Tandem MS Analysis; Li-Kang Zhang1; Merck Research Laboratories, Kenilworth, NJ

MP 203  
Prospecting for Aqueous Gold Clusters [37.6-kDa Au144(pMBA)60, 26.8-kDa Au102(pMBA)44] using a High-Resolution Extended-Mass-Range(EMR) Orbitrap MS; Marcos Alvarez1; German Plascencia-Villa1; Wendell P. Griffith1; David M. Black1; Miguel José Yacamán1; Jenny Chen2; Robert Loyd Whetten1;  
1University of Texas at San Antonio, San Antonio, TX;  
2Thermo Fisher Scientific, San Jose, CA

MP 204  
Increased Identification of Extractables and Leachables Compounds by the Use of Chemical Ionization and Custom Databases; Syed Salman Lateef1; Siji Joseph1;  
Ravindra Gudihal1;  
2Agilent Technologies India Pvt. Ltd, Bangalore, India

MP 205  
Molecular Depth Profiling with a New Hybrid 3D SIMS Instrument for Improved Molecular Identification; Alexander Pirkl1; Rudolf Moellers1; Henrik Arlinghaus1;  
Ewald Niehuis1; Alexander Makarov1; Stevan Horning2;  
3Natarajan Bhanu1; Simone Sidoli1; Zuo-Fei Yuan1; Benjamin A Garcia1;  
1Agilent Technologies India Pvt. Ltd, Bangalore, India;  
2University of Wisconsin Madison, Madison, WI;  
3University of California - San Diego, La Jolla, CA  

MP 206  
LC-Quadrupole/Orbitrap MS/HRMS Enables Stable Isotope Resolved Simultaneous Quantification and Metabolistic Isotope Tracing of Acyl-Coenzyme A Species;
MP 207
Quantitative Evaluation of Immunosuppressant Drugs by High Resolution Accurate Mass using Selected Ion Monitoring Analysis; Keeley Murphy1; Jonathan L Josephs2; Maciej P Bromirski2; 1Thermo Fisher Scientific, San Jose, CA; 2University of California, San Diego, CA

MP 208
Parallel Untargeted and Targeted Quantitative Metabolomics for Microbiome Research; Alexey V. Melnik1; Fernando Vargas3; Amina Boussilmani3; Ivan Protsyuk3; Theodore Alexandrov1,2,3; Pieter C. Dorrestein1; 1Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, CA; 2European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; 3Morgan Hill, CA

MP 209
Simultaneous Determination of Phthalic Acid Esters, Organotin, Perfluorochemicals and Flame Retardants in Plastics by HPLC-LTQ/Orbitrap Mass Spectrometry; Li Zhang1; Xin Luo1; Zengyuan Niu1; Xiwen Ye1; Zhikun Tang1; Shuwei Xie1; 1Ocean University of China, Qingdao, China

MP 210
Acceptance Criteria for Confirmation of Identity of Chemical Residues Using Exact Mass Data; Hiranthi Jayasuriya1; Philipp K Kjäkaj1; Sherrri Turnipseed1; Timothy R Croley2; Jon Wong1; Bryan Gamble4; Hui Li1; Nathaniel W Snyder1; Alexander J Frey1; Sophie Trefely1; 1University of Texas at Austin, TX; 2Oak Ridge National Laboratory, Oak Ridge, TN; 3Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, China; 4Veterinary Medicine, FDA, Laurel, MD

MP 211
Topographical and Chemical Imaging Using a Combined Atomic Force Microscopy/Infrared Spectroscopy/Mass Spectrometry Platform; Vilmos Kertesz1; Tamin Tai2; Orsolya Karacsony1; Vera Bocharova1; Kevin Kjoller2; Gary J Van Berkel1; Oak Ridge National Laboratory, Oak Ridge, TN; 1Anasys Instruments, Santa Barbara, CA

MP 212
Development of Nanopipettes as Probes for Scanning Electrospay Microscopy (SESM); Elizabeth M Yuill1; Robert Burleigh1; Julia Laskin1; Son N Nguyen1; Melinda J Prosser1; 1Protea Biosciences, Inc. Ithaca, NY; 2Thermo Fisher Scientific, Bremen, DE

MP 213
A Reflectron Microscope-Mode Imaging Mass Spectrometer Capable of Achieving High Mass Resolution; Ang Guo1; Michael B. Burleigh1; Robert Burleigh1; Steve Thompson1; 1University of Oxford, UK; 2University of California, Berkeley, CA

MP 214
Combining Scanning Ion Conductance Microscopy and Nanospray Desorption Electrospray Ionization Mass Spectrometry for Multiomoldal Imaging of Biological Samples; Julia Laskin1; Son N Nguyen2; Venkateshwarlu Prabahakaran3; Andrew L. Liu1; Ruichuan Yin1; 1Pacific Northwest National Lab, Richland, WA; 2Oak Ridge National Laboratory, Oak Ridge, TN; 3Oak Ridge National Laboratory, Oak Ridge, TN

MP 215
Combining Imaging Mass Spectrometry with Infrared Spectroscopy/Microscopy Screening: A New Approach to Studying Biological Tissues; Antoine Masson1; Matthew J DiTuccio2; Anna Susa3; Jeremy T O’Brien1; Evan R Williams1; 1University of California, Berkeley, CA; 2Protea Biosciences, Inc. Ithaca, NY; 3Oak Ridge National Laboratory, Oak Ridge, TN

MP 216
Ambient Submicron Mass Spectrometry Imaging by Combining AFM with MS; Jonathan Brauer1; Jacob Berenbeim2; Mattanjah de Vries2; 1Analyticon Instruments, Santa Barbara, CA; 2University of California Santa Barbara, Santa Barbara, CA

MP 217
Microscope Ion Imaging of Complex Surfaces Using the Pixel Imaging Mass Spectrometry Camera; Robert J Burleigh1; Ang Guo2; Edward Halford1; Michael Burt1; Steve P Thompson3; Mark Brouard1; 1University of Oxford, Oxford, UK; 2Scientific Analysis Instruments, Manchester, UK

MP 218
Development of Laser Capture Microdissection-MS (LMD-LVC/ESI-MS) for Quantitative and Sub-Micrometer Mass Spectral Surface Sampling and Imaging; John F. Cahill1; Vilmos Kertesz1; Gary J Van Berkel1; Oak Ridge National Laboratory, Oak Ridge, TN

MP 219
Liquid Extraction Surface Analysis (LESA) Combined with Nano-Liquid Chromatography (nLC) for In-Depth Analysis of Biological Surfaces; Daniel Eikel1; Rasmus Havelund1; Jean-Marc Kowalski1; Sören-Oliver Deininger1; 1Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, China; 2Thermo Fisher Scientific, Manchester, UK

MP 220
Transmission Geometry MALDI Imaging MS: Assessing Ion Generation/Collection Efficiency at Sub-micron Laser Spot Sizes; Andre Zavalin1; Junhui Yang1; 1Richard M Caprioli1; 2Vanderbilt University, Nashville, TN

MP 221
Desorption Electrospray Ionization for Ambient Mass Spectrometry Imaging; Shuai Guo1; Zhili Li2; 1Shandong Entry-Exit Inspection and Quarantine Bureau, Qingdao, China; 2INSS GmbH, Bremen, Germany

MP 222
Improved Reproducibility in MALDI Imaging using a Scanning Laser Beam; Dagmar Niemeyer1; Michael Becker1; Shannon D Connell1; Paul J Kowalski1; Jane-Marie Kowalski1; Sören-Oliver Deininger1; Bruker Daltonik GmbH, Bremen, Germany; Bruker Daltonics, Inc., Billerica, MA

MP 223
Laser Ablation Electrospray Ionization Mass Spectrometry Imaging (LAESI-MSI) Using an Er:YAG Laser for Improved Spot Size Resolution and Tunable Ablation; Matthew Powell1; Trust T Razunguzwa1; Holly Henderson1; Heather Anderson1; Nicholas J. Morris1; Todd W. Ornduff1; David W. DuBois1; Protea Biosciences, Inc. Morgantown, WV

MP 224
3D nanoSIMS: A Novel High-Mass Resolution Instrument for 3D Molecular Imaging with Sub-Micron Resolution; Melissa K. Passarelli1; Alexander Pirkl2; Rudolf Moellers1; Ewald Niehuis2; Alexander A Makarov3; Henrik Arlinghaus2; Rasmus Havelund2; Paulina D. Rakowska1; Alan M. Race1; Alex Shard1; Andy West1; Steven Horning1; Peter S. Marshall1; Morgan R. Alexander2; Colin Dollery2; Ian Gilmore6; National Physical Laboratory, Teddington, United Kingdom; 1ION-TOF GmbH, Muenster, Germany; 2Thermo Fisher Scientific, Bremen, DE; 3GlaxoSmithKline, Stevenage, UK; 4The University of Nottingham, Nottingham, UK; 5National Physical Laboratory, Teddington, Middlesex UK; 6Development of a Time and Position Sensitive Ion Detector for a Stigmatic Imaging Mass Spectrometer; Jun Aoki1; Yosuke Kawai1; Yowichi Fujita1; Hisanao Hazama1; Toshinobu Hondo1; Kunio Awazu1; Michisato Toyoda1; Yasuo Arai1; 1Osaka University, Toyonaka, Japan; 2High Energy Accelerator Research Organization, Tsukuba, Japan; 3Osaka University, Suita, Japan

MP 225
Three Micron Resolution MALDI-MS Imaging Without Transmission Geometry or Oversampling and Its Application to Maize Root Cross-section; Adam Feenstra1,2; Young-Jin Lee1,2; 1Ames Laboratory-US DOE, Ames, Iowa; 2Iowa State University, Ames, IA

MP 226
Rapid Laser Desorption Imaging MS with Submicron Spatial Resolution; Jerome Moore1; J Albert Schultz2; Valerie Steen2; 1Ares Laboratory-US DOE, Ames, Iowa; 2Iowa State University, Ames, IA
GENERAL INFORMATION

MP 230
Maximizing Performance of Spatial Proteomics through the Fusion of Ultra-High Speed MALDI-TOF and High Mass Resolution MALDI FTICR IMS; Jeffrey Spraggen1, 2, 3; R. Van de Plas1, 2, 3; J. Moore1, 2; D. Ryan1; R. Caprioli2; M. Setou1; E. Takats2; R. M. Caprioli2; E. Claude2; M. Towers1; B. Shrestha2; P. Hart1; 1Hamamatsu University School of Medicine, Hamamatsu, Japan; 2Waters Corporation, Wilmslow, UK; 3University of Manchester, Manchester, UK; 4Imperial College, London, United Kingdom

IMAGING MS: SAMPLE PREPARATION

MP 234
Ammonium Sulfate Improves Detection of Hydrophilic Quaternary Ammonium Compounds through Decreased Ion Suppression in Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging; S. Matsuhashi1; N. Masaki1; K. Sat01; T. Hayasaka1; Y. Sugiyama1; T. Iida1; H. Ito1; N. Kato1; 1Biomedical Research Center, University of Tokyo, Tokyo, Japan

MP 236
Using MALDI Depth Profiles to Understand the Effect of ESD Sample Preparation Parameters on MALDI IMS Samples; B. James Malys1; K. G. Owens1; Drexel University, Philadelphia, PA

MP 237
University, Ambler, PA; Drexel University, Philadelphia, PA

A Combined Enzymatic Digestion and Matrix Application Approach for High Throughput MSI of FFPE Tissue; H. E. Goodman1; E. H. Seeley1; 1Protein Biosciences, Morgantown, WV

MP 239
Utilization of Soft-landing Ion Mobility for the Deposition of Clusters as Matrix Substitutes for Matrix-assisted Laser Desorption/Ionization Mass Spectrometry Imaging; Roberto Aguilar1; G. Verbeck2; 1University of North Texas, Denton, TX

MP 240
Optimal Sample Preparation Method for Visualizing Global Endogenous Metabolites by Mass Spectrometry Imaging in Arabidopsis; T. Ichinose1; Y. Fujiwara1; S. Nakayama1; J. Yamazaki2; N. Nakamura1; E. Hayakawa1; H. Wariishi1; D. Miura1; K. University, Fukuoka, Japan; Shimadzu Corporation, Kyoto, Japan

MP 241
Investigation into the use of Tissue Washing Procedures and the Subsequent Outcomes for DESI-MS Imaging Analyses; P. Hart1; M. Towers2; E. Claude2; M. Setou1; J. Langridge2; P. Pringle2; J. Kramer2; J. List2; M. Spetalon1; S. Caprioli2; 1Hamamatsu University School of Medicine, Hamamatsu, Japan; 2Waters Corporation, Wilmslow, UK

MP 242
Investigation of Aging of Chemically Fixed Mammalian Cells via ToF-SIMS; J. Kokkech-Himmelreich1; D. J. Graham1; L. J. Gamble2; 1University of Washington, Seattle, WA

MP 243
Mass Spectrometry Imaging to Better Understand the Mycoparasitic Interaction of Biocontrol Agents; M. Holzlechner1; Z. Samuele1; S. Reitschmidt1; M. Takats2; J. K. Nicholson2; 1Vienna University of Technology, Vienna, Austria; 2Imperial College, London, UK

IMAGING MS: SOFTWARE

MP 244
High-Performance Visualization and Multivariate Analysis Software for Mass Spectrometric Imaging; D. Yukihiro1; M. Kazawa1; 1Reifys Inc., Tokyo, Japan

MP 245
Finding Patterns in Mass Spectrometry images; D. J. Graham1; L. J. Gamble2; 1University of Washington, Seattle, WA

MP 246
Software for Distributed MALDI Imaging Workflows; S. Spraggins1; S. Spraggins1; K. Spraggins1; K. Spraggins1; 1Drexel University, Philadelphia, PA

MP 247
Absolute Quantification and Customizable Database Integration for Molecular Identification with MSReader; K. Garrard1; T. Bokhart1; M. Nazari1; D. C. Muddiman1; 1North Carolina State University, Raleigh, NC

MP 248
Translational Data Analytics for Large Mass Spectrometry Imaging Datasets in Clinical Research; K. Veselkov1; M. Reza2; E. Claude3; J. Kinross2; M. Spraggins2; N. Inglese4; K. Baston1; 1Vanderbilt University, Nashville, TN; 2Drexel University, Philadelphia, PA; 3Imperial College, London, UK; 4University of California, San Diego, La Jolla, CA

MP 249
Characterization of Data-driven Image Fusion for Imaging MS: Exploring Image Modality Combinations that Maximize Predictive Performance for Distinct Biomolecular Classes; R. Van de Plas1; J. Spraggins2; N. Verbeek2; J. Yang2; R. M. Caprioli2; 1Delft University of Technology, Delft, Netherlands; 2Vanderbilt University, Nashville, TN
MP 250

**IFrid: A Novel In-Source Fragmentation Detection and Deconvolution Algorithm for LC-MS Metabolomics Data**

Tytus Mak; Maryam Goudarzi; Stephen Stein; National Institute of Standards and Technology, Gaithersburg, MD; Georgetown University Medical Center, Washington, DC

MP 251

**Exploring Spectral Relationships and Peak Redundancy in API Mass Spectra**

Nathaniel Mahieu; Gary J Patti; Washington University in St. Louis, St. Louis, MO

MP 252

**Accurate Mass Retention Time Locked Metabolomics**

El Library and Workflows for Accurate Mass GC/Q-TOF Metabolomics Data Processing; Sofia Nieto; Zijuan Lai; Mine Palazoglu; Hong Chen; Aditi Koul; Vadim Kalmeyer; Oliver Fiehn; Agilent technologies Inc, Santa Clara, CA; UC Davis, Davis, CA

MP 253

**Rapid MS1 Formulae to Isotope Pattern Matching Using a Novel MS1 Search Engine for Metabolomics**

Scott Walmesley; Hyungwon Choi; Samantha Bokatzian; Richard Reisdorph; Nichole A Reisdorph; Dept. of Pharmaceutical Sci., University of Colorado Denver-Anschutz, Aurora, Colorado [CO]; UCD Computational Biosciences Program, Aurora, Colorado [CO]; National University of Singapore, Singapore, Singapore

MP 254

**Optimus + iii: Software for LC-MS Based Spatial Metabolomics in 2D, 3D, and Virtual Reality**

Ivan Protsyuk; Sergey Ryazanov; Garg Neha; Tal Luzzatto-Knaan; Amina Bouslimani; Clifford Kapporn; Alexey Melnik; Dimitri Flores; Luca Rappez; Prasad Phapale; Pieter Doorsteijn; Theodore Alexandrov; EMBL, Heidelberg, Germany; Skaggs School of Pharmacy, UC San Diego La Jolla, CA

MP 255

**Building High Confidence Metabolite Libraries for Fast Identification in Targeted Profiling Experiments**

Gina Tan; Ralf Tautenhahn; Andreas Huhmer; Thermo Fisher Scientific, San Jose, CA

MP 256

**The 1-StOAP Approach to Annotation of LC-MS Metabolomics Data**

Corey D Broeckling; Andrea Ganna; Mark Layer; Brown Kevin; Ben Sutton; Erik Ingelsson; Graham Peers; Jessica E Premni; Colorado State University Proteomics and Metabolomics Facility, Fort Collins, Co; Broad Institute of MIT and Harvard of Minnesota, Minneapolis, MN; Uppsala University, Uppsala, Sweden; Institute of Standards and Technology, Gaithersburg, MD; University of Minnesota, Minneapolis, MN; National University of Singapore, Singapore, Singapore

MP 257

**Utilizing Advanced Multivariate Analysis Features with Automated Database Searching Algorithms to Simplify Metabolomics Study Conduct and Understanding**

Christopher Colangelo; Phillip Seiler; Rick Schneider; Primary Ion, Old Lyme, CT; Proteome Software, Portland, OR; Pfizer, Groton, CT

MP 258

**Automatic CCS and MS/MS Library Creation and Application for Large Scale Metabolic Profiling**

Jonathan P Williams; David Eaton; Lee A Gethings; Christopher J. Hughes; Mark Towers; Leanne Nye; Steven Lai; Richard Tyldesley-Worster; Johannes PC Vissers; Waters Corporation, Wilmslow, United Kingdom; Waters Corporation, London, United Kingdom; Waters Corporation, Beverly, MA

MP 259

**Algorithm for Metabolite Identification Based on MS/MS for Untargeted Metabolomics**

Guoan Zhang; New York University, New York, NY

MP 260

**A Generalizable Method for False-Discovery Rate Estimation in Mass Spectrometry-Based Lipidomics**

Grant Fujimoto; Jennifer E Kyle; Kevin Crowell; Richard D Smith; Thomas O Metz; Sam Payne; Pacific Northwest National Lab, Richland, WA

MP 261

**Assessing Metabolic Pathways Using Chemical Kinetics Theory**

Ismael Zamora; Guillem Plasencia; Laura Goracci; Lead Molecular Design, S.L.; Sant Cugat del Valles, Barcelona; Lead Molecular Design S.L., Sant Cugat de Valles, Spain; Perugia University, Perugia, Italy

MP 262

**A Computational Platform for Analysis of Stable Isotope Assisted Metabolomics Data Acquired on GC-MS**

Xiaoli Wei; Imhoi Koo; Biyun Shi; Pawel Lorkiewicz; Ramandeep Rattan; Shailendra Girl; Xiang Zhang; Department of Chemistry, University of Louisville, Louisville, KY; University of Louisville, Louisville, KY; University of Louisville, Louisville, KY; Pharmacology & Toxicology, University of Louisville, Louisville, KY; Institute of Molecular Cardiology, University of Louisville, Louisville, KY; Henry Ford Health System, Detroit, MI

MP 263

**Analysis of Stable Isotope Assisted Metabolomics Data Acquired by High Resolution Mass Spectrometry**

Pawel Lorkiewicz; Xiaoli Wei; Joshua Safalbi; Biyun Shi; Bradford Hill; Seongho Kim; Craig James McClain; Xiang Zhang; University of Louisville, Louisville, KY; Wayne State University; Detroit, MI; Robley Rex Louisville VAMC, Louisville, KY

MP 264

**metaX: an Automatic and Comprehensive Pipeline for Processing Metabolomics Data**

Bo Wen; Zhenyu Guo; David Broadhurst; Yanqun Fan; Chunwei Zeng; Hui Jiang; Xin Xu; Siqi Liu; BGI-Shenzhen, Shenzhen, China; University of Alberta, Edmonton, Canada

**INFORMATICS: MULTIMICS INTEGRATION**

MP 265

**A Multi-omics Visualization Platform (MVP) Plug-in for Galaxy-based Applications**

Thomas Mogwan; James Johnson; Pratik Jagtap; Getira Onsongo; Candace Guerrero; Timothy Griffin; University of Minnesota Supercomputing Institute, Minneapolis, MN; University of Minnesota, Minneapolis, MN; Center for Mass Spectrometry and Proteomics, UMN St.Paul, MN

From Start to Finish: a Complete Proteogenomic Informatics Environment Implemented in the Galaxy Platform: Getira Onsongo; Pratik D Jagtap; James E Johnson; Thomas McGowan; Mohammad Heydarian; Karen Reddy; Timothy J Griffin; University of Minnesota, Minneapolis, MN; University of Minnesota at Twin Cities, Saint Paul, MN; University of Minnesota Supercomputing Institute, Minneapolis, MN; Johns Hopkins University, Baltimore, Maryland; Johns Hopkins University, Baltimore, MD

A Multi-Omic Approach to Reveal the Effect of Low-Level Gamma Radiation on Rice Seeds: Gohei Hayashi; J Shibato; T Imanaka; G Oros; M Fukumoto; Garg Neha; T Imanaka; G Oros; Randeep Rakwall; Sa Deepak; Gundimeda Seetaram; Upendra Simha; Padmanaban Arunkumar; Institute of Developement, Aging and Cancer, Tohoku University, Sendai, Japan; Hoshi University, Tokyo, Japan; NIES, Tsukuba, Japan; TRABB, Kathmandu, Nepal; Tohoku University, Sendai, Japan; Plant Protection Institute, Budapest, Hungary; Tsukuba University, Tsukuba, Japan; Agilent Technologies, Bangalore, India; Agilent Technologies, Bangalore, India; Agilent Technologies (India) Pvt. Ltd., Bangalore, India

Global Analysis of Lipidomics, Oxylin and Metabolomics Data Sets in Paediatric Plasmidium Falciparum Malaria: Izabella Surowiec; Sandra Gouveia-Figueira; Tomas Skotare; Judy Orikiiriza; Elisabeth Lindquist; Sven Bergström; Johan Normark; Johan Trygg; Computational Life Science Cluster (CLIC), Umeå University, Umeå, Sweden; Infectious Diseases Institute, School of Medicine and Health Sciences, Makerere University, Kampala, Uganda; Department of Molecular Biology, Umeå University, Umeå, Sweden
MP 269 An NGS-Independent Strategy for Proteome-Wide Identification of Single Amino Acid Polymorphisms by Mass Spectrometry: Wengong Shu1; Yun Xiong2; Yufeng Guo3; WeiDi Xiao4; 1Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, Tianjin; 2Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, CN; 3Nankai university, Tianjin, China

MP 270 The Fragmentarium: A Universal Query Service Enabling Partial Matching of Unidentified Spectra across the Full Gamut NIST MS Spectral Libraries; Manor Askenazi; Stephen Stein; 1Biomedical Hosting LLC, Arlington, MA; 2NIST, Gaithersburg, MD

MP 271 Precise Label-Free Quantitative Proteomes in High-Throughput Using microLC-SWATH-MS; Jakob Vowinckel1; Aleksei Zalezniak1,2; Markus Raiser1,2
1University of Cambridge, Cambridge, UK; 2The Francis Crick Institute, London, UK

MP 272 ProteoGenomics: Linking between Ensembl and PRIDE using ProteoAnnotator; Fawaz Ghali1; Simon Perkins2; Tobias Ternenti3; Juan Antonio Vizcaino2; Henning Hermjakob2; Andy Yates2; Paul Flicek2; Andy Jones1; 1University of Cambridge, Cambridge, UK; 2EMBL-EBI, Hinxton, UK

MP 273 Crosstalk: A Biological Network Analysis Platform With an Emphasis on Openness; Sean Maxwell; 1Mark R Chance1; 2Case Western Reserve University, Cleveland, OH; 3NeProteomics, Inc. Cleveland, OH

MP 274 Looking for Black Sheep: Identifying Significant Proteogenomic Outliers; Emily Kawai1et1; Kelly V Ruggles2; David Fenyo2; 1Center for Health Informatics and Bioinformatics, New York University Medical School, New York, NY

MP 275 proBAMsuite Bioinformatics Framework for Genome-Based Representation and Analysis of Proteomics Data; Xiaoqing Wang1; Robbert J Slebos1; Matthew C. Chambers1; David L. Tabb2; Daniel C. Liebler2; Bing Zhang3; 1Vanderbilt University, Nashville, TN

MP 276 Systematic Analysis of Phospho-signaling-affected Mutations in a Large Clinical Breast Cancer Cohort; Karsten Krug1; Philip Merlins2; Lauren Tang3; Jana Qiao4; Filip Munth5; Karl R Clauser6; Michael A Gillett7; Li Ding8; Kelly V Ruggles2; David Fenyo2; Matthew Ellis4; D.R. Mani3; Steven A Carr1; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2Washington University School of Medicine, St. Louis, MO; 3New York University, New York, NY; 4Vanderbilt University, Nashville, TN

MP 277 Detection of Colorectal Cancer Related Antibody Peptides Using Proteogenomics; Seong Won Chae1; Vincen Batra1; 1UCSD, La Jolla, California; 2UCSD, La Jolla, CA

MP 278 A Comprehensive Proteogenomic Workflow Reveals Novel Insights into Leukemogenesis; Jarrod Sandow; The Walter & Eliza Hall Institute, Parkville, VIC

MP 279 Taxonomic Characterization of Metaproteomes Using Databases of Translated Metagenomic Sequencing Reads; Damon May1; Emma Timmins-Schiffman1; Molly Miklan2; Rodger Harvey1; Elhanan Borenstein1; Brook Nunn1; William S Noble1; 1University of Washington, Seattle, WA; 2Old Dominion University, Norfolk, VA

MP 280 Integrating Global Proteome and Phosphoproteome Expression into the Cancer Cell Line Encyclopedia; David Nusinow1; John Szpyt1; Christopher M Rose1; Mahmood Ghandi2; Levi A Garraway2,3; Steven P Gygi1; 1Harvard Medical School, Boston, MA; 2Broad Institute of MIT and Harvard, Cambridge, MA; 3Dana Farber Cancer Institute, Boston, MA

MP 281 Microfabrication and Evaluation of the T-Probe: A Novel Device for Online in Situ Live Single Cell MS Analysis; Ren nemg Liu1; Yanlin Zhu1; Ning Pan1; Zhibo Yang1; 1University of Oklahoma, Dept. of Chem & Biochem Norman, OK

MP 282 An Alternative to a Direct Insertion Probe using a Traditional GCMS Pyrolyzer Instrument; Ben Peters1; Karen Sam2; Gary Deger1; 1CD3 Analytical, Oxford, PA

MP 283 Development of Automated Screening and Quantitation Method on Novel On-Line SPE-SFC-MS/MS Platform – (I) For 24 Restricted Perfluoro compounds; Jie Xing1; Jun Xiang Lee1; Peiling Zeng1; Zhaqoi Zhan1; 1Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore

MP 284 Facilitating Disulfide Bond Assignments in a Bottom-Up Proteomics Procedure Combined with Online LC–Electrochemistry–MS; Linda Switzer; Arno de Ru1; Agnieszka Kraj1; Jean-Pierre Chervet1; Annemieke Artama-Rus1; Yuri EM van der Burgt1; Peter A van Veelen1; 1Leiden University Medical Center (LUMC), Leiden, The Netherlands; 2Antec, Zoeterwoude, The Netherlands

MP 285 Novel Ion Optics Boosting the Sensitivity of Proton-Transfer-Reaction - Time-of-Flight Mass Spectrometry (PTR-TOFMS); Alfons Jordan1; Christian Lindinger1; Stefan Feil1; Paul Mutschlechner1; Gernot Hanel1; Eugen Hartungen1; Jens Herbig1; Lukas Märk1; Simone Jürschik1; Philipp Sulzer1; 1IONICON Analytik GmbH, Innsbruck, Austria

MP 286 Digitally-Driven Ion Funnels to Enhance High Mass Ion Collection; Bojana Opacic1; Liang Wang1; Brian H Clowers1; Peter Ta Reilly1; 1Washington State University, Pullman, WA

MP 287 A Segmented Linear Quadrupole Ion Trap for Enhanced Activation and Storage; Dimitris Papanastasiou1; Emmanuel Raptakis1; Diamantis Kounadis1; Ioannis Orfanopoulos1; Alexander Lekkas1; Andreas Mpozatzidis1; 1Fasmatech, Athens, Greece

MP 288 Analysis of Species of N2 in Environmental Samples and H2 in Inorganic Samples by New Type of Quadrupole Mass-Spectrometer; Adolf Goetz Dr.1; Michael Laessig1; Thimo Post1; Bernd Apelt1; Peter Paplewski1; 1Inoprox Instruments, Bremen, Germany; 2Bremen, Bremen, Germany; 3Bremen, Bremen, Germany; 4Helmholtz Centre for Environmental Research - UFZ; 5Leipzig, Germany; 6Brüker, Karlsruhe, Germany

MP 289 A Simple Ion Funnel-Based Device for the Thermalization and Transmission of Megadalton Ions; Staci N Anthony1; Benjamin E Draper1; Martin F Jarold1; 1Indiana University Dept. Chemistry, Bloomington, IN

MP 290 Ion Confinement in a Fourier Transform Electrostatic Linear Ion Trap via Mirror-Switching: Correction of a Voltage-Induced Frequency Drift; Eric Dziekan1; Joshua T.K. Johnson1; Santini Robert1; Scott A McLuckey1; 1Purdue University-Department of Chemistry, West Lafayette, IN

MP 291 Mass Manipulation of Ions in a Cryogenic Linear Ion Trap: Simulations and Experiment; Larry Tesler1; Nicolas C Poller2; 1University of Florida, Gainesville, Florida; 2University of Florida, Gainesville, Florida

MP 292 Ion Journey in a Mass Spectrometer: Simulation of the Ion Trajectories from an Atmospheric Pressure Source to the mass analyzer; Xiaoyu Zhou1; Zheng Ouyang2; 1Purdue University, west lafayette, Indiana; 2Purdue University, West Lafayette, IN

MP 293 Maximizing Linear Quadrupole Resolution and Sensitivity Using Digital Waveform Manipulation; Zachary Philip Gotlib1; Gregory Forrest Brabec1; Peter Ta Reilly1; 1Washington State University, Pullman, WA

MP 294 Mapping the Pseudopotential Well at all Points in...
the Stability Diagram; Peter Ta Reilly1; Gregory Forrest Brabec2; Washington State University, Pullman, WA

Lead-Free Ceramic Continuous Dynode Electron Multiplier; Hiroshi Kobayashi1; Motohito Suyama2; 1Hamamatsu Photonics K.K., Iwata, Shizuoka; 2Hamamatsu Photonics K.K., Iwata, Japan

MP 296

Vacuum Ultra-Violet (VUV) Detection as a Complement to Mass Spectrometry (MS) Analysis of Biological Metabolites; Shinjiro Kenneth Strain1; James Diekmann2; Brooke Barnette3; Mark Emmett4; 1Dep of Neuroscience and Cell Biology, University of Texas Medical Branch, Galveston, TX; 2VUV Analytics, Austin, TX; 3Dep of Biochemistry and Molecular Biology, University of Texas Medica Branch, Galveston, TX; 4Dep of Pharmacology & Toxicology, University of Texas Medical Branch, Galveston, TX; 5Dep of Radiation Oncolog, University of Texas Medical Branch, Galveston, TX; 6UTMB Cancer Center, University of Texas Galveston, USA

MP 297

A Modular Data Station for Radio-Frequency Ionization FT-ICR Mass Spectrometry Built on Robust and Expandable Commercial Architectures for Imaging Applications; Matthew R Brantley1; Solouki Touraj2; 1Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, Shanghai; 2Shimadzu Research Laboratory (Europe) Ltd., Manchester, Manchester

MP 298

Multiplexed Targeted Assays Using Ion Trap Waveform Isolation; Philip M Remes; Thermo Fisher Scientific, San Jose, CA

MP 299

Deconvolution Method for Multiple Harmonics FTMS Spectra; Sergey Smirnov1; Aleksandr Rusinov2; Li Ding1; 1Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom; 2Shimadzu Research Laboratory (Europe) Ltd., Manchester, Manchester

MP 300

Novel Tandem Ionization GCxGC-TOF MS for Characterization of Allergens in Cosmetics; Matthew Edwards1; Joe Blanch1; Laura McGregor2; Nick Bukowski2; Pete Grosshans3; Chris Hall4; Massimo Santoro5; 1David Wevill6; 2Markes International, Cardiff, UK; 3Markes International Inc., Cincinnati, OH

MP 301

Design and Simulation for a Novel Wedge Ion Guide (WIG) to Achieve Ion Compression and Ion Bending; Yupeng Cheng1; Xiaqiao Zhang2; Wenjian Sun3; 1Shimadzu Research Laboratory (China) Co., Ltd., Shanghai, Shanghai; 2Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China

MP 302

SCOUT-MRM: a Method to Acquire Large Numbers of MRM without Predefined Retention Time; Cox Dave1; Blandine Rougemont2; Romain Carriere2; 1J.C. YVES LEBLANC3; Lemoine Jerome4; 1SCIEX, Concord ON, Canada; 2Institut des Sciences Analytiques - UMR CNRS, Villerbanne (Lyon), France; 3Institut des Sciences Analytiques - UMR CNRS, Villerabnne (Lyon), France; 4SCIEX, Concord, ON

INTACT PROTEINS

MP 303

Making Heavy Peaks With a Pinch of Sugar: A Strategy for Intact Protein MS Quantitation in Any Feed; Jennifer Quijada1, 2; Jared R. Auclair1, 2; Joseph P. Salisbury1, 2; Jeffrey Agar1, 2; 1Barnett Inst., Northeastern University Boston, MA; 2Northeastern University, Boston, MA

MP 304

An LC-MS based method for monitoring the activation of Mestotryptsin and a Strategy for Quantitation in Cellular Secretions; Derek Wachtel1; Sushmit Maitra2; Keith Goodman2; Dan Warren2; Lyle Burton2; Marco Kessler1; Sanjeev Forsyth1; Maria Ribadeneira1; 1Ironwood Pharmaceuticals, Cambridge, MA; 2SCIEX, Concord ON, Canada

MP 305

Separation of Native Proteins and Protein Complexes using Capillary Electrophoresis Coupled with Mass Spectrometry; James Wilkins1; Jonathon Johnston1; Michael J Trinka2; Alma Burlingame1; 1UCSF, San Francisco, CA; 2UCSF, San Francisco, CA

Development of a high quality intact protein standard for LC and MS quality control and application development; Helene Cardassi1; Rosa Viner2; Vikrant Gohil2; Kay Opperman1; John Rogers1; Kelly Flook2; Alexander Cherkasky3; Jim Stephenson3; Egle Cakauskas3; Kestutis Bargaila3; Agne Alminaite3; Viktorija Vitkovske6; Juozas Siurkus3; 1Thermo Fisher Scientific, San York, NY; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Cambridge, MA; 4Thermo Fisher Scientific, Rockford, IL; 5Thermo Fisher Scientific, Sunnyvale, CA; 6Thermo Fisher Scientific, Vilnius, Lithuania

MP 307

Novel Strategy for Quality Assessment of Glycosylation on a Biotherapeutic Glycoprotein by Intact Protein Analysis; Unyong Kim1, 2; Myung Jin Oh1, 2; Hyun Joong Kim2; Youngsuk Seo1, 2; Hyun Joo An1, 2; 1Asia Glycomics Reference Site, Daejeon, Korea; 2Graduate School of Analytical Science and Technology, Daejeon, Korea

MP 308

The Use of Methionine Sulfoxide Reductases to Reverse Oxidized Methionine for Mass Spectrometry Application; Robert Cunningham1; Kratika Singhal2; Ryan T Fellers2; Luca Forcelli3; Henrique Dos Santos Seckler2; Bhavin Patel1; Egle Cakauskas3; Juozas Siurkus4; Philip Compton5; John C Rogers6; Neil L Kelleher7; 1Thermo Fisher Scientific, Rockford, IL; 2University of Illinois at Chicago; 3Rockford, IL; 4Northwestern University, Evanston, IL; 5Thermo Fisher Scientific, Vilnius, Lithuania

MP 309

Top-Down sequence-specific copper and zinc retenction from ECD and ETD of superoxide dismutase for ALS spinal cord; Joe Beckman1; Yury V Vasili2, 3; Nathan I Lopez4; Valery G Voyniv5; 1Linus Pauling Institute, Corvallis, OR; 2-eMion, Inc. Corvallis, Oregon; 3Oregon State University, Corvallis, OR; 4Linus Pauling Institute, Oregon State University Corvallis, OR

MP 310

Two-Dimensional Time-Resolved LC-MS Deconvolution for Intact Mass Analysis of Biological Drugs; Peter Habert1; Joe Shambough2; David Bush3; Maurizio Bronzetti2; Cassandra Wigmore4; Amit Brandenburg4; 1Genedata GmbH, Munich, Germany; 2Genedata Inc, Lexington, MA; 3Genedata AG, Basel, Switzerland

MP 311

Development of LC/MS/M Bioanalytical Method for Quantitative Determination of Intact Insulin Glargine and Human Insulin in Plasma; ZHAOQI ZHAN1; Zhe Sun2; Jie Xing2; Edwin Zhi Wei Ting3; 3Shimadzu (Asia Pacific) Pte Ltd, Singapore, Science Park 1; 4Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd 79 Science Park Drive #02-01/08, Singapore

MP 312


MP 313

Is Online Detection by Native ESI MS Beneficial to Size Exclusion Chromatography?: Cedric Bob1; Igor A Kaltashov; 1University of Massachusetts Amherst, Amherst, MA

MP 314

BAC-PAGE: A Novel Proteomics Workflow Using Dissolvable Polyacrylamide Gel Electrophoresis; Nobuaki Takemori1; Ayako Takemori2; 1Ironwood Pharmaceuticals, Cambridge, MA; 2Shimoto Scientific, New York, NY; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher Scientific, Cambridge, MA

MP 315

Impact of Phosphorylation on the Ionization Efficiency of Intact Proteins: A Systematic Investigation; Zhijie Wu1; Wenxuan Cai2; Bifan Chen1; Ziqing Lin1; Zachery Gregorich1; Ying Ge1; 1Department of Chemistry, UW-Madison Madison, WI; 2University of Wisconsin Madison, Madison, WI
| MP 316 | Magnetic Resin Microreactor for Affinity-Capture Top-Down Mass Spectrometry: Delafield Daniel1; Zhe Wang2; Woodward Toni3; Si Wu4; 1University of Oklahoma, Dept. of Chem & Biochem Norman, OK |
| MP 317 | High Resolving Power Isoelectric Focusing for Routine and Comprehensive Proteoform Interrogations: Michael Tran1; John Corbett1, 2; Daniel A Plymire1; Casey Wing3; Steven M Patrie1, 2; 1University of Texas at Dallas, Richardson, TX; 2University of Texas Southwestern, Dallas, TX |
| MP 318 | On the Reliability and Reproducibility of 2D Isoelectric Focusing and Reversed-Phase Chromatography with FTMS for Intact Label-free Proteoform Quantitation: John Corbett1, 2; Michael Tran1; Casey Wing3; Daniel Plymire1; Steven Patrie1, 2; 1University of Texas at Dallas, Richardson, TX; 2University of Texas Southwestern Medical Center, Dallas, TX |
| MP 319 | Data Independent Characterization of Proteins from 2D CID Fingerprints Generated through Collision Energy Scanning: Boris Kozlov1; Jeff Brown1; John Hoyes1; 1Waters, Wilmslow, United Kingdom |

**ION ACTIVATION/DISSOCIATION 320 - 340**

| MP 320 | Potential Fragmentation of the Hydroxy Carbene; Sabyasachi Mistry; Purdue University, West Lafayette, IN |
| MP 321 | Photodissociation of Triethylphosphonium Charge Tagged Peptides: Nick DeGraan-Weber1; James P Reilly1; 1Indiana University Dept. Chemistry, Bloomington, IN |
| MP 322 | Structural Determination of Peptides Containing Multiple Acceptors using Action-EET: Lance E Talbert1; Ryan R Julian1; 1Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany |
| MP 323 | Implementation and Bench-Marking of Dual-Polarity 193 nm UVPD for Bottom-Up Proteomics on the Thermo Orbitrap Fusion Tridend Mass Spectrometer: Sylvester Greer1; Jennifer S Brodbelt2; 1Univ of Texas at Austin, Austin, Texas; 2University of Texas at Austin, Austin, TX |
| MP 324 | Reaction Dynamics of Small Sulfur-Containing Molecules with a Hydrated Electron in the Gas Phase; Chi-Kit Su1; Wai-Kit Tang2; 1City University of Hong kong; Hong Kong; 2City University of Hong Kong, Hong Kong SAR, Hong Kong |
| MP 325 | Kinetic Energy Release and Fragmentation Pattern of Substituted Anilines after Collision Activation: Sarah Seulen1; Tassilo Muskat1; Jürgen Grotemeyer1; 1Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany |
| MP 326 | Photodissociation Action Spectroscopy of Fluorescent Dye Molecules in the Gas Phase; Elena Mitrofanov1; Tassilo Muskat1; Claus Gernert1; Jürgen Grotemeyer1; 1Institute for Physical Chemistry, Christian-Albrechts-University at Kiel, Kiel, Germany |
| MP 327 | Difference of Electron Capture and Transfer Dissociation Mass Spectrometry on Zn2+-Polyhistidine Complexes in the Absence of Remote Protons: Daiki Asakawa1; Edwin De Pauw1; 1AIST, Tsukuba, Ibaraki |
| MP 328 | Glycan and Peptide Analysis with Iron Oxide Nanoparticle MALDI Matrices; Joseph Mercer Wilson1; Qiadi Liang1; Jennifer Sherwood1; Thomas Macher1; 1University of Alabama, Tuscaloosa, AL |
| MP 329 | Characterized Fragmentation of Neutral Carbohydrates Induced by Quartz-Tungsten-Halogen Light Prior to MALDI Mass Spectrometry: Yu-Meng Ou1; Yin-Hung Lai1; Yi-Sheng Wang1; 1Genomics Research Center, Academia Sinica Taipei, Taiwan |
| MP 330 | Optimizing Production of Selected Product Ions for SRM Analysis in a Quadrupole Collision Cell; Bennett Kalafut1; Harold Oser1; 1Thermo Fisher Scientific, San Jose, California |
| MP 331 | Cationized Polymer Fragmentation: Energetic and Mechanistic Effects of End-group Substitution: Jordan M. Rabus1; Benjamin Bytheil1; 1University of Missouri-St. Louis, St. Louis, MO |
| MP 332 | The Collision of a Hypervelocity Massive Projectile with Free-Standing Graphene: Investigation of Secondary Ion Emission and Projectile Fragmentation: Sheng Geng1; Stanislav S Verkhoturov1; Michael J Eller1; Emilie A Schweikert1; 1Texas A&M University, College Station, TX |

**ION ACTIVATION/DISSOCIATION**

| MP 333 | Comparison of Ion Temperatures in a Linear Trap using the Ambient Ionization Techniques: ESI, DART and APCI; George N. Khairallah1; Morphy Dumlao2; Richard A J O’Hair2; William A Donald2; 1Bio21 Inst, Uni of Melbourne and Accurate Mass Scientific P/L, Melbourne, VIC; 2University of New South Wales, Sydney, Australia; 3University of Melbourne, Victoria, Australia |
| MP 334 | Exploring the Combination of Helium Charge Transfer Dissociation (He-CTD) and Hydrogen Deuterium Exchange Tandem Mass Spectrometry (HDX-MS/MSn): Gregory C. Donohoe1; Li Pengfei1; Glen P. Jackson1; Stephen J Valentine1; 1West Virginia University, Morgantown, WV |
| MP 335 | Dissociation of Gas-Phase, Triply-Charged Lanthanide and Doubly-Charged Actinide Complexes by Multiple-Stage Tandem Mass Spectrometry: Cassandra Hanley1; Michael Van Stipdonk1; 1Duquesne University, Pittsburgh, PA |
| MP 336 | Chemical Derivatization to Enhance 266 nm Ultraviolet Photodissociation for Proteomics: M. Montana Quick1; Rachel Mehaffey1; Lucas D. Akin1; 1University of Texas at Austin, Austin, TX |
| MP 337 | Dissociation of Gas-Phase, Doubly-Charged Uranyl-Acetone and Uranyl-Dimethyl Sulfoxide Complexes by Collisional Activation and Infrared Photodissociation: Theodore Corcovilos1; Cassandra Hanley1; Evan Perez1; Benjamin J Bytheil1; Michael J. Van Stipdonk1; 1Duquesne University, Pittsburgh, PA; 2University of Missouri-St.Louis, St. Louis, MO |
| MP 338 | General Rules of Fragmentations Evidencing Lasso Structures in CID and ETD: Kevin Jeanne Dit Fouque1; Helene Lavanan1; Severine Zirah2; Julian D. Hegemann3; 1University of Texas at Arlington, Arlington, TX; 2University of Oklahoma, Dept. of Chemistry; 3University of Alabama, Provo, UT |
| MP 339 | A Novel Macrocylic Polyether with Carbon Bridgehead Atoms: Complexation with AlkalI Metals; Anupriya Anupriya1; David V Dearden1; 1Brigham Young University, Provo, UT |
| MP 340 | Ab Initio Prediction of Collision-Induced Dissociation Mass Spectra: LLI1; Rodger Mensing1; Benjamin Janesko1; 1University of Texas at Arlington, Arlington, TX; 2Texas Christian University, Fort Worth, TX |

**ION MOBILITY: APPLICATIONS (OTHER/INSTRUMENTATION) 341 - 373**

| MP 341 | Characterization of i-motif DNA Kinetically Trapped Folding Intermediates Using nanoESI-TIMS-MS and Molecular Dynamics: Alvyasa Garabedian1; David Butcher1; Jennifer Lippens2; Jaroslava Miksovskova1; Prem Chapagain1; Daniele Fabs1; Mark E Ridgeway2; Melvin Park2; Francisco Fernandez-Lima1; 1Florida International University, Miami, FL; 2The RNA Institute, University at Albany Albany, NY; 3Bruker Daltonik, Billerica, MA |
MP 342  Analysis of Synthetic Nucleotides using Accurate Mass and Ion Mobility,  Cynthia Sanderson1; Sushmit Maitra1; Keith Goodman1; 1SCiEX, Concord ON, Canada

MP 343  High Resolution Ion Mobility-Mass Spectrometry for Separation of isomers in Natural Products and Complex Mixtures; Michael Groessl1; Sonia Klee1; Stephan Graf1; 2OFWERK, Thun, Switzerland

MP 344 Frequency Encoding the Mobility of Isomeric Glycans: Separations Using Drill Tube Ion Mobility and Tandem Mass Spectrometry; Kelsey A Morrison1; Brad K Bendik1; Brian H Clowers1; Washington State University, Pullman, WA; 1University of Colorado, Denver - Anschutz Medical Campus, Denver, CO

MP 345 Rapid and High-Throughput Detection and Quantitation of Radiation Biomarkers in Human and Nonhuman Primates by Differential Mobility Spectrometry-Mass Spectrometry; Zhidan Chen1; Stephen L. Coy1; Evan L. Pannuki1; Evagelia C. Laiaikas1; Adam B. Hall1; Albert J Jr Furnace1; Paul Younis1; 1Northeastern University, Boston, MA; 2Georgetown University, Washington, DC

MP 346 Enhancing Carbohydrate Isomer Separation with Ion Mobility Spectrometry-Mass Spectrometry; Xueyun Zheng1; Xing Zhang1; Nathaniel S Schocker1; Roger A Ashmus1; Igor C Almeida1; Keji Tang1; Catherine E Costello1; Richard D Smith1; Katja Michael1; Erin Baker1; 1Pacific Northwest National Laboratory, Richland, WA; 2University of Colorado, Denver, CO; 1University of Texas, El Paso, TX; 2Boston University School of Medicine, Boston, MA

MP 347 Evaluation of Collision Cross Section Calibrants for Structural Analysis of Lipids by Traveling Wave IM-MS; Kelly M Hines1; Jody C May1; John A McLean1; Libin Xu1; 1University of Washington, Seattle, WA; 2Vanderbilt University, Nashville, TN

MP 348 Rapid Differentiation of Bile Acid Isomers Using Sodiated Multimer Complexes with Ion Mobility - Mass Spectrometry; Robin H J. Kemperman1; Christopher D Chouinard1; Richard A Yost1; 1University of Florida, Gainesville, FL

MP 349 Machine Learning-Enabled Collisional Cross Section Predictor (CCSP) for Identification of Unknown Lipids; Molly T Soper-Hopper1; Nga Lee Ng1; Nicholas V Hud1; Charles Liotta1; Facundo M Fernandez1; 1University of Florida, Gainesville, FL; 2Vanderbilt University, Nashville, TN

MP 350 Reducing Isobaric Species by Differential Mobility Spectrometry (DMS) for infusion-based lipidomics; Goncalo Vale1; Jeff McDonald1; Paul RS Baker1; 1UT Southwestern Medical Center, Dallas, TX; 2Sciex, Framingham, MA

MP 351 Characterization of Exposome Components in Human Bloodfluids Using LC-ESI-Ion Mobility QTOF Mass Spectrometry; Yunia Li1; Mine Palazoglu1; Olivier Fiehn1; 1UC Davis Genome Center, Davis, CA

MP 352 Increasing the Resolving Power of Differential Mobility to Supplement (or Eliminate) LC Separation; J.C. Yves Leblanc1; Chang Liu1; Larry J Campbell1; Brad Schneider1; 1SCiEX, Concord, ON, ON; 2SCiEX, Concord, ON, Canada

MP 353 Enhanced Ion Mobility Separation of Derivatized Isobaric Isotopes by DESI and MALDI TOF Mass Spectrometry; Mark Towers1; Michalagination Khan1; C.Logan C Mackay1; Ruth Andrew1; Emmanuelle Claude1; 1Waters Corporation, Wilmslow, UK; 2Queen’s Medical Research Institute, University of Edinburgh, Edinburgh, UK; 3SIRCAM, University of Edinburgh, Edinburgh, UK

MP 354 Rapid separation of Vitamin D epimers in human serum by Liquid Chromatography Ion Mobility Mass Spectrometry; Nicholas Oranz1; Christopher D Chouinard1; Richard A Yost1; 1University of Florida, Gainesville, FL

MP 355 Combining Rapid Isomer Separations and Physicochemical Property Predictions for Drug Molecules with Differential Mobility Spectrometry; CHANG LIU1; Yves J C LeBlanc1; Jeffry Shields1; Hui Zhang1; John S Janiszewski1; Christian Ieritano1; Luke Melo1; Evan Shepherson1; Mitch Verbuyst1; Moaraj Hasan1; Dalia Naser1; Scott W Hopkins1; Larry J Campbell1; Tim Hoffman1; 1SCiEX, Concord, ON; 2Pfizer, Groton, CT; 3University of Waterloo, Waterloo, Ontario (ON)

MP 356 Complicated Natural Product Analysis Using Liquid Chromatography (LC) – Drill Tube Ion Mobility (DTIM) Mass Spectrometry (MS); Xin Ma1; Tao Bo1; 1Agilent Technologies, Beijing, China; 2Agilent Technologies (China) Limited, Beijing, China

MP 357 Structural Database of Secondary Metabolites for Natural Product Discovery: Ion Mobility-Mass Spectrometry Measurements in Nitrogen and Helium Drift Gases; Andrezej Balinski1; Jody C May1; Brian O Bachmann1; Sarah M Stow1; John A McLean1; 1Vanderbilt University, Nashville, TN

MP 358 Determining Molecular Modifications by ESI Ion Mobility Mass Spectrometry (ESI IM-MS); Alfred L. Yergey1; Paul S Blank1; Stephanie M Cologna1; Peter S Backlund1; Allan Darling1; 1NIH, Bethesda, MD; 2University of Illinois, Chicago, IL; 3Vtess Inc, Gaithersburg, MD

MP 359 Analysis of Propolis Extracts and Isomeric Flavonoid Mixtures Using Trapped Ion Mobility QTOF-MS; Sven Wolfgang Meyer1; Alexander Harden1; Detlev Suckau1; Peter Sander1; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker Daltonik GmbH, Bremen, Germany

MP 360 Investigation of the Cu(I) and Zn(II) Binding Characteristics of Methanobactin from Methylosinus trichosporium OB3b; Jacob Watson McCabe1; Rajpal Vangala1; Laurence Ambrose Angel1; 1Texas A&M University – Commerce, Commerce, TX

MP 361 Single Oligomer Polyurethane Synthesis: Characterization by Ion Mobility-Mass Spectrometry and Computational Strategies; Tiffany Crescentini1, 2; Sarah M Stow1, 2; Robert W. Davis1, 2; Gary A. Sulikowski1, 2; David M. Hercules1, 2; John A McLean1, 2; 1Vanderbilt Dept. of Chemistry, Nashville, TN; 2Vanderbilt University, Nashville, TN; 3Vanderbilt Institute of Chemical Biology, Nashville, TN

MP 362 Characterization of Conformational Isomers of Bisthenylethenes (BTEs) Using Ion Mobility Mass Spectrometry; Xu Wang1; Ming Wang1; Alejandro Cisneros1; Xiaopeng Li1; 1Texas State University, San Marcos, TX

MP 363 Enhancing Analytical Characterization Workflows of Complex Synthetic Polymeric and Small Molecule Mixtures through Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS); Sarah M Stow1, 2; Robert W. Davis1, 2; Gary A. Sulikowski1, 2; David M. Hercules1, 2; John A McLean1, 2; 1Vanderbilt University, Nashville, TN; 2Vanderbilt University, Nashville, TN; 3Vanderbilt Institute of Chemical Biology, Nashville, TN

MP 364 Comparison of Ion Mobility Mass Spectrometry Applications on Commercial Drift-Tube and Differential Mobility Based Instruments; Jeffrey Gilbert1; Jesse L Balcer1; John O’Brien1; David McCaskill1; Yelena Adelfinskaya1; Gerrit J Deboer1; Cassie Frander1; Krishnamoorthy Kuppannan1; Mary D Evenson1; Lisa Buchholz1; Bruce M Bell1; Jeffrey R Gilbert2; Bruce M Bell2; 1The Dow Chemical Company, Midland, MI; 2Dow AgroSciences, Indianapolis, IN

MP 365 Separation of Positional Isomers of PAHs Using LC-MS/MS Coupled with Differential Ion Mobility Mass Spectrometry; Shaokun Pang1; Liling Liu1; Xiaorong Liang1; Amos Baruch1; Leo Wang2; Brian Dean2; Yuzhong Deng1; 1SCiEX, Redwood City, CA; 2Genentech Inc, South San Francisco, CA
MONDAY POSTERS

MP 366 Structural Dependent Section of Calibrants for Accurate Measurement of CCS Values Obtained with Ion Mobility Mass Spectrometry: Dongwan Ling1; Arif Ahmed1; Sungahn Kim1; Kyungpook National University, Daegu, Republic of Korea

MP 367 Enantiomer Separation of Amino Acids through Binuclear Copper Bound Complex by Travelling Wave Ion Mobility Mass Spectrometry: Xiang-Ying Yu1; Zhong-Ping Yao1, 2; State Key Laboratory of Chinese Medicine and Molecular Pharmacology (Incubation), Shenzhen Research Institute of the Hong Kong Polytechnic University, Shenzhen, China; Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China

MP 368 Maintaining Speciation of Reactive Gas-Phase Complexes for the Metals Uranyl, Barium, Cesium and Lanthanum with Sulfoxides using AP-IMS-MS: Austen Davis1; Brian H Clowers1; Washington State University, Pullman, WA

MP 369 Ion Mobility Mass Spectrometry of Polyoxometallate Anion Assemblies: Helene Lavranos1; Sebastien Hupin; Michael Grossi2; Madeleine Pilot2; Guillaume Izzet3; Carlos Afonso3; Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; TOFWERK, Thun, Switzerland; Sorbonnes Univ, CNRS UMR 8332 IPMC Paris, France

MP 370 Ion Mobility Quadrupole Time-of-Flight Mass Spectrometer Modified for Electron Capture Dissociation of Glycans, Glycoconjugates, Peptides, and Proteins: Rebecca S. Glaskin1; Kenneth Newton2; Afonso1; Michael Tawiah1; Sunghwan Kim1; Chicago, IL

MP 371 On-line Parallel Accumulation – Serial Fragmentation (PASEF) for Shotgun Proteomics on a Modified UHR-QTOF Platform: Scarlet Beck1; Florian Meier1; Jürgen Cox1; Markus Lubeck2; Stephanie Kaspar-Schoenefeld3; Nicole Drechsler4; Niels Goedecke5; Melvin Park2; Oliver Raether6; Matthias Mann7; Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; Bruker Daltonics GmbH, Bremen, Germany; Bruker Daltonic, Billerica, MA

MP 372 Bio-Molecule Characterization Using a Novel Ion Mobility Orbitrap Mass Spectrometer: Sung Hwan Yoon1; Thomas Schneider2; Tao Liang1; Yue Huang2; Robert K Ernsth1; Mikhail E Belov3; David Dixon2; Kirk A. Peterson3; 1University of Maryland, Baltimore, MD; 2Deurion LLC, Seattle, WA; 3Spectrolymph LLC, Kennenwick, WA; 4University of Maryland Baltimore, Baltimore, MD

MP 373 Improvement of Selectivity and Detection Capabilities in Non-Targeted Metabolomics Using Liquid Chromatography with Drift Tube Ion Mobility Mass Spectrometry: Tim Causon1; 2Teresa Mairinger1; 2Stephan Hann1, 2; 1University of Natural Resources and Life Sciences (BOKU Vienna), Vienna, AT; 2Austrian Centre of Industrial Biotechnology (acib), Vienna, AT

MP 374 Radical Cations of Nucleobases: A Gas-Phase Reactivity and Structural Elucidation Study: Michael Lesslie1; Lawler T John1; Courtney Kanak1; Ryszow Victor1; 1Northern Illinois University, DeKalb, IL

MP 375 Gas-Phase Reactions of the Deprotonated Nucleobases with H, N, and O Atoms: Charles Nichols1; Zhe-Chen Wang1; Carl W Lineberger1; Veronica M Bierbaum1; 1University of Colorado, Boulder, CO

MP 376 Charge Transfer Dissociation (CTD) of Phosphocholines: Gas-Phase Ion/Ion Reactions between Helium Cations and Phospholipid Cations: Pengfei Li1; Glen P Jackson1; 1West Virginia University, Morgantown, WV

MP 377 DNA/Peptide Complex Ion Dissociations: Survivor Non-Covalent Sites in “Three-Body” Product Ions Independent on Charge Polarity: Bessem Brahim1; Sandra Alves2; Jean-claude Tabet3; 1University Paris VI (UPMC) case 45 UMR 8323 CNRS, Paris Cedex 05, France; 2CEA/IBiTeC-S SPI LEMM Gil Sur Yvette, France; 3University Paris VI (UPMC) case 45 UMR 7201 CNRS, Paris Cedex 05, Ile de France; 4CEA, IBiTeC-S SPI LEMM Gil-sur-Yvette, France

MP 378 Origin of the Regioselective [NH3+CO2] Concomitant Losses from Aspartate Predicted by Calculations and Evidenced by 13C and D Labeling: Pierre Saint Hilaire1; Anna Wamet2; Ulli Martin Hohenester2; Yves Gimbert; Marie-Françoise Olivier1; Francois Fenaille1; Benoit Colsch1; Christophe Junot1; Jean-Claude Tabet1; 1CEA, IBiTeC-S, SPI, LEMM, Gil Sur Yvette Cedex, France; 2Université Grenoble Alpes et CNRS UMR 5052, Grenoble, France; 3University Paris VI (UPMC) case 45 UMR 7201 CNRS, Paris Cedex 05, Ile de France; 4CEA, IBiTeC-S SPI LEMM Gil-sur-Yvette, France

MP 379 Cation Influence on the Competitive Ion-Dipole and Ion-Ion Interaction: Distinction of Hexose Phosphate Structural Isomers Using Basic Amino Acids: Ekaterina Daryi1; Sandra Alves2; Alain Perret1; Jean-claude Tabet1; 1CEA-Genoscope/UMR8030, Evry, Ile-de-France; 2UPMC-IPCM/CSOB/UMR8232, Paris Cedex 05, France; 3CEA-Genoscope/UMR8030, Evry, France

MP 380 Distinguishing Hexose Isomers by Lithiated Ion Adduction to Water: Matthew Campbell1; Chen Dazhe2; Gary L. Glish3; 1UNC, Chapel HIll, NC; 2UNC-Chapel Hill, Durham, NC; 3UNC-Chapel Hill, Chapel Hill, NC

MP 381 Ion-Molecule Reactions of Fe+ and FeO+ with Ozone: Temperature Dependent Kinetics and Reaction Pathways: Tri Le1; Gregory Miller1; Joshua Melko1; 1University of North Florida, Jacksonville, FL

MP 382 Bipimolecular Reactions between Water and Metal Dioxide Cations, MO2+: Energetics and Mechanisms of Hydration, Hydrolysis and o xo-Exchange: Phuong D. Dau1; John Gibson1; David Dixon2; 1University of Alabama, Tuscaloosa, AL; 2Washington State University, Pullman, WA; 3Argonne National Laboratory, Argonne, IL

MP 383 Dual-Electrospray Synthesis and Reactions: Shaan Rashid1; Paul Michael Mayer2; 1University of Ottawa, Ottawa, Canada; 2University of Ottawa, Ottawa, ON

MP 384 Efficient and Direct Amide Bond Formation Using a Novel Alcohol/Amine Cross-Coupling Reaction Mediated by Electrospray-Based Photo-catalysis: Savithra Jayaram1; Qiongqiong Wan1; Abraham Badu-Tawiah1; 1The Ohio State University, Columbus, OH

ION MOLECULE, ION/IION, ION/ELECTRON INTERACTIONS

MP 385 Phenylintryon ions: Gas-phase Synthesis, Properties in Selective Alkane Activation, Gas-phase acidity, Hydride Affinity, Electron Affinity, and Electronic states: Lei Yue1; Pan Yuanjiang1; Ding Chuanfan2; Zhejiang University, Hangzhou, China; 2Fudan University, Shanghai, China
ION SPECTROSCOPY

MP 399 - 411

MP 399 Calculation of Average-Dipole-Orientiation Rate Constants for Proton Transfer Reactions between H3O+ and Organic Compounds Using Molecular Mass and Elemental Composition: Kanako Sekimoto1; Shao-Meng Li2; Bin Yuan1; Abigail Koss1-2; Matthew Coggon1-4; Carsten Warnke1; Joost De Gouw1; NOAA Earth System Research Laboratory, Boulder, CO; Yokohama City Univ., Yokohama, Japan; Environment Canada, Tronto, Canada; Cooperative Institute for Research in Environmental Sciences, University of Colorado Boulder, Boulder, CO

MP 400 Action-Excitation Energy Transfer Illuminates the Impact of Amino Acid Epimerization and Isomerization on Peptide Structure: Dylan Riegs; University of California - Riverside, Riverside, CA

MP 401 Thermochromic Differences in Isomeric Oligopeptides: Structural Insights Using IRMPD Spectroscopy: Patrick Henry Batoon; Jianhua Ren; Jos Oomens; Giel Berden; University of the Pacific, Stockton, CA; University of Berlin, Germany.

MP 402 Deep Molecular Structure Probing in MSn by IR Ion Spectroscopy: Deamidation Reaction Networks of Gin and Asn-Containing Dipeptides: Jos Oomens; Lisanne JM Kemkes; Jonathan Martens; Josipa Grzetic; Giel Berden; Radboud University, Nijmegen, Netherlands.

MP 403 Infraredspectroscopy of Protonated and Radical Cationic Triphenylamine: Giel Berden; Md. Musleh Uddin Munshi; Jonathan Martens; Jos Oomens; FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands.

MP 404 The Remarkable Ionic Coordinating Ability of All-cis 1,2,3,4,5-Cyclohexane in the Gas Phase: Terry Memhorn; Blake Ziegler; Michael Lecours; Rick Marta; Eric Gillion; Scott W Hopkins; David O'Hagan; Keddie Neil; University of Waterloo, Waterloo, ON; University of Waterloo, Waterloo, Ontario, Canada; University of Waterloo, Waterloo, Ontario (ON); University of St. Andrews, St. Andrews, UK.

MP 405 Laser Spectroscopic Investigation on Dichlorofluorobenzenes by Means of Resonance Enhanced Multiphoton Ionization and Mass Analyzed Threshold Ionization: Sascha Krüger; Jürgen Grotemeyer; Institute for Physical Chemistry; Christian-Albrechts-University at Kiel, Kiel, Germany.

MP 406 New Insights into the Combustion Chemistry of Butane Isomers in Premixed Low-Pressure Hydrogen Flames by Imaging Photoelectron Photoion Coincidence Spectroscopy: Thomas Bierkandt; Yasin Karakaya; Dominik Krüger; Patrick Hemberger; Patrick Oßwald; Markus Köhler; Tina Kasper; University of Duisburg-Essen, Duisburg, Germany; Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany.

MP 407 VUV Spectroscopy Group, Swiss Light Source: Deamidation Reaction Networks of Gin and Asn-Containing Dipeptides: Jos Oomens; Lisanne JM Kemkes; Jonathan Martens; Josipa Grzetic; Giel Berden; Radboud University, Nijmegen, Netherlands.

MP 408 Förster Resonance Energy Transfer as a Distance Probe for Gas-phase Ubiquitin Ions: Jocky Chun Kui Kung; Martin F Czar; Benjamin Schuler; Rebecca A Jockusch; University of Toronto, Toronto ON, Canada; University of Zurich, Zurich, Switzerland.

MP 409 Alkaline Cation Cationelation in Cold β-0-4 Tetralinol Complexes: Andrew F DeBlase; Eric T Dziekonski; John R Hopkins; Nicole L Burke; Huaming Sheng; Hilika I Kenttamaa; Scott A McLuckey; Timothy S Zwier; Purdue University-Department of Chemistry, West Lafayette, IN.


MP 411 Photodissociation Dynamics in Infrared Multiple Photon Dissociation Monitored by Time-of-Flight Mass Spectrometry: Matthew Bell; Nicolas C Polfer; University of Florida, Gainesville, FL.

MP 412 Gas Phase Fluorescence Spectroscopy for the Study of Catalytic Nitrogen-Containing Heterocycles: Alessandra Berzocco; Vaishnavi Rajagopal; Rowland Institute at Harvard, Cambridge, MA.

LC-MS: CHROMATOGRAPHY AND SOFTWARE (PART 1) 412 - 440

MP 412 Demonstration of Automated On-The-Fly Retention Time Updating and SRM Method Visualization for Targeted Peptide Quantitation: Susan Abbatiello; Qingyu Song; Mary Blackburn; Jacek W Sikora; Paul
MP 413 An Interactive Skyline Tool for Flagging Incorrectly Chosen Peptide Peaks Across Data-Independent Acquisition Experiments: AT-Peptide Peak Picking (AT-P3); Andy Lin1; Jarrett D Egerton1; Brooke Nuøn1; Michael J MacCoss1; 1University of Washington, Seattle, WA

MP 414 Column Performance: Comparison of Superficially Porous Porous Particle (SPP) to Fully Porous Particles (FPP); Robert Freeman1; Sharon Luo1; Shun-Hsin Liang1; Frances Carroll1; Ty Kahler1; Susan Steinike1; 1Resekt Corporation, Bellefonte, PA

MP 415 High Resolution LC/MS analysis of Therapeutic Oligonucleotides on a New Porous Polymer-Based Reversed Phase Column; Shanhui Lin1; Julia Baek1; Jim Thayer1; Hongxia Wang1; Jonathan L Josephs1; Xiaodong Liu1; 1Thermo Fisher Scientific, Sunnyvale, CA; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Sunnyvale, CA

MP 416 Slightly Bigger is Better: Nano-LC/MS with 100um ID columns; Brett Larsen1; Joshua Sandor1; Meghan McFadden1; Anne-Claude Gingras1,2; 1LTRI, Toronto, Canada; 2Department of Molecular Genetics, University of Toronto, Toronto, Canada

MP 417 Improving Sensitivity in LC/MS with Multi-Dimensional Chromatography; Thomas E. Wheat1; Amanda B. Dlugasch1; Patricia R. McConville1; 1Waters Corporation, Hopedale, MA; 2Waters, Milford, MA

MP 418 Maximizing Flexibility: A Gas and Temperature Enabled Chip-Based Solution for Nanoflow and Microflow LC-MS; Helena Svobodová1; Aaron Dewberry1; Amanda Berg1; Gary A Valaskovic1; 1New Objective, Inc., Woburn, MA; 2New Objectives, Inc., Woburn, MA

MP 419 Achieving High Proteome Coverage by Miniaturization of HPLC Columns; Annie Moradian1; Roxana Eggleston-Rangel1; Michael Sweredoski1; Sonja Hess1; 1California Institute of Technology, Pasadena, CA

MP 420 Sphingolipid Profiling Using Robust and Sensitive LC-MS-MS Method; Shachi Saluja1; Dipankar Malakar1; Manoj Pillar1; Avinash Bajaj1; Ujjaini Dasgupta1; 1Regional Centre for Biotechnology, Faridabad, India; 2Sicce, Gurgaon, India; 3Amity University, Gurgaon, India

MP 421 Evaluation of Critical Column Parameters for Use in Supercritical Fluid Chromatography by SFC-MS; Alison Wicker1; Doug D. Carlton Jr.1; Ty Kahler1; Kevin A Schug1; 1University of Texas at Arlington, Arlington, TX; 2Restek Corporation, Bellefonte, PA

MP 422 Advancing Separation Sciences under Alkali Conditions Using a Novel C18 Column for LC-MS; Haru Yazawa1; Yasuo Yamamori1; Hiroshi Tachikawa1; 1Imtakt Corporation, Kyoto, Japan; 2Imtakt Corporation, Kyoto, Japan

MP 423 Analysis of Antioxidants in Yam (Dioscorea alata L. var. Purpurea (Roxb.) M. Pouch.) by HILIC-UV-ECD-MS; Jaiswal1; David M Good2; Marc Browning1; Benjamin J Burns1; Ashley T Jordan1; Jeremy L Norris1; Richard M Castrillon1; 1Imtakt Corporation, Kyoto, Japan; 2Vanderbilt University MSRC, Nashville, TN

MP 424 Complementary ERLIC and RPLC Online Separations Significantly Expand Sequence Coverage in MS-Based Proteomic and Proteogenomic Studies; Candece Guerrero1; Pratik D Jagtap1; James Johnson2; Thomas F McGowan1; Tim Griffin1; 1University of Minnesota, Minneapolis, MN; 2University of Minnesota Supercomputing Institute, Minneapolis, MN; 3University of Minnesota at Twin Cities, Saint Paul, MN

MP 425 Combined New Approaches for Improved Quantitative and Qualitative LC-MS; Stephan Altmair1; Hans Griesinger1; Michael Schulz1; 1Merck, Darmstadt, Germany

MP 426 Rapid Separation and Determination Of 25-Hydroxy Vitamin D2 / D3 in Serum By UHPLC-MS/MS Using A Novel C18-PFP Stationary Phase; Geoffreay Faden1; Alan P McKeeown1; 1MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; 2Advanced Chromatography Technologies Ltd, Aberdeen, -

MP 427 Separation and Low Level Determination Of Catecholamines: Epinephrine, Norepinephrine and Dopamine from Plasma By UHPLC-MS/MS Using A Novel C18-PFP Column; Edward Faden1; Alan P McKeeown1; 1MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; 2Advanced Chromatography Technologies Ltd, Aberdeen, -

MP 428 LC/MS as a Monitoring Technique for (semi) Preparative Electrochemical Metabolite Synthesis; Lisa Frensemeier1; Uwe Karst1; 1University of Münster, Münster, DE

MP 429 Increased MS Protein Identification Rates Using 75 cm Long nano LC C18 Separation Columns: Pushing the Limits of Bottom-Up Proteomics; Daniel Lopez-Ferrerr1; Michael Blaik1; 1Ernst Medingen1; Aran Paulus1; Romain Huguet1; Remco Swart2; Andreas FR Huhmer1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Germering, Germany

MP 430 Maximizing Throughput of Shotgun Proteomics by Increasing the Internal Diameter of Nano-Capillary Columns; Yuan-wei Nie1; Danielle B Gutierrez1; William J Burns1; Ashley T Jordan1; Jeremy L Norris1; Richard M Castrillon1; 1Imtakt Corporation, Kyoto, Japan; 2Imtakt Corporation, Kyoto, Japan

MP 431 Extraction and Ionization Efficiency in On-line Supercritical Fluid Extraction and Chromatography—Mass Spectrometry for Protease Inhibitors and Steroids in Blood; Laura Kabal1; Michael Raetz2; Kyoko Watanabe2; Yasuhiro Funada3; Gerhard Hopfgartner3; 1University of Geneva, Geneva, Switzerland; 2Shimadzu, Kyoto, Japan

MP 432 Improved Sensitivity for Characterization of Sulfonylamides and Trimethoprim in Honey Using QuEChERS Extracts with LC-MS/MS; Hernando Escobar1; Jeffrey H Dahl1; Eddie Medina1; Christopher T Giles1; Shimadzu Scientific Instruments, Inc., Columbia, MD

MP 433 LC/MS-MS Method

MP 434 Quantitative Analysis of Oligonucleotides Using Liquid Chromatography Coupled with High Resolution/Accurate Mass (HR/AM) Mass Spectrometry; Niclí Jaiswal1; David M Good1; Marc Browning1; Benjamin Johnson1; Emily Measom1; Cassidy Hatch1; Min Meng1; Scott A Reuschel1; Troy Voelker1; 1Coverge, Salt Lake City, UT; 2Coverge, Madison, WI

MP 435 Rapid Separation and Determination Of 25-Hydroxy Vitamin D2 / D3 in Serum By UHPLC-MS/MS Using A Novel C18-PFP Stationary Phase; Geoffreay Faden1; Alan P McKeeown1; 1MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; 2Advanced Chromatography Technologies Ltd, Aberdeen, -

MP 427 Separation and Low Level Determination Of Catecholamines: Epinephrine, Norepinephrine and Dopamine from Plasma By UHPLC-MS/MS Using A Novel C18-PFP Column; Edward Faden1; Alan P McKeeown1; 1MACMOD Analytical Inc., 103 Commons Court PO Box 587 Chadds Ford, PA 19317; 2Advanced Chromatography Technologies Ltd, Aberdeen, -

MP 428 LC/MS as a Monitoring Technique for (semi) Preparative Electrochemical Metabolite Synthesis; Lisa Frensemeier1; Uwe Karst1; 1University of Münster, Münster, DE

MP 429 Increased MS Protein Identification Rates Using 75 cm Long nano LC C18 Separation Columns: Pushing the Limits of Bottom-Up Proteomics; Daniel Lopez-Ferrerr1; Michael Blaik1; 1Ernst Medingen1; Aran Paulus1; Romain Huguet1; Remco Swart2; Andreas FR Huhmer1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Germering, Germany

MP 430 Maximizing Throughput of Shotgun Proteomics by Increasing the Internal Diameter of Nano-Capillary Columns; Yuan-wei Nie1; Danielle B Gutierrez1; William J Burns1; Ashley T Jordan1; Jeremy L Norris1; Richard M Castrillon1; 1Imtakt Corporation, Kyoto, Japan; 2Imtakt Corporation, Kyoto, Japan

MP 431 Extraction and Ionization Efficiency in On-line Supercritical Fluid Extraction and Chromatography—Mass Spectrometry for Protease Inhibitors and Steroids in Blood; Laura Kabal1; Michael Raetz2; Kyoko Watanabe2; Yasuhiro Funada3; Gerhard Hopfgartner3; 1University of Geneva, Geneva, Switzerland; 2Shimadzu, Kyoto, Japan

MP 432 Improved Sensitivity for Characterization of Sulfonylamides and Trimethoprim in Honey Using QuEChERS Extracts with LC-MS/MS; Hernando Escobar1; Jeffrey H Dahl1; Eddie Medina1; Christopher T Giles1; Shimadzu Scientific Instruments, Inc., Columbia, MD

MP 435 Quantitative Analysis of Oligonucleotides Using Liquid Chromatography Coupled with High Resolution/Accurate Mass (HR/AM) Mass Spectrometry; Niclí Jaiswal1; David M Good1; Marc Browning1; Benjamin Johnson1; Emily Measom1; Cassidy Hatch1; Min Meng1; Scott A Reuschel1; Troy Voelker1; 1Coverge, Salt Lake City, UT; 2Coverge, Madison, WI

MP 436 Complementary ERLIC and RPLC Online Separations Significantly Expand Sequence Coverage in MS-Based Proteomic and Proteogenomic Studies; Candece Guerrero1; Pratik D Jagtap1; James Johnson2; Thomas F McGowan1; Tim Griffin1; 1University of Minnesota, Minneapolis, MN; 2University of Minnesota Supercomputing Institute, Minneapolis, MN; 3University of Minnesota at Twin Cities, Saint Paul, MN

MP 437 A Direct Comparison between Ultrafiltration and Online Size Exclusion Affinity Selection Mass Spectrometry Methods; Christopher Reutter1; Manuel Molina-Martín1;
LIPIDS: GENERAL

MP 441 Selective Extraction of Phospholipids from Biological Sample with Metal Oxide Chromatography for Mass Spectrometry-Based Analysis; Shota Miyazaki1; Yuko Yui1; Shigenori Ota1; Kosuke Osaka1; Mamoru Kyogashima1; Atsushi Sato1; GL Sciences Inc., Saitama, Japan; 2GL Sciences Inc., Tokyo, Japan; 3Nihon Pharmaceutical University, Saitama, Japan

MP 442 Evaluation of Docosahexaenoic Acid Derived Lipid Mediators after Traumatic Brain Injury by a Global LC-MS/MS Method; Taelvan Selvan Anthonythurai1; Lewis Jesse1; Andrew A Amoscato1; Patrick M Kochanek1; Department of Chemical and Biomolecular Engineering, University of Cincinnati, Cincinnati, OH; 2University of Washington, Seattle, WA; 3Department of Chemical Engineering, University of Detroit Mercy, Detroit, MI

MP 443 Lipidomic Analyses of CEACAM1 Knockout Mouse Liver and Adipose Tissue; Gabriel Guiqu1; Deirdre La Placa1; Zhifang Zhang1; John E. Shively1; City of Hope, Duarte, CA

MP 444 Multiclass Lipid Profiling Using Liquid Chromatography High Resolution Mass Spectrometry with Dielectric Barrier Discharge Ionization; Felice J Lura-Ortega1; José Robles-Molina1; Bienvenida Gilbert-López1; Juan F Garcia-Reyes1; Antonio Molina-Díaz1; Alexander Schütz1; Sebastian Brandt2; Joachim Franzke3; University of Jaen, Jaen, Spain; 2Csc-Cial, Madrid, ES; 3University of Jaen, Jaen, Spain; 4Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany

MP 445 Comparison of Different Stationary Phases for Gangliosides Separation; Ashita Lakshmi Prasad1; Anuradha Prasad1; Gobburu1; Renliang Zhang1; Denise Imman1; Anderson J David1; Cleveland State University, Department of Chemistry, Cleveland, OHIO; 2Cleveland Clinic Lerner Research Institute, Cleveland, OH; 3Northeast Ohio Medical University, Rootstown, Ohio; 4Cleveland State University, Department of Chemistry Cleveland, OH

MP 446 High Throughput Solid Phase Microextraction: A New Alternative for Lipid Analysis and Cellular Lipidomics; Alsoon Pajand-Birjandi1; Vincent Bessonneau1; Pawlizyn Janusz1; University of Waterloo, Waterloo ON, Canada

MP 447 Characterization of Triglycerides and Lipogenesis of Serum Lipids from Dietary or Hepatic Origin: A LC-MS/MS and GC/MS Stable-Isotope Tracer Approach; Sergio P Palli1; Grace M Jones2; Russell Caccavelli3; Alejandro Gugliucci4; Jean-Marc Schwarz5; 6Department of Research, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; 7Department of Basic Sciences, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; 8Department of Medicine, University of California San Francisco, San Francisco, CA

MP 448 Steroid Profiling Method for Rat Serum and Plasma by Gas Chromatography/Tandem Mass Spectrometry with Large Volume Injection; Udi Jumahwani1; Toshiyuki Yamashita1; Motonao Nakao1; Kuniyo Sugitake1; Takeshi Serino1; Ryoiichi Sasaono1; Yoshihiro Izumi1; Takeshi Bamba2; Kyushu University, Fukuoka, Japan; 3Osaka University, Suita, Japan; 4Agilent Technologies Co. Ltd, Hachioji, Japan; 5AISTI SCIENCE CO., Ltd., Wakayama, Japan; 6Kyushu University, Fukuoka, Fukuoka

MP 449 Unsaturated Cholesterol Ester Analysis from Human Plasma via Online Photochemical Reaction and nanoESI-MS/MS; Jia Ren1; Elissia Franklin1; Yu Xia1; 2Purdue University, West Lafayette, IN

MP 450 Discovery of Endocannabinoids by Untargeted All-Ions Fragmentation High Resolution LC-MS/MS Screen; Mesut Bilgin1; Petra Born1; Fezza Filomena1; Michael Heimes1; Nicolina Maistrangelo1; Nicolai Wagner1; Carsten Schultz1; Mauro Maccarrone1; Suzanne Eaton1; Andre Nadler1; Matthias Wilm2; Andrej Shevchenko3; Danish Cancer Society Research Center, Copenhagen, DK; 4Max Planck Institute for Cell Biology and Genetics, Dresden, DE; 5Department of Experimental Medicine and Surgery, University of Rome Tor Vergata, Rome, IT; 6European Center for Brain Research/Fondazione Santa Lucia, Rome, IT; 7European Molecular Biology Laboratory (EMBL), Heidelberg, DE; 8Department of Medicine, Campus Bio-Medico University of Rome, Rome, IT; 9European Center for Brain Research/Fondazione Santa Lucia, via del Fosso di Fiorano 65, Rome, IT; 10Conway Institute of Biomolecular and Biomedical Research, University College Dublin, Dublin, IE

MP 451 Role of Ammonium Salts in the Ionization and Fragmentation of Phosphatidylcholines Found in Krill Oil; Michael Rush1; Richard van Bremen1; University of Illinois College of Pharmacy, Chicago, IL

MP 452 Determination of β-Glucocerebrosidase (GBA) Activity through Global and Targeted Lipid Profiling; Yi Zeng1; Sangwon Min2; Baris Bingol1; Wendy Sandoval1; 2Genentech Inc, South San Francisco, CA

MP 453 Separation of Metalated Lipid Isomers Using Linear and Nonlinear Ion Mobility Spectrometry; Andrew Bowman1; Julia Kaszycki2; Rinal Abzalimov3; Gordon A Anderson4; Alexandre A Shvartsburg1; 2Max Planck Institute for Cell Biology and Genetics, Dresden, DE; 3Department of Research, College of Osteopathic Medicine, Touro University California, Vallejo, CA 94592; 4City University of New York, New York City, NY; 5GAA Cancer Society Research Center, Copenhagen, DK; 6Department of Medicine, University of California San Francisco, San Francisco, CA

MP 454 Analysis of Lipids from Biological Samples by Laser Desorption Ionization from Silicon Nanopost Arrays; Andrew Korte1; Akos Vertes1; George Washington University, Washington, DC

MP 455 Polar Lipids from Insect and Tick Cuticle. Analysis and Discovery of their Roles in Semiochemical Signaling; Robert Renthal1; University of Texas at San Antonio, San Antonio, TX

MP 456 Natural Variation of Blood Plasma Lipids in Healthy Asian Individuals; Husna Begum1; Fedorio Torta1; Pradeep Narayanawamy1; Piyushkumar Mundra2; Yi-King Teo1; Peter Little1; Peter Meikle1; Markus Wenk1; 2Life Sciences Institute, National University of Singapore,
METABOLIC FLUIDS: GENERAL

MP 457 Validating the Roles of FraD and FraB in the Metabolism of F-Asn by Salmonella; Jikana Wu1; Anindita Sengupta1; Anice Sabag-Dagli2; Pradip Biswas1; Brian Ahmer2; Venkati Gopalani3; Edward Behrman4; Vicki Wysocki1; 1Ohio State University, Columbus, OH

MP 458 Exploiting the Sensitivity of Structural Mass Spectrometry as a Next Generation Platform for Metabolomics; Olga Gorlova1; Conrad Wolke1; Sean Spectrometry as a Next Generation Platform for Exploiting the Sensitivity of Structural Mass Spectrometry; 2Department of Pathology, University of Florida Gainesville, FL; 3IROA Technologies, Ann Arbor, MI

MP 459 Globally Optimized Targeted Mass Spectrometry (GOT-MS): Reliable Metabolomics Analysis with Broad Coverage; Dany Frape1; University of Washington, Seattle, WA; 2Fred Hutchinson Cancer Research Center, Seattle, WA

MP 460 Targeted Metabolomics to Characterize Lipoplysaccaridic Biosynthetic Intermediates in Gram-Negative Bacteria in Response to Chemical and Genetic Perturbations; William Sawyer1; Jade Bojkovic1; Charles R. Dean2; Brian Y. Feng3; Daryl L. Richie4; David A. Six5; Lisha Wang6; Christopher M. Rith7; 1Novartis Institutes for Biomedical Research, Emeryville, CA

MP 461 Internal Extractive Electrospray Ionization Mass Spectrometry based- Metabolomics for Lung Cancer Analysis; Yun Li1; Zhizhan Wang1; Qian Li1; Yiping Wei2; Dany Frape1; Huanwen Chen1; 1East China Institute of Technology, Nanchang, China; 2Department of Cardiothoracic Surgery of Second Affiliated Hospital to Nanchang University, Nanchang, China; 3East China University of Technology, Nanchang, Mainland

MP 462 Study of Untargeted Metabolite Degradation in Plasma using Isotopic Ratio Outlier Analysis by uHPLC-MS/MS; Elizabeth Dhummakupt1; Casey Chamberlain2; Chris Beecher3; Timothy Garrett4; 1University of Florida, Gainesville, FL; 2Department of Pathology, University of Florida Gainesville, FL; 3IROA Technologies, Ann Arbor, MI

MP 463 A Step Forward in GC-HRMS-MS Based Metabolomics - A Novel Atmospheric Pressure GC-APCI Source Increases Quantitative and Qualitative Performance; Christian J. Wachsmuth1; Aiko Barsch2; Christoph Schelli1; Joshua Rutowski1; Britt Holmén2; Jiangjiang (Chris) Zhu1; 1Department of Chemistry and Biochemistry, Miami University, Oxford, OH; 2Civil & Environmental Engineering, School of Engineering, University of Vermont, Burlington, VT

MP 464 Novel Strategies for the Analysis of Isotopologue and Isotopomer Fractions of Primary Metabolites in 13C Based Metabolomic Flux Analysis Experiments; Teresa Mairinger1; 1Austrian Centre of Industrial Biotechnology (acib), Vienna, Austria; 2Department of Chemistry, University of Natural Resources and Life Sciences - BOKU Vienna, Vienna, Austria; 3Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria

MP 465 13C-Metabolic Flux Analysis of Microbes by Using Novel Fragmentations of tert-Butyldimethylsilyl (tBDMs)-Amino Acid Derivatives with GC-MS/MS; Nobuyuki Okahashi1; Shuichi Kawanami1; Junko Iida2; Hiroshi Shimizu1; Fumio Matsuda1; Osaka University, Suita, Japan; 2Shimadzu Corporation, Kyoto, Japan

MP 466 Analysis of Plasma Metabolites Using Gas-Chromatography Tandem Mass Spectrometry System with Automated TMS Derivatization; Shuichi Kawanami1; Yumi Unno2; Yukihiko Kudo2; Takero Sakai1; Takashi Kobayashi1; Shin Nishiumi2; Masaru Yoshida3; Noriyuki Ojima1; 1Shimadzu Corporation, Osaka, Japan; 2Shimadzu Corporation, Kanagawa, Japan; 3Shimadzu Corporation, Kyoto, Japan; 4Kobe University Graduate School of Medicine, Kobe, Japan; 5Shimadzu Corporation, Tokyo, Japan

MP 467 LC-HRMS Metabolic Flux Analysis Reveals Mechanistic-Based Changes after Muscle AMPK Activation; John Keni Meissner1; Russell Alan Miller2; Matt Blatnik2; 1Pfizer, Groton, CT; 2Pfizer, Cambridge, MA

MP 468 Metabolic Analysis of Single Human Cells in Different Mitotic Phases by Capillary Microsampling Electrospray Ionization Mass Spectrometry; Linwen Zhang1; Akos Vertes1; 1The George Washington University, Washington, DC

MP 469 Evaluating the Impact of Environmental Ultrafine Particles to Gut Bacterial Metabolism by targeted LC-MS/MS Metabolic Profiling; Julia Roubidoux1; Kate Schell1; Joshua Rutowski1; Britt Holmén2; Jiangjiang (Chris) Zhu1; 1Department of Chemistry and Biochemistry, Miami University, Oxford, OH; 2Civil & Environmental Engineering, School of Engineering, University of Vermont, Burlington, VT

MP 470 Ion-pairing LC-MS with Automated Sample Prep for Metabolomics; Jason L. Richardson1; Bhavana Shah1; Zhongqi Zhang1; Jinhua Zhang1; Anjen, Inc., Thousand Oaks, CA

MP 471 Application of Data-Dependent MS/MS in Structural Analysis of Isomeric Acylsugar Metabolites from Solanaceous Plants; Xiaoxiao Li1; 1A. Daniel Jones1; 2Department of Chemistry, Michigan State University, East Lansing, MI; 3Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI

MP 472 Probiotic Lactobacillus Reuteri Strains Produce L-Ethionine via a Two-Carbon-Transferring Alternative Branch of the Folate Cycle; Daniel Raftery1, 2; Teresa Hopfgartner1; Gunda Koellensperger3; Stephan Hann1, 2; 1Austrian Centre of Industrial Biotechnology (acib), Vienna, Austria; 2Department of Chemistry, University of Natural Resources and Life Sciences - BOKU Vienna, Vienna, Austria; 3Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria

MP 473 Using Isotopic Ratio Analysis (IROA) and Non-negative Matrix Factorization (NMF) to Sort Mixtures in Metabolic Analyses; Chris Beecher1; Timothy J Garrett2; Elizabeth Dhummakupt3; Vanessa Y. Rubio4; 1IROA Technologies, Gainesville, Florida; 2University of Florida, Gainesville, FL

MP 474 MS Profiling of Molecular Composition Inside live 3D Artificial Tumors Using the Single-Probe Device; Wei Rao1; Ning Pan1; Haiqing Yu1; Xuewei Qu2; Chuanbin Mao3; Zhibo Yang3; 1University of Oklahoma, Dept of Chem & Biochem Norman, OK

MP 475 5a-Reductase Type 3 (SRD5A3) ∆4-3-keto Steroid Metabolism Using Triple Quadrupole Mass Spectroscopy; sumankalai ramachandran; Division of Genitourinary Medical Oncology, David H. Koch Center for Applied Research of Genitourinary Cancers, The University of Texas MD Anderson Cancer Center, Houston, Texas., Houston, TX

MP 476 LC-SWATH/MS Metabolomics Platform with Hyphenation of Extraction and Analysis of Polar and Non-Polar Metabolites in Plasma and Urine; Michel Raetz1; Renzo Picenoni2; Guenter Boehm3; Gerard Hopfgartner4; 1University of Geneva, Geneva, Switzerland; 2CTC Analytics AG, Zwingen, Switzerland

MP 477 What Are We Eating? Differential Metabolomic Profiles Reveal an Insight into our Dietary Habits; Paul Clemens1; Baljit Ubbi1; 1SCIEX, Redwood City, CA
Chromatographic performance for high resolution
Berkeley National Lab, Berkeley, CA
Toronto ON, Canada; 3Department of Molecular Genetics,
Cellular and Biomolecular Research, University of Toronto,
Jay Kirkwood1, 2; Corey Broeckling1, 2; Jordan Steel1, 3;
Development of an LC-MS Method for the Kinetic
Anastasia Kalli1; Bryson Bennett2; Junhua Wang1; Caroline
Spectrometry and Compound Discoverer Software
Utilizing High Resolution Orbitrap™ Mass
Metabolomic Analysis of 13C/15N Labeled Metabolites
Liang Li1; Jose, CA; 2Calico Labs, South San Francisco, CA
Lanthanide-Chelator Barcode for Combinatorial
University of Toronto, Toronto ON, Canada
Metabolic Phenotyping of Platelet-Rich Plasma Using
Collection and Chemical Isotope Labeling LC-MS
in VHL (-) Clear Cell Renal Carcinoma (ccRCC);
Collin Wetzel1; Megan Bischoff1; Johnson Chu1; Patrick
A Limbach1; David R Plas1; Maria F Czyzyk-krzeska1;
1University of Cincinnati, Cincinnati, OH

An Optimized Acquisition Database and LC-MS/MS Method Targeting Central Carbon Pathway Metabolites;
Mark Sartain1; Amy Caudy2, 3; Adam Rosebrock2, 3; Agilent
Technologies, Santa Clara, CA; 3Donnelly Centre for
Cellular and Molecular Research, University of Toronto,
Toronto, ON, Canada; 2Department of Molecular Genetics,
University of Toronto, Toronto ON, Canada

Lanthanide-Chelator Barcode for Combinatorial Screening Applications; Todd Duncombe1; Kai Deng1;
Paul D Adams2; Anup K Singh1; Trent R Northen1; 3Sandia National Laboratories, Albuquerque, NM;
4Lawrence Berkeley National Lab, Berkeley, CA

Chromatographic performance for high resolution metabolomics; Vilinh Tran1; 2; Ken Liu1; 2; Dean Jones1, 2;
Clinical Biomarker, Emory School of Medicine Atlanta, GA;
Emory University School of Medicine, Atlanta, GA

Development of Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry for Metabolomic Analysis of Small Numbers of Mammalian Cells; Xian Luo1; Liang Li1; University of Alberta, Edmonton, Alberta; 2University of Alberta, Edmonton, Canada

Cow Milk Metabolome Profiling and Determination of its Dietary Effects on the Human Urine Metabolome Using Chemical Isotope Labeling LC-MS; Dorothea Mung1; Liang Li1; University of Alberta, Edmonton, Canada

Metabolic Profiling of Human Sweat from Various Epidermal Locations Using Non-occlusive Sample Collection and Chemical Isotope Labeling LC-MS; Kevin Hooton1; Liang Li1; University of Alberta, Edmonton, Canada

Metabolic Phenotyping of Platelet-Rich Plasma Using the AbsoluteIDQ™p180 kit; Lisa ST John Williams1;
Guido Dallmann2; Will J Thompson1; Therese Koal1; Duke University Medical Center, Durham, NC; 3Bioclates Life Science AG, Innsbruck, Austria

Metabolomic Analysis of 13C/15N Labeled Metabolites Utilizing High Resolution Orbitrap™ Mass Spectrometry and Compound Discoverer Software; Anastasia Kalli1; Bryson Bennett1; Junhua Wang1; Caroline Ding1; Ralf Tautenhahn1; 2Thermo Fisher Scientific, San Jose, CA; 2Calico Labs, South San Francisco, CA

Development of Ion Pair-Reverse Phase Chromatography Mass Spectrometry Method to Maximize Isomer Separation and Coverage of Endogenous Metabolite Classes; Yuqin Dai1; Agilent
Technologies, Santa Clara, CA

Formate Tetrahydrofolate Ligase of Lactobacillus reuteri: A Multifaceted Player of the Folate Cycle?; Abby
Chiang1; Daniel Röth1; James Versalovic2; Markus Kulkum1; 3City of Hope, Duarte, CA; 4Texas Children’s Hospital,
Baylor College Houston, TX

Development of a MR-Mediated Detection of the Plant Metabolome Using Liquid Chromatography/Tandem Mass Spectrometry; Satoshi Yamaki1; Junichi Masuda2; Yoshishiro Hayakawa1; Munee Sato1; Yuji Sawada2; Masami Yokota Hira1; Shimadzu Corporation, Kanagawa, E; Shimadzu Corporation, Kanagawa, Japan; 2Shimadzu Corporation, Kyoto, Japan; 3RIKEN, Yokohama, Japan

Fractionation and Untargeted Metabolomics of Human Plasma by Off-Line Coupling of Reversed-Phase and Hydrophilic Interaction Liquid Chromatography LC/MS; Stefanie Wernisch1; 2Sonja Penza Marnaj1; 3University of Michigan, Ann Arbor, MI; 1University of Michigan Medical School, Ann Arbor, MI

Wine Flavonoids Identified and Analyzed by Composite Neutral Loss Scan and Novel Data-Dependent Scans for Metabolomics Discovery by LC/MS/MS; Bennett Kalafut1; Rina Ana Snyder1; Mark Dreyer1; 2Thermo Fisher Scientific, San Jose, CA

MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION

Utility of Random Forest Combined with Infusion Electrospray MS and MALDI-TOF MS for Rapid Classification of Neisseria Meningitidis Strains; Adrian R Woofitt1; Hercules Moura1; Bryan A Parks1; Ramnath Gowrishankar1; Conrad P Quinn1; Brian H Harcourt1; Xin Wang1; John R Barr1; 2CDC, Atlanta, GA

Identification of Microorganisms in Biofluids and Saliva of Individuals with Periodontitis and Chronic Kidney Disease Using MALDI Biotyper; Levy Anderson Cesar Alves1; Rafael Celestino Souza1; Taizana Maria Cauto Silva1; Marcelo Fava1; Meriellen Dias1; Maria Anita Mendes1; Ana Lidia Ciamponi1; 1Orthodontics and Paediatric Department – Dental School – University of São Paulo, São Paulo, SP - BR; 2Paediatric Nephrology Department – Medical School – University of São Paulo (USP), São Paulo, SP; 3BRAZIL; 4LSCP - Chemical Engineering Department - Polytechnics School – University of São Paulo (USP), São Paulo, SP/ Brazil

A Peptide-Based LC-MS/MS Method for Detection and Identification of Salmonella serovars; Shu-Hua Chen1; Christine H. Parker1; Melinda A. McFarland1; Timothy R Croley1; 2FDA/CFSAN, College Park, MD

Detection of Penicillin Binding Protein 2a for the Identification of Methicillin Resistant S.aureus Using Top-down Proteomics; Jason Neil1; James Jr L Stephenson1; Alexander Cherkeskysky1; 2Thermo Fisher Scientific, Cambridge, MA; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher Scientific, San Jose CA, CA

Reliable Biomarkers for Identification of Mycobacterium Tuberculosis Complex in Broth Culture Media with Nanodiamond; Hsi-An Chen1; Ya-Chin Chin1; Po-Chi Soo1; Wen-Ping Peng1; 1National Dong Hwa University, Shoufeng Hualien, Taiwan; 2Tzu Chi University, Hualien, Taiwan
Deciphering Multifactorial Resistance in Acinetobacter baumannii Combining Whole-Genome Sequencing and Targeted Label-Free Proteomics; Tiphaine Cecchin1; Eun-Jeong Yoon1; Corinne Beaujolle1; Yannick Charrelier2; Chloe Bardet1; Xavier Lacoux1; Zack Blair1; Patrice Courvalin1;
MP 502

Novel Genetic Determinants for Complex Head Composition in a Giant Salmonella Phage; Susan T. Weintraub1; Adriana Coll2; Martine Bosch2; Kevin Hakala1; Sammy Pardo1; Dana Molleur1; Stephen C Hardies1; Lindsay W Black1; Julie A Thomas2; 1Univ. of Texas HSC, San Antonio, TX; 2Rochester Institute of Technology, Rochester, NY; 3Thermo Fisher Scientific, San Jose, CA; 4University of Maryland School of Medicine, Baltimore, MD

MP 503

Thermal Desorption Electrospray/Ionization Mass Spectrometry Combined with Principal Component Analysis for Rapid Characterization of Bacterial Species; Shiang Jian Lin1; Sung Pin Tseng2; Hung Su1; Yang Kuang Pan1; Jentia Shiea1; 1National Sun Yat-Sen University, Kaohsiung, Taiwan; 2Kaohsiung Medical University, Kaohsiung, Taiwan

MP 504

Application of Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry for Differentiation of Cacao Phytopathogen Strains Growing in Different Tissues and Hosts; Fábio Santos1; Adriana Coll2; Martine Bosch2; Kevin Hakala3; Rickards2; Kate Hardiman1; Adam Burke1; Julia Balog3; Philippe Charrier1; Fábio Santos1; 1MO BIO Laboratories, Carlsbad, CA; 2MO BIO Laboratories, Carlsbad, CA

MP 505

MALDI Profiling of Cyanobacteria by Monitoring Large Molecules; Hirohiko Asukabe1; Takuma Nakayama1; Ken-ichi Harada1; Susumu Y. Imanishi2; 1Meijo University, Nagoya, Japan; 2Department of Biology, University of California, Santa Cruz, CA

MP 506

Identification of Fungi using Rapid Evaporative Ionisation Mass Spectrometry; Frances Bolt1; Simon Cameron1; Ali Abdolrasouli1; Johanna Rhodes1; Tony Rickards1; Kate Hardiman1; Adam Burke1; Julia Balog1; 1University of Birmingham, Birmingham, United Kingdom; 2University of Campinas, Campinas SP, Brazil; 3CEPLAC, Ilhéus Bahia, Brazil

MP 507

Identification and Species Delineation of Bacteria Using MALDI-TOF MS Based on Ribosomal Protein Sequences in DNA Databases; Kenneth Parker1; SimulTOFI/ VIC Instruments, Marlborough, MA

MP 508

Differentiation of Bacteria at the Strain Level by MALDI-MS of Proteins >15kDa; Dina L. Bai1; Mark Cobbold3; Jeffrey Shabanowitz1; Donald F Hunt1; Cameron1; 1University of Campinas, Campinas SP, Brazil; 3McKusick-Nathans Institute of Genetic Medicine, Johns Hopkins University, Baltimore, MD

MP 509

Liquid Extraction Surface Analysis Mass Spectrometry for Protein Analysis Directly from Escherichia coli and Staphylococcus epidermidis; Klaudia I Kocurek1; 2; Josephine Bunch1; Robin C May1; Helen J. Cooper1; 1University of Birmingham, Birmingham, United Kingdom; 2National Physical Laboratory, Teddington, United Kingdom

MP 510

High-velocity Impact Survival and Bouncing Kinetics of Electrospayed Bacterial Spores Studied using Novel Asymmetric Image Charge Detectors; Brandon Barney1; Daniel Austin2; 1Brigham Young University, Provo, UT

MP 511

Probing Protein Interaction Dynamics between Asian Citrus Psyllid and Candidatus Liberibacter asiaticus by Chemical Crosslinking Mass Spectrometry; Xuefei Zhong1; John Ramsey1, 2; Juan Chavez1; Arti Navara1; Jared Mohr2; Michelle Cilia1, 2, 3; James Bruce1; 1University of Washington, Seattle, WA; 2USDA Agricultural Research Service, Ithaca, NY; 3Boyce Thompson Institute for plant research, Ithaca, NY; 4Cornell University, Ithaca, NY

MP 512

High Yielding Spin Column Isolation of Total Proteins from Microbial Cultures for Proteomic Applications; Victoria Nieciecki1; Heather Callahan1; Eddie Adams1; 1MO BIO Laboratories, Carlsbad, CA - California; 2MO BIO Laboratories, Carlsbad, CA

MP 513

Simultaneous DNA, RNA, and Protein Extraction from Microbial Cells: Sequential Isolation of Complex Biomolecules from a Single Source; Victoria Nieciecki1; Eddie Adams1; 1MO BIO Laboratories, Carlsbad, CA

MP 514

Characterizing the Formation of Electrophilic Fatty Acid Derivatives During Influenza Infection and Determining their Role in Pathogenesis; Greg Buchanan; University of Pittsburgh, Pittsburgh, PA

MP 515

Integrated Omics Reveals Dynamic Nature of the Arabidopsis Rhizosphere Microbiome; Lillian Pasa-Tolic1; Abigail Ferrer1; Charles K. Ansorg1; Heatherr M. Brewer2; Angela D. Norbeck2; Yaya Cui2; Christopher Staley3; Malak Tfally4; Rosalie Chua4; Jared Shaw4; Meng L. Markilie2; Richard A. Ferrieri2; Susannah G. Tringe5; Michael J. Sadowsky2; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of California, Berkeley, CA; 3University of California, Santa Cruz, Santa Cruz, CA

MP 516

Development of Metaproteomics Methods for Characterization of Soil Microbial Communities; ZHOU Li1; Cristina N. Butterfield1; Susan Spaulding2; Brian C. Thomas3; Andrea Singh1; K. Blake Suttle4; Robert Hettlie1; Jillian Banfield1; Chongle Pan1; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of California, Berkeley, CA; 3University of California, Santa Cruz, Santa Cruz, CA

PHOSPHOPEPTIDES: ENRICHMENT METHODS 518 - 529

MP 518

Enrichment and Identification of MHC-Associated Phosphopeptide Neoantigens in Hepatocellular Carcinoma for the Development of Novel Cancer Immunotherapeutics; Gemma E Hardman1; Claire E Eyers1; 1University of Liverpool, Liverpool, United Kingdom

MP 519

Phosphoproteome Changes in Altered Cholesterol Metabolism Revealed by SCX Tip Based Fractionation of Batch-Enriched Phosphoproteomes; Alireza Dehgani1; Markus Gödderz2; Volkmar Gieselmann1; Dominic Winter1; 1University of Bonn, Bonn, Germany

MP 520

Development of Enrichment Strategies for the Analysis of Phosphohistidine-Containing Peptides; 1University of Bonn, Bonn, Germany

MP 521

Enrichment of Phosphorylated Peptides Using Metal-Loaded Polymeric Reverse Micelles for MALDI-MS Analysis; Meizhe Wang1; Bo Zhao2; Sankaran Thayumanavan1; Richard Vachet1; 1University of Massachusetts Amherst, Amherst, MA
**Fabrication of MnFe2O4 Magnetic Nanoparticles for the Enrichment of Phosphopeptides in Combination with Mass Spectrometric Analysis:** Yung-Yun Huang1; He-Hsuan Hsiao2; *Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; *Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan

**Dual Wield nanoLC-ESI-MS for Simultaneous Detection of Singly and Multiply Phosphorylated Peptides:** Chia-Feng Tsai1; Kosuke Ogata1; Masaki Wakabayashi1; Natsuyuki Sugiyama1; Yasushi Ishihara1; *Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan

**Metal Ion-Immobilized Magnetic Nanoparticles for Global Enrichment and Identification of Phosphopeptides by Mass Spectrometry:** Yangjun Zhang1, 2; Rui Zhai2; XiaoHong Qian2; *Beijing Proteome Research Ctr, Beijing, Beijing; *Beijing Institute of Radiation Medicine, Beijing, C.N.

**Excellent Sensitivity through Excellent Recovery – ERLIC Outperforms TiO2─Affinity Purification in Excellent Sensitivity through Excellent Recovery:** Stefan Loroch1; Albert Sickmann1, 2, 3; Rene P Zhang1, 2; Rui Zhai2; XiaoHong Qian2; *Beijing Proteome Research Ctr, Beijing, Beijing; *Beijing Institute of Radiation Medicine, Beijing, C.N.

**ESI Tandem Mass Spectrometric Analysis of Phosphopeptide Modified by Cyclic Quaternary Ammonium Tags:** Hyo Kyong Kweon1; Kristina Hakansson1; Philip Andrews1; *University of Michigan, Ann Arbor, MI

**Method Development and Evaluation of the Protein Phosphatase 2 Phosphoproteome Using the Chip iFunnel QTOF Platform:** Brooke Thompson1; Vadiraja Bhat1; Chelsea E. Cunningham2; Paulos Chumala1; Frederick S. Vizeacoumar2; Franco J. Vizeacoumar3; George S. Katselis1; *CHCSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada; *Agilent Technologies, Wilmington, DE; *Department of Pathology, Cancer Cluster, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada

**Acid-Based SCX Fractionation for In-Depth Proteome and Phosphoproteome Analysis:** Jun Adachi1; Hashiguchi Kazunari1; Nagano Maiko2; Sato Misako1; Sato Ayako1; Fukamizu Kazuna1; Ishihama Yasushi1; Tomonaga Takeshi2; *National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Osaka; *National Institute of Biomedical Innovation, Health and Nutrition, Osaka, Japan; *Kyoto University, Kyoto, Japan

**Two-Step Elution of Phosphopeptides from TiO2 Microparticles – an Improved Detection of Multiphosphorylated Peptides:** Rudolf Kuptcik1; Pavel Rehulka1; Ivo Fabrik1; Jana Klimentova1; Helena Rehulkova1; Jiri Stulik1; Pavla Krulisova1; Zuzana Bilkova1; *Department of Biological and Biochemical Sciences, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic; *Department of Molecular Pathology and Biology, Faculty of Military Health Sciences, University of Defence, Hradec Kralove, Czech Republic

**Characterization of Bromine Functionalized Alternating and Random Copolymers by Tandem Mass Spectrometry:** Selim Géraldoug1; Xiaoglin Yin1; Coleen Pugh1; Chrys Wesdemiotis2; *The University of Akron, Akron, OH; *The University of Akron, Akron, OH

**The Characterization of Polymeric Methylene Diphenyle Disocyanates (PDMs) Using UHPSFC and FT-ICR APPI-MS:** Julie M Herriman1; Robert Carr2; John G Langley1; *University of Southampton, Southampton, United Kingdom; *Huntsman (Europe), bvba, Everberg, Belgium

**An APCl LC-MS-MS Method for the Determination of Octamethylcyclotetrasiloxane (D4), Decamethylcyclopentasiloxane (D5), and Dodecamethylcyclodecasiloxane (D6) in Silicone Emulsions:** Ron Tecklenburg1; Tanya M Habitz1; *Dow Corning Corporation, Auburn, MI

**Supramolecular Fractal Architectures Using ESI-MS Assembling and Characterization of Discrete Supramolecular Fractal Architectures Using ESI-MS and Ion Mobility-Mass Spectrometry:** Shiva Ahmadi1; Dominic Winter1; *University of Bonn, Bonn, Germany

**Mass Spectrometry Characterization of Isomeric Biodegradable Polymers:** Sahar Sallam1; Chrys Wesdemiotis1; Yuyuan Luo1; Mathew L. Becker1; *The University of Akron, Akron, OH

**MALDI-MS Signal Enhancement of Peptides from Donor-Acceptor Interactions between Amphiphilic Polymers and MALDI Matrix:** Mahalia Serrano1; Huan He1; Sankaran Thayumanavan1; Richard W Vachet1; *University of Massachusetts Amherst, Amherst, Massachusetts

**Investigating the Effect of Sample Preparation Parameters on the Cationization of Synthetic Polymers Using Matrix-Assisted Laser Desorption Ionization Mass Spectrometry and NMR Characterization of Plasma Polymeric Strene:** Lee Elliott1; Kris Micheal Kinness1; Gary Ray Kinsel1; *Southern Illinois University Carbondale, Carbondale, IL

**Characterization of Residual Monomers in Adhesives Using HSGC/MS:** Sanket Chiplunkar1; Durvesh Sawant1; Dheeraj Handique1; Prashant Hase1; Ankush Bhone1; Ajit Date1; Jitendra Kelkar1; Pratap Rasam1; *Shimadzu Analytical (India) Pvt. Ltd., Mumbai, Maharashtra; *Shimadzu Analytical (India) Pvt. Ltd.,
Mumbai, India

MP 554  
Polymer and Adhesive Tape Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time (DART) Mass Spectrometry; Cody Robert B.; Chi Ngu, Tsay; Harau Shimada; Yasuo Shida; Akiko Kusai; JEOA USA, Inc. Peabody, MA; 2Biochromato, Inc. Fujisawa, Japan; 3Shiseido Research Center, Yokohama, Japan; 4University of Yamanashi, Kofu, Japan; 5JEOL Ltd., Akishima, Japan

MP 555  
Proteomic Characterization of Cell Architecture and its Preparatory Biochemical Extractions; Li-Hua Li; Cheng-Chih Richard Hsu; Cheng-Hsien Yang; Cheng Meng; Yeou-Guang Tsay; 5, 6; 1Taipei Veterans General Hospital, Taipei, Taiwan; 2Department of Chemistry National Taiwan University, Taipei, Taiwan; 3Institute of Biochemistry and Molecular Biology, Taipei, Taiwan; 4Chair of Proteomics and Bioanalytics Technische Universitaet Muenchen, Munich, Germany; 5Proteomics Research Center, Taipei, Taiwan; 6Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan

The Interactions between N-Heterocyclic Carbene Silver Complex and Cytochrome C Studied by Electrospray Ionization Mass Spectrometry; Yan Pan; 2Morgantown, WV
A Chemical Proteomic Method for the Discovery of Novel LPA-binding Proteins; Xuejiao Dong; Yinsheng Wang; 1University of California - Riverside, Riverside, CA

MONDAY POSTERS

Proteins: General and Membrane

549 - 571

MP 549  
Biophysical Characterization of the Interactions between Membrane Proteins and Lipids; Xiao Cong; Yang Liu; Wen Liu; David H Russell; Arthur Lagowski; 1Albert Eye Research Institute, Duke University; 2IMMM, CBM CNRS UPR4301, Orleans, France; 3IMM CNRS UPR3401, Orleans, France; 4University of California, Davis, CA 95616, USA, Davis, CA

MP 550  
Protein Mass Spectra Database for Rapid Identification of Field-Caught Phlebotomine Sand Flies; Kristyna Hlavackova; Daniel Kavan; Vit Dvorak; Petr Volf; Petr Honing; 1DSM Resolve, Geleen, Netherlands; 2Bruker Daltonics, Billerica, MA; 3VU University, Amsterdam, Netherlands

MP 551  
Developments in Analysis of GPCRs: Monitoring Protein Movement by Means of Mass Spectrometry; Krzysztof Okraska; James Errey; Rob Cooke; 1Heptares Therapeutics Ltd., Welwyn Garden City, UK

MP 552  
Improving the Efficiency and Rapidity of Tryptic Proteolysis: from Blood to “Unknown Stains”; Eka Patel; Paola Cicatiello; Lisa Deininger; Malcolm R Clench; 1Centre for Mass Spectrometry Imaging, Biomolecular Research Centre, Sheffield, South Yorkshire; 2Universita’ di Napoli Federico II, Dipartimento di Scienze Chimiche, Naples, Naples; 3GlaxoSmithKline, Stevenage, UK

MP 553  
How Sequence Variant Analysis can be Hampered by Trypsin Side Reactions; Georg Drabner; Marco Boettger; 1Roche Innovation Center Penzberg, Penzberg, Germany

MP 554  
Mass spectrometry of Collagen and Casein in the Remains of the 5th to 7th Century Bamiyan Buddhas; Takashi Nakazawa; Kazuki Kawahara; Shunsuke Fukuskai; Mao Karino; Mioh Takashima; Yoko Taniguchi; 1Nara Women’s University, Nara, Nara; 2Osaka University, Suita, Japan; 3Nara Women’s University, Nara, Japan; 4The National Museum of Western Art, Tokyo, Japan; 5University of Tsukuba, Tsukuba, Japan

MP 555  
Proteomic Characterization of Cell Architecture and its Preparatory Biochemical Extractions; Li-Hua Li; Cheng-Chih Richard Hsu; Cheng-Hsien Yang; Cheng Meng; Yeou-Guang Tsay; 5, 6; 1Taipei Veterans General Hospital, Taipei, Taiwan; 2Department of Chemistry National Taiwan University, Taipei, Taiwan; 3Institute of Biochemistry and Molecular Biology, Taipei, Taiwan; 4Chair of Proteomics and Bioanalytics Technische Universitaet Muenchen, Munich, Germany; 5Proteomics Research Center, Taipei, Taiwan; 6Department of Biotechnology and Laboratory Science in Medicine, National Yang-Ming University, Taipei, Taiwan

The Interactions between N-Heterocyclic Carbene Silver Complex and Cytochrome C Studied by Electrospray Ionization Mass Spectrometry; Yan Pan; 2Morgantown, WV
A Chemical Proteomic Method for the Discovery of Novel LPA-binding Proteins; Xuejiao Dong; Yinsheng Wang; 1University of California - Riverside, Riverside, CA

Exploring the Differences in Endocytic Vesicles with the Aid of Mass Spectrometry Based Protein and Lipid Profiling; Bini Ramachandran; Krishnamurthy H; Satyajit Mayor; 1National Centre for Biological Sciences, Bangalore, India, Bangalore, Karnataka; 2Centre for Imaging and Flow Cytometry Facility, National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; 3National Centre for Biological Sciences, Tata Institute of Fundamental Research, GKVK, Bangalore, India; 4Institute for Stem Cell Biology and Regenerative Medicine, Bellary Road., Bangalore, India

Quality by Design (QbD) Based Development of a Peptide Mapping UPLC Method for Recombinant Human Serum Albumin (HSA); Ashraf Madian; Irish Gibson; Janet G. De Los Reyes; Cassandra Norton; Shen Chen; Lisa Cherry; 1Global Technology Services, Hospira, a Pfizer Company, Lake Forest, IL; 2One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, McPherson, KS; 3Global Established Products R and D, Hospira, a Pfizer Company, McPherson, KS; 4Global Technical Supply, Hospira, a Pfizer Company, McPherson, KS; 5One2One® Global Pharmaceutical R and D, Hospira, a Pfizer Company, Lake Forest, IL

Using LC-MS Based Methods for Testing the Digestibility of a Non-Purified Membrane Protein in Simulated Gastric Fluid; Dave Hatcher; 1Canadian Grain Commission, Winnipeg, MB; 2Canadian Grain Commission, Winnipeg, Canada

Towards a Prediction of Protein Reactivity Against Electrophile Ligands: 1. Ranking Amino Acid Side Chain Nucleophilicities; Guillaume Gabard; Yoann Richer; Solene Motteau; Emmanuelle Membot; Martine Cadene; 1CBM CNRS UPR4301, Orleans, France; 2IMM CNRS UMR6283, Le Mans, France

Evaluation of N-Terminus Labelling Protocols for Determination of Protein Cleavage Sites by Mass Spectrometry; Michelle Gadush; Maria D. Person; 1University of Texas at Austin, Austin, TX

Identification of Unique Rod Outer Segment Plasma Membrane Proteins Using a Label-Free Protein Correlation Profiling; Nikolai P Skjenga; Vadim Y Arshavsky; 1Albert Eye Research Institute, Duke University Medical Center, Durham, NC
PROTEINS: PTMS (PART 1)

**MP 561** Identification of Polyglutamylation of C-Terminal Tails of Tubulin from In-Gel Double Digests with Trypsin and Subtilisin; Hang-Gyeong Chun1; Colleen McClung2; Srirarsa Pradhan3; Christopher J. Noren1; Cristian I. Ruse1; 1New England Biolabs, Ipswich, MA

**MP 566** Disulfide Bond Reduction on TiBlue Electrodes – a Breakthrough in Protein Analysis; Jean-Pierre Chervel1; Agnieszka Kraj2; Hendrik-Jan Broecker2; Nico Reinhoud2; Martin Eysberg3; Antec, Zoeterwoude, The Netherlands; Antec LLC, Boston, MA

**MP 567** Rapid Analysis of Proteins on High-Resolution Mass Spectrometers Using Matrix-Assisted Ionization; Shamsheer Thawoos6; Casey Daniel Foley1; James Rapid1; 6Wayne State University, Detroit, MI; 1Indiana University Dept. Chemistry, Bloomington, IN

**MP 568** A New Thiol Derivatization Reactions with 2,1,3-Benzotriazolindiazole Studied by Mass Spectrometry; Chang Xu1; Qilu Sun2; Kehua Xu2; Bo Tang2; Hao Chen3; Ohio University, Athens, OH; 3Shandong Normal University, Jinan, China

**MP 569** Native Mass Spectrometry Analysis of Membrane-Bound Reaction Center from Blastochloris viridis; Yuan Lu4; Zhang Hao1; Michael L Gross1; Robert E Blankenship1; Washington University in St. Louis, St. Louis, MO

**MP 570** Improved Proteolytic Digestion under High Pressure Cycling: Rapid Digestion with Improved Sensitivity and Sequence Coverage; Vera S. Gross1; John Wilson2; Alexander Lazarev3; Pressure BioSciences, South Easton, MA; 2Profil, LLC, Huntington, NY

**MP 571** Fully Automated Digestion, Separation and Analysis of the Human Prolactin Receptor Transmembrane Protein by LC-MS/MS; Joshua Emory1; Nishi Rochelle1; Boutaghou Nazim1; Feld J Brian1; Shimadzu Scientific Instruments, Inc. Columbia

**MP 572** Proteomic Analysis of Protein S-Sulfhydration in Staphylococcus aureus; Xianzhang Zhang1; Hui Peng1; David Peter Giedroc2; Jonathan Cyboski Trinidad1; 1Department of Chemistry, Indiana University, Bloomington, IN; 2Department of Molecular and Cell Biochemistry, Indiana University, Bloomington, IN

**MP 573** Deep Coverage of the Mouse Cysteine Sulfenome in vivo; Shinf-Cheng Tzeng1; Jeroen Van der Post1; Nelmi O Devarie-Baez2; Cristina M Furdui1; Jason Held1; Washington University in St. Louis, St. Louis, MO; Wake Forest School of Medicine, Winston-Salem, NC

**MP 574** Quantifying Oxidation in Peptides Containing Multiple Methionine Residues; Joshua T Shepard1; Eden P Go1; Heather Desaire1; University of Kansas, Lawrence, KS

**MP 575** Quantifying Reversible Oxidation of Protein Thiolis in Arabidopsis Thaliana; Evan Mc Connell1; Leslie M Hicks2; 1University of North Carolina, Chapel Hill, NC

**MP 576** Energetics of S-Palmitoylation: Role of Palrine and Neighboring Cysteines; Neelam Khanal1; Vikas Pejaver1; Zhu Li3; Predrag Radivojac1; David E Clemmer1; Sucheta Mukhopadhyay1; Indiana University Dept. Chemistry, Bloomington, IN; 3Novillyc, West Lafayette, IN; 1Indiana University, Bloomington, IN

**MP 577** Elevated Level of S-Glutathionylation of Hemoglobin in Mole-Rats Detected by LC-MS; Kuanshy Kabytaev1; Christiane Vole1; Dmitry Shin1; Philip Dammann1; Alexandre Stoyanov1; 1Department of Pathology & Anatomical Sciences, University of Missouri, Columbia, MO; 2Department of General Zoology, University of Duisburg-Essen, Essen, Germany

**MP 578** Difference Gel Electrophoresis for Phosphoproteomics (DIGEP); Mavank Srivastava1; Linna Wang2; Weiguo Andy Tao3; 1Purdue University, West Lafayette, IN

**MP 579** Intact Phosphorylated Protein Analysis by Microfluidic CE-ESI-MS; Esmé Candish2; Michael E Pacold2; Scott Mellors2; Michael J Ramsey1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2Whitehead Institute for Biomedical Research, Cambridge, MA; 3908 Devices Inc., Boston, MA

**MP 580** Elucidating Kinase Substrate Networks in Chlamydomonas reinhardtii; Alex Chao1; Chris A Broberg1; Megan C Connor1; Leslie E Hicks1; 1UNC Chapel Hill, Department of Chemistry Chapel Hill, NC

**MP 581** Studies of the Molecular Mechanisms in the Regulation of PRL-3 Phosphatase Activity in the Endothelial Cells; Xinggui Shen1; Christopher G. Kevill2; 1LSU Health-Shreveport, Shreveport, LA

**MP 582** Phosphoproteomic Evaluation of Chimeric Proteins; Katerlyn I Ludwig1; Nirmalya Sen1; Natasha J Caplen1; Amanda B Hummon1; 1University of Notre Dame, Notre Dame, IN; 2NIH, Bethesda, MD

**MP 583** The Functions of Serine 687 Phosphorylation of Human DNA Polymerase h in UV Damage Tolerance; Xiaoxia Dai1; Changjun You1; Yinsheng Wang1; UC Riverside, Riverside, CA

**MP 584** Phosphorylation Dynamics and Interacting Proteins of MAP Kinase 4 Revealed by Proteomics; Tong Zhang1; Jacqueline D Schneider1; Craig P Dufresne2; Alice C Harmon1; sixue chen3; 1University of Florida, Gainesville, FL; 2University of Florida, Gainesville, Florida; 3Thermo Fisher Scientific, West Palm Beach.

**MP 585** A Panoramic Survey of Cellular Signaling in Human Gastric Cancer Cells by Monitoring both Phosphoryrosine and Acetyl-Lysine Post-Translational Modifications. Jeffrey C Silva1; Cammarata John1; Hamza Ghaith1; Manor Askenazi1; Jun Zhu1; Zhongyi Cheng1; 1Lighthouse Proteomics, Beverly, MA; 2Adeptrix Corporation, Beverly, MA; 3PTM BioLab (Hangzhou) Co. Ltd, Hangzhou, China

**MP 586** Updating and Expanding the PTM Catalog of Acid-Soluble Tau: A Case for Multiplexed Proteomic Analysis; Gooze Crynen1; Robert Peol2; Craig P Dufresne1; Jon M Reed1; Prashanti Vallabhaneni1; Benoit Mouzon1; Laila Abdullah1; James E Evans2; Fiona Crawford3; 1Roskamp Institute, Sarasota, FL; 2Thermo Fisher Scientific, West Palm Beach, FL

**MP 587** Identification of Cross-Linked Peptides in Proteins Subjected to Photo-Oxidation; Michele Marotti1; Fabian Leinisch1; Diana Julie Oersens-Leeming2; Michael J Davies2; Birte Svensson3; Per Hägglund3; 1Technical University of Denmark, Kongens Lyngby, Denmark; 2University of Copenhagen, Copenhagen, Denmark; 3Nordic Bioscience, Herlev, Denmark; 4Technical University of Denmark, Lyngby, Denmark

**MP 588** msViz, a Zero Learning Curve Graphical Software Tool for Detailed Manual Validation and Quantitation of Post-Translational Modifications; Manfredo Quadrini1; Roman Mylonas1; Trinidad Martin Campos2; 2Alessandro Masselot1; Patrice Waridel1; Ioannis xenarios2; 1CIG - University of Lausanne, Lausanne, Switzerland; 2Vital-IT Group - Swiss Institute of Bioinformatics, Lausanne, Switzerland; 3University of Geneva, Geneva, Switzerland
MP 590  Sequential Immunoaffinity Purification of Post-Translationally Modified Peptides for Improved Enrichment Specificity. Matthew P. Stokes1; Charles L Farnsworth1; Jian Min Ren2; Kimberly A Lee1; Xiaoying Jia1; Hongbo Gu1; Vicky Yang1; 1Cell Signaling Technology, Inc. Danvers, MA

MP 591  Metabolomics-Assisted Proteomics Reveals the Function of Lysine Succinylation and SIRT5 in Regulation of β-Oxidation of Long-Chain Fatty Acids. Sushabhan Sadhukhan1; Xiaoqiang Li1; Omerla D Nelson1; John A Stupinski1; Sheng Zhang1; Robert S Weiss1; Jason W Locasale1; Hening Lin1; 1Cornell University, Ithaca, NY; 2Cornell University, New York, NY

MP 592  Mass Spectrometry Based Identification and Characterization Studies of Post Translational Modification Citrullination. Mandvi Sharma1; Damagard Dres1; Anne Christian-Bay Jensen2; Claus Nielsen3; Birte Svensson1; Per Hagglund4; 1PhD, Department of Systems Biology, Denmark Technical University, Copenhagen, Denmark; 2Institute for Inflammation Research, Department of Infectious Diseases and Rheumatology, Copenhagen University Hospital, Rigshospitalet, Copenhagen, Denmark; 3Principal Scientist, Head of Rheumatology, Consultant Physician, Head of Department of Rheumatology, Rigshospital, Copenhagen, Denmark; 4Professor Enzyme and Protein Chemistry Department of Systems Biology The Technical University of Denmark, Copenhagen, Denmark; 5Professor, Consultant Physician, Head of Department of Rheumatology, Rigshospitalet, Copenhagen, Denmark; 6Professor Enzyme and Protein Chemistry Department of Systems Biology The Technical University of Denmark, Copenhagen, Denmark; 7Associate Professor, Department of Systems Biology, Technical University of Denmark, Copenhagen, Denmark.

MP 593  Characterization of Non-Heme Iron Enzymes Using Mass Spectrometry. Yi Pu1; Cheng-Hsuan Wu1; Deborah R. Leon1; Pinghua Liu1; Catherine E. Costello1; 1Boston University, Boston, MA

MP 594  Evolutionary Conservation of Sirtuin Lipoamidase Activity from Bacteria to Human Mitochondria. Elizabeth A Rowland1; Todd M Greco1; Caroline K Snowden1; Ileana M. Cristea1; 1Princeton University, Princeton, NJ

MP 595  Detecting Changes in the Epimerization of Water-Soluble and Water-Insoluble Crystallopin Proteins Using Tandem LC-MS. Yana Lyon1; Riversinde, CA

MP 596  Measurement of the Dynamics of Histone Methylation by One-Carbon Metabolic Isotope Labeling and HCD Methylation-Signature-Ions Detection. Hui Tang1; KANGLING ZHANG1; 1University of Texas Medical Branch at Galveston, Galveston, TX

MP 599  Targeted Proteomic Analysis of FFPE Bone Metastases from Lung Cancer and Other Malignancies. Chao Gong1; Fabiola Cecchi1; Adele Blackler1; Wei-Li Liao1; Marlene Darfler1; Todd Hembrough1; 1NantOmics, Rockville, MD

MP 600  Comprehensive Proteome Characterization of Pancreatic Cyst Fluid from Intraductal Papillary Mucinous Neoplasm (IPMN) by LC-MS/MS. Joohnho Park1; Dohyun Han1; Misol Do1;hee Joo Kang1; Jin-Young Kang2; Youngsoo Kim2; 1Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; 2Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; 3Department of Biomedical Science, Seoul National University College of Medicine, Seoul, Korea; 4Department of Surgery, Seoul National University College of Medicine, Seoul, Korea

MP 601  Epitope Identification of Human α-Galactosidase A to a Monoclonal Antibody by Affinity Mass Spectrometry. Zdenek Kukacka1; Marius Iurascu1; Yannick Baschung1; 1Division of Endocrinology, Diabetes and Metabolism, Department of Medicine, University Medical Center Zurich, Switzerland; 2Department of Immunology, University of Toronto, Canada; 3Department of Ophthalmology, University of Toronto, Canada; 4Department of Surgery, University of Pennsylvania, Philadelphia, PA

MP 602  Proteomics Identifies Three New Types of Amyloidosis Associated with Distinctive Clinical Phenotypes. Surendra Dasari1; Jason D Theis1; Julie A Vrana1; Samih H Nasr1; Sanjeev Sethi1; Paul J Kurtin1; 1Mayo Clinic, Rochester, MN

MP 603  Minimal Residual Disease in Multiple Myeloma by LC-MS/MS by Analysis of Immunoglobulin Heavy and Light Chain CDR Tryptic Peptides. Linda M Benson1; Angela Dispenzieri1; David L Murray1; H. Robert Bergen2; 1Mayo Clinic, Rochester, MN; 2Mayo Clinic, Rochester, MN

MP 604  Pharmacoproteomics Identifies the Drug Efficacy Mechanism in Acamprosate Treatment of Alcoholism. Caroline M Germany1; Ashile N Reker1; Hyung W Nam1; 1LSU Health Science Center, Shreveport, LA

MP 605  A Network Based Approach to Understand the Brain Proteome in Alzheimer’s Disease. Nicholas Safvold1; Eric B Dammer1; Vivek Swarup1; Duc Duong1; Luming Yin1; Juan C Troncoso1; Madhav Thambisetty1; Daniel Geschwind1; James Lah1; Allan Levey1; 1Emory University School of Medicine, Atlanta, GA; 2UCLA, Los Angeles, CA; 3Johns Hopkins University School of Medicine, Baltimore, MD; 4National Institutes of Health, Bethesda, MD

MP 606  To Pool or Not to Pool: Discovery of Biomarkers for Šjögren’s Syndrome Using Mass Spectrometry-Based Proteomics. Wanlu Qu1; Driss Zoukhri2; Athena Papas2; Markus Hardt1; 1The Forsyth Institute, Cambridge, MA; 2Tufts University, Medford, MA

MP 607  Analysis of Monoclonal Immunoglobulins from Multiple Myeloma Patients by Use of 21 Tesla FT-ICR MS/MS. Lidong He1; Lisa Anderson2; David R Barnidge1; David L Murray1; Christopher L Hendrickson2; Alan G Marshall1; 1Center for Interdisciplinary Cardiovascular Science, DLMP, Rochester, MN

MP 608  Understanding the Molecular Mechanisms Underlying Cisplatin Resistance in Ovarian Cancer Cells. Yi Hu1; Yuling Chen2; Chao Yang3; Zhenyu Zhang3; HAITENG DENG4; 1MOE Key Laboratory of Bioinformatics, Tsinghua University, Beijing, China; 2Tsinghua University, Beijing, China; 3Chaoyang Hospital Affiliated to Capital Medical University, Beijing, China; 4Tsinghua University, Beijing

MP 609  Apolipoprotein Kinetics Measured in Human HDL by HR/AM-PRM Unveils a Novel Picture of HDL Metabolism. Lang Ho Lee1; Allison B Andraski2; Brett Pieper1; Frank M Sacks1; Masanori Akawa1; Sashia A Singh1; 1Center for Interdisciplinary Cardiovascular Science, 2Tufts University, Medford, MA

PROTEOMICS: CLINICAL APPLICATIONS (APPLIED PROTEOMICS) 597 - 621
MP 610
Relevance of Albumin Bound Iron in Ovarian Cancer as Determined by ICP-MS; Lindsay Schambue1; Lauren Amabile2; Jana Rocker3; Michael Finan4; Rodney Rocconi5; Lewis Pannell5; Mitchell Cancer Institute, Mobile, AL; National Institutes of Health, Bethesda, MD

MP 611
Proteomic Analysis of an ALDH Sub-Population in Colorectal Cancer Identified by Liquid Chromatography-Mass Spectrometry; Rui Yang1; Xinhua Liu1; Smithahthakolwiboon1; Jianhui Zhu2; Xiaohong Pei3; Zhihong Tan4; Mingrui An5; Jun Cao5; Jing Wu5; David M Lubman6; 1University of Michigan Medical Center, Ann Arbor, MI; 2Shanghai University, Shanghai, CHINA; 3Mahidol University, Bangkok, Thailand

MP 612
Ion Current-based Proteomic Profiling in Understanding the Mechanism of Tumor Necrosis Factor Alpha on Myogenic Differentiation; Chengjian Tu1; Jun Li2; Jun Qu3; 1University at Buffalo, Buffalo, NY; 2University at Buffalo SUNY, Williamsport, NY

MP 613
Characterization of O- and N-Glycosylations of Immunoglobulin A in IgA Nephropathy; Jean-Marie Schmitter1; Katell Bathany2; Christelle Oblet3; Jean-Claude Aldigier1; Anne Drulhi4; 1University of Bordeaux, Bordeaux, France; 2University of Bordeaux, Bordeaux, France; 3University of Limoges, Limoges, France

MP 614
Effect of Radiotherapy on Protein Levels in Blood Plasma Collected from Breast Cancer Patients; Catherine C Going1; Marta Vitala2; Marjan Rafat3; Melissa Jenkins4; Kathleen C Horst5; Edward E Graves6; Sharon J Pitter7; 1Stanford University School of Medicine, Palo Alto, CA

MP 615
Prions in Nutritional Supplementation Therapy?; Tanja Panic-Jankovic1; Maria Zellner2; Göran Milutovic3; Medizinische Universität Wien, Vienna, Austria; 2Medical University of Vienna, Vienna, Austria

MP 616
Mass Spectrometry Based Proteomic Investigation of Anulhus Fibrosus and Nucleus Pulposus of the Mature Bovine Intervertebral Disc; Willem Duckworth1; Ashley Brisbin2; Kelly L Wormwood3; Emilayn J Dupree3; Jessica Roberge1; Devika Channaveerapapa4; Petra Kraus5; Thomas Luft6; Costel C Darie7; 1Clarkson University, Potsdam, NY

MP 617
Single Amino Acid Variation Profiles of the MCF7 Breast Cancer Cell Line Using LC-MS/MS; Zhihong Tan1; Song Nie1,2; Mingrui An3; Rui Yang4; Jun Cao5; Xiaohong Pei6; David M Lubman7; 1The University of Michigan, Ann Arbor, MI; 2Northwest National Laboratory, Richland, WA

MP 618
Evaluation of Undifferentiated State of Human iPSC Cells by Non-Invasive LC-MS/MS Analysis Approach Using Cell Culture Supernatant as Samples; Takashi Suzuki1; Gamo Kento2; Hatabayashi Kunilada3; Takahashi Masatosh4; Kagawa Kenichi5; Ogura Taira6; Hiramaru Daiauke7; Toyota Kenichi1; Oaki Shigenori1; Shimadzu Corporation, Kyoto, Japan; 2Tokyo Electron Limited, Kobe, Japan; 3Shimadzu Scientific Instruments, Inc. Columbia

MP 619
Quantitative Proteomics Analysis Reveals Molecular Signatures Associate with LPS, Betamethasone, and Magnesium Sulfate Treatment in E15 Murine Gastrointestinal Tract; Elizabeth Yohannes1; Jessica L. Slack2; Vivek Ramachandran3; Andrew S. Thagard4; Mark Wingerd5; Avedis Kazanjian6; 1Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, Washington; 2Maternal Fetal Medicine, Madigan Army Medical Center, Tacoma, Washington

MP 620
Proteomics of Globo H High/Low BxPC-3 Pancreatic Cancer Cell Line; Sheng-Ta Tsai1; Hsin-Ying Han1; Shok-Li Ng2; Chia-Ning Shen3; Chung-Hsuan Chen4; 1Genomics Research Center, Academia Sinica Taipei, Taiwan

MP 621
Proteomic Analysis by SILAC to Distinguish between Salmonella Lipopolysaccharide (LPS) and Monosodium Urate (MSU) Crystals Induced Inflammation in Macrophages; Sarbieet Makkar1; Rohana Liyanage1; Jackson O Lay1; 1University of Arkansas, Fayetteville, AR

PROTEOMICS: QUANTITATIVE

MP 622
Quantitation of Immunoglobulin Alpha from Whole Gut Lavage Fluid Using the Thermo Q-Exactive Plus; Joseph Otto1; Crystal Daniels1; Lindsay Schambue1; Jana Rocker2; Mitchell Cancer Institute, Mobile, AL

MP 623
Targeted Quantification of CrbpI in Cancer Cells through a Bottom-Up Approach; Wenjiong Li1; Jianshi Yu2; Claire Louise Carter1; Jace W Jones1; Maureen A Kane1; 1University of Maryland School of Pharmacy, Baltimore, MD; 2Kinase Activity Profiling of Lung Adenocarcinoma to Understand Cancer Signaling and Select Targeted Therapeutics; Melissa A. Hoffman1,2; Bin Fang3; Christopher Hirtz2; Sylvain Lehmann1; Shimadzu MS/MS; New York, USA; 2Tokyo Electron Limited, Kobe, Japan; 3University of South Florida, Tampa, FL

MP 624
Label-Free Quantitative Proteomics Profiling of Human Osteoclast Activation, Differentiation and anti-TNF Biologics Treatment; Chenqi Hu1; Bohdan Harvey2; Zehra Kaymakcalan1; Edt Tarsca2; Dongdong Wang3; Yu Tian4; 1Abbvie Bioresearch Center, Worcester, MA

MP 625
In Depth Quantification of Extracellular Matrix Proteins from Human Pancreas for Tissue Engineering; Fengfei Ma1; Christopher Lietz2; Sara Sackett3; Dan Trembrel4; Jon Orodi5; Lingjun Li6,7; 1School of Pharmacy, University of Wisconsin-Madison, Madison, WI; 2Department of Chemistry, University of Wisconsin-Madison, Madison, WI; 3Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; 4Identification of Interaction Networks of Mutant and Wild-Type IDH1 in Gioma Cell Lines; Nina Overbeck1; Anja Stefanski1; Vanessa Scherbaum1; Christiane Knobbe-Thomsen1; Kai Stuhler2; 1Molecular Proteomics Laboratory, Heirich-Heine-University, Düsseldorf, Germany; 2Department of Neuropathology, Heirich-Heine-University, Düsseldorf, Germany

MP 626
Quantitative MRM Assays of Salivary Proteins for Biomarker Assessment Studies; Andrew J Percy1; Darryl B Hardie2; Juncung Yang3; Armando Jardim4; Yassene Mohammed5,6; Monica H. Elliott7; Christoph H. Borchers4,8; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2Institute of Parasitology, McGill University, Montreal, QC, Canada; 3Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; 4University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 5Institute of Parasitology, McGill University, Montreal, QC, Canada; 6Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

MP 627
Toward the Development of a Scheduled GeLC-MRM Method for High-Throughput Quantitative Profiling of Small GTPases in Cancer Cells; Ming Huang1; Yinsheng Wang2; 1University of California, Riverside, Riverside, California; 2University of California, Riverside, Riverside, CA

MP 628
TARGETED PROTEOMICS:

MP 629
Method for High-Throughput Quantitative Profiling of Small GTPases in Cancer Cells; Ming Huang1; Yinsheng Wang2; 1University of California, Riverside, Riverside, California; 2University of California, Riverside, Riverside, CA

MONDAY POSTERS

MP 630
Targeted Proteomic Analysis Using Parallel Reaction
Monetary Monitoring Revealed Longitudinal Change in Level of Proteins in Activation of BV2 Mouse Microglia: Woo Jengam 1, Hann H. Hwang 2, 3, Hyunmin Park 4, 5, 6, Donghan Yoo 4, 5, 6, Institute of Biomedical Sciences, Seoul National University, College of Medicine, Seoul, Korea; 2Department of Biomedical Engineering, Seoul National University, College of Medicine, Seoul, Korea; 3Biomedical Research Institute, SNUH, Seoul, Korea

MP 632 Changes in Lipid Raft Proteome upon TNF-α Stimulation of Cytotoxic Fibrosis Cells Using SILAC; Cerina Chhuon 1; Iwona Pranke 2; Florence Borot 2; Danielle Tondelier 2; Joanna Lipecka 2; Janine Fritsch 2; Marc Chanson 2; Aleksander Edelman 3; Mario Ollero 3; Chiara Ida Guerra 4; 1Proteomic Platform Necker, PPN-3P5, Structure Fédérative de Recherche SFR Necker US24, 75015, Paris, France; 2Institut Necker Enfants Malades, INSERM, U1151, Paris, France; 3The CPN Proteomics Facility – 3PS, Center of Psychiatry and Neuroscience, UMR INSERM 894, 75014, Paris, France; 4Geneva University Hospitals and University of Geneva, 1211, Geneva, Switzerland; 5Institut Mondor de Recherche Biomédicale, INSERM, U955, and Université Paris Est Créteil, 94010, Créteil, France

MP 633 MRM Quantitation of an In-depth Panel of Candidate Disease-linked Proteins in Various Mouse Tissues; Sarah Michaud 1; Andrew Percy 2; Nicholas Sinclair 2; André LeBlanc 2; Suping Zhang 3; Christoph H. Borchers 4; MRM Proteomics Inc, Victoria, BC, Canada; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

MP 634 The Proteomic Landscape of Breast Patient-Derived Xenografts Reveals Tumor-Specific Education of the Xenograft - Genome BC Proteomics Centre, Victoria, BC, Canada; 2University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

MP 635 The Pathway Activity of Fatty Acid β-Oxidation is Up-regulated in the Skeletal Muscle Mitochondria of T2DM Mouse Model; Zhou Yang 1; Petra Erdmann-Gilmore 1; Rosa Viner 2; Matthew R Meyer 2; Timothy J Stuhlmiller 2; Sherri R Davies 2; Shunqiang Li 3; Qiang Zhang 3; Arshag D Mooradian 4; Kuan-lin Huang 5; Ryan Bonggardien 6; Li Ding 6; Matthew J Ellis 6; John C Rogers 6; Gary L Johnson 6; Reid R Townsend 7; Andrew Percy 8; Nicholas Sinclair 8; André LeBlanc 8; Suping Zhang 9; Christoph H. Borchers 10; MRM Proteomics Inc, Victoria, BC, Canada; and 1Department of Pharmacology, University of North Carolina, Chapel Hill, NC; 2The Genome Institute Washington University, Saint Louis, MO; 3Thermo Fisher Scientific, Rockford, IL; 4Baylor College of Medicine, Houston, TX; 5Department of Anesthesiology Washington University, Saint Louis, MO

MP 636 In-Depth Quantitative Proteomic Analysis of Human Breast Cancer Cells in Response to Nicotinamide; Dohyun Han 1; Ji Young Kim 2; Joonho Park 3; Han Suk Ryu 3; 1Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea; 2Department of Biomedical Engineering, Seoul National University Hospital, Seoul, Korea; 3Department of Pathology, Seoul National University Hospital, Seoul, Korea

MP 637 iTRAQ Based Quantitative Proteomics of a Brain-Enriched Cytosolic Protein Fraction in Schizophrenia; Erika Velásquez 1; Daniel Martins-de-Souza 1; Ingrid Velásquez 2; Andrea Schmitt 2; Fabio Cs Nogueira 2; Gilberto B Domont 3; 1Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; 2Unicamp, Campinas, SP; 3University of Carabobo, Valencia, Venezuela; 4Ludwig Maximilian University of Munich, Munich, Germany; 5UF RJ, Rio de Janeiro, Brazil

MP 638 Challenges of Using Isobaric Labeling for In-Depth Analysis of Large Numbers of Plasma Samples in a Cardiotoxicity Biomarker Discovery Study; Pengyuan Liu 1; Lynn A. Beer 2; Bonnie Ky 2; David W Speicher 2; 1The Wistar Institute, Philadelphia, PA; 2University of Pennsylvania, Philadelphia, PA

MP 639 Quantitative Multiplexed Isobaric Tag-Based Proteomic and Phosphoproteomic Profiling Reveals Nicotine and Cigarette Smoke Extract-Induced Alterations in Human Pancreatic Stellate Cells; Joo-A Park 1; Steven P Gygi 2; 1Harvard, Boston, MA; 2Harvard Medical School, Boston, MA

MP 640 SILAC-based Phosphoproteomic Analysis of PTH1R Signaling in Proliferating Osteoblasts; Lauren E Ball 1; Grace Williams 1; Jennifer Bethard 1; Louis Luttrell 1; 1Medical Univ of S Carolina, Charleston, SC

MP 641 Quantitative Temporal Proteomics of Flow Cytometry Isolated Virus-Driven MDSCs; Derek Clements 1; Patrick Murphy 2; Youra Kim 3; Andrea Sterea 4; Shekoufeh Almasi 5; Namit Holay 6; Prathyusha Konda 6; Joao Paulo 6; Steven P Gygi 6; Shashi Gujjar 6; Patrick Lee 6, 7; 1Department of Pathology, Dalhousie University, Halifax, NS, Canada; 2Department of Microbiology & Immunology, Dalhousie University, Halifax, NS, Canada; 3Department of Biology, Dalhousie University, Halifax, NS, Canada; 4Harvard University, Boston

MP 642 Down Regulation of Glycolysis Pathway in PICCALM Depleted Cells; Barsam Mirfattah 1; Hui Tang 1; Cheryl F Lichti 2; Fernanda Laeza 3; Kangling Zhang 4; 1University of Texas Medical Branch at Galveston, Galveston, TX

MP 643 Phosphoproteomic and Glycoproteomic Studies of Tonic and Activated B Cell Receptor Signaling in Burkitt’s Lymphoma; Jasmin Corso 1; Kuan-Ting Pan 2; Roland Walter 2; Carmen Dobele 2; Sebastian Mohr 1; Christof Lenz 1, 3; Hubert Serve 3; Henning Uralb 1, 3; Thomas Oellrich 2, 4, 5; Bioanal. MS Group, Max Plank Inst for Biophys Chem, Gottingen, Germany; 2Department of Hematology/Oncology, Johann Wolfgang Goethe University, Frankfurt, Germany; 3Bionanoflytics, University Medical Center Göttingen, Institute for Clinical Chemistry, Gottingen, Germany; 4German Cancer Consortium/ German Cancer Research Center, Heidelberg, Germany; 5Department of Haematology, University of Cambridge, Cambridge, United Kingdom

MP 644 Quantitative Profiling of Peroxisome Proliferation in the Heart by Selected Reaction and Selected Ion Monitoring. Effects of High Fat Diets; Caroline Kinter 1; Maria Thomas 2; David Gutierrez 3; Szweda Luke 1; Michael Kinter 1; Oklahoma Medical Research Foundation, Oklahoma City, OK

MP 645 MS1-Based Quantitative Proteomics Investigation of Mechanisms Underlying Gmcctinib and Trabectedin Synergism with High Multiplexing Capacity and Extremely Low Missing Value; Shichen Shen 1; Xin Mao 2; Jun Li 3; Xiaomeng Shen 3; Xue Wang 3; William Jusko 1; Kishore 2; Shailendra Rane 3; Deepti Bhandarkar 3; 1Biomedical Research Institute, Seoul National University, College of Medicine, Seoul, Korea

MP 646 Understanding Proteomic Alterations in GBM Tumors Associated with the Subventricular Zone: a Quest for Better Prognostic Markers; S Kishore Sai Sainthala 1; Shivani Kishore 2; Deepthi Bhandarkar 2; Sanjeewa Sripivastava 2; Aliasgar Moidiyyadi 2; 1Indian Institute of Technology, Bombay, Mumbai, India; 2Indian Institute of Technology, Bombay, Mumbai, India; 3Shimadzu Analytical (India) Pvt. Ltd., Mumbai, INDIA; 4Tata Memorial Centre’s-Advanced Centre for Research, Training and Education in Cancer, Kharghar, Navi Mumbai, India
**MONDAY POSTERS**

**MP 647**

Exploration of Novel Mechanisms for Synergy of Paclitaxel and Brinapant through Large-scale Quantitative Label-free LC/MS Proteomics; Xue Wang1; Jin niu2; Jun Li3; Shichen Shen2; Xiaomeng Shen2; Jun Qu2; 1University at Buffalo, Buffalo, NY; 2Center of Excellence in Bioinformatics&Life Sci., Buffalo, NY

**MP 648**

ProteOMZ: Development of Biogeochemically Relevant Peptide Biomarkers for High-Throughput Marine Microbial Ecosystem Characterization in Oceanic Oxygen Minimum Zones; Mak Saito1; Matt Mclvain2; Dawn Moran2; Alyson Sartoro2; Chris Dupont1; Michael Rappe1; 1Woods Hole Oceanographic Institution, Woods Hole, MA; 2University of Maryland Horn Point Laboratory, Cambridge, MD; 3J.C. Venter Institute, La Jolla, CA; 4Hawaii Institute of Marine Biology, University of Hawaii, Manoa, HI

**SMALL MOLECULES: QUALITATIVE ANALYSIS 651 - 680**

**MP 651**

Identification of Chemical Ingredients from Ginkgo biloba Extract Using UHPLC-QTOF/MS Coupled with PCDL Library; Guoqiang Liu1; Shan-An Chan2; 1Agilent Technology, Inc. Shanghai, China; 2Agilent Technology, Inc. Taipai, Taiwan, Taiwan

**MP 652**

Collision-Induced Dissociation MS/MS of Citrumpyrazepines, A New Class of Alkaloids from Black Cohosh (Actaea racemosa); Dejan Nikolic1; David C Lankin1; Richard van Breemen1; 1Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; 2University at Buffalo, Buffalo, NY; 3J.C. Venter Institute, La Jolla, CA; 4Hawaii Institute of Marine Biology, University of Hawaii, Manoa, HI

**MP 653**

Dereplication of Fungal Secondary Metabolites by UPLC-PDA-HRMS-MS/MS and Mass Defect Filtering; Noemi Paguigan1; Tamam M. El-Elimat1, 2; Diana Kao1; 1University at Buffalo, Buffalo, NY; 2Center of Excellence in Standards and Technology, Gaithersburg, MD; 3J.C. Venter Institute, La Jolla, CA; 4Hawaii Institute of Marine Biology, University of Hawaii, Manoa, HI

**MP 655**

Formation of m/z 92 Ion During Fragmentation of Deprotonated N-butyl Benzenesulfonamide; Chongming Liu1; Athula B. Attygalle1; 1Stevens Institute of Technology, Hoboken, NJ

**MP 656**

Gas-phase Methylation of Benzene by an Internal Electrophilic Aromatic Addition Mechanism Mediated by in-situ Generated Methylcarbenium Ion; Hanxue Xia1; Athula Attygalle2; Yong Zhang3; 1SIT, jersey city, New Jersey; 2Stevens Institute of Technology, Hoboken, NJ

**MP 657**

Non-Targeted Screening of Tattoo Ink Contaminants Using Liquid Chromatography/High-Resolution Mass Spectrometry and Chemometrics; Caitlin N. Kneapler1; Ann M. Knollhoff2; Clark Ridge1; Fred Fry3; Timothy R Croyle1; 1FDA/CFSAN, College Park, MD

**MP 658**

Applications of Infrared Ion Spectroscopy in Bioanalytical Chemistry; Jonathan Martens1; Giel Berden1; Jos Oomens1; 1FELIX Laboratory - IMM - Radboud University, Nijmegen, The Netherlands

**MP 659**

A Bayesian Prior Probability Model to improve the Confidence of Chemical Identification; Tyler A Zimmerman1; Richard Sablier2; 1Sorbonne Universités, UPMC; 2Muséum National d'Histoire Naturelle, Paris, France; 3Sciex, Lorraine, QC

**MP 660**

Investigation of the Metabolites of the HIF-Stabilizer FG-4592, Formed by Four in vitro Models, Using High Resolution Mass Spectrometry; AnneLise Hansson1; Mario Thevis2; Geoff Miller1; Daniel Eichner1; Ulf Bondesson1; 1Uppsala University, Uppsala, SE; 2German Sport University, Cologne, DE; 3Sports Medicine Research and Testing Laboratory, Salt Lake City, UT; 4National Veterinary Institute, Uppsala, SE

**MP 661**

The ETD-Like Fragmentation for Small Molecules; Romain Huguet1; Chad R Weisbrod1; Mark Berhow2; Vad Vlad Zabroukov3; Jae Schwartz4; Tim J Stratton1; 1Thermo Fisher Scientific, San Jose, CA; 2USDA, ARS NCAUR, Peoria, IL

**MP 662**

Application of TOF MS instrument in Bioanalysis – A Case Study; Shaokun Pang1; Weixing Sun2; Adrien Musuku3; Xavier Misonne4; 1Sciex, Redwood City, CA; 2PharmaSciences, Montreal, Canada; 3Sciex, Lorraine, QC

**MP 663**

On-Line Chiral Identification of Reaction Mixtures Using the Kinetic Method; Ryan M Bain1; Xin Yan2; Shannan A Raab3; 1SIT, Jersey City, New Jersey; 2Tennessee Tech, Cookeville, TN; 3University of Wisconsin, Madison, WI

**MP 664**

Automated Correlation between Structural Isomers and Fragment Ion Spectra Using a Novel Fragmentation Prediction Engine; Kiril Tzvetkov1; Stephen Stein1; Anzor Mikaia1; 1Pharmascience, Montreal, Canada; 2Sciex, Lorraine, QC

**MP 665**

Understanding Paper Degradation: Identification of Products of Cellulosic Paper Decomposition at the Wet-Dry "Tideline" Interface Using GC-MS and LTQ Orbitrap; Sergey Sladkevich1; Anne-Laurence Dupont2; Michel Sablier2; Richard T Gallagher2; 1Uppsala University, Uppsala, SE; 2UMPC Univ Paris 06, Paris, France; 3Muséum National d'Histoire Naturelle, Paris, France

**MP 666**

Development of a GC-MS Method for Structure Elucidation of Disubstituted Naphthalenes; Kirill Tretyakov1; Stephen Stein1; Anzor Mikaia1; 1National Institute of Standards and Technology, Gaithersburg, MD

**MP 667**

Substituting Atmospheric Solid Analysis Probe Ionization for Direct Probe Electron Impact Ionization for Analysis of Alcohols and Hydrocarbons; Martha M Vestling1; Trevor C. Christenson; Stephanie N. Knezez; 1University of Wisconsin, Madison, WI

**MP 668**

Dosing Syringe Extractables Analysis Using Bench-top Orbitrap Mass Spectrometer; Kenneth Wong1; Dujuan Lu2; 1Kate Comstock3; 2SGS, Fairfield, NJ; 3Thermo Fisher Scientific, San Jose, CA
MP 671 Identification and Quantitation of IV Bag Extractables Using LC-HRMS and GCMS; Dukuan Lu; Kenneth Wong; Kate Comstock; SGS, Fairfield, NJ; *Thermo Fisher Scientific, San Jose, CA

MP 672 The Application of Electrochemistry/MS to Pharmaceutical Stability Testing and Degradant Synthesis; Martin Eysberg; Jean-Pierre Chervet; Nico Reinhold; Mark Taylor; Susana da Silva Torres; *Antec LLC, Boston, MA; *Antec, Zoeterwoude, The Netherlands; 2Pfizer World Research and Development, Kent, United Kingdom

MP 673 Determining between Leachates and Process Related Compounds in Drug Substance Using Accurate Mass LC-MS and LC-MS/MS; George L Perkins; Lorraine Hill; Gary Campbell; Matthew Balmer; *Sanofi Pasteur Inc, Swiftwater, PA

MP 674 Analysis of Celestrol in Rat Brain Tissue and Plasma Samples Using TSQ Quantum Access MAX; Usha Mishra; Minmass(Minnesota Mass Spec), Minneapolis, MN

MP 675 Determination of Limaprost, an Analogue of PGE1 in Human Plasma by QTQRT® 6500+ and Seleion®+ Technology; Sanjoy Li; Chao Zhang; Wenhai Jin; 1Kuhui Center Hospital, Shanghai, China; 2SCIEX Asia Pacific Application Support Center, Beijing, China; 3SCIEX Asia Pacific Application Support Center, Shanghai, China

MP 676 Effects of Temperature and Anticoagulant on the Stability of Tetracyclines in Whole Blood: Drug-Matrix Equilibrium; Vinicio Vasquez; Richard Lavalleé; Nikolay I Youhovniski; Milton Furtado; Anahita Keyhani; 1Algorithme Pharma Inc., Laval, Canada

MP 677 Extremely Low LC-MS/MS Lithium Adduct Detection of Ramapycin in Animal Blood and Tissues; Alexandre Pimenov; Timothy Samuels; 1Charles River Bioanalyses, Senneville, Canada

MP 678 Analyzing Zn-BDPA Probes to Detect Apoptotic Cells in Three-Dimensional Cell Culture System via Mass Spectrometry; Jessica K Lukowski; Eric M Weaver; Kasey Clear; Bradley D Smith; Amanda B Hummon; 1University of Notre Dame, Notre Dame, Indiana

MP 679 LC-MS Based Approach to Characterize Non-Specific Binding Inhibitors to Mycobacterium tuberculosis Shikimate Kinase (MtkSK); Mansour Alturki; Madison Jarrard; Rene Ngouli; Douglas Goodwin; Angela Calderon; 1Auburn University, Auburn, AL; 2Washington University, St Louis, MO

MP 680 Synthesis and Characterization of Tetraphenylpyrrophenyl Manganese(III) Siloxides by Silyl Group Transfer from Silanethiols; Zachary J Tonzetich; Daniel J Meininger; Wendell P. Griffith; 1University of Texas at San Antonio, San Antonio, TX

MP 683 Proteomic and Metabolomic Comparative Analyses of Plasma and Vasculature Tissue from TiO2nanoparticle Exposed Rats; Megan M. Maurer; Jinghai Yi; Carroll McBride; Timothy R. Nurkiwicz; Stephen J Valentine; 1West Virginia University, Morgantown, WV

MP 684 Combined Metabolomics-Proteomic Profiling Reveals Intermittent Hypoxia to Result in Lower Productivity on Scale-Up to a 5000-Liter Industrial CHO Bioprocess; Yuanyei Gao; Somak Ray; Shujia Dai; Alexander R. Ivanov; Nicholas R. Abu-Absi; Amanda M. Lewis; Zhuangrong Huang; Xing Zhizhou; Michael C. Borys; Zheng Jian Li; Barry L Karger; 1Northeastern University, Boston, Massachusetts; 2Bristol-Myers Squibb, Devens, MA

MP 685 Triomics Analysis from Cancer Cells and Tumors: Modeling the Biology of Disease through The Integration of Metabolomics, Lipidomics and Phosphoproteomics; Susanne Breitkopf; Min Yuan; Ying Xu; John M Asara; 1Beth Israel Deaconess Medical Center, Boston, MA; 2Harvard Medical School, Boston, MA

MP 686 Integrated Multi-Omic Analysis of Chinese Hamster Ovary Cells: Joseph Longworth; Javier Gonzalez; Paul Dobson; Josselin Noirel; Neil Lawrence; Mark Dickman; David James; 1The University of Sheffield, Sheffield, United Kingdom; 2The University of Manchester, Manchester, United Kingdom; 3Conservatoire National des Arts et Métiers, Paris, France

MP 687 Systematic Integration of Multiple ‘Omics Data for Yeast Strains Isolated from Different Environments; Rohith Srivasa; Barbara Dunn; Andreas Humer; Daniel Lopez Ferrer; Michael Snyder; 1Dept. of Genetics, Stanford University, Palo Alto, CA - California; 2Thermo Fisher Scientific, San Jose, CA; 3ThermoFisher, Palo Alto, CA

MP 688 Integrative Analysis of Proteome, Transcriptome, and MHC Class I Ligandome of Human Cancer Cell Lines; Pedro Navarro; Sebastien Boegel; Jennifer Hahlbrock; John C Castle; Meike Wagner; Hansjorg Schild; Ugrur Sahin; Stefan Tenzer; 1Institute for Immunology, JG University Medical Center, Mainz, Germany; 2TRON – Translational Oncology at the University Medical Center of Johannes Gutenberg University, Mainz, Germany; 3Agenus, 4-Antibody AG, Basel, Switzerland

MP 689 Differential Dynamics of the Mammalian mRNA and Protein Expression Response to Misfolding Stress; Zhe Cheng; Guoshou Teo; Sabrina Krueger; Tara Rock; Hiromi Koh; Hyungwon Choi; Christine Vogel; 1New York University, New York, NY; 2National University of Singapore, Singapore, Singapore; 3Max-Delbruck-Center, Berlin, Germany

MP 690 High Resolution Mass Spectrometry-Based Subcellular Proteomics of a Human Cell Line; Alkaterina Geladaki; Claire Mulvey; Jake Beech; Kathryn S Lilley; 1Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom

MP 691 A Multi-Molecular Omics Approach to Study Metabolic Shifts in Caveolin-3 Transgenic Mice; Cristina Coman; Denis Gabriela Hathazi; Andreas Roos; Robert Ahrends; 1Leibniz-Institut für Agrar. Wissens. - ISAS -, Dortmund, Germany

SYSTEMS BIOLOGY (MULTIOMICS AND OTHER) 681 - 707

MP 681 Trans-omics Analysis of Yeast Central Carbon Metabolism by Integration of Metabolome, Proteome and Fluxome Data; Fumio Matsuda; Syunyuke Nishino; Taro Ogura; Atsumi Tomita; Ichiro Hirano; Hiroshi Shimizu; Osaka University, Osaka, Japan; Osaka University, Osaka, Japan; Shimadzu Corporation, Kyoto, Japan

MP 682 Proteomics and Metabolomics Demonstrate Inheritance of Key Energy Pathways in Red Blood Cells; Erin M. Weißenhorn; Thomas J. van't Erve; Michael S Westphall; Thomas J. Raifer; Joshua J Coon; 1Integrated Program in Biochemistry, University of Wisconsin-Madison, Madison, WI; 2Immunity, Inflammation and Disease Laboratory, National Institute of Environmental Health Sciences, Research Triangle Park, NC; 3University of Wisconsin-Madison Genome Center of Wisconsin, University of Wisconsin-Madison, Madison, WI; 4Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI; 5Departments of Chemistry and Biomolecular Chemistry, University of Wisconsin–Madison, Madison, WI

MP 683 Proteome and Metabolomic Comparative Analyses of Plasma and Vasculature Tissue from TiO2nanoparticle Exposed Rats; Megan M. Maurer; Jinghai Yi; Carroll McBride; Timothy R. Nurkiwicz; Stephen J Valentine; 1West Virginia University, Morgantown, WV

MP 684 Combined Metabolomics-Proteomic Profiling Reveals Intermittent Hypoxia to Result in Lower Productivity on Scale-Up to a 5000-Liter Industrial CHO Bioprocess; Yuanyei Gao; Somak Ray; Shujia Dai; Alexander R. Ivanov; Nicholas R. Abu-Absi; Amanda M. Lewis; Zhuangrong Huang; Xing Zhizhou; Michael C. Borys; Zheng Jian Li; Barry L Karger; 1Northeastern University, Boston, Massachusetts; 2Bristol-Myers Squibb, Devens, MA

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MP 690 High Resolution Mass Spectrometry-Based Subcellular Proteomics of a Human Cell Line; Alkaterina Geladaki; Claire Mulvey; Jake Beech; Kathryn S Lilley; 1Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom

MP 691 A Multi-Molecular Omics Approach to Study Metabolic Shifts in Caveolin-3 Transgenic Mice; Cristina Coman; Denis Gabriela Hathazi; Andreas Roos; Robert Ahrends; 1Leibniz-Institut für Agrar. Wissens. - ISAS -, Dortmund, Germany
Inhibition.

Carcinoma with ARID1A Knockdown and EzH2

In-Depth Secretome Analysis of Ovarian Clear Cell

Wright-Patterson AFB, OH; 3The Henry M. Jackson

Brain Injury Therapeutic Development

Human Performance Wing, Air Force Research Laboratory,

Data-independent Quantitative Mass Spectrometry in

OR

Texas HSC, San Antonio, TX; 2Proteome Software, Portland,

Emmons2; Susan T Weintraub1; Nicolas Musi1;

Olivier1; Ottar Rolfsson1, 2; Michael Gardner2; Bryan A Parks2; Christopher Toth3; Jeffrey

Stacy D Sherrod1; James C Pino1; Jamie L Allen1; Jeffrey

Rugang Zhang1; David W Speicher1; 1The Wistar Institute,

Philadelphia, PA

Ranwez1; Claudia Fortes1; Jon Rees2; Lisa G McWilliams2; James L. Pirkle1; CDC, Atlanta, GA;

“Center for Disease Control and Prevention, Atlanta, GA;

“Battelle Memorial Institute, Atlanta, GA

Analysis of Liver and Heart Spheroids in Drug-Induced

Hepatotoxicity and Cardiotoxicity; Nathalie Selevsek1;

Bemrd Roschitzki1; Jens Kelm2; Olivia Rose Clayton3;

Claudia Fortes1; Vitold Wolski1; Jonas Grossmann1; Laura

Kunz1; Paolo Nanni1; Adrian B. Roth1; Ralph Schlapbach1;

“Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; InSphero AG,

Schlieren, Switzerland; Roche Innovation Center Basel,

Grenzacherstasse Basel, Switzerland

Label Free Proteomics Profiling Unveils Down

Regulation of Thrombin Mediated Signaling and

Aggregation of Human Platelets upon Treatment

with Thrombin Inhibitors; Cristina Clement1; Ebeenerze

L.V. Ewul1; Anna Babinska1; Janet Gonzalez2; Monika

Dzieciatkowska1; Moro Salifu1; Manfred Philipp2; “Albert

Einstein College of Medicine, Bronx, NY; “Chemistry Department Lehman College,CUNY, Bronx, NY; “Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY; “Department of National Sciences, LaGuardia Community College, Queens, NY; “Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Colorado; “Biological Mass Spectrometry Core Facility, University of Colorado at Denver, Aurora, Denver, CO; “Division of Nephrology, Department of Medicine, State University of New York, Downstate Medical Center, Brooklyn, NY

Validation of a Unified Sample Preparation Platform

for Multi-Omics Technologies; Danielle Gutierrez1; Stacy

D Sherrod1; Jeremy L Norris1; Carrie E Romer1; Melissa A Farrow1; Simona Codreanu1; Randi Lee Gant-Branum1; Yuan-wei Nie1; John A McLean1; Richard M Caprioli1; 1Vanderbilt University, Nashville, TN

ChIP-MS/TMT: A Quantitative Proteomic Analysis of

Steroid Hormone Receptor Activation; Andrew Holding; 2Cambridge, Cambridgeshire

Proteome-wide Profiling of Geranylgeranyl

TopDownLab – Proteoform-Specific Monitoring of

Phosphoprotein-Protein Interaction Network in Liver via

Click Chemistry-Based Affinity Purification and Mass

Spectrometry; Lei Fang1; Jingzi Zhang1; Di Shen1; Bin

Xue1; Lan Huang2; Chaojun Li1; 1Nanjing University, Nanjing,

China; 2University of California-Irvine, Irvine, CA

Novel Method to Process Proteomics for Identification of

Pathways Associated with Anti-Colon Cancer Properties of Anthocyanin-Rich Purple-Fleshed

Potato in Mice; Venkata Charepalli1; Vadiraja Bhat1;

Lavanya Reddivari1; Jairam Vanamala1; 1Pennsylvania State University, University Park, Pennsylvania; 2Agilent Technologies, Wilmington, DE; 3The Pennsylvania State University, State College, PA; 4The Penn State Hershey Cancer Institute, Hershey, PA

TOP DOWN PROTEIN ANALYSIS (APPLICATIONS)

TopDownLab – Proteoform-Specific Monitoring of

Multi-Site Protein Phosphorylation; Andrea Mizzi,

Brunner1; Philip Lüsli1; Albert J R Heck2; Maarten A F

Allelaar1; Richard A Scheltema1; Utrecht University, Utrecht, Netherlands

Top-Down Proteomic Study of Sarcocere Protein

Post-Translational Modifications in Aging Skeletal

Muscle; Liming Wei1; Ziqing Lin1; Yutong Jin1; Wenchuan

Cai1; Zachery R. Gregorich1; Ying Ge1; “Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison; 2Department of Chemistry, University of Wisconsin-Madison, Madison
MP 710  Ultra-Fast Analysis of Hemoglobin Isoforms Using Capillary Electrophoresis Coupled to Mass Spectrometry and Ultraviolet Photodissociation; Andreas Krupa1; Chien-Hsun Chen1; Xiaolei Xie1; Chad R Weisbrod1; Romain Huguet1; Shiaw-Min Chen2; Achim Karger1; Steve Williams2; Michael Wenz2; Andreas Huhmer2; Aran Paulus3; Daniel Lopez-Ferrer1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, South San Francisco, CA

MP 711  Evaluation and Application of Top-Down Mass Spectrometry for Exploring the Low Molecular Weight Proteome of Osteosarcoma Cells; Leping Yang1; Zifeng Song1; Claudia S Maier1; 1Oregon State University, Corvallis, OR

MP 712  Top-Down Mass Spectrometry Applications for Detection of N-Terminal Sequence Heterogeneity and PTMs for a Therapeutic Molecule; Bao Quoc Tran1; Shivangi Awasthi1; Mohd M Khan1; David R Goodlett1; Young Ah Goo2; 1University of Maryland Baltimore City; 2University of Maryland, College Park

MP 713  Targeted Intact Protein Fragmentation in Complex Mixtures Using a Charge State Scheduled Precursor List of Regulated Proteoforms; Jim Kapron1; Rainer Paape2; Markus Lubeck3; Schmit Pierre-Olivier1; 1Bruker Ltd, Vancouver, Canada; 2Bruker Daltonic GmbH, Bremen, Germany; 3Bruker Daltonique S.A., Wissembourg, bas-rhin, France

MP 714  Investigating Binding Sites of Metal Drugs to Ubiquitin Using Free-Access cheminfo.org Algorithms; Laura Menin1; Ronald F.S. Lee2; Luc Patiny3; Daniel Ortiz3; Paul J. Dyson4; 1EPFL SB ISIC-GE, Lausanne; 2EPFL, Lausanne, Switzerland

MP 715  Human Proteoform Identification by Top-Down LC-MS/MS Utilizing a 21 Tesla FT-ICR Mass Spectrometer; Lisa C Anderson1; Caroline J DeHart1; Nathan K Kaiser1; Donald F Smith1; Christopher L Hendrickson1; 1NHFML, Tallahassee, FL

MP 716  Top-down MS/MS Analysis of Canonical Histone H2A Phosphorylation During the Cell Cycle; Xibei Dang1; Michael E Hoover2; Chen Yu1; Alan G Marshall1; 1Indiana University Dept. Chemistry, Bloomington, IN; 2Ohio State University, Columbus, OH

MP 717  Comprehensive, Quantitative Intact Proteoform Measurements of Patient-Derived Breast Tumor Xenografts Using an Improved Top-down Proteomics Pipeline; Tao Liu1; Paul D Piehowski2; Samuel H Payne2; Sangtae Kim1; Jungkap Park1; Christopher S Wilkins1; Carrie D Nicora2; Yufeng Shen1; Rui Zhao1; Anil K Shukla2; Ronald J Moore1; Shemi R Davies3; Shunqiang Li2; Reid R Townsend4; Matthew J Ellis1; Emily S Boja1; Henry Rodriguez1; Karin D Rodland1; Richard D Smith1; 1Pacific Northwest National Laboratory, Richland, WA; 2Washington University, St Louis, MO; 3Baylor College of Medicine, Houston, TX; 4National Cancer Institute, Bethesda, MD

MP 718  Top-Down LC/MS Analysis of Myofilament Proteoforms Using Top-Down Proteomic Measurements of Patient-Derived Breast Tumor Xenografts; Yumin Lian1; Ziqing Lin1; Yi-Chen Chen1; Nicole Marie Lane1; Takashi Kohmoto1; Ying Ge1; 1University of Wisconsin-Madison, Madison, WI

MP 719  Yahb Protein as a Calibrator For Top-Down Proteomic Identification of Shiga Toxin Using MALDI-TOF-TOF-MS/MS and Post-Source Decay; Clifton K. Faederquist1; William James Zaragoza1; USDA/ARS, Albany, CA

MP 720  Label-Free Quantitative Analysis of Mouse Brain Proteoforms Using Top Down Proteomics; Roderick G. Davis1; Kyunggon Kim1; Paul M Thomas1; Ryan T Fellers1; Richard D Leduc2; VanNispen J Alexandra2; Jonathan Sweedler2; Justin Rhodes2; Neil L Kelleher1; 1University of Texas at Dallas, Richardson, TX; 2University of Illinois at Urbana-Champaign, Urbana, IL

MP 721  Assessing Organismal and Spatial MBP Proteoform Diversification in Healthy Rats by Top-Down Mass Spectrometry (TDMS); Casey E Wing1; Micheal Tran1; Daniel A Pylime2; John Corbett1; Steven M Patrie1; 1University of Texas at Dallas, Richardson, TX; 2University of Texas Southwestern Medical Center, Dallas, TX

MP 722  Top-Down Proteomics can Differentiate Closely Related Pathogenic Enterobacteria; Mathieu Dupré1; Valeria Calvaresi1; Christian Malosse1; Magalie Duchateau1; Dominique Clermont1; Julia Charnot-Rooke1; 1Institut Pasteur, Paris, France

MP 723  Analysis of Proteoforms in Membrane Protein Complexes by Top-Down Proteomics; Hans JCT Wessels1; Sergio Guerrero-Castillo1; Roel Tans1; Schmit Pierre-Olivier2; Stuart Pengelley1; Alain J Van Gool1; 1Radboudumc, Nijmegen, Netherlands; 2Bruker Daltonic GmbH, Bremen, Germany

MP 724  Top Down 3D Spatial Mapping of Myelin Basic Protein Proteoforms: Organism and Spatial Diversification and its Potential Impact on Auto Immunity; Daniel Pylime1; John Corbett1; Casey Wing2; Michael Tran1; Steven Patrie1; 1University of Texas Southwestern Medical Center, Dallas, TX; 2University of Texas at Dallas, Richardson, TX

MP 725  Preparing to Read the Ubiquitin Code: Top-Down Analysis of Polyubiquitin Chains; Amanda Lee1; Lucia Geis-Asteggianite1; Emma Dixon1; Tanuja Kashyap1; Yan Wang1; David Fushman1; Catherine Fenselau1; 1University of Maryland, College Park, MD

MP 726  Identification of Secretory Virulence Factors in S. aureus by Combination of Proteomics Methods; Santsosh Misal1; Shital D Ovhal2; Jonathan A Karty1; James P Reilly1; 1Indiana University Dept. Chemistry, Bloomington, IN

MP 727  Top-Down High Resolution Accurate Mass-Mass Spectrometry for Identification of Clinical Yeast Species; Joanna Freeke1; Azadeh Jamalian1; Mansoureh Vatanshenassan2; Bert Gerrits van den Ende1; Helene L Cardasis3; Johan Fei11; Ping F. Yip1; Scott R. Kronewitter2; James Jr L Stephenson3; Alexander Y. Cherkerassky2; J. Benjamin Stielow1; Sybren de Hoog1; 1Thermo Fisher Scientific, Utrecht, Netherlands; 2CBS/KNAW Fungal Biodiversity Center, Utrecht, Netherlands; 3Thermo Fisher Scientific, Cambridge, MA; 4Thermo Fisher Scientific, Vantaa, Finland
| TP 001 | Characterization of Antibody Drug Conjugate: Intact, Fragment and Peptide Mapping using Reversed Phase Columns; Suresh Babu CV; Tanng Ning; Anne Blackwell; Agilent Technologies, Bangalore, Karnataka, India; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Little Falls, DE |
| TP 005 | Comparison of Innovator and Biosimilar by Peptide Mapping using HPLC Coupled to Time-of-Flight Mass spectrometry; Ravindra Guditahl; Ning Tang; Agilent Technologies India Pvt. Ltd, Bangalore, Karnataka, India; Agilent Technologies, Santa Clara, CA |
| TP 006 | Towards the Complete Characterization of Host Cell Proteins in Biotherapeutics via Affinity Depletions, LC-MS/MS, and Multivariate Analysis; Jennifer Murphy; A. Madsen; Victor Farutin; Yan Yin; Stephen Smith; James Anderson; Ishan Capilla; Momenta Pharmaceuticals, Cambridge, MA; Momenta Pharmaceuticals, Cambridge, MA |
| TP 007 | Reversed-Phase Separation of Therapeutic Monoclonal Antibodies Using Superficially Porous Column: LC/MS Analysis; Suresh Babu CV; Ning Tang; Anne Blackwell; Agilent Technologies, Bangalore, Karnataka, India; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Little Falls, DE |
| TP 008 | Rapid Automated LC-MS/MS Glycan Analysis for Monoclonal Antibodies; Bhavana Shah; Jason Richardson; Zhongqi Zhang; Amgen Inc., Thousand Oaks, CA; Amgen, Inc., Thousand Oaks, CA |
| TP 009 | Towards the Automated Monoclonal Antibody Sequencing and Characterization from LC-MS data; Lin He; Mohammad Zaur Rahman; Ngoc Hieu Tran; Baozhen Shan; Ming Li; Bioinformatics Solutions Inc., Waterloo, Canada; David R. Cheriton School of Computer Science, University of Waterloo, Waterloo, ON |
| TP 010 | Development of a Non-Toxic Antibody Drug Conjugate Mimic to Enable LC-MS Method Development Without Risk; Kevin Ray; Brian Gaul; John Dapron; Nicolas Caffarelli; Jeffrey Turner; Millipore Sigma, St. Louis, MO |
| TP 011 | Characterisation of Antibody Conjugates under Denaturing Liquid Chromatography Mass Spectrometry (MS) and Native MS Conditions; Karsi Karu; Mauricio Morais; James R Baker; UCL Chemistry Mass Spectrometry Facility, London; Department of Chemistry, Christopher Ignold Building, London, UK |
| TP 012 | Electrospray-Ionization Time-of-Flight Mass Spectrometry Coupled to Online, Comprehensive Two-Dimensional Liquid Chromatography for the Characterization of Therapeutic Monoclonal Antibodies; Matthew Sorensen; David Christopher Harmes; Gregory O Staples; Szabolcs Fekete; Alain Caffarelli; Jeffrey Turner; MilliporeSigma, St. Louis, MO |
| TP 013 | Native Liquid Chromatography-Mass Spectrometry Applied to the Validation of Drug to Antibody Ratio LC-UV Methods and Antibody Drug Conjugates Development; Lieza Daman-Leon; Guillaume Tremintin; Stemcentrx, South San Francisco, CA; Bruker Daltonics, Fremont, CA |
| TP 014 | Direct Analysis of Intact mAb’s and Low Abundant Variants by Advanced LC-MS Approaches; Xiaomei (Annie) He; Janet Lau; Shiv-Min Wu; BioAnalyx, Cambridge, MA |
| TP 015 | Mass Spectrometric Characterization of Half-mAb Separated from Intact Monoclonal Antibody and Fragments using Analytical Size Exclusion Chromatography Column; Crystal Benner; William Evans; Cesar Zurn; Kyle Root; Kemey Jebrel Glover; |
TP 016 LC-MS Characterization of Proteolytic Cleavage Sites in Therapeutic Monoclonal Antibodies; Pavel V. Bondarenko1; Thomas M Dillon1; Gang Xao2; Nicole Ball3; Deirdre M Piedmonte1; Michael J Treuheit1; ‘Amgen, Inc., Thousand Oaks, CA; ‘Amgen, Inc., Thousand Oaks, CA

TP 017 Probing Higher-Order Structural Changes of a Lysine-linked Antibody-Drug Conjugate by Hydrogen-deuterium Exchange Mass Spectrometry (HDXMS), Lintao Wang1; Alexandre C. Lazar2; ImmunoGen Inc., Waltham, MA; ‘ImmunoGen, Inc., Waltham, MA

TP 018 A New Workflow for Characterization of Antibody Mixtures via Slip Flow Chromatography and Ultraviolet Photodissociation for Top-Down Mass Spectrometry; Luca Fornelli1; Philip Compton1; Ximo Zhang2; Mary Wirth2; Neil Kelleher1; ‘Northwestern University, Evanston, IL; ‘Purdue University, West Lafayette, IN

TP 019 Glycoform Separation and Characterization of Cetuximab Glycoforms by Middle-Down Off-line CE-UV/ESI-MS; Nasser Said1; Michael Biachchi1; Rabah Ghahoui1,2; Charly Renard1; Alain Beck1; Yannis-Nicolas Francois1,3; Emmanuelle Leize-wagner1; ‘Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; ‘Division of BioAnalytical Chemistry, ALIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherlands; ‘Centre d’Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France

TP 020 High-order Structural Interrogation of Antibody-drug Conjugates by a Combination of Intact, Middle-up and Bottom-up Techniques using Sheathless Capillary Electrophoresis-Mass Spectrometry; Nasser Said1; Rabah Ghahoui1,2; Laurianne Kuhn1; Alain Beck1; Yannis-Nicolas Francois1,3; Emmanuelle Leize-wagner1; ‘Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS), CNRS – UMR7140, University of Strasbourg, Strasbourg, France; ‘Division of BioAnalytical Chemistry, ALIMMS Research Group BioMolecular Analysis, VU University Amsterdam, Amsterdam, The Netherlands; ‘Institut de Biologie Moléculaire et Cellulaire (IBMC), University of Strasbourg, Strasbourg, France; ‘Centre d’Immunologie Pierre-Fabre, Saint-Julien-en-Genevois, France

TP 021 Microchip Electrophoresis with Integrated ESI-MS for the Detailed Analysis of Intact Biotherapeutic Antibodies and ADCs; J. Scott Mellors1; Erin Anne Redman1; J. Michael Ramsey1,2; Qi Wu1; ‘Medarex, Inc., Andover, MA; ‘Thermo Fisher Scientific, San Diego, CA

TP 022 Capillary Electrophoresis – Mass Spectrometry for Top Down Proteomics; Andreas Krupe1; Shiaw-Min Chen1,2; Achim Karger1; Michael Wenz1; Daniel Lopez-Ferrer1; Aran Paulus2; ‘Thermo Fisher Scientific, South San Francisco, CA; ‘Thermo Fisher Scientific, San Jose, CA

TP 023 Intact Immunoglobulin Gamma Analysis by CE/MS; Bryan Fonslow1; Olga Friese2; Ying Zhang3; John Yates1,2; K. Steven Cook1; Jason Rouse1; ‘SCIEX, San Diego, CA; ‘The Scripps Research Institute, La Jolla, CA; ‘Pfizer, Chesterfield, MO; ‘Pfizer, Inc. Andover, MA

TP 024 Characterization of Monoclonal Antibody Charge Variants using OffGel Fractionation and Mass Spectrometry; Alyssa Neil1; Yeekatrina Kori1; Guilong Charles1; Hongcheng Liu1; ‘Alexion Pharmaceuticals Inc., New Haven, CT; ‘University of Massachusetts Amherst, Amherst, Massachusetts

TP 025 Bioanalytical Challenges of Next-Generation Antibody-Drug-Conjugates Case Study: Developing a 2nd-Generation Affinity Capture LC-MS to Improve In Vivo Stability Assessment; Dian Lu1; Genentech Inc, South San Francisco, CA

TP 026 Novel Microfluidic Chip with In-line Deglycosylation for Rapid Mass Analysis of Reduced Monoclonal Antibodies; Loredana Serafini1; John Corbin1; Victoria Smith1; Mark Nagel1; Leanna Lagpacan2; Debi Jin3; Andy Gieschen2; Caroline S. Chu2; Katherine Brendza1; ‘Gilead Sciences, Foster City, CA; ‘Agilent Technologies, Santa Clara, CA

TP 027 Multidimensional IonKey/MS for Antibody Drug Conjugate Analysis; Greg Roman1; James P Murphy1; ‘Waters, Milford, MA

TP 028 Using Hydrophilic Interaction Chromatography-Mass Spectrometry for Heightened Product Characterization to Overcome Challenges with Hydrophobic Antibodies and Antibody Drug Conjugates; Jacquelynn Smith1; Matthew Lauber1; Stephan Koza2; Erin Chambers2; Jason C Rouse3; Olga Friese4; ‘Senior Associate Scientist at Pfizer, Chesterfield, MO; ‘Waters, Milford, MA; ‘Pfizer, Inc. Andover, MA; ‘Pfizer, Chesterfield, MO

BIOMARKERS: QUANTITATIVE ANALYSIS (PART 1)

TP 029 Towards Absolute Quantification of Protein Expression in 3D Tissue Culture Samples by MALDI-IMS-MS Imaging; Rebecca Day1; Amanda Harvey1; Laura M Cole1; Neil Cross1; David Smith1; Malcolm Clench2; ‘Sheffield Hallam University, Sheffield, United Kingdom

TP 030 Double Standards in Proteomics: DOSCATS: Engineered Peptide/Epitope Concatenations for SRM or Western Blotting; Robert Beynon1; Richard J Bennett1; Deborah M Simpson1; Stephen W Holman1; Daniel S Spellman1; ‘Merck & Co., Inc., West Point, PA; ‘Merck & Co, Kenilworth, NJ

TP 031 Development of New LC-MS Methodologies to Assess Liver Function in a Clinical Setting using Plasma and Dried Blood Spot; Lei Guo1; Raymond Gonzalez1; Kara Pearson1; Elizabeth Joshi1; Kevin P Bateman1; Daniel S Spellman1; ‘Merck & Co., Inc., West Point, PA; ‘Merck & Co, Kenilworth, NJ

TP 032 Serial Lectin Affinity Chromatography for Comparative Serum Glycoproteomics on Colorectal Cancer Biomarker Discovery; Jinwook Lee1; Wonryeon Cho1; ‘wonkwang University, Iksan, Jeonbuk

TP 033 Between Good, Fast and Cheap: Method Development for Large-Scale Plasma-Proteome Analysis between the Antagonizing Poles of Sensitivity, Through-put and Costs; Christoph Stirling1; Lennard Dekker1; Diana A T Nijholt1; Coskun Güzel1; Martijn M. van Duijn1; Theo M. Luider1; ‘Erasmus Medical Center, Rotterdam, The Netherlands

TP 034 Comparative Proteomic Analysis of Kidney Distal Convoluted Tubule and Cortical Collecting Duct Cells following Long-Term Hormonal Stimulation; Qi Wu1; Trairak Pisutkin1; Robert Fenton1; ‘Center for Interactions of Proteins in Epithelial Transport, Department of Biomedicine, Aarhus, Denmark; ‘Faculty of Medicine, Chulalongkorn University, Bangkok, Thailand

TP 035 Higher Protein Identifications and Coverage May Not Correlate with Higher Numbers of PSMs or Peptides in Quantitative Proteomic Analyses; Lauren Devine1; Tatiana Borolina1; Robert N O’Meally1; Robert N Cole1; ‘Johns Hopkins University School of Medicine, Baltimore, MD

TP 036 Identification of Pathologico-Synuclein Forms in Brain Extracts from Patients with Parkinson’s Disease by Selected Reaction Monitoring; Pavel Bhattacharjee1; Ann Brinkmalm1; Annika Öhrfelt1; Kai Blennow1; Henrik Zetterberg1; ‘University of Gothenburg, Mölndal, Sweden

TP 037 Development of a TFPI (Tissue Factor Pathway Inhibitor) Protein Quantification Assay; Katherine Wright; Pfizer, Andover, MA
**TP 039**
Development of Plasma Protein Biomarkers for Effects of Radiation Exposure Using Quantitative Mass Spectrometry; Kate Liu1; Dyna Shirasaki2; Elizabeth Singer3; William McBride4; Julian Whitelegge5; Joseph A. Loo6; 1UCLA, Los Angeles, CA

**TP 040**
Phosphoproteomic Analysis of Differential Protein Expression in BRaf-Mutated Melanoma Cells with Acquired Resistance to BRaf, MEK1/2, or ERK1/2 Inhibitors; Shiviann Awasthi1; Jacob Sheenstra2; Bao Tran3; Young Ah Goo4; Paul Shapiro5; David R Goodlett6; 1University of Maryland Baltimore, Baltimore, USA

**TP 041**
Identification of Novel Glycoprotein Biomarkers for Distinguishing Intestinal Inflammation from Fibrosis in Crohn’s Disease by LC-MS/MS; W. David M Lubman1; Jing Wu2; Ryan G. Stidham3; Henry Appelman4; 1University of Michigan Medical Center, Ann Arbor, MI

**TP 042**
LC-MS/MS Method for Quantitation of Seven Biomarkers in Human Plasma for the Assessment of Impaired Glucose Tolerance; Qibo Zhang1; Lisa A Ford2; Kelli D Goodman3; Tiffany A Free4; Deirdre M Hauser5; 1University of Rochester, Rochester, NY

**TP 043**
A Robust Analytical LC-MS/MS Method to Quantitate Plasma Itraconazole and Hydroxy-Itraconazole in Patients with Solid Tumors; Claudia Meek1; Eding Beck2; Richard Leff2; 1Texas Tech University, Dallas, TX; 2Texas Tech University Health Sciences Center, Dallas, TX

**TP 044**
Investigation of the Quantitative Properties of Micro Flow LC-MS/MS for Direct Analysis of Frataxin in Human Biopsy; Qihan Lin1; Jinghua Zhu2; 1University at Albany, Rensselaer, NY; 2University at Albany, Rensselaer, NY

**TP 045**
Ultra high Performance Liquid Chromatography-Tandem Mass Spectrometry (UHPLC-MS/MS) Platform for Clinical Diagnostics within Diabetes Care; Linda Ahonen1; Sirkku Jäntti2; Matej Orešič3; Tuula Hyötyläinen4; 1Steno Diabetes Center A/S, Gentofte, Denmark; 2University of Helsinki, Helsinki, Finland

**TP 046**
Quantitative Discovery of the Alterations of the Entire Human Kinome in Human Cells upon Methyglyoxal Treatment; Wei Li1; Lei Guo2; Yongsheng Xiao3; Xiaogang Jiang4; Yinhwang Wang5; 1University of California, Riverside, Riverside, CA

**TP 047**
A Comprehensive Investigation towards the Indicative Proteins of Bladder Cancer in Urine: From Surveying Cellular Secretomes to Verifying Urine Proteins; Jiao Guo1; 1Beijing, Beijing

**TP 048**
Development of MS Based Clinical Assays for Measuring Cerebrospinal Fluid Levels of Pre-Synaptic Proteins in Alzheimer’s Disease; Ann Brinkmalm1; Gunnar Brinkmalm2; Henrik Zetterberg3; Kai Bjelland4; 1University of Gothenburg, Malmö, Sweden; 2UCI Institute of Neurology, London, UK

**TP 049**
Quantification of Heptadin-25 in human Cerebrospinal Fluid using LC-MSRM; Jerome Vialaret1; Costance Delaby2; Pauline Bros3; Amandine Moulinier; Vincent Delatour4; Audrey Gabelle5; Sylvain Lehmann1; Christophe HIRTZ6; 1LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; 2Laboratoire National de Métrologie et d’Essais, Paris, France; 3Laboratoire National de Métrologie et d’Essais, Paris, France; 4Centre Mémoire Ressources CHRU Montpellier, Montpellier, France

**TP 050**
Measurement of DNA Repair Protein Apurinic/Apyrimidinic Endonuclease 1 (APE1) in Human Tissues by Liquid Chromatography/Tandem Mass Spectrometry with Isotope Dilution; Pawel Jaruga1; Fatos Guldikali2; Prasad T. Reddy3; Alessandro Tona4; Bryant C. Nelson5; Mengxia Li6; David M. Wilson, III7; Erdem Coskun8; Miral Dizdar9; 1NIH/NCI (National Cancer Institute), Bethesda, MD; 2NIH/NCI/IRP, Baltimore, MD; 3NIH/NCI (National Institute on Aging), Baltimore, MD; 4Rochville, MD

**TP 051**
Phosphoproteome Analysis Reveals Differential Mode of Action of Sorafenib in Wildtype and Mutated FLT3 AML Cells; Catrin Roof1; Nikolay Dybowskij2; Anett Sekora1; Stefan Mueller3; Gudrun Knuebel1; Hugo Murua Escobar4; Klaus Godi5; Andreas Tebbe6; Christian Juengel8; Christoph Schaab9; 1Rostock, University Medical Center, Department of Hematology/Oncology/Palliative Care, Rostock, Germany; 2Evotec (München) GmbH, Munich, Germany

**TP 052**
Improved Quantification of Rat Plasma NNK and NNAL Using Protein Precipitation and Phospholipid Removal in UFLC-ESI/MS/MS; Estafa Seneh1; Matthew S Bryant1; 1National Center for Toxicological Research, FDA, Jefferson, AR; 2National Center for Toxicological Research - FDA, Jefferson, AR

**TP 053**
Accurate Quantification of Peptide using Multiple Internal Standards in Conjunction with parallel reaction monitoring; Sebastian Gallien1; Bruno Domon1; 1Luxembourg Clinical Proteomics Center, Strassen, Luxembourg

**TP 054**
Precise MRM-based Quantitation of 200 Proteins from Dried Blood Spots and Single Drops of Blood; Jingxi Pan1; Suping Zhang2; Albert Chou3; Christoph H. Borchers4; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2MRM Proteomics, Inc., Victoria, BC, Canada; 3University of Victoria - Genome BC Proteomics Centre, Victoria, BC; 4Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

**TP 055**
The Synaptic Vesicle Cycle is Governed by Heterogeneous and Macromolecular Protein Microdomains; Carla Schmidt1; HALOmem, University of Halle, Halle / Saale

**TP 056**
Structure of α-Synuclein determined by Structural Proteomics and Constraint-Driven Discrete Molecular Dynamic Modeling; Nicholas I Brodie1; Konstantin I Popov2; Evgeniy V Petrochanko2; Nikolay V Dokholyan3; Christoph H. Borchers4; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2University of North Carolina, School of Medicine, Chapel Hill, NC; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

**TP 057**
Profiling Yeast Mitochondrial Protein-Protein Interactions in a Whole-Organelle Scale by Cross-Linking Mass Spectrometry; Chung-Tien Lee1; 2; Peter Rehling1; Henning Urlaub1; 1Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; 2University Medical Center (UMG), Göttingen, Germany

**TP 058**
Transcription Factor-DNA Interaction Studied by Structural Mass Spectrometry; Lukas Slavata1; 2; Michal Rosulek1; 2; Daniel Kavan1; 2; Alan Kadek1; 2; Hynek Mrazeck1; 2; Petr Man1; 2; Petr Novák1; 2; 1Institute of Microbiology CAS, Prague, Czech Republic; 2Faculty of Science, Charles University in Prague, Prague, Czech Republic
TP 059 Assessing the Performance of CID-cleavable cross-linkers and Subsequent Data Analysis Strategies; Rebecca Beveridge1; Karl Mechtler2; 1Research Institute of Molecular Pathology (IMP), Vienna, Austria

TP 060 Improving Cross-linked Peptide Identification in Large Protein Complexes on Quadrupole-Orbitrap and Quadrupole-Orbitrap-Ion Trap Platforms; Chung-Tien Lee1; Oxandry Dybvik1; Christof Lenz1; 1, 2Thomas Monecke2; Ralf Ficner1; Yue Xuam; Henning Urlaub2; 1Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; 2University Medical Center (UMG), Goettingen, Germany; 3Georg August University, Goettingen, Germany; 4Thermo Fisher Scientific, Bremen, DE

TP 061 Optimization of Crosslinked Peptide Analysis on an Orbitrap Fusion Lumos Mass Spectrometer; Ryan Bomgardner1; Erun Raja1; Chris Etienne1; Fan Liu2; Albert J R Heck2; Mathias Mueller2; Rosa I Viner3; 1Thermo Fisher Scientific, Rockford, IL; 2Utrecht University, Utrecht, The Netherlands; 3Thermo Fisher Scientific, Bremen, DE; 4Thermo Fisher Scientific, San Jose, CA

TP 062 Structural Proteomics Analysis of the Native Tau Protein; Karl A T Makepeace1; Evgeniy V Petrotchenko1; Christoph H. Borchers2, 3; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, CANADA; 2University of Victoria - Genome BC Proteome Centre, Victoria, BC; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, CANADA

TP 063 Evaluation of a Photo-Activatable Unnatural Amino Acid Engineered Into Proteins To Crosslink And Identify interaction partners; Robert Heitlich1; Chen Qian2; Steven King1; Melinda Hauser2; Jeffrey Becker2; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Tennessee, Knoxville, TN

TP 064 Analysis of UV-induced DNA-protein cross-links in a chromatin model by mass spectrometry; Alexandra Stuetz1; Christin Kappert1; Aleksandr Chernyev1; Wolfgang Fischen1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Bremen, DE; 3Thermo Fisher Scientific, Rockford, IL

TP 065 RNAPx 2 - Protein-RNA Interaction Site Localization from UV Cross-linked Peptide-RNA Oligonucleotides in Proteome Discoverer 2.1; Timo Sachsenberg1; Johannes Veit1; Aleksandr Chernyev1; Kundan Sharma1; Romina Hofele1; Saadia Qamar2; Christin Kappert1; Katharina Kramer1; Juliana Pfeiffer2; Xiaolong Yang1; Knut Reinert1; 2Christof Lenz2; Henning Urlaub2; Oliver Kohlbacher1, 2; 1Eberhard Karls University, Tübingen, Germany; 2Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; 3KUAST, Thuwal, Saudi Arabia

TP 066 Novel Workflow for Characterization of Non-Disulfide Protein Crosslinks in Normal and Cataractous Human Lens; Rujiang Chen1; 1Stevens Institute of Technology, China, Beijing, China; 2School of Life Science, Beijing Institute of Technology, China, Beijing, China

TP 067 New Methodology for the in vivo Identification of Protein Partners using Genetically Encoded Unnatural Amino Acids and Mass Spectrometry; Mariana Fioramonte1; Bing Yang2; Ana Gisele C Neves-Ferreira1; Lei Wang2; Fabio César Gozzo1; 1University of Campinas, Campinas, Brazil; 2UCSF, San Francisco, CA; 3Thermo Fisher Scientific, Rio de Janeiro, RJ

TP 068 Systematic Determination of Nuclear Pore Complex Protein Interfaces by XL-MS; Joseph Glav1; 1EMBL Heidelberg, Heidelberg, Germany

TP 069 Quantitative Cross-linking/LCMS (CX-MS) to Investigate Allosteric Regulation of Phosphodiesterase 6 (PDE6); Donna Hogan1; Xiongzhao Gao2; Suzanne Matte1; Rick Cole1; FeiXia Chu1; 1University of New Hampshire, Durham, NH

TP 070 Developing a Novel Multiplexed Quantitative Cross-linking Mass Spectrometry Strategy to Define the Structural Dynamics of Cullin-RING Ligase Complex; Clinton Yu1; Haibin Mao2; Alex Huszagh1; Rosa I Viner3; 1University of California, Irvine, Irvine, CA; 2University of Washington, Seattle, WA; 3Thermo Fisher Scientific, San Jose, CA

TP 071 Developing A Novel Acidic Residue Reactive and Sulfoxide-containing MS-cleavable Homobifunctional Cross-linker for Studying Protein-Protein Interactions; Craig Bryant Gutierrez1; Clinton Yu1; Alex Huszagh1; 1UC-Irvine, Irvine, CA

TP 072 Structural Analysis of a Myotoxin-antimyotoxin Complex by Cross-linking, Mass Spectrometry and Bioinformatics; Barbara S. Soares1; Surza L. G. Rocha1; Diogo B. Lima1; Bruno Lomonte1; Gilberto B Domont1; Jonas Perales1; Richard H. Valente1; Francisco Gomes-Neto1; Ana Gisele Neves-Ferreira1; 1Oswaldo Cruz Institute, Fiocruz, Rio de Janeiro, Brazil; 2Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; 3Cldomio Picado Institute, Universidade de Costa Rica, San José, Costa Rica; 4Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

TP 073 Photocrosslink Coupled with Mass Spectrometry on a Transmembrane Protein Pump using an Unnatural Amino Acid, Benzoylphenylalanine; Thao Nguyen1; Grzegorz Sabat1; Michael Sussman2; 1UW Madison, Madison, WI; 2UW-Madison, Madison, WI

TP 074 In vivo Conformational Dynamics of Hsp90 and Its Interactors; Juan Chavez1; Devin K Schweppe1; Jimmy K Eng1; James E Bruce1; 1University of Washington, Seattle, WA

TP 075 An Integrated Workflow for Analysis of Proteins and Protein Complexes based on Cross-Linking/Mass Spectrometry with an MS/MS Cleavable Cross-linker; Christian Art1; Michael Goetze1; Christian Ihling1; Christoph Hage1; Mathias Schaefer2; Andrea Sinz2; 1Martin-Luther-Universität, Halle-Wittenberg, Germany; 2Universität zu Köln, Greinestrasse, Germany

DATA INDEPENDENT ACQUISITION (SWATH)

TP 076 Large-scale Quantitative Measurements of Rat Brain Hippocampus Membrane Proteome in Prolonged Simulated Microgravity Model by 2D-SWATH® Mass Spectrometry; Peibin Qin1; Yun Wang2; Lihai Guo; Yongqian Zhang1; Wenhai Jin2; Yulin Deng3; 1Shanghai AB Sciex Analytical Instrument Trading Co., Ltd., China, Beijing, China; 2School of Life Science, Beijing Institute of Technology, China, Beijing, China

TP 077 An Novel Alignment Strategy for SWATH-MS to Generate Comprehensive Proteomics Data Matrices; Hannes Luc Rößl1; 1Yansheng Liu; Giuseppe D’Agostino1; Matteo Zanella1; Pedro Navarro1; George Rosenberger1; Ben Collins1; Ludovic Gillet1; Giuseppe Testa1; Lars Malmström1; Ruedi Aebersold1; 1ETH Zurich, Zürich, Switzerland; 2Stanford University School of Medicine, Palo Alto CA; 3Department of Experimental Oncology, European Institute of Oncology (Istituto di Ricovero e Cura a Carattere Scientifico, IRCCS), Milan, Italy; 4Institute for Immunology, University Medical Center of the Johannes Gutenberg University Mainz, Mainz, Germany
TP 078 Assessing Proteome Organization by Native SEC Coupled to SWATH-MS; Moritz Heused1; George Rosenberger1; Robin Hafen1; Ben C. Collins1; Matthias Gstaiger1; Ruedi Aebersold2;2 Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; 3Faculty of Science, University of Zurich, Zurich, Switzerland

TP 079 Understanding the Square-Wave Nature of Q1 Ion Formation for Data Independent SWATH® Acquisition; Randy J. Arnold1; Leroi Desouza2; Christie Hunter2; Patrick Pribil2;3 SCIEX, Concord ON, Canada; 3SCIEX, Redwood City, CA

TP 080 Extending the Depth of Coverage in SWATH® Acquisition with Deeper Ion Libraries; Joerg Doleah1; Nick Monnca2; Christie Hunter2;3 SCIEX, Darmstadt, Germany; 2SCIEX, Warrington, UK; 3SCIEX, Redwood City, CA

TP 081 The Use of Smaller Q1 Ion Formation Windows Improves Reproducibility in SWATH Based Protein Quantification Even at Higher Spectral Acquisition Rate; Dipankar Malak1; Faraz Rashid1; Manoj Pillai1;3 SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India

TP 082 Identification and Quantitation of Glycopeptides by SWATH Acquisition; Chi-Hung Lin1; Christoph Krepis1; Mark Molloy1;2 Macquarie University, Sydney, Australia; 2Australian Proteome Analysis Facility, Sydney, Australia; 3Australian Proteome Analysis Facility, Sydney, Australia

TP 083 Using Scanning SWATH Windows to Improve both Quantitative and Qualitative Data over Conventional SWATH and IDA Methodologies; Nic Bloomfield1; Michael Murphy1; Gordana Ivosev2; Stephen Tate1; 3SCIEX, Concord ON, Canada

TP 084 Glycopeptide SWATH Analysis – a Workflow for Quantification of Glycopeptides in Complex Samples; Miloslav Sanda1;2; Nathan Edwards3; Radoslav Goldman1;3 Georgetown University, Lombardi Cancer Center Washington, DC; 2Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC

TP 085 Scrutinization of Library Building for SWATH Analysis; Katleen Van Steendam1; Elisabeth Govaert1; Maarten Dhaenens1; Liesbeth Vossaert1; Dieter Deforce1; Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, BELGIUM

TP 086 SWATH-MS Proteomics and Chemometrics to Study the Cardiovascular Disease; Marcello Manfredi1; Eleonora Conte2; Carmela Chiariello1; Elisa Robotti1; Elia Ranzato1; Simona Martinotti1; Eleonora Mazzucco1; Fabio Gosetti1; Annalis Castagna1; Daniela Ceccon1; Oliviero Olivieri1; Emilio Marengo1; 1ISALIT-DISIT, University of Piemonte Orientale, Alessandria, Italy; 2ISALIT, spin-off DISIT, ISALIT-DISIT, University of Piemonte Orientale, Alessandria, Italy; 3Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; 4Department of Biotechnology, University of Verona, Verona, Italy; 5Department of Biotechnology, University of Verona, Verona, Italy

TP 087 Make Love, Not War: Towards a Comprehensible Workflow for the Integrated Analysis of Transcriptomics and Proteomics Data; Katleen Van Steendam1; Elisabeth Govaert1; Liesbeth Vossaert1; Maarten Dhaenens1; Filip Van Nieuwerburgh1; Laura De Clerck1; Dieter De Coninck1; Dieter Deforce1; Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, BELGIUM

TP 088 Single Shot Deep DIA Methods with Optimal Coverage, Reproducibility and Quantification Precision; Roland Bruderer2; David Gomez-Valera1; Oliver M Bernhardt1; Tejas P Gandhi1; Lukas Reiter1; 1Biogynos AG, Schlieren, Switzerland; 2Max Planck Institute for Biophysical Chemistry, Goettingen, Germany

TP 089 Accelerating Data Independent Acquisition with Microflow Chromatography; Christie Hunter3; Nick Monroe1; 1SCIEX, Redwood City, CA; 3SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK

TP 090 Proteome-wide Turnover Analysis Quantifies Genetic Impact in Down Syndrome; Yansheng Liu1; Christelle Borel1; Li Li1; Torsten Mueller1; Paul Boersema1; Pierre-Luc Germain1; Giuseppe Testa2; Andreas Beyer3; Stylianos Antonarakis1; Ruedi Aebersold;1 Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; 2Department of Genetic Medicine and Development, University of Geneva Medical School, and University Hospitals of Geneva, Geneva, Switzerland; 3University of Cologne, Cologne, Germany; 4Institute of Biochemistry, Department of Biology, ETH Zurich, Zurich, Switzerland; 5Department of Experimental Oncology, European Institute of Oncology, Milan, Italy

TP 091 Rapid Ion Mobility Deconvolution for High-throughput Analysis of Structural Isomers; Michael E Pettit1; Matthew R Brantley1; Touradj Solouki1; 1 Baylor University, Waco, TX

TP 092 Phospholipid Analysis Utilising a Novel, Data Independent, Mode of Acquisition on a QToF Instrument with a Scanning Quadrupole Mass Filter; Jayne Kirk1; Steven La1; Jason Wildgoose1; Keith Richardson1; Martin Green1; Paul Doorbar1; Witold Niklewski1; Kirsten Craven1; Mark Wrona1; Waters Corporation, Waltham, MA; 2Waters Corporation, Milford, MA

TP 093 MS1 Based Quantification Optimization on DIA Methods on a Quadrupole-Orbitrap Mass Spectrometer; Roland Bruderer1; Yue Xuan1; Oliver M Bernhardt1; Tejas Gandhi1; Thomas Moehring1; Lukas Reiter1; 1Biogynosy AG, Schlieren, Switzerland; 2Thermo Fisher Scientific, Bremen, DE

TP 094 Data-independent Acquisition Mass Spectrometry-Based Proteomics of Thyroid Cancer Allows Comprehensive Identification of Malignancy-Associated Changes; Juan Martinez-Aguilar1;2; Roderick Clifton-Bligh1; Mark Molloy1;3 National Autonomous University of Mexico, Mexico city, MEXICO; 2Macquarie University, Sydney, Australia; 3Kolling Institute of Medical Research, Sydney, Australia; 4Australian Proteome Analysis Facility, Sydney, Australia

TP 095 Touch Paper Spray Ambient Mass Spectrometry for Paper-based Immunoassays: Towards On-demand Diagnosis; Sungming Chen1; Qiongqiong Wan1; Abraham Kwarne Badu-Tawiah1; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

TP 096 Real Time and Accelerated Stability Studies of Testosterone Calibrators; Linda Nagara1; Ravi Oungury1; Isil Dilek1; Uma Sreenivasan1; 1Cerilliant Corporation, Round Rock, TX

TP 097 Automated Sample Preparation of Whole Blood for Therapeutic Drug Monitoring and Diagnostics by LC-MS using a Commercial Autosampler; Guenther Boehm1; Christian Berchtold1; Götz Schlotterbeck2; Reto Bolliger2; 1CTC Analytics AG, Zwingen, Switzerland; 2Department of Genetic Medicine and Development, University of Geneva Medical School, and University Hospitals of Geneva, Geneva, Switzerland; 3Waters Corporation, Waltham, MA; 4Waters Corporation, Milford, MA

TP 098 Pharmacotherapy Monitoring and Clinical Diagnosis of Patients with APRT Deficiency Utilizing UPLC-MS/MS Assay; Unnur Anna Thorsteinsson1;2; Finnur Freyr Eiriksson1;2; 1Hafnarhildur Runolfsdottir1; Vidar Edvardsson1; Runolfur Palsson2;3; Margret Thorsteinsson4;2 University of Iceland, Reykjavik, Iceland; 2ArcticMass, Reykjavik, Iceland; 3The National University Hospital of Iceland, Reykjavik, Iceland

TP 099 DIAGNOSTIC CLINICAL CHEMISTRY (GENERAL) 096 - 112

TP 100 Touch Paper Spray Ambient Mass Spectrometry for Paper-based Immunoassays: Towards On-demand Diagnosis; Sungming Chen1; Qiongqiong Wan1; Abraham Kwarne Badu-Tawiah1; Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

TP 101 Automated Sample Preparation of Whole Blood for Therapeutic Drug Monitoring and Diagnostics by LC-MS using a Commercial Autosampler; Guenter Boehm1; Christian Berchtold1; Götz Schlotterbeck2; Reto Bolliger2; 1CTC Analytics AG, Zwingen, Switzerland; 2Department of Genetic Medicine and Development, University of Geneva Medical School, and University Hospitals of Geneva, Geneva, Switzerland; 3Waters Corporation, Waltham, MA; 4Waters Corporation, Milford, MA

TP 102 Pharmacotherapy Monitoring and Clinical Diagnosis of Patients with APRT Deficiency Utilizing UPLC-MS/MS Assay; Unnur Anna Thorsteinsson1;2; Finnur Freyr Eiriksson1;2; 1Hafnarhildur Runolfsdottir1; Vidar Edvardsson1; Runolfur Palsson2;3; Margret Thorsteinsson4;2 University of Iceland, Reykjavik, Iceland; 2ArcticMass, Reykjavik, Iceland; 3The National University Hospital of Iceland, Reykjavik, Iceland
General Information

TP 101

Breath and Exhaled Breath Condensate Analyses for Disease Diagnosis and Monitoring of Newborns by Mass Spectrometry; Vladimir Frankевич; Vitaly Chagovets; Natalia Starodubtseva; Alexey Kononikhin; Anna Bugrova; Andrey Ryndin; Oleg Ionov; Gennady Sukhikh; Federal State Budget Institution "Research Center for Obstetrics, Gynecology and Perinatology" Ministry of Healthcare of the Russian Federation, Moscow, RUSSIA

TP 102

Using Mass Spectrometry to Identify IgG Fc and Fab Fragments Produced by Plasmin in Patient Serum; David Barnidge1; David Murray1; 1Mayo Clinic / DLMP, Rochester, MN

TP 103

Analysis of Sweat Volatiles using Solid Phase Microextraction in Conjunction with Gas Chromatography – Mass Spectrometry; Courtney Weston1; Changling Qiu1; Kevin A. Schug1; The University of Texas, Arlington, TX

TP 104

Exploratory Study of NQO1 Expression in Advanced Solid Tumors; Yuan Tian1; Fabiola Cecchi1; WEI-LI Liao1; David E. Gerber2; David A. Boothman3; William Hoos3; Todd Hembrough1; Nantomics, Rockville, MD; 2University of Texas Southwestern Medical Center, Dallas, TX; 3NQ Oncology, INC, Chapel Hill, NC

TP 105

Quantification of MET by mass spectrometry for status assessment in prescreening of tumors for targeted therapies; Kerry Scott1; Fabiola Cecchi2; Paolo Nuñolof3; Wei-Li Liao1; OncoPlex/NantOncins, Rockville, MD; 2Vall d’Hebron Institute of Oncology, Barcelona, Spain

TP 106

Approach to Implementing LC-MS/MS Plasma Metanephrines : Calibrators, Sample Prep, Workflow; Wai-Yoong Ng1; Jin Shya Yap2; Janelle SJ Chin3; Chin Pin Yeo4; 1Singapore General Hospital, Singapore; 2Singapore General Hospital, Singapore; 3Singapore General Hospital, Singapore

TP 107

Identifications of Candidate Breast Cancer-Specific Biomarkers in Fresh Frozen Breast Tissue Sections by the MALDI-imaging Coupled with On-tissue Digestion; Toyofumi Nakaniishi; Osaka Medical College, Takatsuki, Japan

TP 108

Accurate Diagnosis for Prostate Cancer by Measuring the Ratio between Two Types of Prostate Specific Antigens by LDI-TOF MS; Minyong Yoo1; Konkuk University, Seoul, South Korea

TP 109

LDTD-MS/MS Method for Quantitative Analysis of Four Immunosuppressant Drugs in Whole Blood and Cost Analysis Comparison to LC-MS/MS; Stephen D, Mergen1; Matthew Lawson2; Serge Auger3; Kamisha L Johnson-Paine4; 1ACUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; 2Utah Public Health Laboratory, Salt Lake City, UT; 3Phytronix Technologies, Quebec, QC; 4University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT

TP 110

Dried Blood Spots, Water-soluble Material and LC-MS based Protein Analysis; Cecilie Rosting1; Trine Granhaug Halvorsen1; Astrid Gjeletad1; Christine Østvik Sæ1; 1Department of Molecular Medicine, Kobe University Graduate School of Medicine, Kobe, Japan; 2Division of Diabetes and Endocrinology, Kobe University Graduate School of Medicine, Kobe, Japan; 3Shimadzu Corporation, Kyoto, Japan

TP 111

The Impact of the Antigen-Antibody Interaction on the Tryptic Digestion in Immunocapture Based LC-MS/ MS; Maren Christin Stillesby Levenæs1; Trine Granhaug Halvorsen1; Léon Reubsaet1; Marianne Nordlund Broughton1; 1School of Pharmacy, University of Oslo, Oslo, Norway; 2Radiumhospitalet, Oslo University Hospital, Oslo, Norway

TP 112

Analyte Sequencing Transport Particle Chromatography As A Front-End to Mass Spectrometry; Fred Regnier1; ZhiYu Li2; JinHee Kim3; 1Purdue University / Noviltycarm, IN; 2Noviltyc, West Lafayette, IN

TP 113

Evaluation of the Pharmacokinetics of a Novel Anti-Diabetic Agent using Conventional LC/MS/MS; Kenji Sugawara1; 1Northide Yokoi2; Ritsuko Hoshikawa3; Toshiya Matusbara3; Susumu Seino4; 1Division of Molecular and Metabolic Medicine, Kobe University Graduate School of Medicine, Kobe, Japan; 2Division of Diabetes and Endocrinology, Kobe University Graduate School of Medicine, Kobe, Japan; 3Shimadzu Corporation, Kyoto, Japan

TP 114

Quantification of Bindings of Organometallic Ruthenium Complexes to Protein Thyios by Mass Spectrometry; Yumiao Han1; 2Yu Lin2; Fuxi Wang3; 1Institute of Chemistry Chinese Academy of Sciences, Beijing, China; 2University of Pennsylvania, Philadelphia, PA; 3Rochester, MN

TP 115

Proteome-wide drug dose response of prostate cancer cell lines exposed to androgen receptor antagonists by microflow-LC SWATH MS analysis; Ludovic Gillet1; Sabine Amon1; Yasuo Uchida1; Nick Morrice2; Christie Hunter2; Ruedi Aebersold3; 1ETH Zurich, Zurich, Switzerland; 2SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA 11 RX; 3SCIEX, Redwood City, CA; 4University of Zurich, Zurich, Switzerland

TP 116

Peptide Metabolism: Identification of Metabolite Structures of GLP-1 Receptor Agonists in Different in vitro Systems Using High Resolution Mass Spectrometry; Andreas Brink1; Alessandra Piranha1; 1Thermo Fisher Scientific, San Jose, CA; 2Yies Siegrist2; Ayun Ekcler3; Nicola Thum1; Fabien Fontaine1; Ismael Zamora4; Marcel Gubler1; Silke Simon1; Nicola Kratchovil2; Simone Schadt2; 1Drug Disposition & Safety, Pharmaceutical Sciences, Pharma Research and Early Development, Roche Innovation Center Basel F. Hoffmann-La Roche Ltd., Basel, Switzerland; 2Royal Melbourne Institute of Technology, Melbourne, Australia; 3School of Life Sciences, University of Applied Sciences and Arts Northwestern Switzerland, Basel, Switzerland; 4Lead Molecular Design, Sant Cugat de Valles, Spain

TP 117

Case Study of Stable-Isotopic Dilution for Accurate Mass Spectrometric Pharmaketic Quantitation of a Small Intact Protein from in vivo Samples; Phillip Chu1; Xinxin Gao1; Susan Crowell1; Leslie Dickmann1; Rami Hannoush1; Yichin Liu1; John Tran2; 1Genentech Inc, South San Francisco, CA

TP 118

Metabolite Profiling and Covalent Binding of TAK-875 in Human Hepatocytes or Mitochondria; Wony W Lam1; Yong Gong1; Rhys Salter1; Mark R Player2; David C Evans1; 1Janssen Research and Development, Spring House, PA

TP 119

High Resolution Accurate Mass Quantitation of Iloperidone and the Hydroxyl Iloperidone Metabolite using Full Scan and Selected Ion Monitoring Modes; David Brant1; Keeley Murphy2; Jonathan L. Josephs3; Maciej P Bromirski4; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Bremen, DE

TP 120

Mechanism and Dynamics of SAMT Analog Inactivation of HIV-1 Gag Polyprotein; Lisa M. Miller Jenkins1; Elliott L Paine1; Kara M. George Rosenker2; Harichandra D Tagad1; Michael T Scerba1; Lilat Deshmukh2; Daniel H Appella1; 1National Cancer Institute, NIH Bethesda, MD; 2National Institute of Diabetes and Digestive and Kidney Diseases, NIH, Bethesda, MD
TP 123 A Strategy for the Discovery and Identification of New Natural Product Metabolites by Orbitrap Mass Spectrometer and Multiple Data-Mining Approaches; Chen Li1; Ying Liu1; Jiayu Zhang2; Siyi Liu1; Wei Cai3; Jianqi Lu4; 1Thermo Fisher Scientific, Shanghai, China; 2Center of Scientific Experiment, Beijing University of Chinese Medicine, Beijing, China; 3Hunan University of Medicine, Huaizhou, China

TP 134 Peptide Screening using Laser Desorption Ionization Mass Spectrometry on Fluorinated Nanopost Array (NAPA) Devices; Trust Rasumoglu1; Nicholas Gill1; Michael N. S. Morris1; Heather Anderson2; Matthew J. Powell2; Marvin YU2; 1Protea Biosciences, Morgantown, WV; 2Protea Biosciences, Inc. Morgantown, WV; 3MS2 Array LLC, Pittsburgh, PA

TP 124 In vitro Hepatic Metabolism of Licocchalcone A, a Chalcone from the Licorice species Glycyrrhiza inflata.; Lingyi Huang1; Dejan Nikolic1; Richard B. van Breemen1; Chittiboyina2; Ikhlas A. Khan2; Larry A. Walker2; Daojing White1; Richard B van Breemen1; Concord, ON; 1Protea Biosciences, Concord, ON, Canada; 2SCIEX, Concord, ON, Canada

TP 125 Efficient and Cost-Effective In Vitro Permeability and Transport Assays Using the CACO-2 Well Kit Assay and DiscoveryQuant 3.0.; Jeffrey Clarke1; Katherine Andersen1; Samuel Sperry1; 1EFECTOR Therapeutics, San Diego, CA - California

TP 126 Effects of Intestinal Microbiota on the Bioavailability of Aspirin in Rats.; In Sook Kim; Shaheed Ur Rehman; Min Sun Choi; Jong Suk Park; Hyun Kim; Young Seok Ji; Hyeong Jun Kim; So Yeong Yun; Hanyang University, Ansan-si, Gyeonggi-do

TP 127 A Validated Method for Anatabine Quantification in Human Plasma using High Resolution Parallel Reaction Monitoring Coupled with Chip-Based Nanospray; Jon M Reed1, 2; Prashanthan Vallabhaneni2; Rosa Ajoy3; Gogce Kan1; Pan Mao1; Bharathi Avula1; Zulfiqar Ali1; Amar G. Chittiboyina1; Ikhlas A. Khan2; Larry A. Walker2; Daojing White1; Richard B van Breemen1; Concord, ON; 1Protea Biosciences, Concord, ON, Canada; 2SCIEX, Concord, ON, Canada

TP 128 A Multiplex Assay for Direct Analysis of Natural Products in Crude Botanical Extracts; Guanchen Gu1; Pan Mao1; Bharathi Avula1; Zulfiqar Ali1; Amar G. Chittiboyina1; Ikhlas A. Khan2; Larry A. Walker2; Daojing Wang1; 1Newomics Inc., Emeryville, CA; 2National Center for Natural Products Research, School of Pharmacy, The University of Mississippi, University, MS

TP 129 Recent Experience on LC-MS/MS Determination of ADC-like Drug Candidates and Corresponding Cytotoxic Agent in Biological Matrices; Xiongfeng Wu1; Weimin Hu1; Weiqun Cao1; Yi Tao2; Xinping Fang1; Xin Zhang1; 1WuXi AppTec Co., Shanghai, China

TP 130 Development of an Automated High Throughput PAMPA Experiment for Permeability Assessment of Small Molecules and Peptides; Xu Wang1; Bernard K Choi1; Hui Wan2; Chen Shiyong2; Bahana Habuliahz2; Gino M. Salturo2; Lucinda Cohen2; 1Merck & Co., Rahway, NJ; 2Merck, Dormstadt, Germany

TP 131 Emerging Bioanalytical Tool to Characterize Drug and Drug-products of Biotherapeutics; Jinal Patel1; Mark Cancilla1; Xiang Yu1; Alina Dindyal-Popescu1; Gordon Payne1; 1Eva Duchoslav2; Suma Ramagiri2; 1SCIEX, Concord, ON; 2Merck & Co., Inc., West Point, PA; 3SCIEX, Concord, ON; 4SCIEX, Concord ON, Canada

TP 133 Development of a Magnetic Micro bead Affinity Selection Screening with UHPLC-MS/MS for the Vitamin D Receptor; Daniel Nosál1; Michael D Rush1; Jerry J White1; Richard B van Breemen1; 1University of Illinois College of Pharmacy, Chicago, IL

TP 122 Implementation of Mass Spectrometry Ligand Binding (MS bind) Assays to Rapidly Identify Molecules for Radioligand Development for New Drug Targets; Nathan G Hatcher1; Rose B Flick1; James W Monahan2; Gary E Adamson3; Nanyan Rena Zhang2; Charles M Harrell2; Victor N Uebele2; 1Merck & Co., Inc., West Point, PA

TP 132 Further Efforts towards Accurately Determining Unbound Fractions for Highly Plasma Protein Bound Compounds by LC-MS; Inhou Chu; Merck & Co., Kenilworth, NJ

TP 121 Development of a Magnetic Micro bead Affinity Selection Screening with UHPLC-MS/MS for the Vitamin D Receptor; Daniel Nosál1; Michael D Rush1; Jerry J White1; Richard B van Breemen1; 1University of Illinois College of Pharmacy, Chicago, IL

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TP 129 Recent Experience on LC-MS/MS Determination of ADC-like Drug Candidates and Corresponding Cytotoxic Agent in Biological Matrices; Xiongfeng Wu1; Weimin Hu1; Weiqun Cao1; Yi Tao2; Xinping Fang1; Xin Zhang1; 1WuXi AppTec Co., Shanghai, China

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TP 131 Emerging Bioanalytical Tool to Characterize Drug and Drug-products of Biotherapeutics; Jinal Patel1; Mark Cancilla1; Xiang Yu1; Alina Dindyal-Popescu1; Gordon Payne1; 1Eva Duchoslav2; Suma Ramagiri2; 1SCIEX, Concord, ON; 2Merck & Co., Inc., West Point, PA; 3SCIEX, Concord, ON; 4SCIEX, Concord ON, Canada

TP 132 Improved Data-Independent Workflow Strategies for Small Molecule Identification Using a High Resolution Q-TOF Mass Spectrometer; Alina Dindyal-Popescu1; Keith Goodman2; Eva Duchoslav2; Suma Ramagiri2; 1SCIEX, Concord, ON; 4SCIEX, Concord ON, Canada; 2SCIEX, Concord ON, Canada

TP 133 A Strategy for the Discovery and Identification of New Natural Product Metabolites by Orbitrap Mass Spectrometer and Multiple Data-Mining Approaches; Chen Li1; Ying Liu1; Jiayu Zhang2; Siyi Liu1; Wei Cai3; Jianqi Lu4; 1Thermo Fisher Scientific, Shanghai, China; 2Center of Scientific Experiment, Beijing University of Chinese Medicine, Beijing, China; 3Hunan University of Medicine, Huaizhou, China

TP 134 Peptide Screening using Laser Desorption Ionization Mass Spectrometry on Fluorinated Nanopost Array (NAPA) Devices; Trust Rasumoglu1; Nicholas Gill1; Michael N. S. Morris1; Heather Anderson2; Matthew J. Powell2; Marvin YU2; 1Protea Biosciences, Morgantown, WV; 2Protea Biosciences, Inc. Morgantown, WV; 3MS2 Array LLC, Pittsburgh, PA

TP 124 In vitro Hepatic Metabolism of Licocchalcone A, a Chalcone from the Licorice species Glycyrrhiza inflata.; Lingyi Huang1; Dejan Nikolic1; Richard B. van Breemen1; Chittiboyina2; Ikhlas A. Khan2; Larry A. Walker2; Daojing White1; Richard B van Breemen1; Concord, ON; 1Protea Biosciences, Concord, ON, Canada; 2SCIEX, Concord, ON, Canada

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TP 126 Effects of Intestinal Microbiota on the Bioavailability of Aspirin in Rats.; In Sook Kim; Shaheed Ur Rehman; Min Sun Choi; Jong Suk Park; Hyun Kim; Young Seok Ji; Hyeong Jun Kim; So Yeong Yun; Hanyang University, Ansan-si, Gyeonggi-do

TP 127 A Validated Method for Anatabine Quantification in Human Plasma using High Resolution Parallel Reaction Monitoring Coupled with Chip-Based Nanospray; Jon M Reed1, 2; Prashanthan Vallabhaneni2; Rosa Ajoy3; Gogce Kan1; Pan Mao1; Bharathi Avula1; Zulfiqar Ali1; Amar G. Chittiboyina1; Ikhlas A. Khan2; Larry A. Walker2; Daojing White1; Richard B van Breemen1; Concord, ON; 1Protea Biosciences, Concord, ON, Canada; 2SCIEX, Concord, ON, Canada
TUESDAY POSTERS

ENERGY: HYDROCARBON AND PETROCHEMICAL (HI RESOLUTION & NOMINAL) 145 - 163

TP 144 Development of a High-throughput Metabolic Soft Spot Assay with Integrated Assessment of Glutathione Adduct Formation; Anthony Paiva; Wilson Shou; Cheryl Klakouski; Tatjana Zvyaga; Benjamin Johnson; Yue-Zhong Shu; Ismael Zamora; Bristol-Myers Squibb Company, Wallingford, CT; Bristol-Myers Squibb Company, Lawrenceville, NJ; Lead Molecular Design S.L., Sant Cugat de Valles, Spain

TP 145 Photoionization as a Soft Ionization Source for Comprehensive Two-dimensional GC (GCxGC) and High-Resolution TOFMS; Masaaki Ubukata; A. John Dane; Robert B. Cody; Toshiyuki Kato; Masahiro Ito; Sebastian Wohlfahrt; Michael Fischer; Thomas Denner; Joe Binkley; Jonathan D. Byer; David E Alonso; Lorne E Fell; LECO Corporation, Saint Joseph, MI; JEOL USA, Inc., Peabody, MA; JEOL Ltd., Akishima, Japan; JEOL Europe B. V., Zaventem, Belgium; JEOL Europe SAS, Crossy-Sur-Seine, France; University of Liège, Liège, Belgium

TP 146 Investigation of the Partial Oxidation of Propane using a jet-Stirred Reactor and Molecular-Beam Mass Spectrometry; Dennis Kaczmarski; Patrick Oßwald; Dominik Krüger; Markus Köhler; Tina Kasper; University of Duisburg-Essen, Duisburg, Germany; Institute of Combustion Technology, German Aerospace Center, Stuttgart, Germany

TP 147 Changing the Paradigm in Petrolemics with Comprehensive Two-Dimensional Gas Chromatography–High Resolution Mass Spectrometry; Joe Binkley; Jonathan D Byer; David E Alonso; Lorne Fell; LECO Corporation, Saint Joseph, MI

TP 148 Analysis of Petroleum Products using Comprehensive Two-Dimensional Gas Chromatography (GCxGC) with Both Time of Flight MS and Flame Ionization Detectors; Christina Kelly; Joseph E Binkley; Lorne E Fell; Jonathan D Byer; David E Alonso; LECO Corporation, Saint Joseph, MI

TP 149 A New Method for Characterizing Heavy Petrochemical Fractions Based on Thermal Analysis and Laser Photoionization Mass Spectrometry; Ralf Zimmermann; Anne Ulbrich; Thorsten Streibel; Mohammad Saraji-Bozorgzad; Sebastian Wohlfihr; Michael Fischer; Thomas Denner; Christoph Grimm; University of Rostock, Rostock; University of Rostock, Rostock, N/A; University of Rostock, Rostock, Germany; Photonion GmbH, Schwerin, Germany; Netzsch Gerätebau GmbH, Selb, Germany

TP 150 Identification of the Byproducts in the Preparation of 2,6-naphthalenedicarboxylic Acid by UPLC-QTOF MS/MS; Jiwen Li; Liyan Jiang; Junyan Liu; Chuan Wang; SINOPEC SRIPT, Shanghai, Shanghai; SINOPEC Shanghai Research Institute of Petrochemical, Shanghai, China

TP 151 High Performance Thin Layer Chromatography (HPTLC) Coupled with DESI-Ion Mobility-Mass Spectrometry: A Novel Approach for Petroleum Characterisation; Eleanor Riches; Caroline Mangote; Delphine Thuault; Pierre Giusti; Carlos Afonso; Peter Hancock; Waters Corporation, Wilmington, United Kingdom; TOTAL Refining and Chemicals, Total Research & Technology Gonfreville, F-76700 Harfleur, France; Normandie Univ, COBRA, UMR6014 and FR3038,Université de Rouen; INSa de Rouen; CNRS, IRCOF, Rouen, France

TP 152 Intrinsic Ion Mobility Peak Width as an Indicator of Isomeric Species Distribution in Petroleum using Ion Mobility - Mass Spectrometry; Mathilde Farenq; Eleanor Riches; Carlos Afonso; Pierre Giusti; TOTAL Refining and Chemicals, TRYG Gonfreville l'Orcher, France; Normandie Univ, CNRS UMR 6014 COBRA Mont St Aignan, France; TOTAL RC - CNRS Joint Laboratory C2MC: Complex Matrices Molecular Characterization, France; Waters, Wilmslow, United Kingdom

TP 153 Petroleomics by Atmospheric Solid Analysis Probe Mass Spectrometry (ASAP-MS); Lilian Teese; Michael Murguia; Boniek Gontijo Vaz; Wanderson Romão; UFES, Vitória, Brazil; waters Corporation, São Paulo, BRAZIL; UFG, Goiânia, Brazil

TP 154 Application of Paper Spray Ionization Mass Spectrometry for the Analysis of Weathered Oil; Dongshui Kim; Purun Kim; Joon Geon An; Un Hyuk Yim; Sangwon Cha; Sunghwan Kim; Kyungpook National University, Daegu, Republic of Korea; Hankuk Univ. Foreign Studies, Yongin, South Korea; Korea Institute of Ocean Science and Technology, Geoje, South Korea

TP 155 UnisprayTM Ion Source Coupled to UHP-SFC for the Detection of Oilfield Additives; Etstathios Andreas Elia; William Durnie; Ed Sarke; John G Langley; Chemistry, University of Southampton, Southampton, United Kingdom; BP Exploration, Sunbury-on-Thames, Middlesex, United Kingdom; Waters, Wilmslow, United Kingdom

TP 156 Insights into Iron Promoted Sugar Conversion to 5-Hydroxymethylfurfural (HMF) and Levulinic Acid (LA) From Tandem Mass Spectrometry; Yuan Jiang; Linan Yang; Christine M Bohn; Guannan Li; Dong Han; Nathan S Mosier; Jeffrey T Miller; Hilkka I Kenttämäa; Mahdi M Abu-Omar; Purdue University, West Lafayette, IN

TP 157 Untargeted Metabolomic Approach for the Management of Microbiologically Influenced Corrosion in the Oil and Gas Industry; Vincent Bonifay; Iwona B Beech; Jan A Sunner; University of Oklahoma, Norman, OK

TP 158 A Fast Mass Spectrometric Approach for the Characterization of Aromatic Compounds Present in Crude oil; Ravikiran Yerabolu; Raghavendra Kotha; Xueming Dong; John Kong; Bryan Clayton; Hilkka Kenttämäa; Purdue University-Department of Chemistry, West Lafayette, IN; Pioneer Oil Company, Lawrenceville, IL

TP 159 GC-MS and SFC-MS Approaches for the Low- level Detection and Quantification of a New Fuel Marker; John G Langley; Julie M Hermiman; Edward M. J. Wilmut; Anastasia C. M. Carter; Jim Barker; University of Southampton, Southampton, United Kingdom; Innospec Inc., Ellersmere Port, United Kingdom; Energy Institute, London, United Kingdom

TP 160 Comparison of GC-MS, GC-UV, and Comprehensive Two-Dimensional GC for the Characterization and Source Identification of Diesel Fuels; Ling Bai; University of Texas at Arlington, Arlington, Texas

TP 161 Using GC/MSD with High Efficiency Source and Hydrogen Cleaning to Detect Low Level Contaminants in Ethylene and Propylene; Angela Henry; Bruce Quimby; Badr Astiphan; Agilent Technologies, Little Falls, DE; Agilent Technologies, Santa Clara, CA

TP 162 Can Elusive Structural Features of Heavy Crude Oil Components be Decoded from FT-ICR-MS Data?; Cristian Blanco-Tirado; Marianne Y Combariza; Cristian Alejandro Blanco-Combariza; Universidad Industrial de Santander, Bucaramanga, Santander; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

TP 163 Highly Specific Biomarker Determination in Biodegraded Petroleum with Gas Chromatography and Triple Quadrupole Detection using Multiple Reaction Monitoring; Andrés González; Taylor Motta; Ivama Calles; Sánchez Carlos; Jairo René Martínez; Shasthenko Elena; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia
TP 164 Rapid Exploration of the Mechanism of Action of Forskolin via Untargeted Proteomics and Knowledge-based Pathway Analysis; Ziad Sahab1; Bindesh Shrestha2; Lida Parvin1; Peter Nemes1; Akos Vertes1; John Vukovic1; Adam Ladak1; Waters, Milford, MA; *MTM Research Centre, Örebro University Örebro, Sweden

TP 165 Determination of Aqueous Film Forming Foam (AFFF) Components using a Multivariate Analysis Approach; Lauren Mullin1; Anna Karmann1; Gareth Cleland2; John Vukovic3; Idna Canton1; Adam Ladak1; Waters, Milford, MA; *MTM Research Centre, Örebro University Örebro, Sweden

TP 166 Characterization of Fa-rich Multi-element Particles by ICP TOF; Joel Kimmel1; Olga Borovinskaya1; Martin Tanner1; TOFWERK, Thun, Switzerland

TP 167 Polycyclic Aromatic Hydrocarbon and Metabolite Analysis of Soils Related to Energy Exploration by On-Line SFE/SFC-MS; Doug D. Carlton1,2; A. Paige Wicker1; Kenichiro Tanaka1; Erin McMallister1; Kevin A Schug1,3; Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; *Affiliate of the Collaborative Laboratories for Environmental Analysis and Remediation, The University of Texas at Arlington, Arlington, TX; 1Shimadzu Scientific Instruments, Inc., Columbia, MD

TP 168 Laser DesorptionSingle Particle Aerosol Mass SpectrometryforDirectAnalysis of Solid Materials; Mei Liu1; Li Xu1; Junguo Dong1; Zhengxu Huang1; Ping Cheng1; Zhen Zhou1; School of Environmental and Chemical Engineering, Shanghai University, Shanghai, China; 1Institute of Atmosphere environment security and Pollution control, Jinan University, Guangzhou, China; 2School of Environmental and Chemical Engineering, Shanghai University, Shanghai, China

TP 169 Development and Validation of a UPLC-MS/MS Method for Mono(2-ethylhexyl)phthalate, a Metabolite of Di(2-ethylhexyl)phthalate, in Rat Plasma, Amniotic Fluid, and Fetus; Melanie A. Rehder Silinski1; Brenda L. Fletcher1; Reshan A. Fernando1; Veronica G. Robinson1; Paul Foster1; Suramya Waidyanatha2; RTI International, Research Triangle Park, NC; 3RTI International, Research Triangle Park, NC; 4Division of National Toxicology Program, NIH, Research Triangle Park, NC

TP 170 An Automated Method for Microcystins Analysis using Two-dimensional Liquid Chromatography-quadrupole Time-of-Flight Mass Spectrometry (2DLC-QTOFMS); Xavier Ortiz Almira1; Marie Meyer-Month1; Eva Korenkova1; Karl Jobst1; Eric Reiner1; Karen McPherson1; Ministry of the Environment and Climate Change of Ontario, Toronto, ON; 1University of Toronto, Toronto ON, Canada

TP 171 Development of an LC-QTOF MS Method for the Non-targeted Analysis of Microcystins; Marie Meyer-Month1; Xavier Ortiz 1; Eva Korenkova1; Ralph Ruffolo1; Karl Jobst1; 2Satyendra Bhavsar1,2,4; André Simpson1; Eric Reiner1,2; 1Ontario Ministry of Environment & Climate Change, Toronto, Canada; 2University of Toronto, Toronto ON, Canada; 3McMaster University, Hamilton, Canada; 4University of Windsor, Windsor, Canada

TP 172 Determination of Trace Microcystins in Aqueous Samples by Solid-Supported Liquid Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry; Chang-Lin Hsu1; Chung-Yu Chen1; Maw-Rong Lee1; 1National Chung-Hsing University, Taichung, TAIWAN (R.O.C.); 2National Chung-Hsing University, Taichung, TAIWAN (R.O.C.)

TP 173 Effect of Analytical Standard Preparation Procedures in the Quantitation of Urinary Monohydroxy-Poly cyclic Aromatic Hydrocarbons (OH-PAHs) by Online SPE-HPLC-MS/MS; Yuesong Wang1; Mei Meng1; Eric N Pittman1; Alisha Ethedrige1; Kendra Hubbard1; Debra A Trinidad1; Xiaoyun Ye1; Antonia M. Calafat1; CDC, Atlanta, GA

TP 174 New 2,4-dinitroanisole (DNAN; Minitions Chemical) (bio)Transformation Products discovered and Bioassayed using High Resolution UPLC-QToFMS; Leif Abliff1; Christopher I. Olavres1; Jon Chorover1; Reyes Sierra-Alvarez1; Jim A. Field1; 1University of Arizona, Tucson, Arizona

TP 175 Investigation of Eicosanoids and Fatty Acids in Pansteatitis-Afflicted Mozambique Tilapia at Loskop Dam, South Africa; theresa cantu1; John Bowden2; Jack McAlhany3; Matthew Guillette4; hannes botha5; Louis J. Guillette6; 1MUSC, Charleston, SC; 2National Institute of Standards and Technology, Charleston, SC; 3college of charleston, charleston, sc; 4Medical Univ of S Carolina, Charleston, SC; 5Mpumalanga Tourism and Parks, Pretoria, South Africa

TP 176 Analysis of Problematic Cyclic Silioxane Compounds in the Atmosphere of the International Space Station; Patti Cheng1; Vanessa de Vera1; Robert Gillispie1; Steven Beck1; William Wallace2; Thomas Limer2; 1Wyle Science, Technology, and Engineering Group, Houston, TX; 2Houston, TX

TP 177 Accurate Mass Spectral Database: Harnessing the Power of High Performance Mass Spectrometry at Long Last; Lorne Feil1; Viatcheslav Artaev1; Kevin McNitt1; Steve Robles1; Albert Lebedev2; 1LECO Corporation, Saint Joseph, MI; 2Moscow State University, Moscow, Russian Federation

TP 178 A Method for Real-Time Monitoring of Acrolein in Air using TAGA Mass Spectrometry; Nicholas Karella; Ontario Ministry of the Environment, Toronto, ON

TP 179 Mass Spectrometry-based Studies on the Association of Organic Dusts and Respiratory Symptoms; Brooke Thompson1; Paulos Chumala2; Shelley Krychuk1; George S. Katseles3; CCHSA/Medicine, College of Medicine, University of Saskatchewan, Saskatoon, SK, Canada

TP 180 Monitoring Fugitive Emissions with a Miniature Ion Trap Mass Spectrometer: Preshious Rearden1; Corey Stedwell1; Parminster Kaur1; Daniel DeBord1; 11st Detect Corporation, Webster, TX

TP 181 Analytical Strategy to Investigate Naphthenic Acids in Atmospheric Aerosols by Ultrahigh-Performance Liquid Chromatography/Quadrupole Time-of-Flight Mass Spectrometry (UPLC/QTOF-MS); Mahmoud Yassine; Environment and Climate Change Canada, Ottawa, ON

TP 182 A Comparison of Thermal- and Valve-based Modulation for the Analysis of Environmental Contaminants by GCxGC-QTOF MS; Tadeusz Gorecki1; Matthew Edwards1,2; Haleigh Boswell1; Pete Grosshans1; University of Waterloo, Ontario, Canada; 1Markes International, Cardiff, UK; 2Markes International Inc, Cincinnati, OH

TP 183 High sensitive quantitation method of perfluorinated compounds by an automated online solid extraction LC/MS/MS; Yoshikane Mitsuha1; Jun Watanabe1; Kagi Noriko1; Minchata Yoshikazu1; Obara Taro1; Nakayama Shig1; 1IDEA Consultants, Inc., Yaidzu, Japan; 2Shimadzu Corporation, Kyoto, Japan; 3JASCO International Co., Ltd., Hachioji, Japan; 4Shimazu Corporation, Kyoto, Japan; 5Shimadzu Scientific Instruments, Inc. Columbia, MD; 6National Institute for Environmental Studies, Tsukuba, Japan

TP 184 A Collaborative EPA Method 625 Update Study using a New Mass Spectrometry Method for Quantification Combined with Stir-bar Sorptive Extraction; Weier Hao1; Andrew Bogess1; Edward Pfannkoch1; Skip Kingston1; 1Duquesne University, Pittsburgh, PA; 2Geretel, Inc. Linthicum, MD
TP 185 Automated Screening of Explosives in Soil Samples by Online SFE-SFC-MS; William A Hedgepeth; Kenichiro Tanaka; Taio Ogura; Jonathan Edwardsen; Shimadzu Scientific Instruments, Inc. Columbia, MD; Shimadzu Scientific Instruments, Inc. Columbia, MD

TP 186 Efficiency Screening of Carbon Nanomaterial or Superoxidant in Advanced Water Treatment by Mass Spectrometry Are They Accurate Enough?; Hugues Preud’homme; Jabier Al-Mari; Pierre Kubiak; Rachid Essellhi; QEERI - HBKU - Qatar Foundation, Doha, QATAR

TP 187 Chromatographic Mass Spectrometric Detection of Arsenic Species in Sulfidic Waters – Method Development; Denzel Bolden; Akeena Harper; Jianye Zhang; Voorhees College, Denmark, NC

TP 188 Fast Detection of Environmental Vapors by Thermal Desorption - Atmospheric Pressure Photoionization - Differential Mobility Analysis - Mass Spectrometry (TD-APPI-DMA-MS); Ross David McCulloch; Amo Gonzalez-Mario; SEADM, Boeicillo, Spain

TP 201 Model FAIMS RF System using Neural Network; Xiaojun Zou; Thermofisher Scientific, San Jose, CA

TP 202 Making FAIMS Faster, More Selective, and More Sensitive; Michael Belford; Satendra Prasad; Jean-Jacques Dunyach; Susan E Abbatiello; Ryan Hemmizen; Hoa Pham; Ann Yadiowsky; Alex Zou; Thermo Fisher Scientific, San Jose, CA

TP 203 Selection-based Detergent Interference Removal for Shotgun-Lipidomics Analyses; Cyrus Papan; Julian D Langer; Scie, Darmstadt, Hessen; Max-Planck-Institute of Biophysics, Frankfurt Am Main, Germany

TP 204 Rapid Analysis of Steroid Metabolites using Field Asymmetric Waveform Ion Mobility Spectrometry Combined with Liquid Chromatography and Mass Spectrometry; Kayleigh Louise Arthur; Matthew Arran Turner; James Christopher Reynolds; Colin Creaser; Loughborough University, Loughborough, United Kingdom

TP 189 Rapid Separation and Quantification of Hydroxyvitamin D3 Epimers by FAIMS-MS, Eliminating the Need for LC Separation for High-throughput Clinical Analysis; Lauren Brown; Danielle Toutoungi; Robert Smith; Billy Boyle; Owlsone Ltd., Cambridge, UK

TP 190 Resolution of Isotopologues and Isotopomers by High-Field Ion Mobility Coupled to Mass Spectrometry: Path to Gas-Phase NMR?; Julia Kaszynski; Matthew A. Baird; Andrew P. Bowman; Alexandre A Shvartsburg; Wichita State University, Wichita, KS

TP 191 Modeling and Characterization of the Ion Transit Time in a FAIMS-MS Interface; Satendra Prasad; Jean-Jacques Dunyach; Michael W Belford; Thermo Fisher Scientific, San Jose, CA

TP 192 On a Multi-physics Computational Model to Understand Heat Exchange between FAIMS Electrode and Ion Transport Gas; Satendra Prasad; Thermo Fisher Scientific, San Jose, CA

TP 193 Efficiency of Ion Transmission between FAIMS Electrodes without a Separation Electric Field; Satendra Prasad; Susan E Abbatiello; Michael W Belford; Jean-Jacques Dunyach; Mary L Blackbum; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Cambridge, USA

TP 194 Comparison of Rectangular Waveform FAIMS/MS to Conventional Sum-of-sines Waveform; Michael Wei; Michael Costanzo; Joaquin Casanova; Jared Boock; Richard A Yost; University of Florida, Gainesville, Florida

TP 195 Glyphosate quantified in Black Tea and Other Food Matrices by Automatically Optimized LC-FAIMS MS/MS; Bennett Kalaft; Rae Ana Snyder; Claudia Martin; Manish Doshi; Mark Hardman; Thermo Fisher Scientific, San Jose, California

TP 196 Rapid FAIMS at Extreme Fields Inside the Mass Spectrometry Envelope with Applications to Peptide and Protein Analyses; Alexandre Shvartsburg; Andrew Entwistle; Roger Giles; Wichita State University, Wichita, KS; Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom

TP 197 Is Differential Mobility Chemically Driven? Evidence and Simulations for Chemical Effects as Primary Separation Factor in DMS; Walter Wissdorf; Bradly B Schneider; Tom Covey; James Hager; Thorsten Benter; Bergische Universität Wuppertal, Wuppertal; SCIEX, Concord, ON; Bergische Universität Wuppertal, Wuppertal, Germany

TP 198 LESA FAIMS Mass Spectrometry for the Spatial Profiling of Proteins from Tissue; Rian L. Griffiths; Alex Dexter; Andrew J Creese; Alan M. Race; Josephine Bunch; Helen Cooper; University of Birmingham, Birmingham, UK; National Physical Laboratory, Teddington, UK; University of Nottingham, Nottingham, UK

TP 199 Analysis of Derivatized Glycans using Differential Mobility Spectrometry; Cathy Lane; Yves J C LeBlanc; J Larry Campbell; SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK, WA1 1RX; SCIEX, Concord, ON

TP 200 Improved Quantitative Measurements for Large Scale Proteomic Analyses using Metabolic Labeling and Ion Mobility; Sibylle Pfammatter; Eric Bonnici; Pierre Thibault; l’IRIC-Université de Montréal, Montréal, QC; Universite de de Montreal, Montreal, QC

TP 201 Improved Quantitative Measurements for Large Scale Proteomic Analyses using Metabolic Labeling and Ion Mobility; Sibylle Pfammatter; Eric Bonnici; Pierre Thibault; l’IRIC-Université de Montréal, Montréal, QC; Universite de de Montreal, Montreal, QC

TP 202 Making FAIMS Faster, More Selective, and More Sensitive; Michael Belford; Satendra Prasad; Jean-Jacques Dunyach; Susan E Abbatiello; Ryan Hemmizen; Hoa Pham; Ann Yadiowsky; Alex Zou; Thermo Fisher Scientific, San Jose, CA

TP 203 Selection-based Detergent Interference Removal for Shotgun-Lipidomics Analyses; Cyrus Papan; Julian D Langer; Scie, Darmstadt, Hessen; Max-Planck-Institute of Biophysics, Frankfurt Am Main, Germany

TP 204 Rapid Analysis of Steroid Metabolites using Field Asymmetric Waveform Ion Mobility Spectrometry Combined with Liquid Chromatography and Mass Spectrometry; Kayleigh Louise Arthur; Matthew Arran Turner; James Christopher Reynolds; Colin Creaser; Loughborough University, Loughborough, United Kingdom

TP 205 Differential Mobility Spectrometry (DMS) Reveals the Elevation of Urinary Acetylcarnitine in Non-Human Primates (NHP) Exposed to Radiation; Nicholas B. Vera; Amol Kaffe; Evan Pannukku; Evagelia C. Laiakas; A.J. Fornace, Jr.; Stephen L. Coy; Derek M Erion; Paul Vouros; Pfizer, Cambridge, MA; Northeastern University, Boston, Massachusetts; Northeastern University, Boston, MA; Georgetown University, Washington, DC

TP 206 Characterization of Variables Affecting Internal Energy Deposition inside a Differential Ion Mobility Spectrometer; Brandon Santiago; Matthew T. Campbell; Gary L. Gish; The University of North Carolina at Chapel Hill, Chapel Hill, NC

TP 207 Analysis of Free Drug in Antibody-Drug Conjugate by Reversed-phase HPLC Coupled with Differential Mobility Mass Spectrometry; Chunang (Christine) Gu; Marie-France Morissette; Loren Y Olson; Shaokun Pang; Yi Li; Colin Medley; David Russell; Genentech, South San Francisco, CA; Genentech Inc, South San Francisco, CA; SCIEX, Redwood City, CA

TP 208 Optimizing DMS Separations by Comparing Alpha Functions; Brad Schneider; Erkionin Nazarov; J C. Yves Le Blanc; Frank Londry; Thomas Covey; SCIEX, Concord ON, Canada

TP 209 Rapid Ion Trap Mass Analysis of Inorganic Water Clusters Separated by Differential Mobility Spectrometry; Theresa Evans-Nguen; Timothy Vazquez; University of South Florida, Tampa, FL

FOOD SAFETY (PESTICIDES IN FOOD) 210 - 235

TP 210 Significant Improvement in GCMS Screening of Pesticides in Scan Mode using a High Efficiency Ion Source and Spectral Deconvolution; Melissa Cherley; Bruce Quimby; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Little Falls, DE

TP 211 A Targeted Quantitative LC-MS/MS Method for 431 Positive and Negative Ion Pesticides in a Single Analysis; Louis Majiers; Zicheng Yang; Bruker Daltonics, Fremont, CA; Bruker Daltonics Inc, Fremont, CA
TP 212  GC/MS/MS Analysis of Pesticide Residues in Cannabis Using QuECHERS Extraction and Cleanup: Kathy Stenerson; Craig Aurand; David Bell; Sara Smith; Emily Barrey; Candace Price; MilliporeSigma, Bellefonte, PA

TP 213  Analysis of Pesticides in Spaghetti Sauce by Direct Immersion Solid Phase Microextraction GC/MS: Kathy Stenerson; Candace Price; Craig Aurand; Dave Bell; Emily Barrey; Sara Smith; Sigma Aldrich, Bellefonte, PA

TP 214  An Optimal Method for the Analysis of Pesticides in a Variety of Matrices: Jessica Westland; Vivian Chen; Agilent Technologies, Wilmington, Delaware; Agilent Technologies, Santa Clara, CA

TP 215  Accurately Identify and Quantify A Hundred Pesticides in a Single GC Run: Jessica Westland; Tom Doherty; Vivian Chen; Agilent Technologies, Wilmington, Delaware; Agilent Technologies, Santa Clara, CA; Agilent, Shanghai, China

TP 216  Maintaining Sensitivity and Reproducibility with the Self Cleaning Ion Source for Pesticides in Food and Feed: Vivian Chen; Jessica Westland; Elizabeth Almasi; Agilent, Shanghai, China; Agilent Technologies, Wilmington, Delaware; Agilent Technologies, Santa Clara, CA

TP 217  “No Dilute” Just Shoot LC-ESI-MS/MS: Feasibility and Robustness of a Maintenance-Free Source for Applications in Low-level Pesticide Residue Analysis: Matteo Medici; Frank A Kero; Joshua Ye; Craig Young; Sharanya Reddy; Mosti Mondiale, Villa Ste Catherine, QC; PerkinElmer, Shelton, CT; Ionics Mass Spectrometry Group, Bolton, ON

TP 218  Rapid Detection of Pesticides in Honey by C18 Pipette-tip Electrospray Ionization Mass Spectrometry: Yi-Ching Choi; Tsz-Tsun Ng; Bin Hu; Zhong-Ping Yao; Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong, China

TP 219  A Single LC-MS/MS Method for Confirmation and Quantification of over 400 Pesticides in Complex Matrix without Compromising Data Quality: Dimple Shah; Emear McCall; Gareth Cleland; Waters Corp., Milford, MA; Waters, Wilmmslow, United Kingdom; Waters Corporation, Milford, MA

TP 220  Determination of Multiple Pesticides Residues in Imported Tea in UAE Using Liquid and Gas Chromatography Tandem Mass Spectrometry: Mohammed Meetani; Sarah Ali Almulla; Nasra M. Ibrahim; United Arab Emirates University, Al-Ain, Abu Dhabi; laboratories Department, Ministry of Environment and Water, Sharjah, United Arab Emirates; chemistry Department, College of Science, UAE University, Al-Ain, United Arab Emirates

TP 221  Multi-residue Analysis of Pesticides in Agricultural Products using QuECHERS and SFC/MS: Yuka Fujito; Kenichiro Tanaka; Taizo Ogura; Kiyo Miyakawa; Yoshinori Hayakawa; Shimadzu Corporation, Kyoto, Japan; Shimadzu Scientific Instruments, Inc. Columbia

TP 222  Supercritical Fluid Chromatography/Tandem Mass Spectrometry (SFC-MS/MS) Analysis of Hundreds of Pesticide Residues in Food Safety: David Baker; Christopher Titman; Jonathan Homer; Neil Lofts; Shimadzu, Manchester, UK; SAL (Scientific Analysis Laboratories), Cambridge, UK

TP 223  Quantitative Analysis of 647 Pesticides (1,929 MRMs) by LC-MS/MS with a Fast 10.5 Minute Cycle Time: David Baker; Laetitia Fages; Eric Capodanno; Neil Lofts; Shimadzu, Manchester, UK; SAL (Scientific Analysis Laboratories), Cambridge, UK

TP 224  Food Residue Screening using Liquid Chromatography Coupled to High Resolution MS/MS (LC-HR-MS/MS) - Multi-Pesticide Identification and Quantitation: KC Hyland; Paul Winkler; Andre Schreiber; SCIEX, Redwood City, CA; AB SCIEX, Concord, ON

TP 225  Screening of Pesticides in Lipid-rich Food Matrices by using High Resolution GC/Q-TOF and Accurate Mass Pesticide Library: Kai Chen; Joan Stevens; Hong Chen; Vadim Kalmykov; Sofia Nielo; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Wilmington, DE

TP 226  Routine Quantitative and Qualitative Methodologies for Food Pesticide Residue Laboratories Using Tandem and High Resolution Accurate Mass (HRAM) LC/MS Instrumentation: Claudia Martins; Ed George; Dipankar Ghosh; Katerina Bousova; Thermo Fisher Scientific, San Jose, CA; Thermo Fisher Scientific, Dreieich, Germany

TP 227  Screening for More than 600 Pesticide Residues and Their Identification in Food Samples using a New LC/MSMS Library Data Base: Houssain El Aribi; Salah A. Almama; Mustafa A. Gassiem; Majed A. Alansari; Saudi FDA, Riyadh

TP 228  Rapid Extraction and Clean-up Kits for the Determination of Pesticide Residues in Food: Shao Kai Lin; Taichung, Taichung

TP 229  Development of Multi-Pesticides in Avocado using Enhanced Matrix Removal by liquid Chromatography-Tandem Mass Spectrometry with Dynamic MRM and Triggered MRM: Wen-Yen Lee; Jin-Lan Sun; Chun-Ye Sun; Shan-An Chan; Agilent, Taipei, Taiwan; Agilent, Shanghai, China

TP 230  Rapid Screening and Quantitation of Pesticide Residues in Cannabis by Modified QuEChERS and LC-MS-MS: Jeff Dahl; Julie Kowalski; Gordon Fagras; Shimadzu, Columbia, MD; Restek Corporation, Bellefonte, PA; Trace Analytics, Spokane, WA

TP 231  Pesticide Analysis in Complex Food Extracts by Multi-transition MRM and Library Searching for Enhanced Residue Confirmation: David Baker; Christopher Titman; Jonathan Homer; Neil Lofts; Shimadzu, Manchester, UK; SAL (Scientific Analysis Laboratories), Manchester, UK

TP 232  Fast Data Acquisition Speed and High quantitative Performance in the Simultaneous Determination of Mycotoxins, Illegal Dyes and Pesticides in Spices: Mark Sartain; Thomas Glauener; Craig Marvins; Andre Santos; Anumol Tarun; Jerry Zweigenbaum; Agilent Technologies, Santa Clara, CA; Agilent Technologies Sales & Services GmbH, Waldbronn, Germany; Agilent Technologies, Wilmington, DE; Agilent Technologies Inc, Barueri, Brazil

TP 233  Multi-Residue Pesticides Analysis by LC-MS/MS using the ODS Column and the Biphenyl Column: Natuyo Asano; David Baker; Yuki Uno; Atsuko Toyama; Jun Watanabe; Shimadzu Corporation, Kyoto, Japan; Shimadzu, Manchester, UK

TP 234  Automated Pressurized Liquid Extraction and Clean Up of Sea Food Samples in the Analysis of Persistent Organic Pollutants (POPs): Hamid Shirkhan; Rudolf Addink; Toxic Report, Watertown, MA

TP 235  Fully Automated Online Sample Extraction and Analysis of Mycotoxins in Foods by Online SFE-SFC-MS: Kenichiro Tanaka; William Hedgepeth; Taizo Ogura; Shimadzu Scientific Instruments, Inc. Columbia

FOOD ’OMICS’ MS CHARACTERIZATION OF FOOD AND NUTRITIONAL SUPPLEMENTS (PART 1) 236 - 250

TP 236  DLLME-Gas Chromatography-Quadrupole Time-Of-Flight Mass Spectrometry for Classification of Botanical Origin of Chinese Honey by Its Volatile and Semi-volatile Compound Profile: Hui Chen; Linghe Jin; Chunlin Fan; Guofang Pang; Shan Zhou; Wenwen Wang; Chinese Academy of Inspection and Quarantine, Beijing, China; Shandong Agriculture University, Tai’an, China; Agilent Technologies Company, Ltd, Beijing, China
TP 237  Discrimination of Honey of Different Botanical Origins using an Untargeted High-Definition Metabolomic Workflow; Joanne B. Connolly1; Sara Stead2; Antonietta Wallace3; Delano Turner4; 1Waters Corporation, Manchester, UK; 2Waters Corporation, Manchester, UK

TP 238  Proteomic and Peptidomic Differences and Similarities between Four Muscle Types from New Zealand Raised Angus Steers; 1Stefan Cleerans1; 2Hedil Thomas; 3Jessica Gathercole; 4Jeffrey E Flowman; 5Tzer-Yang Yu; 6Alita J Grosvener; 7Stephen R Haines; 8Peter Dobbie; 9Kevin Tauri; 10Katja Rosenvold; 11Jolon M Dyer; 12Santanu Deb-Choudhury; 13AgResearch, Lincoln, New Zealand; 14Biomolecular Interaction Centre, Christchurch, New Zealand; 15AgResearch, Ruakura, New Zealand

TP 239  The Modernisation of Fish Fraud Detection using Rapid Evaporative Ionisation Mass Spectrometry (REIMS); Connor Black1; Olivier Chevallier1; Julia Balog2; Nicolas Sommerer1; 1INRA, UMR1083 SPO, Montpellier, France; 2IFV, INRA, UMR1083 SPO, Montpellier, France

TP 240  Solid Phase Mesh Enhanced Sorption from Headspace (SPMESH) Coupled to DART-MS/MS for Quantification of Trace-level Odor-active Volatiles in Foodstuffs; Jillian Jastrzembski; Cornell University, Ithaca, New York

TP 241  Headspace Analysis of E-Cigarette Liquid Flavorings by Vacuum Thermal Desorption; Eric Knappenberger; Corey Stedwell; J. Daniel DeBord; 11st Detect, Webster, TX

TP 242  Direct Analysis of Anthocyanins (a Class of Flavonoid Pigments in Red Wine) by Characteristic Components Profiling using Discrimination of Wine Cultivars and Geographic Origins by Characteristic Components Profiling using UHPLC-ESI/QTOF-MS Combined with Chemometric Analysis; 1Nicolas Sommerer; 2Marine Lambert; 3Emmanuelle Meudec; 4Marie-Agnès Ducasse; 5Jean-Claude Boulet; 6Gérard Mazerolles; 7Gilles Masson; 8Véronique Cheynier; 9INRA, UMR1083 SPO, Montpellier, France; 10IFV, UMT QUALINNOV, Gruissan, France; 11IFV, centre du rosé, Vidauban, France

TP 243  LC/MS Metabolomic Profiling of an Amber Ale Fermented with Four Different Yeast Strains; 1Kearney M Foss; 2Karen Fortmann; 3Christine A. Hughney; 4James Madison University, Harrisonburg, VA; 5White Labs, San Diego, CA; 6James Madison University, Harrisonburg, VA

TP 244  Rapid Preparation for Quantitative Analysis of Volatile and Semi-Volatile Compounds in Scotch Using Gas Chromatography Mass Spectrometry; Yashawini Nagaranjan; 1Doug D Carlton; 2Evelyn H Wang; 3Jillian Melbourne; 4Kevin A Schug; 5Department of Chemistry and Biochemistry, UTA Arlington, tx

TP 245  Analysis of the Oligosaccharide and Protein Content of Beer Using Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry (MALDI TOFMS); Elsa Gorr; 1Ashley Phetsanthad; 2Jon Soffer; 3Kevin G Owens; 4Drexel University, Philadelphia, PA

TP 246  Cryogenic-Focusing Fast Gas Chromatography Isootope Ratio Mass Spectrometry for Anti-Doping; Herbert Tobias; 1Thomas J Brenna; 1Cornell University, Ithaca, NY

TP 247  Data Quality Control Measures for Forensic Mass Spectral Libraries; William E. Wallace; Weihua Ji; Karen W Phinney; 1National Institute of Standards & Technology, Gaithersburg, MD; 2National Institute of Standards and Technology, Gaithersburg, MD; 3Cryogenic-Focusing Fast Gas Chromatography Mass Spectrometry for Anti-Doping; Herbert Tobias; 1Insititute of Forensic Science, Ministry of Justice, Shanghai, China; 2PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China

TP 248  High-throughput LDTD-MS/MS for Quantification of GHB in Hair, Urine and Saliva; 1Institue of Forensic Science, Ministry of Justice, Shanghai, China; 2PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China

TP 249  Tracking the Ages of Latent Fingerprints using Triacylglycerols as an Age Marker; Kelly O’Neill; 1Young Jin Lee; 2Iowa State University, Ames, IA; 3Iowa State University, Ames, Iowa

TP 250  Detection and Mapping of Proteomic Blood Signatures in Fingerprints for Forensic Analysis; Lisa Deininger; 1Ekta Patel; 2Malcolm R Clench; 3Vaughn Sears; 4Chris Sammon; 5Simona Francese; 6Sheffield Hallam University, BMRC Sheffield, United Kingdom; 7Centre for Applied Science and Technology, Home Office, St Albans, United Kingdom; 8Sheffield Hallam University, MERI, Sheffield, United Kingdom

TP 251  Investigating Environmental Degradation of Trace Explosives with Thermal Desorption DART-MS; 1Edward Sisco; 2Marcela Najarro; 3Jeffrey Lawrence; 4Katherine Schilling; 5NIST, Rockville, MD; 6Defense Forensic Science Center, Gillem Enclave, GA

TP 252  Metallic Muzzle Discharge Gunshot Residue Analysis by DART-TOF-MS; 1Emily Lenner; 2Candice Bridge; 3National Center for Forensic Science, Orlando, FL

TP 253  Laser Ablation Sample Transfer with Vacuum Capture for Forensic Sampling; Fabrizio Donnarumma; 1Kermit K Murray; 2Louisiana State University, Baton Rouge, LA

TP 254  Impact of Energetic Particles on Proteinaceous Specimens; 1Christopher Rollman; 2Mehdi Moini; 3George Washington University, Washington, DC

TP 255  Rapid Screening of Methylamphetamine Hair of Drug Addicts using DSA-TOF; 1Bachua Shen; 2Xianyi Zhuo; 3Jingchao Lin; 4Chengyuan Cai; 5Lizhong Yang; 6Yongming Xie; 7Institute of Forensic Science, Ministry of Justice, Shanghai, China; 8PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China

TP 256  High-throughput DART-MS for Quantification of Triacylglycerols as an Age Marker; Kelly O’Neill; 1Young Jin Lee; 2Iowa State University, Ames, IA; 3Iowa State University, Ames, Iowa

TP 257  Tracking the Ages of Latent Fingerprints using Triacylglycerols as an Age Marker; Kelly O’Neill; 1Young Jin Lee; 2Iowa State University, Ames, IA; 3Iowa State University, Ames, Iowa
TP 263  Species Identification using Bayesian Modeling and Mass Spectrometry: Jennifer Teubl1; Heyi Yang2; Donald Siegel1; David Fenyo2; 1NYU Langone Medical Ctr, NY, NY; 2Office of Chief Med Exam, New York, NY; 3NYU Langone Medical Center, New York, NY

TP 264  Tackling the Sensitivity using an Improved Proteomics Methodology: from Cultural Heritage to Forensic Studies; Fabrice Bray1; Stephanie Devassine1; Nicolas Garnier2; Christian Rolando4; Caroline Tokarski1; 1USR CNRS 3290 MSAP, Villeneuve d’Ascq, France; 2SARL Laboratoire Nicolas Garnier, Vic le Comte, France

TP 265  In-Depth Analysis of Saliva N-glycans Found in Live Human and Corpse for the Discovery of Post-mortem Interval (PMI) Marker; Bum Jin Kim1; 2; Dong-Gi Lee3; Jong-Soon Choi1; 3; Hyun Joo An1; 3; 1GRAST, Chungnam National University, Daejeon, Republic of Korea; 2AGRS, Chungnam National University, Daejeon, Republic of Korea; 3Division of Life Science, Korea Basic Science Institute, Daejeon, Republic of Korea

TP 266  Postmortem Identification of Metabolizer Type through CYP Quantification and Polymorphism Identification; Brigitte Desharnais1; 2; Pascal Mireault1; Cameron D. Skinner1; 1Laboratoire de sciences judiciaires et de médecine légale, Montréal, QC; 2Concordia University, Montreal, Canada

TP 267  Protein Profiling of Decedent Scalp Hair Segments Exhibiting a Post-Mortem Hair Root Band; McKay B. Allred1; Brian A. Eckenrode1; Traci L. Carlson1; Jamie N. Buist1; 1National Center for Forensic Science, Orlando, FL; 2Centers for Disease Control and Prevention (CDC), Atlanta, GA; 3Centers for Disease Control and Prevention, Atlanta, GA

TP 268  Quantification of Seven Nerve Agent Compounds by ESI and APCI-MSMS; Kathleen Housman1; Jonathan Oyler1; 1USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD

TP 269  Validation of a GC/MS/MS Method for the Analysis of Chemical Warfare Agents (CWAs); Thomas Russe1; Benjamin L Oyler1; 1USAMRICD, Aberdeen Proving Ground, MD; 2U. Maryland, Baltimore, MD; 3USAMRICD, Aberdeen Proving Ground, MD

TP 270  Rapid and Unambiguous Identification of Ricin in Complex Matrices using a High Throughput, Integrated Immunoaffinity, Proteolyis and Mass Spectrometry Approach; Bao Quoc Tran1; Kathleen J. Housman1; Samir V. Deshpande2; James D. Wright2; Mary M. Wade2; Jonathan M Oyler2; Raymond F. Sullivan3; 1Science and Technology Corporation, Belcamp, MD - Maryland; 2US Army Medical Research Institute for Chemical Defense, Aberdeen Proving Ground, MD - Maryland; 3US Army Edgewood Chemical and Biological Center, Aberdeen Proving Ground, MD - Maryland

TP 271  DART-TOF-MS and ATR-FTIR Analysis of Silicone Based Personal Lubricants; Lauren Harvey1; Candice Bridge1; 1National Center for Forensic Science, Orlando, FL

TP 272  Analytical Validation of a Portable, Ambient Sampling Mass Spectrometer for High Throughput, Forensic Evidence Screening; Zachary E. Lawton1; William L Fatigante1; Jamie R Wieland1; 1University of Georgia, CCRC, Athens, GA; 2University of Georgia, CCRC Athens, GA

TP 273  Transportable GC/MS for the Rapid Detection and Identification of Suspected Drug Compounds in Field Operations; Phillip Tackett1; Mitch Wells2; 1FLIR Systems, Inc., West Lafayette, Indiana; 2FLIR Systems, Inc., West Lafayette, IN

TP 274  Detection and On-Site Presumptive Testing of a Clandestine Drug Laboratory using a Portable Mass Spectrometer; Ethan McBride1; Phillip Mach1; Kenneth C Wright3; Guido F Verbeck1; 1University of North Texas, Denton, TX; 2Infinon, Syracuse, NY

TP 275  Portable Drug Systems vs. the Daubert Standard: Anticipating the Admissibility of a New Technology for Forensic Investigation; Angelica Traub1; Zachary E. Lawton1; Jamie R. Wieland1; 1National Center for Forensic Science, Orlando, FL; 2Department of Chemistry, Illinois State University, Normal, IL; 3Department of Technology, Illinois State University, Normal, IL; 4Department of Criminal Justice Sciences, Illinois State University, Normal, IL

TP 276  Examining the Legality of using Ambient Sampling, Portable Mass Spectrometers in Criminal Justice Applications; Alessandra Bruno1; Michael C Gizzi1; Jamie R Wieland1; 1Department of Criminal Justice Sciences, Illinois State University, Normal, IL; 2Department of Criminal Justice Sciences, Illinois State University, Normal, IL; 3Department of Technology, Illinois State University, Normal, IL; 4Department of Chemistry, Illinois State University, Normal, IL

TP 277  Chiral Separation and Quantitation of Cathinone Related Drugs by Gas chromatography Mass spectrometry: Rashid Alrumaithi1; Mohammad Meetani1; Sajid Elidn Khali1; Khalid Alsumaili2; Dubai Police, Dubai, Dubai; 1United Arab Emirates University, Al Ain, United Arab Emirates.; 2Dubai Police, Dubai, Dubai, United Arab Emirates.

TP 278  Improved Sensitivity for the Qualitative and Quantitative Analysis of Active Ricin by MALDI-TOF Mass Spectrometry; Donoxia Wang1; Jakub Baudys2; John R Barr2; Suzanne R Kalt2; 1Institute of Forensic Sciences, Cleveland, Ohio; 2Centers of Disease Control and Prevention (CDC), Atlanta, GA; 3Centers for Disease Control and Prevention, Atlanta, GA

TP 279  A SPEG coupled Mass Spec Approach for Understanding the Glycosylated and Sialylated Proteome of CHO Mutants: Ozgo Can1; 2; Deniz Baycin Hizal1; A. Emin Atik2; R. Serdar Alpan3; Sharon Krag4; Hui Zhang5; Michael Batenbaugh5; 1Acibadem University, Istanbul, Turkey; 2Turgut Biotechnology Group, Istanbul, Turkey; 3Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; 4Johns Hopkins University School of Medicine, Baltimore, MD; 5Johns Hopkins Bloomberg School of Public Health, Baltimore, MD

TP 280  Studying the Effect of Glycan and Peptide Backbone Structures on Kinetics of N-glycan Release by PNGase F with MRM Quantization; Yining Huang1; Ron Orlando2; 1University of Georgia, CCRC, Athens, GA; 2University of Georgia, CCRC Athens, GA

TP 281  Mass Spectrometry-based Quantitative Analysis for Decoding Site-specific Alteration of Sialo-glycoproteome in EGFR-subtype of Non-small Cell Lung Cancers; Yi-Ju Chen1; Yu-Hsien Lin2; 1University of Georgia, CCRC, Athens, GA; 2University of Georgia, CCRC Athens, GA

TP 282  Features of N-Glycosylation of Immunoglobulins from Two Knockout Pig Models; Emy Komatsu1; Marjone Buist1; Paul Gabriel Lopez2; Apolline Salama1; David Sachs3; 1Institute of Legal Medicine, Innbruck Medial University, Innbruck, Austria; 2Acibadem University, Istanbul, Turkey; 3Johns Hopkins Bloomberg School of Public Health, Baltimore, MD
Uncovering Single Glycoprotein Signatures using a One-pot Dual Nanoprobe-based Mass Spectrometry Assay. Mira Anne C. dela Rosa1,2, Wei-Chun Chen3, Yi-Ju Chen4, Rofeamor P. Obena5, Chih-Hsiang Chang6, Rey Y. Capangangan7, Tung-Hung Su8, Chi-Ling Chen9, Pei-Jer Chen9, Yu-Ju Chen9. Department of Chemistry, National Taiwan University, Taipei, Taiwan (R.O.C.); 3National Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan, TAIWAN (R.O.C.); 4Nanofabrication Laboratory Di Tecnologia Della Riproduzione, Cremona, Italy; 5Fondazione Avanetta, Cremona, Italy; 6University of Bologna, Bologna, Italy; 7Université de Nantes, Nantes, France; 8Université de Paris-Descartes, Paris, France.

Serum N-Glycome and Glycoproteome Analysis for Oral Cancer Patients. Chuan Fa Chang1; Shu-Jie Chang1; Orac Lee1,2; Gun Wook Park1,2; Heeyoun Hwang1; Chuan Fa Chang1; Shu-Jie Chang1; University of Nebraska-Lincoln, Lincoln, NE; 2University of Nebraska-Lincoln, Lincoln, NE.

The Role of N-Glycosylation in Receptor Tyrosine Kinase (RTK) Signaling: Kevin B Chandler1; Deborah R Leon1; Rosana D Meyer2; Nader Rahimi1; Catherine E Costello1; Boston University School of Medicine, Boston, MA.

MALDI-MS Characterization of Glycan Multivalency in Synthetic Glycan-Protein Conjugates. Christopher C. Lai1; David Farnsworth2; Jeffrey C. Gildersleeve3; James A. Kelley4; CBL, CCR, NCI-Frederick, NIH, Frederick, MD - National Institutes of Health, Frederick, MD.

Glycoproteomic Analysis of HIV Latently Infected Cells and Plasma from Elite Suppressor Identify Important Glycoproteins in virus-host Interaction. Weiming Yang1; Hui Zhang1; Johns Hopkins University School of Medicine, Baltimore, MD.

Revealing the Functions of Glycosylation Genes in Breast Cancer Cell Brain Metastasis with Gene Silencing Coupled to LC-MS/MS Glycomics. Wenjing Peng1; Yehia Mechref2; Ling Hao1; John Young Kim1; Jong Shin Yoo1,2; Texas Tech University, Lubbock, TX.

Deciphering Glycemics and Neuroproteomic Alterations in Experimental TBI: Comparative Analysis of Aspirin and Clopidogrel Treatment. Hisham Bahmad1; Rui Zhu2; Nafyi Ramadan1; Hussein Abou Abbass3; Shiyue Zhou4; Xue Dong5; Firas Kobeissy6; Yehia Mechref7; American University of Beirut, Beirut, Lebanon; Texas Tech University, Lubbock, Texas.

Effect of Aspirin on Platelet Glycoproteins in Presence of Collagen. Punit Shah1; Weiming Yang1; Shisheng Sun1; John Young Kim1; Jong Shin Yoo2; Texas Tech University, Lubbock, TX.

Comparative Transcriptomic and Proteomic Analysis of Productively HIV-1-infected and Bystander Monocyte-derived Macrophages during HIV-1 Infection of Uninfected Donors. Isabel Martinez Ferrando1; Johns Hopkins University School of Medicine, Baltimore, MD.

HIGH MASS ACCURACY/HIGH PERFORMANCE MS METHODS & DEVELOPMENTS.

TUESDAY POSTERS.

TP 287 N-Glycoproteomic Characterization of Recombinant Human Cytomegalovirus Glycoprotein B using Multienzymatic Proteolysis Coupled to LC-MS/MS and CZE-MS/MS. Nicolas Smargiasso1; Johann Far1; Catherine Navarre2; Gabriel Mazuccelli1; Dominique Biaivi3; Marc Boutry3; Edwin De Pauw4; University of Liege, Liege, Belgium; 2University of Louvain, Louvain-la-Neuve, Belgium.

Ultrasensitive Glycoproteomics pairing Liquid Phase Isoelectric Focusing and Data Independent LC-MS reveals Site Specific N-glycosylation Alterations in Gastric Adenocarcinoma. Josh Smith1; Colin Clarke1; Stefan Mittemayr1; Jonathan Bones2; National Institute of Bioprocessing Research and Training (NIBRT), Dublin, Ireland.

Glucosyl Profiling of Human Hyaluronidase 1. Abby S. Gelb1; Christine Booth1; Melanie A Simpson2; Eric D Dodds2; Carle Lab.

The Universality of Nebraska-Lincoln, Lincoln, NE; 2University of Nebraska-Lincoln, Lincoln, NE; 3University of Wisconsin Madison, Madison, WI; 4University of Wisconsin-Madison, Madison, WI.
TP 301 Using Simultaneous Waveform Averaging and Ion Counting Techniques to Expand the Quantitative Measurement Range in a Time-of-Flight Mass Spectrometer; Toshinobu Hondo1,2; Yuki Miyada2; Yosuke Kawai3; Kentaro Terada3; Michisato Toyoda4,4; 4MS-Cheminformatics, Inabe-gun, Mie; 2Project Research Center for Fundamental Sciences, Graduate School of Science, Osaka University, Osaka, Japan; 3Department of Earth and Space Science, Graduate School of Science, Osaka University, Osaka, Japan; 4Department of Physics, Graduate School of Science, Osaka University, Osaka, Japan.

TP 302 Computer Modeling of Trapped-Ion Cell Capacitance for Optimization of Ion Image Charge Detection Mass Spectrometry; Steven C Beu1; Nathan K Kaiser2; Donald F Smith2; Christopher L Hendrickson2,3; 1S C Beu Consulting, Austin, TX; 2Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; 3Department of Chemistry and Biochemistry, Tallahassee, FL.

TP 303 Static Harmonization of Dynamically Harmonized FT ICR Cell. High Order Contributions to the Electric Field; Ekaterina Zhdanova1,2; Gleb Vladimirov1,2; Yury Kostyukevich1,2; Eugene Nikolaev1; 1Moscow Institute of Physics and Technology, Dolgoprudny Moscow Oblast, Russia; 2Institute for Energy Problems of Chemical Physics, Moscow, Russia; 3Skolkovo Institute of Science and Technology, Skolkovo Moscow Oblast, Russia.

TP 304 Setup and Application of Gas-phase APCI Coupled to Ultra-high Resolution Mass Spectrometry for Gas Chromatography and Thermal analysis; Martin Stutz1; Christopher Paul Rüger2; Theo Schwemer1,2; Toni Miersch1; 1Arthen-Engeland1; Ralf Zimmermann1,2,4; 2University of Rostock, Analytical Chemistry, Rostock, Germany; 3HICE - Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health, Munich, Germany; 4Bruker Daltonic GmbH, Bremen, Germany; 5Helmholtz Zentrum München, Cooperation Group “Comprehensive Molecular Analytics”, Munich, Germany.

TP 305 Charge Ordered Parallel Ion aNalysis (CHOPIN) Mass Spectrometry Enhances Global Sequence Coverage, Deep Proteomics and PToMics; Simon Davis1; Philip Charles1; Lin He1; Benedikt M Kessler1; Roman Fischer1; 1Oxford University, Oxford, United Kingdom; 2Bioinformatics Solutions Inc., Waterloo, Canada.

TP 306 Implementation of the All Ion Fragmentation Analysis for Targeted/Untargeted Metabolomic Approaches; Marie Stoud1; Shannon R Sweeney1; Jennifer Chiou1; Stefano Tiziani2; Dell Pediatric Research Institute, Austin, TX.

TP 307 Accurate FT-ICR MS with Fluctuating Ion Sources; Konstantin O Nagornov1; Anton N Kozhinov1; Yury O Tsybins1; 1Spectroswiss Sàrl, Lausanne, Switzerland.

TP 308 Characterization of a Modified Dynamically Harmonized FT-ICR Cell at High Magnetic Field; Christopher L Hendrickson1,2; Nathan K Kaiser1; Steven C Beu1; Greg T Blakney1; John P Quinn1; Donald J Smith1; Alan G Marshall1,2; 1Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory, Tallahassee, FL; 2Department of Chemistry, Florida State University Tallahassee, FL; 3S C Beu Consulting, Austin, TX.

TP 309 Boosting FTMS Performance via Advanced Data Acquisition Electronics and Signal Processing; Yury O Tsybin1; Konstantin O Nagornov1; Anton N Kozhinov1; 1Spectroswiss Sàrl, Lausanne, Switzerland.

TP 310 Implementation of a High-performance FPGA-based Data Acquisition System for FTMS; Anton Kozhinov1; Konstantin Nagornov1; Yury Tsybin1; 1Spectroswiss Sàrl, Lausanne, Switzerland.

TP 311 Design of Automated Quantitative Optimization Software for Hi-Resolution Analysis; Eugene F. Ciccarino1; Asoka Ranasinghe2; Timothy Olah3; Richard Baran4; Mark Sanders5; Jonathan L Josephs6; 1Bristol-Myers Squibb, Princeton, NJ; 2Bristol-Myers Squibb, Princeton, NJ; 3Thermo Fisher Scientific, San Jose, CA.

TP 312 9-plex Metabolic Labeling with NeuCode SILAC; Katherine A Overmyer1; Elyse C Freiberger1; Stefa Tyanova1; Anna E Merrill1; William Wood2; Marwan Elmasri1; Alexander S Hebert1; Michael S Westphall1; Joel C Bradley1; Jürgen H Coxe1; Joshua J Coon1; 1Wolfson Molecular Imaging Centre, Manchester, UK; 2Waters Corporation, Wilmslow, UK; 3Bruker Daltonik GmbH, Bremen, Germany; 4Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany.

IMAGING MS: DISEASE MARKERS 313 - 344

TP 313 New Insights into the Microenvironment of Cancerous Tissue by Combined Mass Spectrometry, Microscopy and Multivariant Analysis; Tina Angerer1; John Stephen Fletcher1; 1University of Gothenburg, Gothenburg, Sweden.

TP 314 Typing of Colon and Lung Adenocarcinoma using High-throughput Imaging Mass Spectrometry; Rita Casadonte1; Mark Kriegsmann1; Rémi Longuespéere1; Petra Wandelwirth1,2; Cristina Moharan1; Tiemo Katzenberger1; Daniela Aust1; Gustavo Barettone1; Jörg Kriengsman1,3; 1Bioinformatics Solutions Inc., Waterloo, Canada; 2University of Heidelberg, Heidelberg, Germany; 3Institute for Energy Problems of Chemical Physics, Moscow, Russia; 4Bruker Daltonic GmbH, Bremen, Germany.

TP 315 MALDI-MS Imaging of Lipid Changes after PI3-K Inhibition in Colorectal Cancer Liver Metastases; Fiona Henderson1; 1Imperial College London, South Kensington Campus London, United Kingdom.

TP 316 MALDI-MS Imaging of Lipid Changes after PI3-K Inhibition in Colorectal Cancer Liver Metastases; Fiona Henderson1; 1Imperial College London, South Kensington Campus London, United Kingdom.

TP 317 Comparative Mapping of PSA and N-glycan Distributions in FFPE Prostate Cancer Tissues using MALDI-FTICR and Rapid MALDI-TOF Mass Spectrometry Imaging; Richard R Drake1; Peggi M Angel1; Hendrik Jan Koolag1; Shannon Corbett1; Medical University of South Carolina, Charleston, SC; 1SCILS GmbH, Bremen, Germany; 2Bruker Daltonic GmbH, Bremen, Germany; 3Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany.

TP 318 Comparative Mapping of PSA and N-glycan Distributions in FFPE Prostate Cancer Tissues using MALDI-FTICR and Rapid MALDI-TOF Mass Spectrometry Imaging; Richard R Drake1; Peggi M Angel1; Hendrik Jan Koolag1; Shannon Corbett1; Medical University of South Carolina, Charleston, SC; 1SCILS GmbH, Bremen, Germany; 2Bruker Daltonic GmbH, Bremen, Germany; 3Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany.

TP 319 Imaging Mass Spectrometry Approach for the Diagnosis of Carcinoma of the Cervix; Rita Casadonte1; Rémi Longuespéere1; Mark Kriegsmann1; Michael Becker2; Sören-Oliver Deininger2; Mike Otto1; Jörg Kriengsman1; 1Bioinformatics Solutions Inc., Waterloo, Canada; 2University of Heidelberg, Heidelberg, Germany; 3Bruker Daltonik GmbH, Bremen, Germany; 4Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany.

TP 320 Imaging Mass Spectrometry Approach for the Diagnosis of Carcinoma of the Cervix; Rita Casadonte1; Rémi Longuespéere1; Mark Kriegsmann1; Michael Becker2; Sören-Oliver Deininger2; Mike Otto1; Jörg Kriengsman1; 1Bioinformatics Solutions Inc., Waterloo, Canada; 2University of Heidelberg, Heidelberg, Germany; 3Bruker Daltonik GmbH, Bremen, Germany; 4Centre for Histology, Cytology and Molecular Diagnostics, Trier, Germany.
TP 321 Molecular Markers of Serous Ovarian Cancer Aggressiveness and Surgical Outcome by Ambient Ionization Mass Spectrometry Imaging: Marta Sans Escorih1; Kshipra Gharpure2; Jialing Zhang1; Jinsong Liu3; Anil K. Soody1; Livia S. Eberlin1; 1University of Texas at Austin, Austin, TX; 2the University of Texas M.D Anderson Cancer Center, Houston, TX

TP 322 Linking Lipid Metabolism, Hypoxia, Radiation Therapy and Metastasis using DESI Imaging Mass Spectrometry; Erik J. Soderblom1; Kathleen Ashcraft2; Matt W. Foster3; and Metastasis using DESI Imaging Mass Spectrometry Linking Lipid Metabolism, Hypoxia, Radiation Therapy
Hospital Johns Hopkins Medicine, Saint Petersburg, FL; 2Waters Corp., Beverly, MA; 3Proteomics and Metabolomics Shared Resource, Duke University School of Medicine, Durham, NC; 4Department of Molecular Biology, University of Duisburg-Essen, Essen, Germany

TP 323 Elemental Analysis and Imaging of Stroke-aﬀected Brain Tissues by Utilizing Laser Ablation-inductively Coupled Plasma-Mass Spectrometry: Diagnostic Study; Khalid A. Al-Saad1; Mohamed H Ali2; MD Fazle Rakib1; Eman M Fayad1; Rick Dijkhuijzen1; Gerald T Viltj1; 1Qatar University, Doha, Doha; 2Qatar Biomedical Research Institute, Doha, Qatar; 3University Medical Center Utrecht, Utrecht, Netherlands

TP 324 Molecular Signature Discovery of Human Chronic Traumatic Encephalopathy Tissues using Mass Spectrometry Imaging: Bo Yan1; Dharmendra B. Goswami1; Deborah R Leon1; Mark E McComb2; Ann C. McKe1; Catherine E Costello1; 1Boston University School of Medicine, Boston, MA; 2United States Department of Veterans Affairs, VA Boston Healthcare System, Boston, MA

TP 325 MALDI Imaging of Neuronal Plasticity: Analysing Fine Adaptations with Large Eﬀects: Jakob Meier-Credo1; Michael Becker2; Alice Ly3; Shahar Or1; Irina Epstein1; Thomas Hagedorn1; Tamas Dalmay4; Johannes J Letzkus5; Erin Schuman1; Julian Langere1; 1Max-Planck-Institute for Brain Research, Frankfurt Am Main, Germany; 2Bruker Daltonik GmbH, Bremen, Germany

TP 326 Nanoparticle Matrix Implantation Mass Spectrometry Imaging Discoveries and Quantifies Lipid Biomarkers of Traumatic Brain Injury and Tracks Therapeutic Response: Aurelle Roux1; Ludovic Muller1; Shelley N Jackson2; Jeremy Post; Katherine Baldwin2; Barry Hoffer3; Carey Balaban4; Damon Barbacci1; Albert J Schultz5; Shawn Gouy6; Brian M Cox7; Amina S Woods1; 1Children’s Hospital Johns Hopkins Medicine, Saint Petersburg, FL; 2NIH/NIDA-IRP, Baltimore, MD; 3Philadelphia College of Osteopathic Medicine, Philadelphia, PA; 4University Hospitals of Cleveland, Cleveland, OH; 5University of Pittsburgh, Pittsburgh, PA; 6Ionwerks, Gaithersburg, MD; 7Ionwerks Inc, Houston, TX; 8Uniformed Services University, Bethesda, MD; 9NIDA-IRP, NIH Baltimore, MD

TP 327 MALDI Mass Spectrometry Imaging in Alzheimer’s disease mouse model Het CRND8 (+/-):Lyna Sellami1; Marcia Roy2; Matthew E O’Hanes1; Luis Mancera1; Omar Belgacem1; ’Shimadzu, Kratos Manchester, United Kingdom; 1University of Edinburgh, Edinburgh, UK

TP 328 Simultaneous MALDI MS Imaging and Quantitation of Multiple Neurotransmitters In Parkinson’s Disease Models; Elva Fridjonsdottir1; Mohammadreza Shariatgoji2; Anna Nilsson1; Patrik Kälflack1; Xiaqiong Zhang1; Per Svenningsson4; 1University of Pennsylvania, University, Sweden; 2Karolinska Institutet, Stockholm, Sweden; 3Uppsala University, Uppsala, SE

TP 329 Detection of Ganglioside Lipid Species in the Brain of Mucopolysaccharidosis Type II Mouse by Imaging Mass Spectrometry: Martin Dufresne1; Daniel Guenyisu1; Martin Marcinkevicz1; Anthony Regina2; Michel Demoule2; Pierre Chaurand2; 1Université de Montréal, St-Hyacinthe, QC; 2Cytochem Inc., Montreal Quebec, Canada; 3Anglochem Inc., Montréal, QC, Canada; 4University of Montreal, Montreal, QC

TP 330 Studying the Sphingolipid Pathway into Co-morbidity of Depression and Alcoholism by MALDI Imaging FT-ICR Mass Spectrometry: Christian P Muller1; Matthias Witt2; Michael L. Easterling4; Jens Fuchs2; Beckmann Janine1; Thomas Stockii1; Eva Sprenger1; Jens Ties1; Sabine E Huber1; Davide Amato1; Ercolino3; Martin Reichel1; Johannes Kornhuber1; 1Department of Psychiatry and Psychotherapy, Friedrich-Alexander-University of Erlangen-Nuremberg, Erlangen, Germany; 2Bruker Daltonik GmbH, Bremen, Germany; 3Bruker Daltonics, Billerica, MA; 4Department of Molecular Biology, University of Duisburg-Essen, Essen, Germany

TP 331 Molecular Mapping of Gangliosides and Related Lipids using Mass Spectrometry Imaging with Ion Mobility Separation: Bindesh Shrestha1; Hernando Olivos2; Khaja Muneevuddin3; Miguel Sena-Esteves4; 1Justus Liebig University, Kalyan, India; 2Munich, Germany; 3University of Massachusetts Medical School, Worcester, MA

TP 332 Evaluating the Viability of Kidney Transplants using High-speed MALDI-Imaging: Shane R Ellis1; Tim C van Smaalen2; Nadine E Masci3; 1Université de Montréal, St-Hyacinthe, QC; 2Cytochem Inc., Montreal Quebec, Canada; 3University of Massachusetts Medical School, Worcester, MA

TP 333 Protemic Mass Imaging of Kidney from Type 2 Diabetes (T2D) Rat Model: Hirata Chie1; Kuzuhara Yuk1; Iwasaki Noriyuki2; Kudo Yoshji1; Nirasawa Takashi1; Masuyama Ke1; Kakuda Nobuto2; Wakazono Hiroshi3; Yanagi Hiroyuki3; Masaya Ikegawa4; 1Doshisha University, Kyoto, Japan; 2Bruker Daltonics K.K., Kanagawa, Japan; 3Ono Pharmaceutical Co., Ltd., Fukui, Japan; 4Doshisha University, Kyoto, Japan

TP 334 Differentiating Macrophages in Atherosclerotic Plaques using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging; Pegah Khamehzari-Sil1; Florian Schnitt1; Andreas H. Wagner1; Sabine Schulz2; Markus Becker2; Bernhard Spengler1; ’Justus Liebig University, Giessen, Germany; 1Ruprecht-Karls-University, Heidelberg, Germany

TP 335 What Can We Learn from the Na+/K+ Ratio in Imaging Mass Spectrometry Experiments?: Roberto Fernandez1; Jone garate1; Sergio Lage1; Silvia Teres1; Pau Gonzalez2; Monica Higuera1; Alfredo Maqueda2; 1Justo Baster-Calearas, Barcelona, Spain; 2Cytochem Inc., Montreal Quebec, Canada; 3University of Massachusetts Medical School, Worcester, MA; 4Cytochem Inc., Montreal, QC; 5University of Montreal, Montreal, QC; 6University of Pennsylvania, University, Sweden; 7Ionwerks, Gaithersburg, MD; 8Uniformed Services University, Bethesda, MD; 9NIDA-IRP, NIH Baltimore, MD
TP 336  Analysis of Retinal Degeneration in a Leber Congenital Amaurosis Mouse Model Using High Spatial Resolution MALDI-Imaging Mass Spectrometry; David M. Anderson1; Zsolt Ablonczy2; Yiannis Koutalos3; Nico Verbeek4; Raf Van De Plas1; Jeffrey Spraggins5; Rosalie K. Crouch6; Richard M Caprioli7; Kevin L. Schey8; Vanderbilt University MSRC, Nashville, TN; 2Department of Ophthalmology, St. Mary’s Eye Institute, Medical University of South Carolina, Charleston, SC; 3Delft Center for Systems and Control (DCSC), Delft University of Technology, Delft, Netherlands

TP 337  Molecular Target Validation in Human Atherosclerosis Based on Mass Spectrometry Imaging and Immunohistochemical Evaluation; Jonathan Stauber1; Gregory Hamm1; Sylvia Ald1; Juliette Masure2; Kim Holstrom3; Serife Arda4; Danielle Van Keulen2; David Bonne1; Ivana Bobeldijk-Pastorova5; Dennie Tempel5; Boye S Nielsen3; Michael Gudo4; Jan NH Lindeman7; Ulf Hedini1; Alain van Gool2; Eva Hult Camo3; ImaBiotec, MS Imaging Dept. Loos, France; 2Department of Molecular Imaging and Surgery, Karolinska Institutet, Stockholm, Sweden; 3Bioneer, Hoersholm, Denmark; 4Morphisto, Frankfurt Am Main, Germany; 5TNO, Metabolic Health Research Leiden, The Netherlands; 6CardioGenx, Rotterdam, The Netherlands; 7Leiden University Medical Centre, Leiden, The Netherlands; 8AstraZeneca R&D, Gothenburg, Sweden

TP 338  Simultaneous Detection of N-glycans and Peptides from a Single FFPE Tissue Section by MALDI FT-ICR Imaging Mass Spectrometry: Peppi Angel1; Rita Casadonte2; Jörg Kriegsmann3; Richard Drake4; Medical University of South Carolina, Charleston, SC; 5Proteopath GMBH, Trier, Germany; 6Medical Univ of S Carolina, Charleston, SC

TP 339  The Effect of Oxygen on the Lipid Composition of Human Chondrocytes using MALDI Imaging: Brenda Bakker1; Gert Eijk2; Ron Heeren3; Marcel Karperien1; Janine Post1; Berta Cillero-Pastor5; Developmental BioEngineering, University of Twente, Enschede, The Netherlands; 3Maastricht Multimodal Molecular Imaging Institute (M4I), Maastricht University, Maastricht, The Netherlands

TP 340  Metabolite Profiling of Intestinal Microbiota by Mass Spectrometry Imaging for Biological Understanding of Gastrointestinal Disease; Gregory Hamm1; Juliette Masure1; Sylvain Normand2; David Bonnel1; Mathias Chamaillard1; Jonathan Stauber1; ImaBiotec, MS Imaging Dept. Loos, France; 2Center of Infection and Immunity of France, 3National Hospital for Paraplegics, Toledo, Spain; 4University of the Balearic Islands, Palma Balearic Islands, Spain; 5Vanderbilt University, Nashville, TN; 6University of the Pais Vasco, Leioa, Spain

TP 341  Differential Human Pancreatic Lipid and Protein Distributions in Normal and Type 1 Diabetes Revealed by Tissue Imaging Mass Spectrometry; Boone M Prentice1; Rachana Haluyur1; Nathaniel J Hart2; Audra M Judd3; Radhika Aramandia4; Marcela Brissova5; Jeffrey M Spraggins6; Jeremy L Norris1; Alvin C Powers7; Richard M Caprioli4; Vanderbilt University MSRC, Nashville, TN

TP 342  Lipid and Metabolite Distribution in Healthy and Diseased Brain Tissue using DESI and High Resolution Mass Spectrometry; Joseph H Kennedy1; Jeff Patrick2; Mariam ENaggar1; Justin M Wiseman2; 1Prosolia, Inc. Indianapolis, IN

TP 343  Imaging Mass Spectrometry for the Pathological Studies of Cardiac Allografts; Terada Megumi1; Iwasaki Noriyuki2; Kudo Toshii2; Nirasawa Takashi3; Bruneval

TP 344  High Spatial Resolution Lipid Imaging Offers Promising Perspectives in Sustaining Diagnosis of Human Lymphoma; Yousef El Aalami1; Arndt Asperger2; Xian Mao3; Wim Waelput4; Thomas Toussey5; Bart De Moor5; Etienne Waelkens6; 1ESAT-STADIUS / Minds Medical IT, KU Leuven, Leuven, Belgium; 2Bruker Daltonik GmbH, Bremen, Germany; 3Dept. of Pathology, UZ-Brussel, Brussels, Belgium; 4Dept. Imaging and Pathology, KU Leuven., Leuven., Belgium; 5Dept. Cellular and Molecular Medicine, KU Leuven, Leuven, Belgium

TP 345  Towards Absolute Quantitative MALDI MS Imaging of Drugs; Patrik Kaliback1; Theodosis Vallianatou2; Anna Nilsson3; Mohammadreza Shariatgorgi4; Per E Andren5; Uppsala University, Uppsala, Uppsala; 6Uppsala University, Uppsala, Sweden

TP 346  Derivatization Strategies for the Quantitation of Triaminocoline Acetamide in Cartilage using Imaging Mass Spectrometry: Florian Bar6; Bryn Flinders2; Joao Garcia1; Laura Creemers3; Ron M A Heeren2; Berta Cillero-Pastor5; 6M4I Institute - Maastricht University, Maastricht, The Netherlands; 7Utrecht University, Utrecht, The Netherlands

TP 347  3D MALDI Mass Spectrometry Imaging to Empower Drug Distribution And Quantitation Studies in Solid Tumors; Silvia Giordano1; Lavinia Morosi2; Pietro Veglianelle1; Simonetta Andrea Licandro1; Roberta Frapolli1; Massimo Zucchetti1; Maurizio D’Incalci1; Enrico Davoli1; 1IRCCS Istituto Mario Negri, Milano, Italy

TP 348  Study of the Blood Brain Barrier Permeability using a Multimodal Imaging Approach; David Calligaris1; Fa-Ke Lu1; Armen Changelian2; Isaiah Norton1; Brett L Carlson1; Jeffrey Agar1; William F Elquist3; Daniel MA4; Jann N Sarkaria5; Nathalie YF Agar4; Department of Neurosurgery, Brigham and Women’s Hospital - Harvard Medical School, Boston, MA; 5Mayo Clinic, Rochester, MN; 6Barnett Institute of Chemical and Biological Analysis, Northeastern University, Boston, MA; 7Department of Pharmaceutics, University of Minnesota, Minneapolis, MN

TP 349  Comparison of LESA-MS to MALDI-MS for Mouse Whole Body Tissue Profiling: Diclofenac and Major Metabolites; Walter Korfmann1; Gargey Yagnik2; Yongyi Luo3; Stacy Ho2; Liduo Shen3; Terry Wilpert; Karen Norton4; Eric Solomon5; Hanlan Liu6; Sara Savage7; Thomas O’Shea8; Genzyme, Waltham, MA; 2Genzyme, a Sanofi company Waltham, MA; 3Sanofi, Waltham, MA; 4Genzyme, Framingham, MA; 5QPS, Newark, DE

TP 350  Matrix Assisted Laser Desorption/Ionisation Mass Spectrometry Imaging of Therapeutic Oligonucleotides: Application to Antisense Therapy; C. Logan Mackay1; John G Swales1; Richard J A Goodwin2; 1SIRCAMS, Edinburgh, UK; 2AstraZeneca, Cambridge, UK

TP 351  Microinjection and High-throughput Alginement of Cellular Spheroids for MALDI Mass Spectrometry Imaging Analysis; Jillian Johnson1; Fengfei Ma1; Weiyuan Liao1; 1University of Wisconsin-Madison, Madison, WI

TP 352  Applications of Single-Probe Device for Ambient Mass Spectrometry Imaging Analysis: Human Corneas and 3D Artificial Tumors; Xiang Tian1; Wei Rao1; Ning Pan1; Hailing Yu1; Dimitrios Karamichos2; Zhibo Yang1; 1University of Wisconsin-Madison, Madison, WI
TP 353 Application of Imaging Mass Spectrometry to Assess Ocular Drug Transport: Kerri Grove1; Viral Kansara2; Melissa Prentiss2; Debby Long2; Muneto Mogi2; Sean Kim2; Patrick Rudewicz2; Novartis Institutes for BioMedical Research, Emeryville, CA; 2Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA

TP 354 MALDI-FTICR Imaging of the Distribution of Terriflunomide in CNS Tissues in an Experimental Model of Multiple Sclerosis; Janacy Rzagalinski1; Carola Meier1; Nadine Hainz1; Thomas Tschernig1; Dietrich Volmer1; 1Saarland University, Saarbrücken, Germany

TP 355 Multimodal Mass Spectrometry Imaging for Detection and Early Prediction of Drug Induced Phospholipidosis; Richard Goodwin1; Anna Nilsson1; Jennifer Barnes1; Julia Sampson1; Hui Zhang1; John G Swales1; Nicole strittmatter4; Alan Race1; Rory Steven1; Logan C Mackay1; Josephine Bunch1; Per E Andren1; 1AstraZeneca, Cambridge, UK; 2Uppsala University, Uppsala, Sweden; 3AstraZeneca R&D, Molndal, Sweden; 4AstraZeneca, Macclesfield, Select State; 5National Physical Laboratory, Teddington, United Kingdom; 6University of Edinburgh, Edinburgh, United Kingdom

TP 356 The Evaluation of Erythroblast Dynamics in Mice Bone Marrows by MALDI FTICR-MS Imaging which Identifies 5Fe-labeled Heme Isotopic Fine Structure; Makoto Kihara1; Yukari Matsuo-Tezuka1; Keigo Yorozu2; Mitsue Kurasawa2; Hideyuki Yasuno2; Yasushi Shimonaka2; Chugai Pharmaceutical Co., Ltd, Kamakura, Japan; 2Chugai Pharmaceutical Co., Ltd Kamakura, Japan

TP 357 Large Scale, Multi-instrument MALDI-MSI Study into Lipidosis in Inhalation Dosed Rats: Rory Thomas1; Alan Race1; Aateka Patel2; Lea Ann Dailey2; Josephine Bunch3,4; National Physical Laboratory, Teddington, UK; King's College London, London, UK; 3University of Edinburgh, Edinburgh, United Kingdom

TP 358 MALDI Imaging Mass Spectrometry of Platinum-Based Drugs in Multicellular Tumor Spheroids (MCTS) using Derivatization with Diethyldithiocarbamate (DDTC): Xin Liu1; Amanda B Hummon1; University of Notre Dame, Notre Dame, Indiana

TP 359 Visualization of Small Molecule and Nanoparticle Anticancer Agents in Tissue and Tumor Sections using IR-MALDESI Mass Spectrometry Imaging: Mark Bokhart1; Allison Schorzman2; Andrew Lucas2; Michael Berens2; Harshil Dhruv3; William Zamboni2; Andrew Lucas2; Michael Berens3; 1University of Southern Denmark, Odense, Denmark; 2Federal University of Minas Gerais, Belo Horizonte, Brazil; 3University of Cape Town, ZA; 4Buck Institute for Research on Aging, Novato, CA; 5Stellenbosch University, Liberty, MO

TP 360 Tissue Distribution of Compound X and its Metabolites in Jck Mouse Polycystic Kidneys using Mass Spectrometry Imaging (MSI); Hanlian Liu1; Cristina Silvescu1; Mandy Crowwell2; Kelly Keefe2; Lindsay Quigley2; Siramas Sudsakon1; Sarah Nserek1; Yang Guo1; Laurie Smith1; Thomas Natoli2; Dinesh Bangari2; Gregory Ham2; Harshil Dhruv3; William Zamboni2; David C Muddiman2; Aateka Patel2; Lea Ann Dailey2; 1University of Münster, Institute of Biochemistry, Mülheim an der Ruhr, Germany; 2National Physical Laboratory, Teddington, UK; 3AstraZeneca, Macclesfield, Select State; 4National Physical Laboratory, Teddington, United Kingdom; 5National Physical Laboratory, Teddington, United Kingdom

TP 361 Visualizing Anti-Retroviral Distribution in Sheep and Human Vaginal Tissue by Imaging Mass Spectrometry; Michelle Reyer1; Mark Marzinke1; Trevelyn Olive1; Richard Pyles2; Kathleen L Vincent2; Manjula Gunawardana2; John Moss3; Marc M Baum3; Richard M Capirol1; Vanderbilt University, Nashville, TN; 1Johns Hopkins University, Baltimore, MD; 2University of Texas Medical Branch at Galveston, Galveston, TX; 3Oak Crest Institute of Science, Monrovia, CA

TP 362 MALDI IMS in Drug Development: Shedding New Light on Toxicology; M. Reid Groseclose1; Stephen Castellino1; 1GlaxoSmithKline, Upper Merion, PA

TP 363 Complementary Elemental And Molecular Mass Spectrometry Imaging to Investigate 5-aminolevulinic Acid, Protoporphyrin IX and Heme Distribution in Human Brain Tumor; Sabrina Kröger1; Ann-Christian Niehoff1; Uwe Karst1; 1University of Münster, Institute of Inorganic and Analytical Chemistry, Münster

INFORMATICS: PEPTIDE ID AND QUANTIFICATION

TP 364 Resolving Complex Glycopeptide Fragmentation Tandem Mass Spectrum; Aying Yu1; Lauren Zacharias1; Rui Zhu2; Kenny Wooding2; Yehia Mechref2; 1Texas Tech University, Lubbock, Texas

TP 365 Recycling Modification Site Information for Improved Glycopeptide Analysis: Robert Chalkley1; Peter R Baker1; 1UCSF, San Francisco, CA

TP 366 Decoding Histone Post-translational Modifications by bottom-up Mass Spectrometry: Zuo-Fei Yuan1; Simone Sidoli1; Shi Lin2; Xiaoshi Wang2; 1National Physical Laboratory, Teddington, UK; 2Translational Clinical Oncology, Novartis

TP 367 Peak Annotation of High Resolution Spectra for Constructing Peptide Mass Spectral Libraries; Xiaoyu Yang1; Pedartsur Neta1; Yuri Mirokin1; Dmitrii Tchekhovskoi2; Yuxue Liang1; Zheng Zhang1; Sergey Sheeltin1; Sanford Markey1; Stephen Stein1; 1NIST, Gaithersburg, MD

TP 368 A New Hope for Label Free Proteomics: moFF for Open-source, Platform-independent, Automated MS1 Intensity Extraction; Andrea Argentini1; 2, 3; Kenneth Verheggen1; 2, 3; Lennart Martens1; 2, 3; 1Medical Biotechnology Center, VIB, Gent, Belgium; 2Department of Biochemistry, Ghent University, Gent, Belgium; 3Bioinformatics Institute Ghent, Ghent University, Gent, Belgium

TP 369 Interconverion of Peptide Spectral Libraries between iTRAQ and TMT Labels; Zheng Zhang1; Xiaoyu Yang1; Yuri A Mirokin1; Dmitrii V Tchekhovskoi2; Weihaa Ji1; Sanford P Markey1; 1University of Oklahoma, Dept. of Chem & Biochem Norman, OK; 2Translational Genomics Institute, Tandem Mass Spectrometry, Horizonte, Brazil

TP 370 Employing Complementary Ions for Deconvolution of Mixture Tandem Mass Spectra; Vladimir Gorshkov1; Stéphanie Yuki Kolbeck Hotta1; Thiago Verano-Braga1; Frank Kjeldsen1; University of Southern Denmark, Odense, Denmark; 1Federal University of Minas Gerais, Belo Horizonte, Brazil

TP 371 Combination of MS3/HCD and MS2/CID Improves Peptide IDs in Addition to Reducing the Precursor Interference of TMT-quantitation Experiment; Wen Y1; Raghothama Chaerkady1; Deniz Bacin-Hizal1; Mathew Woodward1; Michael A Bowen1; 1MedImmune, Gaithersburg, MD - Maryland; 2MedImmune, Cambridge, UK

TP 372 The Benefits of Recycling – Protein Prospector: the Eco-Friendly Search Engine; Peter R Baker1; Juan A Oses1; Robert J Chalkley1; 1UCSF, Rokietnica; 2UCSF, San Francisco, CA

TP 373 Evaluating Software for Precursor Ion Chromatograms in Label-Free Data-Dependent Acquisition Sets through Differentiation, Quantification, and Clustering; Yasset Perez-Riverol1; Chao Liu1; Bridge Calder2; Suereta Fortuin3; Alexander Giddey3; Birgit Schilling3; 1EMBL-EBI, Horixton, UK; 2Institute of Computing Technology, CAS Beijing, CHINA; 3University of Cape Town, Cape Town, ZA; 4Buck Institute for Research on Aging, Novato, CA; 5Stellenbosch University, Liberty, MO
TP 374 Identification of Host Cell Protein Impurities using Spectral Libraries; Meghan Burke; Yuxue Liang; Kelly H. Telu; Jenny Heidbrink Thompson; Chris Larkin; Stephen Stein; "National Institute of Standards and Technology, Gaithersburg, MD; "MedImmune, Gaithersburg, MD

TP 375 Negative Electron Transfer Dissociation Fragmentation in a Full-Featured Proteomics Search Engine; Yong J Kim; Wilfred Tang; Nicholas M Riley; Michael S Westphall; Joshua J Coon; Marshall W. Bern; "Protein Metrics, San Carlos, CA; "Protein Metrics, Palo Alto, CA; "University of Wisconsin Madison, Madison, Wisconsin

TP 376 Fast and Comprehensive Peptide Identifications through Index-based Database Search; Andy Kong; Felipe de Veiga Leprevost; Alexey I Nesvizhskii; "University of Michigan, Ann Arbor, MI

TP 377 A Graph-Centric Approach for Metagenome-Guided Peptide Identification in Metaproteomics; Sukin Li; Yuzhen Ye; Haixu Tang; "Indiana University, Bloomington, IN

TP 378 Large Scale Silac Based Quantitative Analysis of Electron Accepter Stressed Azobenzyl Sulillium PS using Retention and Drift Time Profiling; Anthony T Lavaroni; Matthew D Youngblut; Emilie Gios; Michael Daly; Hans K Carlson; Ulla N Andersen; "Johannes PC Vissers; John D Coates; "UC Berkeley, Berkeley, California; "Waters, Inc. Pleasanton, CA; "Waters, Wilmslow, United Kingdom

TP 379 PGA: an R Package for Identification of Novel Peptides by Customized Database Derived from RNA-Seq; Bo Wen; Shaohang Xu; Ruo Zhou; Bing Zhang; Wang Xiaojiang; Xin Liu; Xin Xu; Siqiu Liu; "BG-Shenzhen, Shenzhen, China; "Vanderbilt University School of Medicine, Nashville, TN

TP 380 The SysteMHC Atlas Project: toward a First Mass Spectrometry-based Draft of the Human Immunopeptidome; Witold Wolski; Etienne Caron; Heiko Schuster; Michal Bassani-Sternberg; Lorenz Blum; Christian Panse; Ruedi Aebersold; "FGCZ ETH Zurich, Zurich, Switzerland; "Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; "UNIL/CHUV Ludwig Cancer Research Center Lausanne, Switzerland, Lausanne, Switzerland; "ETH Zurich, Zurich, Switzerland; "FGCZ, Univ Zurich Zurich, Switzerland

TP 381 An Approach to Explore Millions of Unidentified MS/MS Peptide Features with Network Modeling and Its Implication for In-depth Proteomics; Paul E Abraham; John C Cushman; Daniel Jacobson; Robert L Hettick; Richard J Giannone; "Oak Ridge National Laboratory, Oak Ridge, TN; "University of Nevada, Reno, Reno, NV

TP 382 Should We Care about Peptide Co-elution?; Jamie Shermag; Stephen Tate; "SCIEX, Concord ON, Canada

TP 383 Solving the "no-enzyme" Problem in MHC-peptide immuno-precipitation Database Searches; Patrick Murphy; Konda Prathyusha; Clements Derek; Heiko Schuster; Daniel Kowalewski; Brian Erickson; Joao Paulo; Alejandro Cohen; Steven P Gygi; Stefano Stevanovic; Shashi Gujar; Patrick Lee; "Dalhousie University Dept of Microbiology and Immunology, Halifax, Canada; "University of Tuebingen, Tuebingen, Germany; "Harvard Medical School, Boston, MA; "Dalhousie University, Department of Chemistry Halifax, Canada

TP 384 New Calibration and Absolute Quantification Features in Skyline; Nicholas Shulman; Clark Henderson; Birgit Schilling; Will J Thompson; Christopher M Shuford; Andy Hoofnagle; Michael J MacCons; Brendan MacLean; "University of Washington, Seattle, WA; "Buck Institute for Research on Aging, Novato, CA; "Duke University, Durham, NC; "Center for Esoteric Testing, Burlington, NC

TP 385 Do novo Sequencing of Peptides from High-resolution Bottom-up Tandem Mass Spectra using Top-down Intended Methods; Kira Vyatkina; Lennard J.M. Dekker; Si Wu; Martijn M. Vanduijn; Xiaowen Liu; Nikolica Tolic; Theo M. Luider; Lijiliana Pasa-Tolic; Pavel A. Pevzner 1; "Saint Petersburg State University, St Petersburg, Russia; "Saint Petersburg Academic University, St Petersburg, Russia; "Erasmus Medical Center, Rotterdam, The Netherlands; "University of Oklahoma, Dept of Chem & Biochem Norman, OK; "Indiana University-Purdue University Indianapolis, Indianapolis, IN; "Indiana University School of Medicine, Indianapolis, IN; "Pacific Northwest National Laboratory - PNNL, Richland, WA; "University of California, San Diego La Jolla, CA

TP 386 Advanced XIC-based Label-free Algorithm for High-Resolution Data; Sung Kyu Robin Park; Rohan Rampuria; Khaterah Motamedchaboki; Jolene Diedrich; Claire Delahunty; John R Yates; "The Scripps Research Institute, San Diego, CA; "The Scripps Research Institute, La Jolla, CA; "Sanford-Burnham Medical Research Institute, La Jolla, CA

TP 387 Pros and Cons of Large Scale MS/MS Clustering - Are We There Yet?; Benjamin Pullman; Nuno Bandeira; "Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; "Computer Science and Engineering, University of California San Diego, La Jolla, CA; "Skaggs School of Pharmacy, UC San Diego La Jolla, CA

TP 388 Combining RNA-Seq Proteogenomics and Global Post-Translational Modification (G-PTM) Search Strategy to Reveal Human Proteomic Variation; Anthony J Cesnak; Michael R Shortreed; Gloria M Shemykman; Brian L Frey; Lloyd M Smith; "Department of Chemistry, University of Wisconsin-Madison, Madison, WI

TP 389 A New Database Format to More Closely Examine Protein Splice Forms; Aparna Nathan; Waltraud Mair; Jan Muntel; Hendrik Wesseling; Judith Steen; Hanno Steen; "Boston Children's Hospital, Boston, MA

TP 390 Challenges and Solutions when Using OpenMS LFQProfiler Node in Proteome Discoverer 2.1 for Feature Comparison in Very Large Datasets; Anna Moerbe Rocker; Lindsay Schambeau; Lewis K Pannell; "University of South Alabama, Mobile, AL

TP 391 New Method for Label-free Quantification in the Proteome Discoverer Framework; David Horn; Torsten Ueckert; Kai Fritzemeier; Carmen Paschke; Katja Tham; Hans Pfaff; Xiaoyue Jiang; Joseph Brown; Iman Mohtashemi; "Thermo Fisher Scientific, San Jose, CA; "Thermo Fisher Scientific, Bremen, DE; "Thermo Fisher Scientific, San Jose, CA

TP 392 Control Software for a Spatially Multiplexed Ion Mobility-Mass Spectrometer; Babatunde H. Belo; Katrina L. Leaptrot; Jody C. May; John A. McLean; "Department of Mechanical Engineering, Vanderbilt University, Nashville, TN; "Department of Chemistry, Vanderbilt University, Nashville, TN; "VIBRE, Vanderbilt University, Nashville, TN

TP 393 Real-Time Instrument Control of the Orbitrap Tribrid Mass Spectrometer; Derek J Bailey; Florian Grosse-Coomans; Manish Dhali; Qingyu Song; Jesse D Canterbury; Qiming Wan; Michael Senko; "Thermo Fisher Scientific, San Jose, CA; "Thermo Fisher Scientific, Bremen, DE

TP 394 High-Sensitive MCP-based Ion Detector for Time of Flight Mass Spectrometry using Triode Structure; Tetsuya Hayashi; Tetsuya Matsuhashita; Joji Sakakiyama; Akio Suzuki; Toshiyuki Uchiyama; Yasuhide Naito; "Thermo Fisher Scientific, San Jose, CA

TP 395 Instrumentation: General

INSTRUMENTATION: GENERAL

392 - 416

TP 396 Control Software for a Spatially Multiplexed Ion Mobility-Mass Spectrometer; Babatunde H. Belo; Katrina L. Leaptrot; Jody C. May; John A. McLean; "Department of Mechanical Engineering, Vanderbilt University, Nashville, TN; "Department of Chemistry, Vanderbilt University, Nashville, TN; "VIBRE, Vanderbilt University, Nashville, TN

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TP 398 High-Sensitive MCP-based Ion Detector for Time of Flight Mass Spectrometry using Triode Structure; Tetsuya Hayashi; Tetsuya Matsuhashita; Joji Sakakiyama; Akio Suzuki; Toshiyuki Uchiyama; Yasuhide Naito; "Thermo Fisher Scientific, San Jose, CA
TP 395
Improved Detection Efficiency of a High Dynamic Range Pulse Counting Detection System; Bruce Collings; Martina Dima; Pascal Martin; Stephen Bruce Locke; SCIEX, Concord, ON

TP 396
Highly Charge-sensitive Device to Enhance the Direct Detection of Molecular Ions; Szu-Wei Chou; Yao-Hsin Tseng; Liang-Chun Fan; Yi-Kun Lee; Chun-Yen Cheng; AcreoMass Technologies, Inc. Taipei, Taiwan

TP 397
A New Method for Measuring Detector Operating Life Performance; Toby Shanley; Cliffon Chey; Russell Jurek; Kevin L Hunter; Peter Raffin; Daen Ekerd; Wayne Sheils; ETP Ion Detec, Clyde, Australia

TP 398
A Method for Controlling Collective Electron Motion in Ion Detectors by Locally Manipulating Magnetic Fields; Toby Shanley; Russell Jurek; Yair Benari; Dick Stresau; Kevin L Hunter; ETP Electron Multipliers, Clyde, Australia

TP 399
Combined Fast Mode and Polarity Switching for Analysis of a Range of Vitamins and Nutritional Supplements in a Single Injections; Lisa Cousins; Heather Gamble; Charles Joliffe; Joshua Ye; Jason Cournoyer; Ionics, Bolton, Canada; PerkinElmer, Waltham, MA

TP 400
Evaluation of RF-phase during Photoionization on the Trapping and Ejection of Ions from a 3D Ion Trap; Laura Bailey; Matthew R. Bell; Nicolas C Polfer; University of Florida, Gainesville, FL

TP 401
Implementation of Ultraviolet Photodissociation using Light Emitting Diodes (LEDs) in an Ion Trap; Dustin D. Holden; Alexander Makarov; Jace C Schwartz; James D. Sanders; Eugene Zhuk; Jennifer S Bordell; University of Texas at Austin, Austin, TX; Thermo Fisher Scientific, Bremen, DE; Thermo Fisher Scientific, San Jose, CA

TP 402
Improving the Performance of a Wysockii SID Cell for Synapt HDMS; Mehdi Shirzadeh; David H Russell; Texas A&M, College Station, TX

TP 403
ECO Analysis of Serine Phosphorylated Peptides using EMS Cell; Valery G. Voinov; Yuri V Vasil'ev; Douglas F Barofsky; Joseph Beckman; Linus Pauling Institute, Oregon State University Corvallis, OR; Oregon State University, Department of Chemistry Corvallis, OR

TP 404
Up Front CID in a Laminar Flow Ion Guide for Performance Enhancement in Biological Samples; Charles Joliffe; Shah Joshua Ye; Heather Gamble; Devanand Pinto; Andrew Leslie; Ionics, Bolton, Canada; National Research Council of Canada, Halifax, Canada

TP 405
Design and Modeling of a Long Distance Low Vacuum Ion Transfer System; Roman Levin; Evgeny Zhvansky; Vasily Elferov; Igor Popov; Alexey Boldyrev; Gleb Vladimirov; Eugene Nikolaev; Moscow Institute of Physics and Technology, Dolgoprudy Moscow Oblast, Russia; Institute for Energy Problems of Chemical Physics, Moscow, Russia; Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation

TP 406
Efficient Ion Transmission and Desolvation Enabled by Vortical Flow in Drift Ion Localization and Locomotion (DRILL) MS Interface; Jung Lee; Peter Kotke; Elizabeth S Hecht; David C Muddiman; Nagender Panyala; Matthew Torres; Andrei Fedorov; Georgia Institute of Technology, Atlanta, GA; NC State University, Raleigh, NC

TP 407
A Mass Selective Transfer Line for Injecting Ions in a Uniform Supersonic Flow; Baptiste Joailland; Ludovic Bienanni; Sophie Carles; Alexander Legkas; Dimitris Papanastasiou; Emmanuel Raptakis; Institut de Physique de Rennes, CNRS - Universite de Rennes 1, Rennes, FR; Fasmatech, Athens, Greece

TP 408
Ion Transport through Zirconia Capillaries; J. A. Jarrell; Waters Corporation, Milford, MA

TP 409
Development of Ultra-High Resolution Biological Target Characterization Mass Spectrometry Instrumentation; Raul Villacobo; Paolo Benigni; Francisco Fernandez-Lima; Florida International University, Miami, FL

TP 410
Coupling Raman Spectroscopy with Laser Desorption-Atmospheric Pressure Chemical Ionization/Mass Spectrometry (LD-APCI/MS) for Polymer Analysis; Yen-Ting Chen; Siou-Sian Jiang; Jentai Sheia; National Sun Yat-Sen University, Kaohsiung, Taiwan

TP 411
Thermogravimetric Analyzer Coupled with Atmospheric Pressure Chemical Ionization/Mass Spectrometry (TGA-APCI/MS) to Characterize Polymers in Biodegradable Plastics Materials; Yao Sheng Zhang; Sheng Hui Chiu; Ming Chen; Siou Sian Jiang; Jentai Sheia; National Sun Yat-Sen University, Kaohsiung, Taiwan

TP 412
Fully Automated Analysis Platform for the Routine Determination of Immunosuppressants in Whole Blood; Davide Vecchiatti; Maura Brambilla; Daisuke Kawakami; Taku Tsuchimoto; Paolo Brambilla; Shimadzu, Milan, Lombardy; Desio Hospital, Toxicology and Mass spectrometry department, Desio, Italy, Shimadzu Corporation, Kyoto, Japan

TP 413
Automated Bottom-up Proteomics Workflow for Liquid AP-MALDI MS/MS Utilising Multiplied Charged Ions; Pavel Ryumin; Jeff Brown; Michael Morris; Rainer Cramer; University of Reading, Reading, United Kingdom; Waters, Wilmslow, United Kingdom

TP 414
A New Conjoined RF Ion Guide for High Efficiency Ion Transmission; Daniel Kenny; David Gordon; Kevin Giles; Waters, Wilmslow, United Kingdom

TP 415
Performance Evaluation and Octopole Maintenance of a First Generation Q Exactive Orbitrap in a Core Facility Setting; John Leszyk; Scott A Shaffer; UMass Medical School, Shrewsbury, MA

TP 416
Building a Next-Generation Platform for Electron-ion Optics Simulations; Russell Jurek; Kevin L Hunter; ETP Ion Detect, Clyde, Australia; ETP Ion Detect, Clyde, Australia

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS

TP 417
Development and Characterization of an FT-QIT with in situ Electron Ionization for Residual and Trace Gas Analysis; Yessica Brachthausen; David Müller; Hendrik Kersten; Klaus Brockmann; Thorsten Benter; Valerie Derppmann; Alexander Laue; Ruediger Reuter; Michel Alimam; Bergische Universität Wuppertal, Wuppertal, Germany; Carl Zeiss SMT GmbH, Oberkochen, Germany

TP 418
Study of Directional Ion Ejection in an Asymmetric Half-Round Rot Electrode Linear Ion Trap Mass Analyzer; Zhang Zaiyue; Yuan Guangzhou; Qian Jie; He Yang; Yao Rujiao; Zhang Shuguang; Xiaoxu Li; Soochow University, Suzhou, China

TP 419
Optimization of the Mesh-electrode Linear Ion Trap Performance by Simulations; Qiankun Dang; Gary Glish; Chuan-Fan Ding; Fudan University, Shanghai, Shanghai; University of North Carolina at Chapel Hill, Chapel Hill, NC; Fudan University, Shanghai, China

TP 420
Improvement of Mass Resolution, Collision Induced Dissociation Efficiency and Low Mass Cutoff by Octopole Field in Linear Ion Trap Mass Analyzer; Chuan-Fan Ding; Fuxing Xu; Xinhua Dai; Xiang Fang; Fudan University, Shanghai, China; National Institute of Metrology, Beijing, China

TP 421
Design and Analytical Performance Evaluation of a Cooling Cell for a Quadrupole Mass Spectrometer with Enhanced Resolution and Sensitivity; Tsung-Chi Chen; Philip M Remes; Raman Mathur; Paul H Gregory;
TP 422  Effects of Hexapole Electric Fields on the Performance of Linear Ion Trap Mass Analyzer; Fuxing Xu1; Xinhua Dai1; Xiang Fang2; Yuanyuan Wang2; Chuan-fan Ding2; 1Fudan University, Shanghai, China; 2National Institute of Metrology, Beijing, China

TP 423  Reducing Space Charge Effects in a Linear Ion Trap by Rhombic Ion Excitation and Ejection; Li Ji1; Xiaohua Zhang1; Yuzhuo Wang2; Dan Guo3; Wei Xu4; 1Beijing Institute of Technology, Beijing, China; 2Fudan University, Shanghai, China; 3National Institute of Metrology, Beijing, China

TP 424  Ion Collision Cross Section Analyses in Quadrupole Ion Traps using Filter Diagonalization Method; A Theoretical Study; Ting Jiang1; He Muyi1; Guo Dan1; Zhai Yanbing1; Xu Wei1; 1Beijing University of Chemical Technology, Beijing, China

TP 425  Ion Trap Fourier Transform Mass Spectrometer with Induced Current Detection and Arbitrary Storage Waveforms; Michael W Schmidt1; Albrecht Brockhaus1; Stefan Butzmann1; Michel Aliman2; Alexander Laue2; Zhang2; Yuzhuo Wang3; Dan Guo1; Wei Xu1; Yury Khasin2; Anatoly Verenchikov2; 1University of Wuppertal, Wuppertal, Germany; 2Carl Zeiss SMT GmbH, Oberkochen, Germany

TP 426  Improved Performance of Ion Trap Mass Spectrometer with Added Octopole and Dodecapole Capsules; Junichi Taniguchi1; Shishadzu Corp., Soraku-gun, Kyoto

TP 427  Demonstration of using Isolation Waveform Beam Type Selected-Reaction-Monitoring on a QqLT Mass Spectrometer; Qingyu Song1; Jae C Schwartz1; Philip M Remes1; Dumitrescu Dean1; 1Thermo Fisher Scientific, San Jose, CA

TP 428  Advancements in Multi Reflecting High Resolution TOF Mass Spectrometry with Folded Flight Path; Viatcheslav Arteya1; Michael Mason1; Peter A Willis1; George Tikhonov1; Yury Khasin1; Anatoly Verenchikov1; 1LECO Corporation, St Joseph, MI; 2MSC-CG, Bar, Montenegro

TP 429  A Study of Ion Acceleration in tightly Curved Collision Cells; Felician Munlean1; Desmond A Kaplan1; Brucker Daltonics, Inc., Billerica, MA

TP 430  Performance of the Orbitrap Fusion Lumos Tribrid in Single-shot Analyses of Human Samples; Guadalupe Espadas1;2; Eva Borras1;2; Cristina Chiva1;2; Eduard Sabidó1;2; 1Proteomics Unit, Center for Genomic Regulation, Barcelona, Spain; 2Proteomics Unit, Universitat Pompeu Fabra, Barcelona, Spain

TP 431  NTOF Geometry for QqTOF; Bill Lloyd1; Robert E. Hauffler2; 1SCIEX, Concord, ON; 2AB Sciex, Concord, ON

TP 432  Optimization of the Performance of Toroidal Ion Trap by Theoretical Simulation; Haoyang Yang1; Chengsheng Xu2; Chuan-Fan Ding2; 1Fudan University, Shanghai; 2Fudan University, Shanghai, China

TP 433  A Mathematical and Simulation Study of General Toroidal Ion Trap Mass Spectrometer Devices; Robert H Jackson1; Steve Lammert2; Daniel Austin3; Karl Warnick4; Jessica Higgs5; Edgar Lee1; 1Instrumental Design Physics, LLC, Littleton, MA; 2PerkinElmer, Inc., American Fork, UT; 3Brigham Young University, Provo, UT; 4Bruker Daltonics GmbH, Bremen, Germany

TP 434  Radio Frequency Trapping of Ions in a Pure Toroidal Potential Distribution; Jessica Higgs1; Brae V. Petersen1; Steven A. Lammert2; Karl F. Warnick3; Daniel E. Austin4; 1Brigham Young University, Provo, UT; 2PerkinElmer, American Fork, UT

TP 435  Simulation of Ion Motion in Non-Ideal Electric Fields Generated by Novel FTICR Mass Analyzers; Joshua Driver1; Andry Kharchenko1; Jon Amster1; 1Univ of Georgia, Athens, GA

TP 436  Cross-field Drift of Ions and Non-Linear ICR Cell Arrays; Sung-Gun Park1; Gordon Anderson2; James Bruce3; 1University of Washington, Seattle, WA; 2GAA Custom Engineering, LLC, Benton, WA

TP 437  Moving Practical Mass Spectrometry Beyond the Molecular Realm; Roland Jertz1; Claudia Kriete1; Matthias Witt1; Jochen Friedrich1; Christopher Thompson1; Michael L Easterling2; Eugene N Nikolaev2; Goekhan Baykut1; 1Bruker Daltonic GmbH, Bremen, Germany; 2Bruker Dalitontics Inc., Billerica, MA; 3Bruker Daltonic, Billerica, MA; 4The Institute for Energy Problems of Chemical Physics Russian Academy of Sciences, Moscow, Russia

TP 438  A Timing Control Method to Prevent Ion Overtake in a Mult-turn Time-of-Flight Mass Spectrometer (infiTOF); Miki Shinichi1; Hirofumi Nagaao2; Michisato Toyoda3; 1MSI, Tokyo, INC, Chofu, Tokyo, Japan; 2Osaka University, Toyonaka, Osaka, Japan

TP 439  Improving m/z Resolution in Charge Detection Mass Spectrometry by Reduction of Ion Trap Energy Dependence; Joanna Hogan1; Martin F Jarrold1; 1Indiana University Department of Chemistry, Bloomington, IN

TP 440  A Novel, Miniaturized Linear Wire Ion Trap Mass Analyzer; Qinghao Wu1; Yuan Tian1; Ailin Li1; Daniel Austin1; Richard N Zare2; 1Brigham Young University, Provo, Utah; 2Stanford University, Stanford, CA

TP 441  New Analysis of the Bradford-Nielsen Gates with Space Charge as Applied to Time-of-flight Analyzers; Robert Jackson; Instrumental Design Physics, LLC, Littleton, MA

TP 442  Addressing the 100 Isotopologue Challenge: Orbitrap Mass Spectrometry as a Means of High-Dimension Clumped and Position-specific Isotope Analysis; John Eller1; Johannes Schwieters2; Dieter Juchelka3; Alexander Makarov4; Jens Grieb-Raming5; 1California Institute of Technology, Pasadena, CA; 2Thermo Fisher Scientific, Bremen, DE

TP 443  CZE-nanoESI-SLIM-IMS-MS Platform for Comprehensive, Ultrasilverative Proteome Analyses; Roza Wocjic1; Ian K Webb1; Yehia M Ibrahim1; Derek F Hopkins1; Spencer A Prost2; Randolph V Norheim1; Daniel J Oron1; Sandilla Giramella1; Liulin Deng1; Ahmed M Hamid1; Ryan T Kelly1; Erin Baker1; Richard D Smith1; 1PNNL, Richland, WA

TP 444  Separation of Protein Conformers by High Resolution Ion Mobility-Mass Spectrometry; Urs Rohner1; Michael Groessl1; Stephan Graf1; 1TOFWERK, Thun, Switzerland

TP 445  Protein Domain Structure Influences the Collision-Induced Ejection of Small Molecule Binders: Implications for the Development of Pharmaceutical Compounds; Rachel Martin1; Joseph Eschweiler1; Brandon T Ruotolo1; 1University of Michigan, Ann Arbor, MI

TP 446  Native and Denatured Protein Structural Studies using Ion Mobility MS and Ion Activation Techniques; Ruwan Kurulugama1; George C Stafford1; Joseph Eschweiler1; Brandon T Ruotolo1; John Fieldsted1; 1Agilent Technologies, Santa Clara, CA; 2University of Michigan, Ann Arbor, MI

TP 447  MS-based Epitranscriptomics: New Roles for Ion Mobility and Fragmentation Techniques; Daniele Fabris1; Rebeca D’Esposito1; Jennifer Lippens2; Michael Miller3; William McIntyre1; Rebecca Rose1; 1The RNA Institute, University at Albany, Albany, NY; 2The RNA Institute, University at Albany, Albany, NY

TP 448  Analysis of Native-Like Protein and Protein Complex Ions using Structures for Lossless Ion Manipulations; Samuel J. Allen1; Rachel M. Eaton1; Matthew F. Bush1; 1University of Washington, Seattle, WA
TP 449 Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Rapidly Detect Subtle Differences in Antibody Glycoforms; Yuwei Tian1; Brandon T Ruotolo1; 1University of Michigan, Ann Arbor, MI

TP 450 Ion Mobility Employed as a Second Dimension Separation of Isomeric Glycoforms in Glycopeptides; Gege Xu1; Elisha Goonatilleke1; Jasmine Davis1; Mariana Barboza1; Carlito B Lebrilla1; 1UC Davis, Davis, CA - California

TP 451 Water-Mediated Dimerization of Ubiquitin Ions Captured by Cryogenic Ion Mobility-Mass Spectrometry; Kelly SERVAGE1; David H Russell2; 1Texas A&M University, College Station, TX; 2Texas A&M University, College Station, TX

TP 452 Structural Investigation and Binding Site Determination of Huntingtin Protein/Peptide-ligand Complexes by IMS-HDX-MS/MS and Molecular Dynamics Simulations; Samaneh Ghasabeh Kondalaj1; Mahdiar Khakinejad1; Stephen J Valentine1; Justin Legleiter1; 1West Virginia University, Morgantown, WV

TP 453 An LC/ESI-IM-MS/MS Assay for Identification and Quantification of Host Cell Proteins in Therapeutic Monoclonal Antibodies; Catalin Doneanu1; Brad J Williams1; Ian Morns1; Andrew Borthwick1; Jackson Pope1; Ying-Qing Yu1; Weibin Chen1; 1Waters Corporation, Milford, MA; 2Waters Corporation, Beverly, MA; 3Waters, Necastle upon Tyne, UK; 4Waters, Necastle upon tyne, UK; 5Waters, Milford, MA

TP 454 Rapid Profiling of Cellular Extracts using Ion Mobility-Mass Spectrometry; Brett Harper1; Brooke BROWN1; Touraj SOLOUKI1; Baylor University, Waco, TX

TP 455 Integrating Ion Mobility Separation into Peptide Mapping for Therapeutic Protein Characterization: Qualitative and Quantitative Aspects; Ying-Qing Yu1; Liuxi Chen1; Henry Y Shion1; Weibin Chen1; 1Waters, Milford, MA

TP 456 Evaluation of Formulation-Induced Aggregation in Peptide Drug Products by IMS-MS; Elizabeth E Pierson1; Nicholas A Pierson1; Paul L Walsh1; 1Merck Research Laboratories, Rahway, NJ

TP 457 Investigation of the Interaction between Antimicrobial Peptides and Lipid Membranes Using Ion Mobility Mass Spectrometry Coupled with Isothermal Titration Calorimetry; Angi Chen1; John W Patrick1; David H Russell1; 1Texas A&M, College Station, TX

TP 458 Monitoring Conformational Landscape of Prion Protein; Guillaume Van der Rest1; Human Rezaei2; 1Université Paris-Sud, Orsay, France; 2INRA, Jouy-en-Josas, France; 3CNRS, Orsay, France

TP 459 Structural transitions of Bovine Serum Albumin Studied by IMS–IMS–MS; Alexander D Jacobs1; Joseph D Eschweiler2; Sugyan Dixi2; Brandon T Ruotolo2; David E Clemmer1; 1Indiana University, Bloomington, IN; 2University of Michigan, Ann Arbor, MI

TP 460 Characterization of Cytochrome c Intramolecular Interactions using nanoESI-HDX-TIMS-MS and Molecular Dynamics; Juan Camilo MOLANO1; Khoa Pham1; Jaroslava Miksovska1; Mark E Ridgway2; Melvin Park2; Francisco Fernandez-Lima2; 1Florida International University, Miami, FL; 2Bruker Daltonic, Billerica, MA

TP 461 Effects of Chain Length on the cis/trans Isomerization Mediated Folding of Polyproline Helices: Daniel W Woodall1; Tarick J El-Baba2; David E Clemmer1; 1Indiana University Dept. Chemistry, Bloomington, IN

TP 462 Introduction of Hydropic Sites: How Physical Modifications Alter the Conformer Preferences of Gramicidin A; John Patrick1; David H Russell2; 1Texas A&M, college station, TX; 2Texas A&M University, College Station, TX

TP 463 Characterization of Kinetically Trapped Intermediates of Microperoxidase-11 using TIMS-MS/MS and Molecular Modeling; Jacob Porter1; Alyssa Garabedian1; Paolo Benigni1; Jaroslava Miksovska1; Francisco Fernandez-Lima2; 1Florida International University, Miami, FL

TP 464 Proline Influences the Binding of Zinc to Oxytocin; Daniel R. Fuller1; Matthew S. Glover2; DuYong Kim2; David H. Russell2; David E. Clemmer1; 1Indiana University, Bloomington, IN; 2Texas A&M University, College Station, TX

TP 465 Determination of the Gas-Phase Energy Landscape of Substance P by IMS-IMS-MS; Chris Cong1; David H Russell2; David E Clemmer1; 1Indiana University, Bloomington, IN; 2Texas A&M, College Station, TX

TP 466 Analysis of Ionic Self-Complementary Peptides by Ion Mobility Spectrometry-Mass Spectrometry; Zhichao Zhang1; Daniel R. Fuller1; Tarick John El-Baba2; David E Clemmer1; 1Indiana University Dept. Chemistry, Bloomington, IN

TP 467 Comparison of Ion Mobility and Capillary Electrophoresis Mass Spectrometry Techniques for Cysteine Connectivity Identification of Peptides Bearing Intra-Molecular Disulfide Bonds; Philippe Massonnet1; Cédric Delvaux2; Gregory Upert1; Jean R. N. Haler1; Jan Jordens2; Maarten Honing2; Ynze Mengerink2; Johann Far1; Nicolas Gilles1; Loic Quinton1; Edwin De Pauw1; 1University of Liége, Liége, Liége; 2Laboratory of Mass Spectrometry - ULG, Liége, Belgium; 3CEA, DSV/IBiTec – SIMOPRO, Gif-sur-Yvette, France; 4DSM Resolve, Geleen, The Netherlands

TP 468 Using Gas Phase Comformations to Understand the Role of Solvent in Establishing Biomolecule Structure in Solution; Tarick El-Baba1; Daniel Fuller1; DoYong Kim2; Dylan Rogers3; Faizan Khan3; David A Hales3; David H Russell2; David E Clemmer1; 1Indiana University Dept. Chemistry, Bloomington, IN; 2Texas A&M, College Station, TX; 3Hendrix College, Conway, AR

TP 469 Separation of Isomers in Lipidomics and Metabolomics Experiments by High Resolution Ion Mobility-Mass Spectrometry; Michael Grossi1; Stephan Graft1; 1TOFWERK, Thun, Switzerland

TP 470 High Resolution Trapped Ion Mobility Mass Spectrometry Analysis of Isomeric Compounds; Sven W Meyer1; Peter Sander1; Alexander Harder1; Detlev Suckau1; 1Bruker Daltonic GmbH, Bremen, Germany

TP 471 Peptide Elution Rate Equation: a Novel Ideal Elution Model to Help Retention Time Prediction; Wenyuan Lu1; Xiaohui Liu1; Pengyuan Yang1; 1Fudan University, Shanghai, China

TP 472 Evaluating Effects of Metagenome Database Quality and and an Optimized LC/LC-MS/MS Approach for Obtaining Deeper Proteome Coverage of Complex Microbial Communities; Rasmunder Iyer1; Richard J Giannone2; Rose S Kantor3; Susan T.L Harrison4; Robert J Hudy4; Jillian F Banfield5; Robert L Hettich6; 1Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN; 2Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; 3Department of Plant and Microbial Biology, University of California, Berkeley, CA; 4Centre for Bioprocess Engineering Research, Department of Chemical Engineering, University of Cape Town, Cape Town, South Africa; 5Department of Earth and Planetary Sciences, University of California, Berkeley, CA

TP 473 Universal Derivatization of Metabolites for Improved Sensitivity in LC-MS; James Edwards1; Saint Louis University, St Louis, MO
TP 474 Optimization of Size Exclusion Chromatography and Atmospheric Pressure Ionization Enabling Characterization of Intact Lignin and Its Degradation Products; Anastasia Artemyeva1; Kubatova Alena1; Evgenii I. Kozliak1; 1University of North Dakota, Grand Forks, ND.

TP 475 Characterization of Electrochemically Decomposed Lignin Using Liquid Chromatography-High Resolution Mass Spectrometry; Tobias Dier1; Sarah Henrikus1; Verlaine Fosso1; Rolf Hempelmann1; Dietrich A Volmer1; 1Saarland University, Saarbrücken, Germany.

TP 476 Deeper Proteomics using Actively Modulated Online HILIC×nRPLC-HRMS; Andrea Gargano1; 1Martin Samonig1; Michael Woldergebril1; Remco Swart1; Gary Corthals1; Peter Schoenmakers1; 1VU University Amsterdam, Amsterdam, Netherlands; 2University of Amsterdam, Amsterdam, The Netherlands; 3Thermo Fisher Scientific GmbH, Germering, Germany; 4University of Amsterdam, Amsterdam, NL.

TP 477 Low-Temperature Mobile Phase for Peptide Trapping at Elevated Separation Temperature Prior to Nano RP-HPLC-MS/MS; Matthias Schöbinger1; Oskar-James Klein1; Goran Mitulovic2; 1Saarland University, Saarbrücken, Germany; 2Medical University of Vienna, Clinical Institute of Laboratory Medicine, Wien, Austria.

TP 478 Porous Graphitic Carbon Packed Capillaries for the LC-MSMS Analysis of RNA Modified Nucleosides; Robert Ross1; Peter Sarin1; Hannes Drexler1; Sebastian Leidel1; Patrick A Limbach1; 1University of Cincinnati, Cincinnati, OH; 2Max Planck Institute for Molecular Biomedicine, Munster, Deutschland.

TP 479 Redesign of Peptide Mapping Gradients to Resolve Complex Biological Samples; Xinli Yang; Rosalind Franklin University, North Chicago, IL.

TP 480 LC/MS/MS Method for the Determination of Tricyclic and Tetracyclic Antidepressants in Human Urine; Amber Awad1; Kendra Parker1; Lawrence Andrade1; 1Dominion Diagnostics, N. Kingstown, RI; 2Dominion Diagnostics, North Kingstown.

TP 481 A Fast and Sensitive Chiral LC-MS/MS Assay for Ketamine and its Metabolites in Human Plasma; Michel Coutou1; Evgenii Fedorov1; Jean-François Larocque1; Simon Bourgeois3; 1Biotrial Bioanalytical Services, Laval, QC; 2University of North Dakota, Grand Forks, ND; 3University of California Los Angeles, Los Angeles, CA.

TP 482 Proteomics Needs Better Chromatography; Evgenia Shishkova1; Alexander S Hebert1; Michael S Westphall1; Joshua J Coon1; 1JJ Coon Research Group, Madison, WI; 2UCLA, Los Angeles, CA; 3University of North Dakota, Grand Forks, ND.

TP 483 A Novel Approach to Studying Thiamine Kinetics: an LC/ESI-MS/MS-based Method for the Analysis of Thiamine and Derivatives in Biological Samples; Jaeah Kim1; Jason Zatre1; Michael G Bartlett1; 1University of Georgia, Athens, GA.

TP 484 A Functional Group Approach to Determining the Effects of Mobile Phase Modifiers on the Negative Ion ESI Ionization Efficiency; Melanie Odenkirk1; 1University of Georgia, Athens, GA; 2Forschungszentrum Jülich GmbH, Zentralinstitut für Engineering, Elektronik und Analytik, Jülich, Deutschland.

TP 485 A Fast LC/MS/MS Method for High Sensitivity Determination of 24 Perfluorocompounds in Textiles; Jun Xiang Lee1; Jun Xiang Lee1; 1University of North Dakota, Grand Forks, ND; 2Shimadzu (Asia Pacific) Pte Ltd, Singapore.

TP 486 Exploring the Effects of Alternative Dynamic Exclusion Algorithms on Peptide Identification Experiments; Nina Solter1; Graeme C McAlist1; Derek Bailey1; Vlad Zabrouskov1; 1Thermo Fisher Scientific, San Jose, CA; 2University of North Dakota, Grand Forks, ND.

TP 487 Targeted Profiling of Oxytrophs and Endocannabinoids in Biological Samples using the Nanoflow ionKey/MS system – Method Development and Validation; Sandra Gouveia-Figueira1; Malin Linder Nordling1; 1Umea University, Umea, SE.

TP 488 The Simultaneous Detection of a Panel of Drugs of Abuse in Post-mortem Hemolyzed Blood Samples (n=40) by LC-ESI-laminar Flow MS/MS; Sabra Botch-Jones1; Raquel LeBlanc1; 1Boston University School of Medicine, Boston, MA.

TP 489 UHPLC Optimization Study for Improved LC-MS Performance and Throughput; Martin Rude1; Thermo Fisher Scientific, Germering, Germany.

TP 490 A Study of the γ-Ray-labelling of Di-Dodecyl Di-Octyl Diglycolamide (D3DODGA) using UHPLC-ESI-MS Analysis; Kristyn M Johnson1; Christopher A Zarzana1; Gary S Groenewold1; Bruce J Mincher1; Andreas Wilden1; Holger Schmidt1; Giuseppe Modolo1; Beatrix Santiago-Schübel1; 1Idaho National Laboratory, Idaho Falls, ID; 2Forschungszentrum Jülich GmbH, Institut für Energietechnik- Nukleare Entsorgung und Reaktorsicherheit, Jülich, Germany; 3Forschungszentrum Jülich GmbH, Zentralinstitut für Experimentelle Medizin, Elektronik und Analytik, Jülich, Deutschland.

TP 491 The Use of a HILIC Peptide Retention Prediction Model to Predict the Presence of Modifications in Histones; Majors Badgett1; Barry Boyes1; Ron Orlando1; 1The University of Georgia, Athens, GA; 2Advanced Materials Technology, Wilmington, DE.

TP 492 Automation and Remote Visualization of Screening Data; David M Cox1; Burkhard Schaefer1; John Gibbons3; Viktor Iassinskii3; 1SCIEX, Concord, ON; 2BSSN Software, Darmstadt, Germany; 3SCIEX, Concord, ON.

TP 493 Long Term Test on a New Four-Channel HPLC; Pengxiang Yang1; BC cha1; Terry N Olney1; John Brann1; Christopher Elicone1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Franklin, MA.

TP 494 New Supercharging Agents for TFA-Based LC-MS of Peptides and Proteins; Michael Nehanian1; Rachel Loo2; Joseph A Loo2; 1University of California Los Angeles, Los Angeles, CA; 2University of North Dakota, Grand Forks, ND.

TP 495 Matrix Effects: Do They Differ between SFC/ESI-MS and LC/ESI-MS?; Alfred Svan1; Mikael Hedeland1; 1; Torbjörn Arvidsson1; 2; Curt E Pettersson1; 1Uppsala University, Uppsala, Sweden; 2National Veterinary Institute (SVA) Dept. of Chemistry, Environment and Food Hygiene, Uppsala, Sweden; 3Medical Products Agency, Uppsala, Sweden.

TP 496 Development of a Novel Nano Separation Device for Robust and Accurate Gradient Delivery with Intelligent Automation and Remote Visualization of Screening Technology; Wilmington, DE.

TP 497 Targeted Profiling of Oxytrophs and Endocannabinoids in Biological Samples using the Nanoflow ionKey/MS system – Method Development and Validation; Sandra Gouveia-Figueira1; Malin Linder Nordling1; 1Umea University, Umea, SE.

TP 498 The Simultaneous Detection of a Panel of Drugs of Abuse in Post-mortem Hemolyzed Blood Samples (n=40) by LC-ESI-laminar Flow MS/MS; Sabra Botch-Jones1; Raquel LeBlanc1; 1Boston University School of Medicine, Boston, MA.

TP 499 UHPLC Optimization Study for Improved LC-MS Performance and Throughput; Martin Rude1; Thermo Fisher Scientific, Germering, Germany.

TP 500 A Study of the γ-Ray-labelling of Di-Dodecyl Di-Octyl Diglycolamide (D3DODGA) using UHPLC-ESI-MS Analysis; Kristyn M Johnson1; Christopher A Zarzana1; Gary S Groenewold1; Bruce J Mincher1; Andreas Wilden1; Holger Schmidt1; Giuseppe Modolo1; Beatrix Santiago-Schübel1; 1Idaho National Laboratory, Idaho Falls, ID; 2Forschungszentrum Jülich GmbH, Institut für Energietechnik- Nukleare Entsorgung und Reaktorsicherheit, Jülich, Germany; 3Forschungszentrum Jülich GmbH, Zentralinstitut für Experimentelle Medizin, Elektronik und Analytik, Jülich, Deutschland.

TP 501 The Use of a HILIC Peptide Retention Prediction Model to Predict the Presence of Modifications in Histones; Majors Badgett1; Barry Boyes1; Ron Orlando1; 1The University of Georgia, Athens, GA; 2Advanced Materials Technology, Wilmington, DE.

TP 502 Automation and Remote Visualization of Screening Data; David M Cox1; Burkhard Schaefer1; John Gibbons3; Viktor Iassinskii3; 1SCIEX, Concord, ON; 2BSSN Software, Darmstadt, Germany; 3SCIEX, Concord, ON.

TP 503 Long Term Test on a New Four-Channel HPLC; Pengxiang Yang1; BC cha1; Terry N Olney1; John Brann1; Christopher Elicone1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Franklin, MA.

TP 504 New Supercharging Agents for TFA-Based LC-MS of Peptides and Proteins; Michael Nehanian1; Rachel Loo2; Joseph A Loo2; 1University of California Los Angeles, Los Angeles, CA; 2University of North Dakota, Grand Forks, ND.

TP 505 Matrix Effects: Do They Differ between SFC/ESI-MS and LC/ESI-MS?; Alfred Svan1; Mikael Hedeland1; 1; Torbjörn Arvidsson1; 2; Curt E Pettersson1; 1Uppsala University, Uppsala, Sweden; 2National Veterinary Institute (SVA) Dept. of Chemistry, Environment and Food Hygiene, Uppsala, Sweden; 3Medical Products Agency, Uppsala, Sweden.

TP 506 Development of a Novel Nano Separation Device for Robust and Accurate Gradient Delivery with Intelligent Automation and Remote Visualization of Screening Technology; Wilmington, DE.
TP 500 Integrated Software for Data Processing and Analysis in Direct Infusion Ultra-High Resolution / Accurate Mass Spectrometry Based 'Top-Down' Lipidomics Workflows: Yasuto Yokoi; Yukihiro Fukamachi; David Peake; Reiko Kiyonami; Eileen Ryan; Gavin E Reid; Mitsui Knowledge Industry Co, Tokyo, Japan; Thermo Fisher Scientific, San Jose, CA; University of Melbourne, Victoria, Australia

TP 501 A Lipid Mass Spectral Library for Human Plasma: Paul D Hutchins; Dain R Braderman; Jason W Russell; Michael S Westphal; Joshua J Coor; University of Wisconsin Madison, Madison, Wisconsin; Genome Center, University of Wisconsin, Madison, WI; Department of Chemistry, University of Wisconsin, Madison, WI; Morgan Institute for Research, Madison, WI; Biomolecular Chemistry, University of Wisconsin, Madison, WI

TP 502 SimLipid: Software Platform for Automating Shotgun, LC-MS and MALDI-MS Based High-Throughput lipidomics: Ningsomban Sanib Meinli; Himani Gupta; Arun Apte; PREMIER Biosoft, India, India; PREMIER Biosoft, Palo Alto, CA

TP 503 Structural Characterization of Membrane Glycolipids from Marine Sponge-associated Bacteria by Mass Spectrometry: Benjamin L Oyler; Courtney E Chandler; Fan Zhang; Christopher J Thompson; Jeremy J Wolff; Michael L Easterling; Robert K Ernst; Russell T Hill; David R. Goodlett; University of Maryland, Baltimore, Whiteford, MD; University of Maryland, Baltimore, Baltimore, MD - Maryland; University of Maryland Center for Environmental Science, Baltimore, MD - Maryland; Bruker Daltonics, Billerica, MA

TP 504 Identification and Quantitation of Unsaturated Glycerolipids from Human Plasma using the Paternò-Büchi Reaction and Tandem Mass Spectrometry: Hilary Brown; Yu Xia; Purdue University, West Lafayette, IN

TP 505 Study and Optimization of online Paternò-Büchi Reactions for Structural Analysis of Unsaturated Lipids using Mass Spectrometry: Xiaoxiao Ma; Pei Su; Zheng Ouyang; Yu Xia; Purdue University-Weldon School of Biomedical Engineering, West Lafayette, IN; Purdue University-Department of Chemistry, West Lafayette, IN

TP 506 Top-down Structural Elucidation of Gram-negative Bacterial Endotoxins by Tandem Mass Spectrometry: Mohd M. Khan; Benjamin L Oyler; Kelsey A. Gregg; Robert K. Ernst; Alan S. Cross; David R Goodlett; University of Maryland School of Pharmacy, Baltimore, MD; Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD; Department of Microbial Pathogenesis, University of Maryland School of Dentistry, Baltimore, MD; Center for Vaccine Development, University of Maryland School of Medicine, Baltimore, MD

TP 507 Structural Characterization of Lipid Biomarkers from Staphylococcus aureus following Microextraction for Mass Spectrometric Phenotyping: Lisa Leung; Benjamin Oyler; Robert Ernst; David R Goodlett; University of Maryland, Baltimore, MD; University of Maryland School of Pharmacy, Baltimore, MD; University of Maryland School of Pharmacy, Baltimore, MD; University of Maryland School of Pharmacy, Baltimore, MD

TP 508 N-Succinylation of L-lysyl-phosphatidylglycerol in Bacillus subtilis: Paulos Chumala; Metin Atila; George Katselis; Yu Luo; University of Saskatchewan, Saskatoon, Canada; University of Saskatchewan, Saskatoon, SK

TP 509 Systematic Fragmentation of Lipid A Variants by Multiple and Hybrid MS/MS Techniques: Christopher Martin Crittenden; William Ryan Parker; Jennifer S. Brodbelt; University of Texas at Austin, Austin, TX

TP 510 In-situ Characterization of Phospholipids Mixture on Tissue Sections using Wide Ion Gate HE-CID Experiment and ASDF MS/MS Spectra: Saiona Salivo; Yuzo Yamazaki; Peter Quinto Tranchida; Luigi Mondello; Omar Belgacem; University of Messina, Messina, Italy; Shimadzu Corporation, Kyoto, Japan; Shimadzu, Kratos Manchester, United Kingdom

TP 511 Using MS/MS and MSn to Distinguish Cytotoxic J-series Prostaglandin Isomers Produced in Tumorigenic Keratinocytes: Robert Kobet; Rukiyah T, Van Dross; Allison S. Daniel; East Carolina University, Greenville, NC

TP 512 Conformational Atlas of 7 Classes of Sphingolipids and Glycerophospholipids Mapped by Ion Mobility-Mass Spectrometry: Katrina L. Leapord; Jody C. May; James N. Dodds; John A. McLean; Vanderbilt Dept. of Chemistry, Nashville, TN

TP 513 Differentiation of Triacylglycerol Rich Oligosaccharides Using Differential Ion Mobility Spectrometry: Jinyuan Wang; Larry J Campbell; Paul RS Baker; SCIEX, Redwood City, CA; SCIEX, Concord, ON

TP 514 Identification of Lipid Metabolites of Docosahexaenoic and Arachidonic Acids in Human Blood Using Stable Isotope Labeled Compounds: Karl R Kevala; Mark Sanders; Hee-Yong Kim; National Institutes of Health, Bethesda, MD; Thermo Fisher Scientific, Somerset, NJ

TP 515 Identification and Characterization of Sulfolipids Found in Nitzschia palea: Larry Sallans; Daniel Betz; Stephen F Macha; Edna S. Kaneshiro; University of Cincinnati, Cincinnati, OH; University of Cincinnati, Cincinnati, OH

TP 516 Role of pH and Mobile Phase Modifiers on Untargeted RP LC-MS Analysis of Lipid Extracts: Elena Sokol; David Peake; Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; Thermo Fisher Scientific, San Jose, CA

TP 517 Identification of Metabolites of Novel Sphingoid Bases in Sphingolipid-depleted Cells using Liquid-Chromatography Electrospray Tandem Mass Spectroscopy: Brandon M Kenwood; Samuel Kelly; Jingting Duan; Alfred H Merrill Jr; Cameron Sullards; Georgia Institute of Technology, Atlanta, GA

TP 518 Identification of a Novel Lipid Family Containing a Modified Head Group: Seetaramanjaneleyu Gundimeda; Anunukumar Padmanaban; Agilent technologies, bangalore, kannataka; Agilent technologies, Bangalore, India

TP 519 Influence of Sampling Techniques on Human Blood Metabolome Stability during the Long-Term Sample Storage: Kristaps Klaivins; Guido Dallmann; Therese Koal; Biocrates Life Science AG, Innsbruck, Austria

TP 520 Determination of Selectivity Influenced by Liquid-Liquid Extraction in Global Metabolomics using UHPLC-qTOF-MS: Albert Elmqist; Mikael Karl Robert Engskog; Jakob Haglöf; Torbjörn Arvidsson; Curt Pettersson; Department of Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; Department Medicinal Chemistry; Analytical Pharmaceutical Chemistry, Uppsala University Uppsala, Sweden; Medical Product Agency, Uppsala, Sweden

METABOLOMICS: SAMPLE PREPARATION

TP 521 - 529
TP 521 Widely Targeted Analysis of Hydrophilic Anionic Metabolites in Mammalian Cells by Ion Chromatography Coupled with High Resolution Mass Spectrometry; Yoshitomo Izumi1; Takahiro Suzuki2; Motokazu Kimura3; Shigeru Sakamoto2; Takeshi Bamba3; Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; 1Thermo Fisher Scientific Japan, Tokyo, Japan; 2Medical Institute of Bioregulation, Kyushu Univ. Fukuoka, Japan

TP 522 Systematic Assessment and Selection of Liquid and Solid-Phase Methods in the Design of Sequential Extraction Protocols for LC-MS Based Metabolomics; Dmitri Silnikov1; Cian S Morin2; Dajana Vuckovic3; 1Concordia University, Montreal, Canada

TP 523 Metabolomic evaluation of conditions favoring mycotoxin production in isolates of Fusarium fungi; Mark Busman1; USDA, ARS, NCAUR, BFP, Peoria, IL

TP 524 Metabolite Phenotyping of Cell Lines by Rapid Evaporative Ionization Mass spectrometry; Emrys Jones1; Emmanuelle Claude2; James Langridge3; Fiona Henderson1; Adam W McMahon2; Zoltan Takats3; Steve Pringle1; 1Waters Corporation, Wilslmow, UK; 2Wolfson Molecular Imaging Centre, Manchester, UK; 3Imperial College London, South Kensington Campus London, United Kingdom

TP 525 Non-targeted Metabolite Profiling and Antioxidant Activity of Genetically Diverse Soybean Seeds; Yongsoo Choi1; Jiuliang Xu2; Jeong-Sook Shin3; Jung-Kyung Moon4; 1Korea Institute of Science and Technology, Gangneung, South Korea; 2Korea Institute of Science and Technology, Geagneung, South Korea; 3National Institute of Crop Science, Cheongu-Si, Chungbuk

TP 526 Detection Enhancement of Small Molecules, Lipids and Peptides by Functionalizing Silicon Nanopost Arrays with Fluorous Monolayers; Heather Anderson1; Nicholas Morris1; Matthew Powell2; Trust T Razunguzwa1; 1Virginia Bioinformatics Institute, Virginia Tech, USA; 2University of Virginia School of Medicine, Charlottesville, VA

TP 527 Characterizing Temporal And Inter-Individual Functional Differences in Infant Gut Microbiome by a Metaproteomics Approach; Weil Xiong1; Michael Morowitz2; Jillian Banfield3; Robert Hetlich1; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Pittsburgh, Pittsburgh, PA; 3University of California, Berkeley, CA

TP 528 Sub-Minute, Comprehensive Metabolomics Measurements for Disease and Exposure Research; Xing Zhang1; Michelle V Romm2; Erika M Zink3; Daniel J Bolster4; Yehia M Ibrahim1; Mark S Wrona2; Giorgis Isaac3; 1Department of Medicine, 2Environmental Sciences, 3Biosciences, 4Bacterium following Introduction of a Novel Pathway; 1Department of Medicine, 2Environmental Sciences, 3Biosciences, 4Bacterium following Introduction of a Novel Pathway; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of North Florida, Jacksonville, FL; 3University of Wisconsin Madison, Madison, WI

TP 529 Online-SPE-HILIC-ESI-MS Analysis of Redox Cofactors in Chlamydomonas Reinhardtii Algae Cells; Alexander Schriewer1; Heiko Hayen2; 1Institute of Inorganic and Analytical Chemistry, University of Muenster, Muenster, Germany

TP 530 Rapid Detection of Pathogenic Amoeba in Water Distribution Systems using UPLC-MS; Zhihao Yu; Haylea Miller1; Geoffrey Fuzon2; Brian H Clowers3; 1Washington State University, Pullman, WA; 2CSIRO Land and Water, Perth, Australia

TP 531 Isolation and Characterization of Marine Natural Products Using UPLC-QToF-MS Coupled to a Novel Informatics Platform; Roger G. Linton1; Jeni L. Kurita2; Jimmy Yuk1; Kate Yu2; Mark Wrona3; Giorgis Isaac2; 1Simon Fraser University, Burnaby, BC, Canada; 2Waters Corporation, Milford, MA

TP 532 Metabolomic Profiling in Pulmonary Arterial Hypertension Disease Models; David P Mariano1; Caiyun grace Li2; Jan K Hennigs3; Marlene Rubinitch4; Michael Snyder1; 1Stanford University School of Medicine, Palo Alto CA, USA

TP 533 Characterizing Temporal And Inter-Individual Functional Differences in Infant Gut Microbiome by a Metaproteomics Approach; Weil Xiong1; Michael Morowitz2; Jillian Banfield3; Robert Hetlich1; 1Oak Ridge National Laboratory, Oak Ridge, TN; 2University of Pittsburgh, Pittsburgh, PA; 3University of California, Berkeley, CA

TP 534 Isotopic Ratio Outlier Analysis (IROA) Global Metabolome Interrogation of an Actinomycete Bacterium following Introduction of a Novel Pathway; Felice de Jong1; Taylor A. Lundy2; Christopher W W Beecher3; Amy L. Langer4; 1IROA Technologies LLC, 2UCLA, Los Angeles, CA; 3NIST, Rockville, MD; 4University of North Florida, Jacksonville, FL

TP 535 Increasing Arginine Production in C. Glutamicum by Rational Strain Design and Discovery Metabolomics; Linking HRA QTOF Data to Biology; Frederik Walter1; Marcus Persicke1; Aiko Barsch1; Christian Ravnborg2; Heiko Neuwege3; Matthias Szesny2; Nikolas Kessler2; Jörn Kalinowski1; Bielefeld University, Bielefeld, Germany; 1IROA Technologies, 2Bruker Daltonics Ltd, Bremen, Germany; 3Bruker Daltonics, Bremen, Germany

TP 536 Isolation and Chemical Characterization of Marine Natural Products Using UPLC-QToF-MS Coupled to a Novel Informatics Platform; Roger G. Linton1; Jeni L. Kurita2; Jimmy Yuk1; Kate Yu2; Mark Wrona3; Giorgis Isaac2; 1Simon Fraser University, Burnaby, BC, Canada; 2Waters Corporation, Milford, MA

TP 537 Metabolite Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDichips; Christopher George1; Haddon Goodman1; Gregory Boyce1; 1Protea Biosciences, Morgantown, WV

TP 538 Metabolomic Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDichips; Christopher George1; Haddon Goodman1; Gregory Boyce1; 1Protea Biosciences, Morgantown, WV

TP 539 Environmental Exposure to Ionizing Radiation Induces DYSbiosis in Gut Microbiome and Fecal Metabolome; Maryam Goudarzi1; Jonathan Jacobs2; Tytus Mak3; Bo-Hyun Moon4; Steve Strawn5; Jonathan Braun6; David Brenner7; Albert Fornace Jr.; 1Molecular Imaging Centre, Manchester, UK; 2University of Wisconsin Madison, Madison, WI; 3University of North Florida, Jacksonville, FL; 4University of Florida, Gainesville, FL

TP 540 Abiotic Stresses Influence Organic Metabolite Profiles in Soils Hosting Populus Trees and a Microbial Community; Charles J. Doktycz1; Collin M. Timm1; Keiji G Asano1; David J Weston2; Dale A. Pelletier3; Greg Hurst4; 1Oak Ridge National Laboratory, Oak Ridge, TN

TP 541 Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway; Loren V Olson1; Baltij Ubi2; 1SCIEX, Redwood City, CA

TP 542 Untargeted Metabolomics with Fungal Artificial Chromosomes (FAC-MS) Allows Discovery and Facile Dissection of Natural Product Biosynthesis; Kenneth D Cleverenger1; Jin Woo Bok2; Rosa Ye3; Galen P Miley4; Thomas Veik5; Cynthia Chen6; KalHoua Yang7; Peng Gao8; Matthew Lamprecht9; Paul M Thomas1; Md Islam2; Chengcang C Wu1; Nancy P Keller1; Neil Kelleher2; 1IROA Technologies, 2Bruker Daltonics Ltd, Bremen, Germany; 3Bruker Daltonics, Bremen, Germany

TP 543 Novel Informatics Platform for the Analysis of Metabolomic Flux, Kinetics and Pathway; Loren V Olson1; Baltij Ubi2; 1SCIEX, Redwood City, CA

TP 544 Isotopic Ratio Outlier Analysis (IROA) Global Metabolome Interrogation of an Actinomycete Bacterium following Introduction of a Novel Pathway; Felice de Jong1; Taylor A. Lundy2; Christopher W W Beecher3; Amy L. Langer4; 1IROA Technologies LLC, 2UCLA, Los Angeles, CA; 3NIST, Rockville, MD; 4University of North Florida, Jacksonville, FL

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TP 546 Metabolomic Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDichips; Christopher George1; Haddon Goodman1; Gregory Boyce1; 1Protea Biosciences, Morgantown, WV

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TP 548 Metabolomic Profiling of Glyphosate Exposed Saccharomyces cerevisiae with REDichips; Christopher George1; Haddon Goodman1; Gregory Boyce1; 1Protea Biosciences, Morgantown, WV

TP 549 Environmental Exposure to Ionizing Radiation Induces DYSbiosis in Gut Microbiome and Fecal Metabolome; Maryam Goudarzi1; Jonathan Jacobs2; Tytus Mak3; Bo-Hyun Moon4; Steve Strawn5; Jonathan Braun6; David Brenner7; Albert Fornace Jr.; 1Molecular Imaging Centre, Manchester, UK; 2University of Wisconsin Madison, Madison, WI; 3University of North Florida, Jacksonville, FL; 4University of Florida, Gainesville, FL

TP 550 Abiotic Stresses Influence Organic Metabolite Profiles in Soils Hosting Populus Trees and a Microbial Community; Charles J. Doktycz1; Collin M. Timm1; Keiji G Asano1; David J Weston2; Dale A. Pelletier3; Greg Hurst4; 1Oak Ridge National Laboratory, Oak Ridge, TN

TP 551 Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway; Loren V Olson1; Baltij Ubi2; 1SCIEX, Redwood City, CA

TP 552 Untargeted Metabolomics with Fungal Artificial Chromosomes (FAC-MS) Allows Discovery and Facile Dissection of Natural Product Biosynthesis; Kenneth D Cleverenger1; Jin Woo Bok2; Rosa Ye3; Galen P Miley4; Thomas Veik5; Cynthia Chen6; KalHoua Yang7; Peng Gao8; Matthew Lamprecht9; Paul M Thomas1; Md Islam2; Chengcang C Wu1; Nancy P Keller1; Neil Kelleher2; 1IROA Technologies, 2Bruker Daltonics Ltd, Bremen, Germany; 3Bruker Daltonics, Bremen, Germany
In vivo Analysis of Metabolites in Single Embryonic Cells in the Developing Frog (Xenopus) Embryo using Microcapillary-Sampling CE-ESI-MS; Erika Portero; Rosemary M Onjiko; Sally A Moody; Peter Nemes; The George Washington University, Washington, DC

Eavesdropping on Marine Microbial Communication: Influence of Quorum Sensing on the Vibrio campbellii Metabolome; Gregory Ellis; Brian J. Eddie; Stefano A. Torres Padua; W. Judson Hervey IV; Gary J. Vora; Dagmar H. Leary; National Research Council NRL Fellow, Washington, DC; American Society of Engineering Education NRL Fellow, Washington, DC; University of Puerto Rico Mayaguez, Mayaguez, PR; Center for Bio/Molecular Science and Engineering, Naval Research Laboratory, Washington, DC

Untargeted 2-Sample-Comparison using High-Resolution Data from LC/ION Mobility Q-TOF Mass Spectrometers via a Novel 4D Molecular Feature Extraction Algorithm; Frank Kuhlmann; Xiangdong Li; Ed Darland; Agilent Technologies, Santa Clara, CA

Metabolic Profiling of Strawberry Leaves Infected by Xanthomonas fragariae using UPLC/QTOF Mass Spectrometry; Min-Sun Kim; Geum-Sook Hwang; Korea Basic Science Institute, Seoul, Republic of Korea; Korea Basic Science Institute, Seoul, Republic of Korea

Global Metabolomics Approach to Identify Pathways Affected by Glyphosate in Yeast; Gregory Boyce; Mark Szewcz; Protea Biosciences, Morgantown, WV

Chemical Profiling of Actaea Species and Commercial Products using UPLC-QTOF-MS; Jimmy Yuki; Maged Sharaf; Kate Yu; Mark Wrona; Giorgis Isaac; Waters, Milford, MA; American Herbal Products Association, Silver Spring, MD

Non-targeted Differential Screening using LC-HRAM-MS as a Tool for Evaluating Differences in Chemical Composition between Samples and Sample Groups; Daniel Arndt; Arno Knorr; Philip Morris International, Neuchâtel, Switzerland

Non-targeted Differential Screening of Complex Matrices using GC/GC-TOFMS for Comprehensive Characterization of Chemical Composition and Determination of Significant Differences; Martin Almstetter; Arno Knorr; Quentin Dutertre; Elliott Martin; Antonio Castellon; Pavel Pospisil; Mark Bentley; Philip Morris International, Neuchâtel, Neuchâtel

Atmospheric Pressure Gas Chromatography Mass Spectrometry (APGC-MS) Based Metabolomics Profiling of Grape Volatiles; Manoj Ghaste; Giuseppe Astarita; Puvlio Mattivi; Vladimir Shulaev; University of North Texas, Denton, TX; Fondazione Edmund Mach, San Michele all’Adige TN, Italy; Waters, Milford, MA

Comparison of Direct Introduction on Orbitrap Fusion and FT-ICR at High-end Resolution for Global Metabolite Screening; Uli Martin Hohenester; Pierre Barbier Saint Hilaire; BenoîtColsch; François Fenaille; Jean-claude Tabet; Christophe Junot; Richard B Cole; Commissariat à l’énergie atomique et aux énergies alternatives, Gil Sur Yvette Cedex, Fr; Sorbonne Universités, UPMC Univ Paris 06, Institut Parisien de Chimie Moléculaire, Paris, Fr

Development of High-Performance Chemical Isotope Labeling LC-MS for Profiling Alcoholic Hydroxyl-Containing Metabolites in Metabolomics; Shuang Zhao; Liang Li; Department of Chemistry, University of Alberta, Edmonton, AB, Canada

Metabolomic Profiling of Food Diets Using Ion Chromatography with High Resolution Orbitrap Mass Spectrometry; Terri Christison; JUNHUA WANG; Linda Lopez; Ralf Tautenhahn; Thermo Fisher Scientific Inc, Sunnyvale, CA; Thermo Fisher Scientific Inc, San Jose, CA; Thermo Fisher Scientific, San Jose, CA

Metabolic Profiling of Bladder Cancer Cell Lines Reveals Molecular Alterations Involved in Methylation and Novel Epigenetic Phenotypes; Feng Jin; Rashmi Krishnapuram; Franklin Gu; Satil Kumar Bhowmik; Suman Malty; Mohan Manikam; Friedrich-Carl von Rundstedt; Vasantia Pulluri; Yair Lotan; Jonathan Levitt; Seth P Lerner; Cristian Coarfa; Benny Abraham Kaiparettu; Arun Sreekumari; Nagireddy Pulluturi; Baylor College of Medicine, Houston, TX; University of Texas Southwestern Medical Center, Dallas, TX

DNA Modification Mapping – Software Development; Ningxi Yu; Patrick A Limbach; University of Cincinnati, Cincinnati, Ohio

Development of a Computational Algorithm to Predict Mobile Phase Additives for Optimal LC-MS Sensitivity of Oligonucleotides; Babak Basiri; Michael G Bartlett; University of Georgia, Athens, GA

A Flow Injection Inductively Coupled Plasma Mass Spectrometry Method for Quantification of Modified Oligonucleotides; Fanyu Meng; Qiay Tu; Erin Guidry; Merck & Co., Inc, Rathway, NJ; Merck, Darmstadt, International R&D, Neuchâtel, Switzerland

Comparison of Q-Tof, Q-Exactive and Triple Quad for Quantitative Bioanalysis of Oligonucleotide Therapeutics; Yuhuan Ji; Qian Liu; Qian Li; Chengjie Ji; Laixin Wang; NovaBioAssays, LLC, Woburn, MA

A Micro-SCES/LCMS/MS Quantitative Assay for Phosphorodiamidate Morpholino Oligomer (PMOplus®) AVI-7288 in Human Plasma; Ahhua Liu; Jianbo Zhang; Qian Guo; Bryce Ashby; Scott Reuschel; Jay S. Charleston; Joe Rutkowski; Min Meng; Covance, Lake City, UT; Sarepta Therapeutics, Cambridge, MA

Determination of a 15-mer Antisense Oligonucleotide in Mouse Plasma by LC/MS/MS; Lili Xing; Ying Han; Yi Tao; Xinping Fang; Xin Zhang; WuXi AppTec Co., Shanghai, CHINA

A Sensitive Liquid Chromatogram/Mass Spectrometry Method for the Determination of a Therapeutic siRNA in Human Plasma; Pei Li; Jianbo Zhang; Qian Guo; Bryce Ashby; Scott Reuschel; Joe Rutkowski; Min Meng; Covance, Lake City, UT; Sarepta Therapeutics, Cambridge, MA

Differential Mass Spectrometry Analysis of Transfer RNA by Stable Isotope Labelling; Mellie Paulines; Patrick A Limbach; University of Cincinnati, Cincinnati, OH

Evaluating the Specificity of RNase U2 Variants By Mass Spectrometry; Beulah Mae Ann Solviso; Ningxi
| TP 581 | On-Line Monitoring of Oligonucleotide Manufacturing Using a Compact Mass Spectrometer; Stilianos G. Roussias; Andrew Rodriguez; Isaiah Cedillo; Josh Brooks; Claus Rentel; Ionis Pharmaceuticals, Inc., Carlsbad, CA; Ionis Pharmaceuticals, Carlsbad, CA |
| TP 582 | Use of Tricationic Ion-Pairing Compounds for the Detection of Nucleotides from Single Cells; ye quan; Rachel Wocwocfski; Wei Rao; Ning Pan; Anthony Burgett; Zhibo yang; University of Oklahoma, department of Chemistry & Biochemistry, Norman, OK |

**PEPTIDES: PTM IDENTIFICATION**

- TP 583 | Ultra-sensitive Motif-targeting Approach for Measurement of Tyrosine Phosphorylation Stoichiometry in EGFRT, Yan-Chen Liao; Chia-Feng Tsa; Miao-Hsia Lin; Pei-Yi Lin; Yasushi Ishihama; Yu-Ju Chen |
- TP 584 | Comprehensive Peptidomapping Analysis Reveals Acetylation-engaged Enhancement of Thermogenesis in White Adipocytes; Hsin-Yi Chang; Kosaku Shinoda; Shingo Kajimura; Yasushi Ishihama; Department of Molecular and Cellular Bioanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; UCSF Diabetes Center and Department of Cell and Tissue Biology, University of California, San Francisco, USA |

**Low-abundance Protein Phosphorylation**

- TP 585 | Identification of Complex Glycosylated and Disulfide-Bonded Peptides Presented by the MHC Class II Processing Pathway in Melanoma; Stacy Malaker; Michael J Ferracane; Florence R Depontieu; Angela L Zalring; Jeffrey Shabanov; Dina L Bai; Engeland H Victor; Suzanne L Topalian; Donald F Hunt; University of Virginia, Charlottesville, VA; University of Florida, Gainesville, Florida; Johns Hopkins University School of Medicine, Baltimore, MD |

**Ultra-sensitive Motif-targeting Approach for Measurement of Tyrosine Phosphorylation Stoichiometry**

- TP 586 | Development of Rapid LC-MS3 Methodology for In-depth Structural Analysis of Lewis Antigens and Their Sialylated Derivative Isomers using Authentic Standards; Yapino Lin; Chein-Hung Chen; Fang-Chi Liu; Chia-Lin Wu; Jung-Lee Lin; Chien-Tai Ren; Chung-Yi Wu; Chung-Hsuan Chen; Academia sinica, Taiwan; Academia Sinica, Taiwan; Academia Sinica, Taipei, Taiwan |

**Sialo-glycoproteomic Profiling using Zwitter-Ionic Hydrophilic Interaction Chromatography (ZIC-chHILIC)**

- TP 587 | Proteome Dynamics Reveal Temporal Regulation of O-GlcNAcylation/phosphorylation in Determining Apoptosis of Activated B Cells; Hsin-Yi Wu; Jung-Lin Wu; Cheng-Tsung Lu; Yi-Ju Chen; Tzong-Yi Lee; Chih-Wei Chien; Yi-Ting Wang; Chun-Cheng Lin; Kay-Hooi Kho; Yu-Ju Chen; Kuo-I Lin; Instiute of Chemistry, Academia Sinica, Taipei, Taiwan; Department of Microbiology and Immunology, National Yang-Ming University, Taipei, Taiwan; Department of Computer Science and Engineering, Yuan Ze University, Taipei, Taiwan; Institute of Chemistry, Academia Sinica, Taipei, Taiwan; TAIWAN (R.O.C.); Department of Chemistry, National Tsing Hua University, Taipei, Taiwan; Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan |

**Proteome Dynamics**

- TP 588 | Identification of Isomeric Mono-Methylated Nucleosides in Ribonucleic Acids by Liquid Chromatography – Mass Confirmation and Impurity Profiling; Yung-Shiong LI; Robert Birdsell; Joe Fredette; Ying-Qing Yu; Waters Corporation, Milford, MA |
| TP 590 | Efficient Enrichment of SUMOylated Peptides from Alpha-lytic Protease Digest Using K-\&GG Remnant Immuno-affinity Purification: Hongbo Gu1; Xiaoying Jia1; Jian Min Ren1; Elizabeth Komives2; Matthew P Stokes1; 1Cell Signaling Technology, Danvers, MA; 2Department of Chemistry and Biochemistry, UCSD, La Jolla, CA |
| TP 591 | An Improved Strategy for In-depth and Site-specific Analysis of the SUMO Proteome: Ivo A Hendriks1; Clifford Young1; Michael L. Nielsen1; 1NFF Center for Protein Research, Copenhagen, Denmark |
| TP 592 | Ubiquitinated Proteins in MDSC Exosomes Analyzed by High Resolution Tandem Mass Spectrometry: Katherine Adams1; Yan Wang1; Suzanne Ostrand-Rosenberg1; Catherine Fenselau1; 1University of Maryland, College Park, MD; 2University of Maryland, Baltimore County Baltimore, MD |
| TP 593 | Low Mass Ions in Peptide CID Spectra are Diagnostic of Lysine Posttranslational Modifications: Tobias Maile1; Tommy K Cheung1; Corey Bakalari1; Marie Classon1; David Arnold1; 1Genentech Inc, South San Francisco, CA |
| TP 594 | Quantitative Profiling of the Enzymatic Activity of the Protein Lysine Mono-methyltransferase SYMYD2 using SILAC-based Proteomics: Jonathan B Olsen1; Xing-Jun CAC1; Bomie Han1; Lisa Hong Chen1; Alexander Horvath1; Timothy I Richardson1; Robert M Campbell1; Benjamin A Garcia1; Hannah Nguyen1; 1El Lilly and Company, Indianapolis, IN; 2University of Pennsylvania, Philadelphia, PA |
| TP 595 | Characterizing Post-Transailationally Modified Peptides by High-Resolution FAIMS Coupled to Electron Transfer Dissociation: Matthew Baird1; Alexandre A Shvartsburg1; 1Wichita State University, Wichita, KS |
| TP 596 | Innovative Characterization of Hair from pre-Hispanic Andean Mummies using Mass Spectrometry: Margaux Fresnai1; Pascale Richardin1; Marcela Sepúlveda1; Emmanuelle Leize-Wagner1; Armelle Charrié-Duhaut1; 1Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes, UMR 7140 CNRS-Université de Strasbourg, Strasbourg, France; 2Centre de Recherche et de Restauration des Musées de France (C2RMF), Paris, France; 3Laboratorio de Análisis e Investigación Arqueométricas, Instituto de Alta Investigación, University of Tarapacá, Arica, Chile |
| TP 597 | Identification and Characterization of Covalent Modification of Catechol Estrogens on Proteins: Hui-Hui Chen1; Chieh-Ming Fang1; Ming-Chun Ku1; Shu-Hui Chen1; 1Chemistry Dept, NCKU, Tainan, Taiwan (R.O.C.) |
| TP 598 | Comprehensive Analysis of Post-translational Modifications in Proteins Exposed to Metal Catalyzed Oxidation: Martin Ryker1; Birte Svensson1; Kim Henriksen1; Per Hägglund1; 1Technical University of Denmark, Kgs Lyngby, Kgs Lyngby; 2Technical University of Denmark, Systems biology, KGS Lyngby, DK; 3Nordic Bioscience A/S, Herlev, DK |
| TP 599 | Quantitative Profiling of Prokaryotic Post Translational Modifications: Charles L Farnsworth1; Jian Min Ren1; Jake A Namaroni1; Xiaoying Jia1; Kimberly A Lee1; Matthew P Stokes1; 1Cell Signaling Technology, Danvers, MA; 2Cell Signaling Technology, Inc, Danvers, MA |
| TP 600 | Charged Isotope Tag Improves Identification of Hydrophobic Peptide-Ligand Adducts: Melissa Budelien1; James Janetka1; Douglas Covey1; Alex Evers1; 1Washington University in St Louis, St Louis, MO |
| TP 601 | Alkylamine Ion-pairing Agents for Improved Positive Mode Electrospray Ionization Analysis of Sulfated Peptides: Philip McClory1; Kristina Hakansson1; 1University of Michigan, Ann Arbor, MI |
| TP 602 | N-Terminal Charged-based Fractional Diagonal Chromatography (ChaFRADIC) to Study Proteolytic Events in Procoagulant Platelets: Fiorella Andrea Solari1; Saskia A. Venne1; Nadine J.A. Matthie1; Julia M. Burkhart1; Frauke Swieringa1; Peter W. Collins1; Judith M.E.M Cosemans3; Albert Sickmann2; Johan W.M. Heemskerk1; René P Zahedi1; 1Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund, Germany; 2Leibniz-Institut für Analyt. Wissenschaft. - ISAS -, Dortmund, Germany; 3Department of Biochemistry, Cardiovascular Research Institute Maastricht (CARIM) Maastricht University Maastricht, Maastricht, Netherlands; 4Arthur Bloom Haemophilia Centre, School of Medicine, Cardiff University, Cardiff, United Kingdom |
| TP 603 | Using TIMS Mass Spectrometry to Resolve Competitive Isomeric Post-Translational Modifications: Joshua Silveira1; Joe Gomez1; Melvin Park1; Kristofer Fritz1; Brucker Daltonic, Billerica, MA; 2University of Colorado, Anschutz Medical Campus, Aurora, CO; 3University of Colorado, Anschutz Medical Campus, Denver, CO |
| TP 604 | Methylyome: Sara C. Larsen1; Kathrine B. Sylvestersen1; Andreas Mund1; Maria V. Madsen1; David Lyon1; Jeremy A. Daniel1; Lars J. Jensen1; Michael L. Nielsen1; 1NFF Center for Protein Research, Copenhagen, DENMARK |
| TP 605 | Method Development for Complete Mutation and Posttranscriptional Modification Characterization of KRAS4b using Recombinant Proteins in Combination with LC-MS/MS: Zhaojing Meng1; William Gillette1; Stephen Andrew1; Ming Zhou1; 1Frederick National Laboratory for Cancer Research, Frederick, MD |
| TP 606 | MULTIPLEXED TARGETED ANALYSIS 606 - 623 | PHOSPHOPROTEOMES: QUANTITATIVE ANALYSIS 606 - 623 |
| TP 607 | Comparative Phosphoproteomic Analysis of Hippocampal Tissue in a Non-Human Primate Model of Type 1 Diabetes Maintained using Exogenous Insulin: Fang-Ko Huang1; Jose Morales-Corraliza1,2,3; Paul M. Mathews2,3; Thomas A. Neubert1; 1Skirball Institute of Biomolecular Medicine, New York University School of Medicine, New York City, NY; 2Center for Dementia Research, Nathan Kline Institute, Orangeburg, NY; 3Department of Psychiatry, New York University Langone Medical Center, New York City, NY |
| TP 608 | Large-scale Targeted Analysis of Post-translational Modifications by Internal Standard-Triggered Parallel Reaction Monitoring: Application to Determination of Phosphorylation Site Occupancy: Bruno Domen1; Sara Rosali1; Adele Bourraud1; Sebastien Gallien1; 1Luxembourg Clinical Proteomics Center, Strassen, Luxembourg |
| TP 609 | Global Phosphoproteomics of Targeted Combinatorial Therapy in Hepatocellular Carcinoma to Identify Molecular Signatures of Effective Therapy: Joseph Capri1; Whitaker Cohn1; Thuc Le1; Kym F Faul1; Julian P Whitelegge1; 1UCLA, Los Angeles, CA |
TP 611 Phosphoproteome Analysis Reveals Rapid Reprogramming of Signaling Networks of Drug Treated Cancer Cells: Heiner Koch,1, 2, 3; Melanie Schoof; Benjamin Ruprecht; Susan Klaeger; Scarlet Beck; Martin Frejno1, 5; Mathias Wilhelm;1 Hannes Hahnhe; Bernhard Kuster1, 2, 3, 7;1 Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 2German Cancer Consortium (DKTK), Munich, Germany; 3German Cancer Research Center, Heidelberg, Germany; 4Max Planck Institute for Biochemistry, Martinsried, Germany; 5Oxford University, Oxford, United Kingdom; 6OmicScouts GmbH, Freising, Germany; 7Center for Integrated Protein Science, Munich, Germany

TP 612 Effect of Exercise on Skeletal Muscle Phosphoproteome in Obese Insulin Resistant Adults: Danjun Ma; Lisa Guth; Yue Qi; Michael Caruso; Xiangmin Zhang; Jeffrey Horowitz; Zhengping Yi; Wayne State University, Detroit, MI; 2University of Michigan, Ann Arbor, MI

TP 613 Quantitative Phosphoproteomic Analysis of Circadian Cycling in Genetically Modified Arabidopsis: Jae Chol; Jenny Chen; John D Rogers; Dotti A Nusinow; Bradley S Evans;1 Thermo Fisher Scientific, Rockford, IL; 2Thermo Fisher Scientific, San Jose, CA; 3Donald Danforth Plant Science Center, St Louis, MO

TP 614 Differential Mass Spectrometry Analysis Reveals Differential Hypoxic Response in Ovarian Cancer Cells with Different Metastatic Potential: Xuemei Zeng; Huang Huang; Xin Huang; Nathan A Yates;1 University of Pittsburgh, Pittsburgh, PA

TP 615 Rapid Quantitative Phosphoproteome by Tandem Mass Tags: Haiyan Tan; Bing Bai; Kxosheng Wang; Yuxin Li; Ji-Hoon Cho; Tim Shaw; Junmin Peng;2 St.Jude Children’s Research Hospital, memphis, TN; 2St Jude Children’s Research Hospital, Memphis, TN

TP 616 High Throughput Multiplexed Phosphoproteomics Identifies Drivers of Resistance to ALK Inhibitor Treatment in Lung Cancer: Amanda L. Edwards;2, 3; Luc Friboulet;2, 3; Vinoth Nallaparthy;2, 3; Kristine Yu;4 David Ruddy;5 Jeffrey A. Engelman;2, 3; Wilhelm Haas;1, 2, 3, 7;1 Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 2German Cancer Research Center, Heidelberg, Germany; 3German Cancer Consortium (DKTK), Munich, Germany; 4Max Planck Institute for Biochemistry, Martinsried, Germany; 5Oxford University, Oxford, United Kingdom; 6OmicScouts GmbH, Freising, Germany; 7Center for Integrated Protein Science, Munich, Germany

TP 617 Inferring Kinase Network Activity from Activation-loop Phosphopeptides by Data-Independent Acquisition MS: Sander Piersma; 1Thermo Fisher Scientific, Rockford, IL; 2University of Alberta, Edmonton, AB, Canada

TP 618 Prediction of Protein Kinase Substrates using Primary Sequence Preference and Quantitative Phosphoproteomics: Haruna Imamura; Pasrawin Taechawattananant;1 Omar Waghi;2 Naoyuki Sugiyama;1 Pedro Beltrao;2 Yasushi Ishihama1; 2Harvard Medical School, Boston, MA; 3Translational Clinical Oncology, Novartis Institutes for Biomedical Research, Cambridge, MA

TP 619 Absolute Quantitation of Site-specific Phosphorylation of Insulin Receptor by a Nano UPLC-MS Method: Zhongping Liao;1 Kyoung-soo Choi;2 Jason X Tang;2 Eli Lilly and Company, Indianapolis, IN

TP 620 Evaluation of Search Engines for Phosphopeptide Identification and Quantitation: Xiaoyue Jiang; David M Horn;2; Ryan D Bomgardner;2 Tara Schroeder;2 Rosa I Viner;2 Andreas Huhmer;3 Steven Danielson;1 Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Rockford, IL; 3Thermo Fisher Scientific, Somerset, NJ; 1Thermo Fisher, San Jose, CA

TP 621 Dimethylated Alanine (DiAla)-assisted Large-scale Protein Phosphorylation Stoichiometry Characterization: Qiong Yu1; Yu Feng;2 Lingjun Li;2 University of Wisconsin-Madison, Madison, Wisconsin; 2University of Wisconsin-Madison, Madison, WI

TP 622 High Resolution-Enabled 12-plex DiLeu Tagging for Quantitative Phosphoproteomics Profiling of Vascular Smooth Muscle Cells: Xiaofang Zhong;2 Christopher Lietz;2 Xudong Shi;2 Amanda Buchberger;2 Dustin Frost;2 Craig Kent;2 Lingjun Li;1 University of Wisconsin-Madison, Madison, WI

TP 623 Sensitive and Accurate Quantitation of Phosphopeptides using TMT Isobaric Labeling Technique: Xiaoyue Jiang;2 Ryan D Bomgardner;2 Rosa I Viner;2 Andreas Huhmer;1 Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Rockford, IL

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS

TP 624 Using Native MS to inform Statistical Thermodynamic Models of Cooperativity: Melody Pepsi Holmquist;1 Elhii C Ihms;2 Vicki H Wysocki;3 Mark P Foster;1 Ohio State University, Columbus, OH

TP 625 Native MS analysis of chemically stabilized protein complexes: evidence for non-covalent stabilization of protein-protein interactions: Roman Subbotin;1 Dominic Paul B Olinares;1 Julio C Padovan;1 Megan Kelley;1 Zheng Ser;2 Brian T Chait;1 The Rockefeller University, New York, NY

TP 626 Probing Nucleotide-dependent Changes in the Oligomeric State of MORC Proteins using Native Mass Spectrometry: Jonathan Johnston;2 Linda Yen;2 Steven E Jacobsen;2 Alma L Burlingame;1 UCSF, San Francisco, CA; 2UCLA, Los Angeles, CA

TP 627 Characterization of a Protein-DNA Complex by Native Mass Spectrometry and Ultraviolet Photodissociation: Jake Rosenberg;1 Alyssa Garabedian;2 Fenei Leng;2 Francisco Fernandez-Lima;1 Jennifer S Brodbelt;1 University of Texas at Austin, Austin, TX; 2Florida International University, Miami, FL

TP 628 Investigating the Gas-Phase Conformation of Fibroblast Growth Factor 1 upon Binding of Heparin/HS Using Traveling Wave Ion Mobility Spectrometry (TWIMS): Yuejie Zhao;1 Jon Amster;1 Arunima Singh;2 Robert Woods;2 Yongmei Xu;2 Jian Liu;2 Chengli Zong;2 Geert-Jan Boons;2 Fuming Zhang;2 Robert Linhardt;2 University of Georgia, Chemistry Department Athens, GA; 2University of Georgia, CCRC Athens, GA; 3University of North Carolina, Chapel Hill, NC; 4Rensselaer Polytechnic University, Troy, NY

TP 629 Screening Glycolipids Against Proteins in vitro using Picodiscs and Electrospray Ionization Mass Spectrometry: Jun Li;1 Xuxin Fan;1 Elena N Ktova;1 John S Klassen;1 University of Alberta, Edmonton, AB, Canada

TP 630 Detecting Protein-Glycolipid Interactions using Glycomicelles and Car-ESI-MS: Ling Han;1 Elena N Kitova;1 John S Klassen;1 University of Alberta, Edmonton, Canada

TP 631 Characterization of Heparin Interactions with its Client Proteins: Mapping Minimal Protein-Binding Domains within Glycosaminoglycan Chains using Top-down mass spectrometry: Yunlong Zhao;1 Igor A Kaltashov;1 University of Massachusetts Amherst, Amherst, MA

TP 632 Screening Human Milk Oligosaccharides Against Proteins using Catch-and-Release Electrospray Ionization Mass Spectrometry: Yaile Chen;1 Km Shams-Ud-Doha;1 Elena N Ktova;1 Lars Bode;2 John S Klassen;1 University of Alberta, Edmonton, Canada; 2University of California, San Diego La Jolla, CA
TP 633  Label Free, LC-MS Based Approaches to Quantitate Small Molecule-Receptor Binding: Kun Chen; Merck Research Labs, Kenilworth, NJ

TP 634  Label-free Size Exclusion Chromatography Mass Spectrometry for the Characterization of Protein Complex Composition and Stability; Paola Cavaliere1; Nadia Iqbal1; Noah E. Dephoure1; ‘Weill Cornell Medical College, New York, NY

TP 635  Information-Rich Gas-Phase Analysis of Non-Covalent Protein Complexes and Released Subunits for Primary and Quaternary Structure Analysis; Deepali Ratthore1; Forouzan Abdazizi1; Eric D. Dodds1; ‘University of Nebraska-Lincoln, Lincoln, NE

TP 636  Study of Noncovalent Interactions of Hydroxylated Polybrominated Diphenyl Ethers with Serum Albumins and Estrogen Receptors Using Ion Mobility Spectrometry-Mass Spectrometry; Qiang Ma1; Liang-Hong Guo2; ‘Chinese Academy of Inspection and Quarantine, Beijing, CHINA; ‘Chinese Academy of Sciences, Beijing, CHINA

TP 637  Investigating the Noncovalent Complex Formation of Proteins with Electolytic Ligands in Gas Phase; Mehmet Atakaya1; Haci Mehmet Kayili1; Bekir Salih1; ‘Hacettepe University, Department of Chemistry, Ankara, Turkey; ‘Cankiri Karatekin University, Cankiri, Turkey

TP 638  Probing the Stability of Noncovalent Interactions Responsible for Covalently Linked Diibiquitin Ion Structure using nESI-TWIMS-MS and CIU; Nicole Wagner1; David H Russell2; ‘Texas A&M University, College Station, TX

TP 639  Identification of Gpr78/BIP Protein Complexes using Affinity Mass Spectrometry; Dapeng Chen1; Yan Wang1; Eva R. Chin1; ‘University of Maryland, College Park, MD

TP 640  Comparison of Affinity-Purification Mass Spectrometry Workflow for Characterisation of Protein Complexes; Lu Yu1; Mercedes Pardo2; Jyoti Choudhary2; ‘Wellcome Trust Sanger Institute, Hinxton, Cambridgeshire; ‘Wellcome Trust Sanger Institute, Cambridge, United Kingdom

TP 641  Application of Affinity-purification Mass Spectrometry Based Predictive Mapping for Identification of RBM45 Protein Interactors in Amyotrophic Lateral Sclerosis; Krystine Garcia1; Yang Li2; Mahlon Collings3; Jiyan An4; Rachel Geiser1; Tony Tegeler1; Kristine Tsantilas1; Tony Tegeler1; Kristine Tsantilas1; Rachel Geiser1; Tony Tegeler1; Kristine Tsantilas1; ‘University of Pittsburgh School of Medicine, Pittsburgh, PA

TP 642  Nanoprobe-based Affinity Mass Spectrometry for Identification of Binding Glycophates and Protein-Protein Interaction of Galectin-8; Pin-Rui Su1; Chen Yi-Ju2; Lin Yu-Hsien3; Chen Yu-Ju4; ‘Department of Chemistry, National Taiwan University, Taipei, Taiwan; ‘Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ‘Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan

TP 643  Site-specific Characterization of Binding Interfaces in Gaseous HIV-1 RNA-protein Complexes; Eva-Maria Schneeberger1; Kathrin Breuker1; ‘University of Innsbruck, Innsbruck, Austria

TP 644  Novel Blue-Native-PAGE and Targeted Mass Spectrometry Strategy Enable robust and Accurate Quantification of the Kinetics of Protein-Ligand Interactions in Plasma; Shichen Shen1; Xiaotao Duan1; Bo An2; Yang Qu3; Joseph Balthasar4; Jun Qu5; ‘University at Buffalo, Buffalo, NY; ‘Beijing Proteome Research Center, Beijing, China

TP 645  A New Carbene Probe for Efficient Protein Footprinting Allows Mapping of Binding Sites by Mass Spectrometry; Lucio Manzi1; Andrew Barrow1; Daniel Scott1; Robert Layfield2; Timothy Wright1; John Moses1; Neil Oldham1; ‘University of Nottingham, Nottingham, UK

TP 646  Charting the Temporal Landscape of EGFR-stimulated EGFR Proteome; Yue Chen1; Sung Yun Jung1; Mei Leng1; Jong Min Choi2; Antrix Jain3; Anna Malovanavanya1; Yi Wang2; Jun Qin2; ‘Baylor College of Medicine, Houston, TX

TP 647  Development of a Novel Bioanalytical Platform for Anti-Drug Antibody using Immunocapture-LC/MS; Lin-Zhi Chen1; David Roos2; Eley Philip2; ‘Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; ‘Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT

TP 648  Novel Regulators of Alternative NF-κB Pathway Identified through Chemical Proteinomics; Bekim Bajrami1; Michelle Ols2; John Anderson3; Benbo Gao4; Brian Lucas5; Erik Het1; Alan Buckler6; Peter Juhass7; Ru Wei8; ‘Biogen Inc., Cambridge, MA

TP 649  Proteomic Analysis Provides Clues about Normal FUS Function and Its Role in ALS; Jing Chen1; Marisa Kamelgarn1; Alexandra Arenas1; Jianjun Zhai2; Haining Zhu1; Jozsef Gall3; ‘University of Kentucky, Lexington, KY

TP 650  Global Analyses of the Oligomerization, Composition, and Dynamics of Membrane-Associated Protein Complexes; Zach McBride1; Ayal P Uma2; Chen Donglai3; Jun Xie4; Daniel Szymanski5; ‘Purdue University, West Lafayette, IN

TP 651  Mass Spectrometry Cleavealbe Cross-linking Approach for Large-scale Identification of Protein-Protein Interactions; Jayanta Kishor Chakrabartty1; Apeksha Bhatt2; Saiful M Chowdhury3; ‘University of Texas at Arlington, Arlington, TX

TP 652  Relative Abundance Comparative Analysis of ROS-induced Poly(ADP-ribose)-Associated Proteins by LC-MS/MS and Spectral Counting; Angel Islas-Robles1,2; Frances M Munoz3; Serrine S Lau4; Terrence J Monks2; ‘University of Arizona, Tucson, AZ; ‘Wayne State University, Detroit, MI; ‘Drexel University, Philadelphia, PA

TP 653  Fourier Transform Algorithm for Analysis of Mass Spectra for Heterogeneous Ions with Repeated Subunits; Sean P Cleary1; Jesse W Wilson2; Avery M Thompson1; James Prell1; ‘University of Oregon, Eugene, OR

TP 654  Development of Mass Spectrometry Method for the Unbiased Detection of Cytomegalovirus Proteins in Human Brain Tumor Specimens; Dhiman Ghosh1; Brian P Milless2; Philip R Gafken3; Charles S Cobbs1; ‘Swedish Neuroscience Institute, Seattle, Washington; ‘Fred Hutchinson Cancer Research Center, Seattle, Washington; ‘Fred Hutchinson Cancer Research Center, Seattle, WA

TP 655  Edgotypes and Quantitative Mass Spectrometry; James Bruce1; Juan Chavez2; Jimmy K Eng3; Arti Navare1; Devin Schwepp1; Xuei Wu1; Xuefei Zhong1; ‘University of Washington, Seattle, WA

TP 656  Histidine, Arginine’s Versatile Cousin; Amina S Woods1; Ludovic Muller1; Aurelie Roux2; Damon Barbacci3; Shelley N Jackson1; ‘NIH/NIDA-IRP, Baltimore, MD; ‘All Children’s Hospital, Johns Hopkins Medicine, Saint Petersburg, FL; ‘Jonas Grunske Inc, Houston, TX

TP 657  Examination of Aptamer-Protein Complex Structure by Mass Spectrometry; Guo-Ming Hung1; Pang-Hung Hsu1; ‘Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan

TP 658  Cross-linked PSMs in pepXML: a Common Format for Storing Cross-linked Search Results; Michael R. Hoopmann1; Luis Mendoza2; Eric W. Deutsch1; David Shteynberg1; Robert L Moritz2; ‘Institute for Systems Biology, Seattle, WA

TP 659  The Analysis and Identification of STAT3 Interactions and Modifications in the Mitochondria of Cancer Cells; Daniel Garama1; Ching-Seng Ang1; Nick Williamson1; Daniel Gough1; ‘Hudson Institute of Medical Research, Melbourne, Australia; ‘Bio 21 Institute, Melbourne, Australia
TP 660 Proteomic Profiling of Human Islets Collected from Pancreatic Tissue Sections using Laser Capture Microdissection; Lina Zhang; Giacomo Lanzoni; Matteo Battarra; Luca Inverardi; Qibin Zhang; 1, Kannapolis, NC; 2Diabetes Research Institute, University of Miami, Miami, FL; 3Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC

TP 661 Using Quantitative Proteomics to Profile Changes in Individual Immune Cell Types during an Immune Response; Allison Galassie; Johannes Golli; Parimal Samir; Travis Jensen; Kristen L Hoek; Leigh M Howard; Tara M Allos; Xinan Niu; Sebastian Joyce; Kathryn M Edwards; Andrew J Link; 1Department of Chemistry, Vanderbilt University, Nashville, TN; 2The EMMES Corporation, Rockville, MD; 3Department of Biochemistry, Vanderbilt University School of Medicine, Nashville, TN; 4Department of Pathology, Microbiology, and Immunology, Vanderbilt University School of Medicine, Nashville, TN; 5Vanderbilt Vaccine Research Program; Division of Infectious Diseases, Department of Pediatrics, Vanderbilt University School of Medicine, Nashville, TN; 6Veterans Administration Tennessee Valley Healthcare System, Nashville, TN

TP 662 LC-MRM Quantification of Protein Biomarkers in Human Saliva: In Saliva Veritas?; Jerome Vialaret; Nora Nowak; Audrey Gabella; Sylvain LEHMANN; Christophe Hirtz; 1LBPC, IRMB CHU Montpellier St. Eloi Montpellier, France; 2Centre Memoire Ressources Recherche Languedoc-Roussillon, CHU Montpellier, Montpellier, France

TP 663 Elucidating Cellular Heterogeneity in Tumors: a Combination of Antibody-Based Cellular Prefractionation and Ultrasensitive Proteomics; Evelyne Maes; Nathalie Cools; Inge Mertens; 1Dirk Valkenberg; 1, 2Patrick Pauwels; 3Qin Fu; 1Nora Nowak; 1Audrey Gabella; 2Sylvain LEHMANN; 3Christophe Hirtz; 1VITO, Mol, Belgium; 2Laboratory of Experimental Hematology, Vaccine & Infectious Disease Institute (VAXINFECTIO), University of Antwerp, Antwerp, Belgium; 3Center for Proteomics, Antwerp, Belgium; 4Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Diepenbeek, Belgium; 5Pathology Department, University Hospital Antwerp (UZA), Antwerp, Belgium; 6Center for Proteomics, Antwerp, Belgium

TP 664 LC-MS Platform for Identifying Protein Targets of Small-Molecule Binding Relevant to Disease and Metabolism; Reid O'Brien Johnson; Brett Lomenick; Jing Huang; Joseph A Luo; 1UCLA, Los Angeles, CA

TP 665 Simple, Robust, Highly Productive Methodology for LC-MS/MS Quantitative Analysis of Laser Capture Microdissected Tissue from FFPE Biopsies Requiring 10,000 Cells; John P Shapiro; 1Hannah Komar; 1Phil Gafken; 1Philip Hart; 1Darwin Conwell; 1Gregory Lesinski; 1Ohio State University, Columbus, Ohio; 2Fred Hutchinson Cancer Research Center, Seattle, WA

TP 666 Quantifying Signalling Pathway Activity using iMALDI (immuno-MALDI); Robert Popp; 1Andrew G Chambers; 1Adriana Aguilar-Mahecha; 2Oliver Pötz; 3Mark Basik; 4Christoph H. Borchers; 1, 2University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3Department of Oncology, McGill University, Montreal, QC, Canada; 4Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; 5University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 6Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada

TP 667 Automation of an immuno-MALDI assay for Quantifying Signalling Pathway Activity; Robert Popp; 1Björn Fröhlich; 2Andrew G Chambers; 1Yassene Mohammed; 2Adriana Aguilar-Mahecha; 2Oliver Pötz; 3Mark Basik; 4Christoph H. Borchers; 5, 6University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 7Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; 8Department of Oncology, McGill University, Montreal, QC, Canada; 9Natural and Medical Sciences Institute (NMI) at the University of Tübingen, Reutlingen, Germany; 10Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; 11Segal Cancer Proteomics Center, Lady Davis Institute, McGill University, Montreal, QC, Canada

TP 668 Can volumetric Absorptive Micro Sampling in the Presence of a Stable-Isotope Labeled Protein Standard Control Pre-Analytical Variability in Proteomics?; Irene van den Broek; Qin Fu; Kevin Millis; Timothy Eckersley; William W Wood; Michael P Kowalski; Tara R Jones-Roe; Stuart Kushb; Bobby Virasangh; Jennifer E Van Eyk; 2Advanced Clinical Biosystems Research Institute, Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA; 3Cambridge Isotope Laboratories, Inc. Tewksbury, MA; 4Beckman Coulter Life Sciences, Indianapolis, IN; 5Neoteryx, Torrance, CA

TP 669 Methodological Advances Applied to a Biomarker Study of Complex Samples from a Diseased Clinical Cohort of Limited Sample Availability; Stephen Kostel; Patricia Cho; Hui Zhou; John Froehlich; Richard Lee; 1Boston Children's Hospital, Harvard Medical School Boston, MA; 2Combined Analysis of Nucleic Acids and Protein for Cancer Research; Jared Isaac; Mazi Mohiuddin; 1Thermo Fisher Scientific, Kalamazoo, MI; 2Thermo Fisher Scientific, San Jose, CA

TP 670 Human Plasma Proteome Analysis using Meter-Long Monolithic Silica Columns with Match-between-Runs; Yi Ting Wang; Chia-Feng Tsai; Kazuhiro Sonomura; 1Yaushi Ishihama; Fumihiro Matsuda; 2Center for Genomic Medicine, Graduate School of Medicine Kyoto University, Kyoto, Japan; 3Graduate School of Pharmaceutical Sciences Kyoto University, Kyoto, Japan; 4Life Science Research Center, Technology Research Laboratory, Shimadzu Corporation, Kyoto, Japan

TP 671 A Chromosome-Centric Protein-Protein Interaction Profiling of MS-Based Proteome Datasets Derived from Laser-Microdissected Cancerous Cells of Lung Cancer Subtypes; Kiyonaga Fuji; Hiroyuki Kimura; Hideki Marushima; 1Rie Tagaya; Hisashi Saji; Noriaki Kurimoto; Sayaka Mikami; Yasuhiro Bando; Noboru Nakayama; 2Harubumi Kato; 3Toshihide Nishimura; 4Harukazu Nakamura; 5St. Marianna University School of Medicine, Meguro-ku, Tokyo; 6Biosys Technologies, Inc., Tokyo, Japan; 7Nizhishi Central General Hospital, Saitama, Japan High-resolution Quantitative Metaproteomics Pipeline: Documenting Effects of Dietary Changes; Boris Zvybavlov; 1Stephanie Byrum; 1Galina Glazko; 1Lisa Orr; 2Dorothy Kieffer; 3Sean Adams; 4Samuel Mackintosh; 5John Arthur; 6Brian D. Piccolo; 7Nosratola D. Vaziri; 8Shuman Liu; 9Wei L. Lau; 10Mahyar Khazaeli; 11Mary E. Moore; 12Roy J. Martin; 13University of Arkansas for Medical Sciences, Little Rock, AR; 14University of California, Davis, Davis, CA; 15Division of Nephrology, University of California, Irvine, Irvine, CA; 16Dept. of Food Science and Technology, University of California, Davis, Davis, CA; 17Obesity & Metabolism Research Unit, USDA, Davis, CA Investigation of Neutrophilic Proteins/Peptides in Periprosthetic Tissue by MALDI Imaging Mass Spectrometry; Rémi Longuepée; 1Rita Casadonte; Mark
TP 675 Generation of High Quality MALDI-TOF Serum Mass Spectra to Detect Hepatocellular Carcinoma in High-Risk Patients: Nicholas F Dupuis1; Maximillian Steers1; Alex A Nickel1; Gary P Pestano1; Fornelli1; Paul M Thomas1; Philip Compton1; John T Risk Patients

TP 676 Correlating Apolipoprotein Proteome Profiles to Cardiovascular Disease Risk Factors: A Translational Top-Down Proteomics Approach to Pathophysiology: Henrique dos Santos Seckler1; Kyungnon Kim1; Luca Forrelli1; Paul M Thomas1; Philip Compton1; John T Wilkins1; Neil L Kelleher1; Northwestern University, Evanston, IL; Northwestern Feinberg School of Medicine, Chicago, IL

TP 677 Application of Tissue Surrogate for Variance Calibration in Mass Spectrometry Based Amyloidosis Diagnosis: Han-Yin Yang1; Andrew N Hoofnagle1; Michael J MacCoss1; 1University of Washington, Seattle, WA

TP 678 Quantitative Analysis of Protein Composition in Amyloid Plaques from FFPE Specimens using Parallel Reaction Monitoring (PRM): Maria Stella Rittoro1; Oana Madalina Mereuta1; Janine Pichardo1; Ahmet Dogan1; Memorial Sloan Kettering Cancer Center, New York, NY

TP 679 Analysis of Native Proteolytic BNP Variants: Simultaneous Separation of Multiple Samples using Capillary Electrophoresis-Mass Spectrometry with Multi-Segment Injection: Shenyang Zhang1; Koen Raadschelders1; Jennifer Van Eyk1; Barbara Streisand Women’s Heart Center, Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA - California

TP 680 Implementation of siKALIP to Identify the Substrates of CDK5, a Kinase Linked to Severe Neurodevelopmental Disorders: Justine Arrington1; Juan Sebastian Paez Paez2; Madalina Mereuta1; Janine Pichardo1; Ahmet Dogan1; 1Memorial Sloan Kettering Cancer Center, New York, NY; 2Northwestern University, Evanston, IL

TP 681 Dried Blood Spots as a Simple Sample Collection Tool for Personalized Medicine: Jeffrey J. Jones1; Ryan Benz1 Phong Cun1; William Smith1; John Blume1; Applied Proteomics Inc., San Diego, CA

TP 682 Characterization of the Host Proteome within Virion Particles of Sindbis Virus: Andrew Kilianaski1; Amanda Piper2; Vancini Ricardo2; Raquel Hernandez2; Trevor Glaros1; 1ECBC, Apg, MD; 2North Carolina State University, Raleigh, North Carolina

TP 683 Mass Spectrometric Analysis of the Human Pathogen Cryptosporidium parvum: John Robert Haserick1; Deborah R Leon1; Yi Pu1; John Crawford Samuelson1; Catherine E Costello1; Boston University School of Medicine, Boston, MA; Boston University, Boston, MA; Boston University School of Dental Medicine, Boston, MA

TP 684 The Detection of a Clinically Relevant β-lactamase: CTX-M-15, Using MALDI-TOF MS: Jonathan B. Thacker1; John Barnwell3; Mary Patton1; Harlan Caldwell3; Alan Gradziel1; 1Memorial Sloan Kettering Cancer Center, New York, NY; 2Chlamydial Diseases Section, Laboratory of Clinical Infectious Diseases, NIAID, NIH, Bethesda, MD - Maryland

TP 685 Pseudomonas aeruginosa Develops Ciprofloxacin Resistance from Low to High Level with Distinctive Proteome Changes: Jianhe Peng1; Jeffrey Hill1; 1Experimental Therapeutics Centre, A-STAR, Singapore, Singapore; 2Experimental Therapeutics Centre, A-STAR, Singapore, Singapore

TP 686 Proteomics Analysis of Chlamydia trachomatis: Virulence-Plasmid Mediated Protein Expression Changes: Christopher C R Grant1; Stuart McCorrister1; Michael Patton1; Harlan Caldwell3; Alan Gradziel1; Grant McClarty1; National Microbiology Laboratory, Public Health Agency of Canada, Winnipeg, Canada; 2Chlamydial Diseases Section, Laboratory of Clinical Infectious Diseases, NIAID, NIH, Bethesda, MD - Maryland

TP 687 Mass Spectrometry Based Studies on Irreversible Inhibition of Recombinant Mycobacterium Tuberculosislissikimate Kinase by the Marine Sponge Metabolite Ilimaquinone: Angela Calderon1; Joharya Simithy1; Douglas Goodwin2; Mark T Hamann1; 1Auburn University, Auburn, AL; 2Auburn University, Auburn, Alabama; 3Medical University of South Carolina, Charleston, SC

TP 688 Determination of Hepatitis B Virus Infection by Means of Targeted Proteomics Strategy: Hsing-Fen Tsai1; He-Hsuan Hsiao1; 1NCHU, Department of Chemistry, Taichung, Taiwan

TP 689 A Key Retromer Trafficking Interactome of Toxoplasma Gondii Brought to Light by Comprehensive Proteomic Analyses: Benoît Westermann1; Lamba Omar Sangaré1; Agnes Hovasse1; Thilabalalo Dilezitoko Alay1; Stan Tomavo1; Alain Van Dorselaer1; Christine Schaeffer-Reiss1; 1IPHC, UDS CNRS UMR 7178 Strasbourg, France; 2CNRS UMR 8204, Lille, France

TP 690 Proteomic Deciphering of Cystic Echinococcosis using Laser Microdissection-based Microproteomics and MALDI Imaging: Rémi Longuespée1; Rita Casadontone1; Mark Kriegsmann1; Gabriel Mazzucchelli1; Edwin De Pauw4; Michael Becker1; Jörg Kriegsmann1; 1Proteopath GmbH, Trier, Germany; 2University of Heidelberg, Heidelberg, Germany; 3University of Liege, GIGA-Proteomics Liege, Belgium; 4Université de Liège, Liège, Belgium; 5Bruker Daltonik GmbH, Bremen, Germany; Center for Histology Cytology and Molecular Diagnostics, Trier, Germany

TP 691 Plasma Proteomic Changes Induced by Salmonella Typhimurium Lipopolysaccharides in an Avian Model of Inflammation: Balamurugan Pakkialakshmi1; Rohana Liyanage1; Jackson O Lay, Jr1; Sarbjeet K Makkar1; Narayan Rath1; University of Arkansas, Fayetteville, AR; 2PPRSU, USDA-ARS Fayetteville, AR

TP 692 Top Down Proteomic Profiling of a Hypervirulent Clinical Isolate of Acinetobacter baumannii: Zack Li1; Kelly Fulton1; Rhonda Kuo Lee1; Howard H Xu1; Patricia Massel1; Susan Twine1; Wangxue Chen1; National Research Council Canada, Ottawa, Canada; 2California State University, Los Angeles, Los Angeles, CA - California

TP 693 Evolutionary Dynamics of Pseudomonas aeruginosa Revealed by Population Proteome Analysis: Xia Wu1; Katherine B Hisert1; Jayanthi Garudath1; Benjamin J Staudinger1; Jimmy K Eng1; Colin Manoil1; Pradeep K Singh1; James E Bruce1; University of Washington, Seattle, WA

TP 694 A Plasmidic Vivalax Trehalose-schizont Stage Transition Proteome: D. C. Anderson1; Stacey A. Lapp1; John Barnwell2; Mary R. Galinski2; 1Emory Vaccine Center, Yerkes National Primate Research Center, Emory University, Atlanta, GA; 2Malaria Branch, Division of Parasitic Diseases, Centers for Disease Control and Prevention, Atlanta, GA; 3Emory Vaccine Center, Yerkes National Primate Research Center, Emory University; Department of Medicine, Division of Infectious Diseases, Emory University School of Medicine, Atlanta, GA
TP 717 Quantitative Proteome Profiling of Marinobacter sp. CP1 enriched from Microbial Fuel Cell Biocathode MCL; W. Judson Hervey IV; Zheng Wang; Brian J. Edie; Anthony P. Malanoski; Baocuan Lin; Sarah M. Strycharz-Glaven; Naval Research Laboratory, Center for Bio/Molecular Science & Engineering, Washington, DC

TP 720 Fast MS/MS Data Acquisition without Dynamic Exclusion Enables Precise and Accurate Quantification of Proteome; Yichu Shan; University of Wisconsin-Madison, Madison, WI; Fudan University, Shanghai, China

TP 721 Combined Discovery- and Targeted-based Proteomic Analysis of Tumor-Associated Antigen Peptides Derived from MAGE Proteins; Darshit Shah; Xunbao Duan; MacDonald Douglas; Robert Salzer; Regeneron Pharmaceuticals Inc., Tarrytown, NY; Regeneron Pharmaceuticals, Tarrytown, NY

TP 722 Application of Mass Spectrometry Profiling to Establish Brusatol as an Inhibitor of Global Protein Synthesis; Taylur Ma; Steffan Vartanian; James Lee; Peter M. Brusatol as an Inhibitor of Global Protein Synthesis in Drosophila Cells by Direct MALDI-TOF MS Quantification of Biogenic Amines from Single Rabbit Plasma; Max Diesner; Susanne Neupert; 1Biocenter Cologne, University of Cologne; 2School of Physical & Mathematical Sciences, Nanyang Technological University (Asia Pacific) Pte Ltd, Singapore; 3Moscow Institute of Physics and Technology, Dolgoprudny, Russia; 4Research Center for Obstetrics, Gynecology, and Reproductive Medicine, Russian Federation; 5Research Center for Obstetrics, Gynecology, and Neonatology, Moscow, Russia; 6Interstudent Mass Spectrometry-Guided Refinement of Chemical Energy Buffers; Ting-Ru Chen; Pawel Lukasz Urban; 1West Virginia University, Morgantown, WV; 2Oak Ridge National Laboratory, TNMS Oak Ridge, TN

TP 723 Development and Validation of a Method to Quantitate Bisphenol AF in Rodent Plasma and Aminioinic Acid for Energy Problems of Chemical Physics, Moscow, Russia; 2Institute of Biochemical Physics, Moscow, Russia; 3Research Center for Obstetrics, Gynecology, and Neonatology, Moscow, Russia; 4Janssen Research & Development, Spring House, PA

TP 724 Quantitative Analysis of Chromatin Proteome Remodeling Mediated by SWI/SNF Complexes; Zhiping Wü; Eun-Ah Cho; Haiyan Tan; Haifeng Yang; Junmin Cai; Zachery Gregorich; Gary M Diffee; Ying Ge; University of Texas A&M College of Medicine, College Station, TX; 2National Institute of Environmental Health Sciences, Research Triangle Park, NC; 3MRIGlobal, Kansas City, MO

TP 725 Use of Variant Proteomics to Inform Genomic Searches for Novel Targets in Gloma; Ekatrina Mostovenko; Melinda Rezelt; Akos Vegvari; Gyorgy Marko-Varga; Yanhong Liu; E. Susan Amirian; Melissa L Bondy; 1Waters Corporation, Milford, MA; 2Waters Corporation, Beverly, MA

TP 726 Determining Isotope Enrichment in Heavy Water Labeling; Jaying Avva; Kwangwon Lee; Taktar Kasumov; Rosvhan Sadagov; University of Texas Medical Branch at Galveston, Galveston, TX; 2Northeast Ohio Medical University, Rootstown, OH; 3Northeast Ohio Medical University, Rootstown, OH

TP 727 Quantitative MS Investigation of the Effect of Amyloid-beta on the Proteome Of Neuronal Cells; Maria I. Indyukha; Evgeny P Barykin; Alexey S Kononikhin; Vladimir Mitkevich; Igor A Popov; Sergey Kozin; Alexander A Makarov; Eugene Nikolaev; 1Emanuel Institute of Biochemical Physics, Moscow, Russia; 2Institute for Energy Problems of Chemical Physics, Moscow, Russia; 3Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; 4Engelhardt Institute of Molecular Biology, Moscow, Russia; 5Research Center for Obstetrics, Gynecology and Neonatology, Moscow, Russia

TP 728 Quantitative Measurement of Carbidoval and Levodopa in Rat Plasma via HPLC with Tandem Mass Spectrometry; Jingduan Chi; Yonghua Ling; Mofikoya Melissa; Fumin Li; 1PPD, Middleton, WI

TP 729 A A Novel Determination for Menthol in Rat Plasma using Salting-Out LLE and Derivatization Coupled with LC-MS/MS Detection; Mingquan Chen; Milton Furtado; Anahita Keyhani; 1Algorithm Pharma Inc., Laval, Canada

TP 730 Challenges and Solutions in the Bioanalysis of Sulprostone, a Prostaglandin E2 Analogue, in Rat and Monkey Plasma using LC-MS/MS; Yifan Shu; Shefali Patel; Naidong Weng; Janssen Research & Development, Spring House, PA

TP 731 A Combined Discovery and Targeted-based Proteomic Analysis of Tumor-Associated Antigen Peptides Derived from MAGE Proteins; Darshit Shah; Xunbao Duan; MacDonald Douglas; Robert Salzer; Regeneron Pharmaceuticals Inc., Tarrytown, NY; Regeneron Pharmaceuticals, Tarrytown, NY

TP 732 Ultra Sensitive Method for Pre-clinical Quantification of Methacholine in Biological Matrices using SPE-HILIC Tandem Mass Spectrometry; Anders Lundqvist; AstraZeneca Gothenburg, Gothenburg, Sweden

TP 733 Validation of a Method for Quantitation of DMSO in Equine Urine using Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry; Matilda Salomonsson; Lena Ekman; Mikael Hedelund; Ulf Bondesson; The National Veterinary Institute (SVA), Uppsala, Sweden; 2The National Veterinary Institute (SVA), Uppsala, Sweden; 3The National Veterinary Institute (SVA), Uppsala, Sweden

TP 734 Simultaneous Determination of Benzocaine, N-acetyl Benzocaine, and Tetracaine in Rabbit Plasma using High Performance Liquid Chromatography-Mass Spectrometry; Wuvi (Charlie) Zha; Runian Huo; Mohamed Osman; Xiping Fang; Xin Zhang; Xebonic Laboratories, Inc. WuXi AppTec Inc Plainboro, NJ; WuXi AppTec Co., Shanghai, China

TP 735 A A Combined MRM and SIM Method for Direct Determining Isotope Enrichment in Heavy Water Labeling; Jaying Avva; Kwangwon Lee; Taktar Kasumov; Rosvhan Sadagov; University of Texas Medical Branch at Galveston, Galveston, TX; 2Northeast Ohio Medical University, Rootstown, OH; 3Northeast Ohio Medical University, Rootstown, OH

TP 736 Determining Isotope Enrichment in Heavy Water Labeling; Jaying Avva; Kwangwon Lee; Taktar Kasumov; Rosvhan Sadagov; University of Texas Medical Branch at Galveston, Galveston, TX; 2Northeast Ohio Medical University, Rootstown, OH; 3Northeast Ohio Medical University, Rootstown, OH

TP 737 Analysis of Mycotoxins in Coix Seed using a Prototype Tandem Quadrupole Mass Spectrometer; Kerri Smith; Kelly D Boering; Mark Wrona; Giorgis Isaac; Jimmy Yuk; Sukhdev Bangar; Waters Corporation, Milford, MA; 2Waters Corporation, Beverly, MA

TP 738 Quantitative Determination of Amino Acids in Various Samples on LC/MS/MS; Zhe Sun; Jing Xing; Pei Yee Khoo; Zhaqi Zhan; 1Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; 2School of Physical & Mathematical Sciences, Nanyang Technological University Singapore; 3Interstudent
TP 742 Obtain sub-ng/mL Levels for Steroids using a Simple, One-step Derivatization and a Novel, High Efficiency El Source; Tim Conjeelke1; Stephan Baumann1; Matthew Curtis1; Agilent Technologies, Santa Clara, CA

TP 743 Novel SPE Extraction Method for Sensitive and High Throughput Quantitative Analysis of Phosphorothioate Oligonucleotides in Human Plasma Using LC-MS/MS; Vuyhuan Ji1; Qian Liu2; Qian Li3; Ji Chengjie3; Laxin Wang3; 1NovaBioAssays, LLC; Woburn, MA; 2NovaBioAssays, LLC, Woburn, MA

TP 744 Quantitation of Four Chiral Drug Compounds Simultaneously Using Normal Phase LC-MS/MS Equipped With an APPI Ion Source; Min Huang; Zhongping (John) Lin1; 1Frontage Laboratories, Exton, PA

TP 745 The Use of Perchloric Acid as a Problem Solving Precipitating Agent to Overcome Method Development Issues; Pierre-Yves Caron1; Nicolas Jean2; Nadine Lafontaine3; Louis-Chare Joint4; Sylvain Lachance3; Nadine Boudreau1; Clark Willard1; inVentiv Health, Quebec, Canada

TP 746 A Novel Approach for Reducing the Isotopic Distribution Impact during Quantitation of Analte by LCMSMS using Quadratic Regression Fit; Nathalie Pelletier1; Genevieve Emond2; Sylvain Lachance3; Nadine Boudreau1; Clark Willard1; inVentiv Health, Quebec, Canada

TP 747 Monitoring and Quantitating Genotoxic Impurities using Mass Detection and UV – Sensitive Analysis Aryl Sulfonic Acid Esters; Mark Wrona1; Janet Hammond; 1inVentiv Health, Québec, Canada

TP 748 Development of a Low Volume Quantitative Plasma Analysis Method Using a Flexible Capillary Microsampling Technique; Larry Mailla1; Wei Zhang2; Li Yuan3; Zhongping (John) Lin1; 1Frontage Laboratories, Exton, PA

TP 749 An Investigation on the Impact on Drug Stability in Biological Matrix when Stored in Multiple Tubes; Nader Youssef1; John Chapdelaine2; Weixing Sun3; Asvinkumar Patel4; Zhao Heng Ge; Adrien Musuku; 1Pharmascience, Montreal, Canada

TP 750 Simultaneously Determination of the Enantiomers of Ketorolac in Human Plasma by Atmospheric Pressure Chemical Ionization LC/MS/MS; Vince Windisch1; Feng Liang; Allan Xu1; 1Keystone Bioanalytical Inc, North Wales, PA

TP 751 Trace Analysis of Potentially Mutagenic Impurities in Pharmaceutical Substances by Electron Ionization LC/MS (EI-LC/MS) with Supersonic Molecular Beams; Christine Fisher1; Ryan Cohen1; Renee Demjenlian1; 1Merck & Co., Rahway, NJ

TP 752 Expanding Horizons in Real Time Analysis: Dual Polarity SIFT-MS; Murray J Mcewan2, 1; David Hera; Harry Gower1; Vaughan S Langford2; Thomas I McKellar3; Daniel B Milligan1; 1University of Canterbury, Christchurch, Canterbury; 2Syt Technologies Ltd, Christchurch, New Zealand

TP 753 Development of LC/MS/MS Method for Screening and Quantitation of 49 Synthetic Dyes in Textiles under Restricted Substance List (RSL); Ying Peng1; Wenxuan Cai2; Yutong Jin2; Liming Wei1; Albert Chen3; Susan McKiernan3; Jie Ren4; 1Agilent Technologies, Santa Clara, CA

TP 754 Isolation, Characterization and Color Stability of natural blue pigments; Andrew G Newsome1; Lu Yun Chen1; Cathy A Culver1; Richard B van Bremen1; 1University of Illinois at Chicago, Chicago, IL; 2Pepsi-Cola Company, Hawthorne, NY

TP 755 Selective Enrichment of Flavonoids Using Pegylated Graphene Oxide and MALDI-TOF MS; J aesung Lee; Konkuk University, Seoul, South Korea

TP 756 Development of a Sensitive Supercritical Fluid Chromatography (SFC)-MS/MS Method for the Analysis of Potential Genotoxic Impurities of Ondansetron; Jennifer Simeone1; Paula Hong1; 1Waters Corporation, Milford, MA

TP 757 Development and Testing of a Gas Generator for Odour Transmission over Data Networks; Stamatis Giamprhoukas; Jeremy Smith1; Alan Marshall2; Stephen Taylor2; 1University of Liverpool, Liverpool, Please Select; 2University of Liverpool, Liverpool, United Kingdom

TP 758 Novel Applications of Paired Ion Electrospray Ionization Mass Spectrometry (PIESI-MS) for Sensitive Analysis of Anionic Compounds; Hongyu Guo1; Daniel W Armstrong1; 1University of Texas at Arlington, Arlington, TX

TP 761 Commutability of LC/MSMS Assays: Calibration by Internal or External Standardization?; R. Brent Dixon; Physican’s Choice Laboratory Services, Rock Hill, SC

TP 762 Evaluation of an Innovative High-Throughput Online Solid Phase Extraction Tandem Mass Spectrometry System for Bioequivalence Studies; jinhui Zhang1; Patrick J. Faustino1; 1FDA, Silver Spring, MD

TP 763 The National Resource for Translational and Developmental Proteomics offers novel opportunities for training and accelerated research in top-down proteomics; Neil L Kelleher1; Caroline J DeHart1; Ryan T Fellera1; Richard D LeDuc1; Paul M Thomas1; 1Northwestern University, Evanston, IL

TP 764 Application of Spectral Counting for Top-down Proteomics Comparisons; Lucia Geis-Asteggiante1; Nathan Edwards2; Suzanne Ostrand-Rosenberg3; Catherine Fenselau1; 1University of Maryland, College Park, MD; 2Georgetown University Medical Center, Washington, DC; 3University of Maryland, Baltimore County Baltimore, MD

TP 765 Increased Fragmentation Efficiency in Middle-down Protein Analysis using Different Collision Gases in a Modified Q-TOF Mass Spectrometer; Christian Klein1; Alex Mordehai1; Mark Werlich1; William E Barry1; 1Agilent Technologies, Santa Clara, CA

TP 766 Protein Supercharging for Enhanced Top-Down Analysis with HCD MS/MS; Natalia Gasilova1; Kristina Szrent1; Yury Tsybin2; Hubert H Girault2; 1EPFL, Sion, Switzerland; 2EPFL, Lausanne, Switzerland; 3Spectroswiss Sàrl, Lausanne, Switzerland; 4EPFL, Sion, Switzerland

TP 767 Difference Mass Spectra for De novo Identification of N- and C-terminal Sequences of Intact Proteins; Harsha Gunawardena1; Dhaneshi Bagal1; Daryl Bulloch1; Ping Cao1; 1Thermo Fisher Scientific, San Jose, CA

TP 768 Top-down Targeted Proteomics Reveals Novel Molecular Mechanism in Sarcopenia; Zachery Gregorie1; Ying Peng; Wenxuan Cai2; Yutong Jin2; Liming Wei1; Albert Chen1; Susan McKiernan3; Judd Aiken1; Richard Moss1; Gary Diffie2; Ying Ge2; 1UW Madison, Madison

TP 769 Development of a Sensitive Supercritical Fluid Chromatography (SFC)-MS/MS Method for the Analysis of Potential Genotoxic Impurities of Ondansetron; Jennifer Simeone1; Paula Hong1; 1Waters Corporation, Milford, MA

TP 770 A Simple Systematic Strategy for Rapid Development of High-throughput and Reliable LC/MS/MS Assays for Regulated Bioanalysis; Long Yuan; Bristol-Myers Squibb, Princeton, NJ

TP 771 Development of a Sensitive Supercritical Fluid Chromatography (SFC)-MS/MS Method for the Analysis of Potential Genotoxic Impurities of Ondansetron; Jennifer Simeone1; Paula Hong1; 1Waters Corporation, Milford, MA

TP 772 Evaluation of an Innovative High-Throughput Online Solid Phase Extraction Tandem Mass Spectrometry System for Bioequivalence Studies; jinhui Zhang1; Patrick J. Faustino1; 1FDA, Silver Spring, MD

TP 773 The National Resource for Translational and Developmental Proteomics offers novel opportunities for training and accelerated research in top-down proteomics; Neil L Kelleher1; Caroline J DeHart1; Ryan T Fellera1; Richard D LeDuc1; Paul M Thomas1; 1Northwestern University, Evanston, IL

TP 774 Application of Spectral Counting for Top-down Proteomics Comparisons; Lucia Geis-Asteggiante1; Nathan Edwards2; Suzanne Ostrand-Rosenberg3; Catherine Fenselau1; 1University of Maryland, College Park, MD; 2Georgetown University Medical Center, Washington, DC; 3University of Maryland, Baltimore County Baltimore, MD

TP 775 Increased Fragmentation Efficiency in Middle-down Protein Analysis using Different Collision Gases in a Modified Q-TOF Mass Spectrometer; Christian Klein1; Alex Mordehai1; Mark Werlich1; William E Barry1; 1Agilent Technologies, Santa Clara, CA

TP 776 Protein Supercharging for Enhanced Top-Down Analysis with HCD MS/MS; Natalia Gasilova1; Kristina Szrent1; Yury Tsybin2; Hubert H Girault2; 1EPFL, Sion, Switzerland; 2EPFL, Lausanne, Switzerland; 3Spectroswiss Sàrl, Lausanne, Switzerland; 4EPFL, Sion, Switzerland

TP 777 Difference Mass Spectra for De novo Identification of N- and C-terminal Sequences of Intact Proteins; Harsha Gunawardena1; Dhaneshi Bagal1; Daryl Bulloch1; Ping Cao1; 1Thermo Fisher Scientific, San Jose, CA

TP 778 Top-down Targeted Proteomics Reveals Novel Molecular Mechanism in Sarcopenia; Zachery Gregorie1; Ying Peng; Wenxuan Cai2; Yutong Jin2; Liming Wei1; Albert Chen1; Susan McKiernan3; Judd Aiken1; Richard Moss1; Gary Diffie2; Ying Ge2; 1UW Madison, Madison
TP 769  Optimisation of intact Protein Sequencing through Testing Thousands of EThC/ETciD MS/MS Fragmentation Conditions; Pavel Shliaha1; Derek Bailey2; Vladimir Gorshkov1; Ole N. Jensen1; Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; 2Thermo Fisher Scientific, San Jose, CA

TP 770  Development of Mass Spectrometry-based Methods for Quality Assessment of Recombinant Proteins; Rosa I Viner1; Nan Liu2; Seema Sharma1; Sergei I Snovida3; Krishna Vattern3; David M Horn1; Thermo Fisher Scientific, South San Francisco, CA; 2Life Technology, South San Francisco, CA; 3Thermo Fisher Scientific, Rockford, IL

TP 771  Higher-order Structure Determines the Native ETD Fragmentation Behavior of Proteins and Complexes; Frederik Lermyte1; Mateusz Krzysztof Łącki2; Albert Konijnenberg1; Dirk Valkenborg1; Anna Gambin2; Frank Sobott1; 1University of Antwerp, Antwerpen, Belgium; 2University of Warsaw, Warsaw, Poland; 3VITO, Mol, Belgium

TP 772  Native Top-down Mass Spectrometry of Tau Proteins; Piriya Wongkongkathep1; Michael Nshanian1; Michael Ehrmann2; Gal Bitan1; Joseph A Loo1; UCLA, Los Angeles, CA; 2University of Duisburg-Essen, Essen, Germany

TP 773  Mapping p53 Proteoforms by Native and Denaturing Top-down Mass Spectrometry; Caroline J DeHart1; Luca Fornelli1; Owen Skinner1; Philip D Compton1; Paul M Thomas1; Galit Lahav2; Jeremy Gunawardena2; Neil L Kelleher1; Northwestern University, Evanston, IL; 2Harvard Medical School, Boston, MA

TP 774  High-throughput Top Down Proteomics of HeLa cell lysates using UVPD; Timothy Cleland1; Ryan Parker2; Jennifer S Brodbelt1; University of Texas Austin, Pflugerville, TX; 2University of Texas at Austin, Austin, TX

TP 775  Quantitative Top Down Proteomics in Translational Research: Markers for Rejection in Peripheral Blood Following Kidney Transplantation; Timothy Toby1; John Savaryn1; Bryan P Early1; Paul M Thomas1; Ryan T Fellers1; Luca Fornelli1; Joseph B Greer1; Richard D Leduc1; Ioanna Ntai1; Zheng J Zhang2; John Friedewald2; Daniel Salomon2; Michael M Abecassis3; Neil L Kelleher1; Philip D Compton1; Northwestern University, Evanston, IL; 2Northwestern Feinberg School of Medicine, Chicago, IL; 3Scripps Center for Organ and Cell Transplantation, La Jolla, CA
WP 005 Applications and Fundamentals of Swab Touch Spray – Mass Spectrometry: Alan K. Jarmusch1, 2, Valentina Pirro1, 2; R. Graham Cooks1, 2; ‘Purdue University-Department of Chemistry, West Lafayette, IN; 1Center for Analytical Instrumentation Development, West Lafayette, IN

WP 006 Coupling Paper Microfluidics with Paper Spray Mass Spectrometry for Improved Versatility and Analytical Performance; Ian Murray1; Glenn Walker1; Michael Bereman1; ‘North Carolina State University, Raleigh, NC

WP 007 In situ Separation and Analysis of Lipids by Paper Spray Ionization Mass Spectrometry; Sangwon Cha1; Purun Kim1; ‘Hankuk Univ. Foreign Studies, Yongin, South Korea

WP 008 High-Throughput Copper-Catalysts Screening and Their Catalytic Activity Studies Using Paper Spray Mass Spectrometry; Yajun Zheng1; Xuan Wang1; Teng Wang1; Yang Hailun1; Zhiping Zhang1; ‘X’ian Shiyou University, X’ian, China; 2Tsinghua University, Beijing, China

WP 009 Molecular Ionization at Low Voltage from One-Dimensional Nanostructures; Rahul Naravanan; Indian Institute of Technology, Chennai, Tamilnadu, India, Chennai, Tamilnadu

WP 010 Dehydrogenation of Tetrahydroquinolines in Corona Discharge Plasma under Ambient Conditions using Graphite-Coated Hydrophobic Paper Surface; Kathyn Davis1; Abraham Badu-Tawiah1; ‘The Ohio State University, Columbus, OH

WP 011 Mass Spectrum Real-Time Online Optimizing Paal-Knorr Spary Reaction Temperature; Xinping Zeng1; Peng Zhou1; Huanwen Chen1; ‘East China Institute of Technology, Nanchang, China; 2East China University of Technology, Nanchang, Mainland

WP 012 Direct and Rapid Detection of Drugs in Urine by Extractive Electrospray Ionization Mass Spectrometry; Peng Zhou1; Tenggao Zhu1; Yongzi Liu1; Huian Zhao1; Huanwen Chen1; ‘East China Institute of Technology, Nanchang, China; 2Jiangxi of Forensic Science Institute, Nanchang, China; 3East China University of Technology, Nanchang, Mainland

WP 013 Coaxial Extractive Electrospray Ionization Mass Spectrometry; Kenneth D Swanson1; Steven L Reeb1; Gary L Glish1; ‘University of North Carolina, Chapel Hill, NC

WP 014 Generating Radical Cations of Aromatic Hydrocarbons through Reactive ESI Using the Single-Probe; Rachel Vowciefski1; Ning Pan1; Zhibo Yang1; ‘University of Oklahoma, Norman, OK; 2University of Oklahoma, Dept. of Chem & Biochem Norman, OK

WP 015 Pinpointing the Source of Droplet Reactivity in Contained-electrospray ionization; Dmytro Kulyk1; Abraham Badu-Tawiah1; ‘Ohio State University, Columbus, OH

WP 016 Solvent Assisted Inlet Ionization of Airborne Nanoparticles; Andy Horan1; Murray V Johnston1; ‘University of Delaware, Newark, Delaware

WP 017 Ionization Efficiency Comparison of ESI, SAI, and vSAI Using Compounds with Different Surface Activities; Madelaine Fenner1; Charles N McEwen1; ‘University of the Sciences, Philadelphia, PA; 2University of the Sciences in Philadelphia, Philadelphia, PA

WP 018 Effects of Volatile Anions and Cations as Spray Solvent Additives on the DESI–MS Analysis of Proteins; Andre Venter1; Elahe Honarvar1; Wisam Alisawi1; ‘Purdue University, West Lafayette, IN

WP 019 Top-down DESI-UVPD of Proteins and Lipopolysaccharides on Polynylidene Difluoride Membranes; Dustin Klein1; Clara Feider1; Livia S Eberlin1; Jennifer S Brodbelt1; ‘University of Texas at Austin, Austin, TX
WP 020 DART Mass Spectrometry and Emission Spectra of Various DART Gas Sources; William A. Harris1; Johnny K Ho2; Douglas B Henderson1; Northrop Grumman, Linthicum Heights, MD

WP 021 Ambient MS Based Analytical Platform for Rapid Identification of Brain Tumor Tissues; Igor A Popov3, 5; Evgeny Zhvanskii1; Nikita Levin1; Vsevolod Shurkhay2; Denis Bormotov4; Maria Indeykina4; Alexey S Kononikhin4; Yury Kostyukievich4; Evgeny Kukaev4; Alexander Potapov4; Eugene Nikolaev3; Moscow Institute of Physics and Technology, Moscow, Russia; Institute for Energy Problems of Chemical Physics, Moscow, Russia; 2Burdenko Neurosurgical Institute, Moscow, Russian Federation; *Emanuel Institute of Biochemical Physics, Moscow, Russia

WP 022 Assessment of Atmospheric Pressure Surface Mass Spectrometers for Improved Characterization and Imaging of Medical Devices; Felicia M Green1; Adam S Spectrometries for Improved Characterization and Assessment of Atmospheric Pressure Surface Mass; Martin R L Paine1; Curved Three-Dimensional Surfaces

WP 023 Liquid Microjunction Sampling for the Analysis of Proteins from Thin Tissue Sections; Rian Griffiths1; Elizabeth C Randall1; Helen J Cooper1; *The University of Birmingham, Birmingham, UK

WP 024 Ambient Bio-Molecular Mass Spectrometric Imaging with Subcellular Spatial Resolution; Jae Young Kim1; Eunsoek Seo1; Hyunmin Kim1; Dong-Kwon Lim1; Dae Won Moon1; Department of New Biology, DGIST, Daegu, South Korea; *Nano and Energy Research Division, DGIST, Daegu, South Korea; *KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea

WP 025 Spot Size, Sensitivity, and Fit for Purpose: Comparative Analysis of Extractive Analysis Techniques; Mariam S Elnagar1; Prosolia, Inc., Indianapolis, IN

WP 026 Point-of-Care Tissue Analysis with Specificity for C=C Bond Lipid Isomers; Rui Zhao1; 1Purdue University, West Lafayette, IN; 2Biomedical Engineering, Purdue University, West Lafayette, IN; 3School of Veterinary Medicine, Purdue University, West Lafayette, IN; 4Chemistry Department, Purdue University West Lafayette, IN

WP 027 Robotic Surface Analysis Mass Spectrometry (RoSA-MS) for Automated Ambient Sampling of Highly-Curved Three-Dimensional Surfaces; Martin R L Paine1; Rachel V Stryffler1; Jake Pawlowski1; Adriana Bajardi-Taccioli2; Damian Houde2; Marina Feschenko2; Igor A Kaltashov3; 1Protein Metrics Inc., San Carlos, CA; 2Janssen Research and Development, Spring House, PA

ANTIBODIES & ANTIBODY DRUG CONJUGATES (SEQUENCING, MODIFICATIONS & HI RES) 030 - 061

WP 030 Protease-Containing Membranes For Controlled Digestion of Antibody Cocktails and Enhancement of Monoclonal Antibody Sequencing; Yongle Pang1; 1Purdue University, West Lafayette, IN; 2Department of Chemistry, Michigan State University, East Lansing, MI

WP 031 Validation of Originator Sequences by Antibody Domain Mass Determination and Top-Down Sequencing; Anja Resemann1; Wolfgang Jabs2; Anja Wiechmann1; Elsa Wagner1; Colas Olivier1; Waltraud Evers1; Eckhard Belau1; Lars Vorweg1; Catherine Evans1; Alain Beck1; Detlev Suckau1; *Bucker Daltonic GmbH, Bremen, Germany; 2Centre d’Immunologie Pierre-Fabre, St. Julien-en-Genevois, France

WP 032 Distinguishing Leucine and Isoleucine Residues in de novo Sequencing of mAbs using Nano LC-MSn: A Potential to Replace Edman Degradation; Dhanashri Bagal1; 1San Diego State University, San Diego, CA; 2University of California, San Diego, CA

WP 033 High Throughput Antibody de novo Sequencing and Its Utility in Biopharmaceutical Discovery; Kadir Ilker Sen1; Darryl Davis2; Wilfred Tang1; Marshall Bern2; Chris Becker2; Janssen Research and Development, Spring House, PA

WP 034 Automated Antibody Sequencing Software; Wilfred Tang1; Marshall Bern2; Chris Becker2; Kadir Ilker Sen1; *Protein Metrics Inc., San Carlos, CA; Janssen Research and Development, Spring House, PA

WP 035 Rapid Quantitation of IgG after Digestion at Elevated Temperature with a Novel Tryptic Peptide Standard; Michael Rosenblatt1; Daniel S Spellman2; Sergei Savelyev1; Kevin P Bateman1; Marijeta Urh1; *Promega Corp, Madison, WI; 2Merck & Co., Inc., West Point, PA

WP 036 Comparison of Various LC/MS Methods for Label-free Relative Quantitation of Site-specific Glycosylation of a Monoclonal Antibody; Pilsoo Kang1; Jianmei Kochling1; Sanofi Genzyme, Framingham, MA

WP 037 Minimizing Method-induced Modifications in the Complementarity Determining Regions (CDRs) of Antibodies to Ensure Optimal Understanding of Product Quality Attributes; Jennifer Idy1; Elaine Stephens1; Michelle A English1; Jason C Rouse1; Lisa A Marzilli1; Pfizer, Andover, MA; Pfizer, Inc. Andover, MA

WP 038 A Method Comparison for Quantifying Trisulfides in Monoclonal Antibodies: Non-Reduced Peptide Mapping LC-MS vs. Hydrophilic Interaction Chromatography-Charged Aerosol Detection; Christopher Cornell1; Genentech, South San Francisco, CA

WP 039 Impact of Fc N-Glycan Sialylation on IgG Structure; Jason Richardson1; Darryl Davis1; Wilfred Tang2; Marshall Bern2; *Pfizer, Inc. Andover, MA; *Bruker Daltonics GmbH, Bremen, Germany; *Bruker Daltonics, Fremont, CA; *Bruker Daltonics, Inc., Billerica, MA

WP 040 Evaluation of a Rapid Method for Deamidation Profiling of Monoclonal Antibodies Suitable for Early Molecular Selection in Drug Discovery; Heather DeGruttola1; Elaine Stephens1; Michelle English1; Keith A Johnson1; Anja Wiechmann1; Guillaume Tremintin2; Jason Wood1; Wolfgang Jabs2; Lisa A Marzill1; Jason Rouse1; Pfizer, Inc. Andover, MA; Bruker Daltonic GmbH, Bremen, Germany; Bruker Daltonics, Fremont, CA; Bruker Daltonics, Inc., Billerica, MA

WP 041 The Effect of Sialylation of IgG’s N-Glycans on FcRn Binding; Jake Pawlowski1; Adriana Bajardi-Taccioli2; Damen Houde2; Marina Feschions1; Igor A Kaltashov3; Tyler Carlage3; UMass Amherst, Amherst, Massachusetts2; Biogen Inc., Cambridge, MA; University of Massachusetts, Amherst, MA

WP 042 Characterization of Relative N-Glycan Occupancy in Antibodies using Mass Spectrometry; Ekaterina G. Deyanova1; Xu Wang1; Richard Huang1; Guodong Chen1; Boston-Myers Squibb, Princeton, NJ

WP 043 Analysis of O-linked Glycan Released from Biopharmaceuticals by using a Chemical Reaction and ASF- incorporated Curved Field Reflection.; Shuichi Nakaya1; Yuzo Yamazaki1; Shimadzu Corporation, Kyoto, Japan

WP 044 Building a High Confidence, Quantitative O-glycopeptide Profile for IgA; Amol Prakash1; Shabab Ahmad1; Scott M Peterman1; Julian A Saba1; Chu-Wei Ku1; Kay-Hoii Khoo1; Rosa I Viner1; Optyx Tech Corporation,
WP 056  Physicochemical Structural Characterization of Innovator and Biosimilar Eculizumab with High Resolution Mass Spectrometry Methods

Maksim Degtirev

Frisher Scie, CA

WP 065

Identification of Nephropathy Prognostic Markers in Urine from Children Affected by type-1 Diabetes

Magagnotti Cinzia; Gianpaolo Zerbini; Isabella Fermo; Ruiqing Zhang; Shirokova Shana; Maria Indeykina; Zulfia Khodzhaeva; Nataliia Starodubtseva; Alexey S Kononikhin; Anna Bugrova; Igor A Popov; Victoria Shirikova; Maria Indeykina; Olga Vavina; Kamila Muminova; Yury Kosutyevich; Vitaly Chagovets; Vadim Lagutin; Evgeny Kukacev; Vladimir E Frankievich; Zulfia Khodzhaeva; Gennady Sukhikh; Eugene Nikolaev; Research Center for Obstetrics and Gynecology, Moscow, Russia; Moscow Institute of Physics and Technology, Moscow, Russia; Emanuel Institute of Biochemical Physics, Moscow, Russia; Institute for Energy Problems of Chemical Physics, Moscow, Russia; Skolkovo Institute of Technology, Moscow, Russia

WP 064

Identification of Serum Protein Biomarkers Associated with Early Heterotopic Ossification Formation following Traumatic Injury

Michael E. Hoover; Claire Llamas; Elizabeth C. Martin; Elaine Boos; Peter C. Krause; Andrew G. King; Harry Molligan; Olivia C. Lee; Vinod Dasa; Thomas A. Davis; Ammar Qureshi; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; 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Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett; Michael, MI; Bennett;
WP 066
Deep Profiling of Extracellular Vesicles in μL-Scale Plasma Samples Using Miniaturized Isolation Combined with Advanced Separation and MS Data Acquisition; Simion Kreimer1; Arseniy M Belov2; Rosa I Viner2; Marcia Santos3; Barry L Karger1; Alexander R. Ivanov1; 1Northeastern University, Boston, MA; 2Thermo Fisher Scientific, San Jose, CA; 3Scripps Research Institute, La Jolla, CA

WP 067
Selection of Protein Biomarkers in Dehalocloccidan Mccartnystrains Enables an MRM-MS Approach for Monitoring Dechlorination Activities in Environmental Samples; Manuel Villalobos1;2; Karuna Chourey1; Frank Loeffler1; Robert Hettich1; 1University of Tennessee-Knoxville, Knoxville, TN; 2Oak Ridge National Laboratory, Oak Ridge, TN

WP 068
Proteome Analysis of Plasma Extracellular Vesicles and the Impact of Sampling Conditions; Ole Østergaard1; Julia Tanas Tannas2; Henrik Niels Helweg Heegaard1; 1Statens Serum Institut, Copenhagen, Denmark; 2Statens Serum Institut, Copenhagen, Denmark

WP 069
Methodological Development for Exosome Enrichment in Serum; Yan Ren1; Jin Zi2; Liang Lin1; Sigi Liu3; 1BGI-Shenzhen, Shenzhen, China

WP 070
Serum N-glycome Analysis of Colorectal Cancer Patients Reveals Association with Survival; Stefan W de Vroome1; Stephanie Holst1; Mar DM Rodriguez Girondo1; 1Statens Serum Institut, Copenhagen, Denmark; 2Statens Serum Institut, Copenhagen, Denmark

WP 071
Identification of Urinary Protein Biomarkers for Diagnosis of Hepatocellular Carcinoma by an Onco-proteogenomics Approach; Thomas S.-H. Chiou1,2; Chun-Hao Huang1;3; Shu-Wen Chi4; Chao-Jen Kuo1; King-Teh Lee1; 1Kaohsiung Medical University, Kaohsiung, Taiwan; 2Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan; 3Weill Graduate School of Medicine, Cornell University, Ithaca, NY

WP 072
The Ascites N-glycome of Epithelial Ovarian Cancer Patients: Karina Biskup1;2; Elena I Braciu3; Jalid Sehoul1; Rudolf Tauber1; Veronique Blanchard1; 1Institute of Laboratory Medicine, Clinical Chemistry and Pathobiology, Charité Medical University, Berlin, Germany; 2Department of Biology, Chemistry and Pharmacy, Freie University of Berlin, Berlin, Germany; 3Department of Gynecology, Berlin, Germany

WP 073
Blood Proteins with Isolelectric Point Close to 7.4 as Alzheimer Disease Biomarker; Mohammed Pirmoradian Najafabadi1; Thorleif Lavold1; Dag Aaasland1; Roman A Zubarev2;1 Karolinska Institutet, Solna, Sweden; 2Biomotif AB, Stockholm, Sweden; 3Karolinska Institutet, Stockholm, Sweden; 4King's College London, London, UK

WP 074
Searching for CSF Biomarkers in PGRN Associated Frontotemporal Dementia; Diana Nijholt1; Lieke Meeter1; Christoph Stingl1; Lennard Dekker1; Jeroen van Rooij1; Shami Melhem1; Theo M. Luider1; John van Swieten1; 1Erasmus Medical Center, Rotterdam, The Netherlands

WP 075
Expanding the CSF Endopeptidomics by High-pH reversed-phase Fractionation and LC-MS/MS; Karl Hanson1; Elin Pernevik2; Silke Kern3; Kaj Blennow1; Henrik Zetterberg1; Johan Gobom1; Gothenburg University; 1Institute of Neuroscience and Physiology, Gothenburg, Sweden

WP 076
Clinical CSF Proteomics and Endopeptidomics for Biomarker Identification in Neurodegenerative Diseases; Johan Gobom1; Karl Hanson1; Elin Pernevik2; Tobias Skillback1; Henrik Zetterberg1; Kaj Blennow1; 1University of Gothenburg, Institute of Neuroscience and Physiology, Gothenburg, Sweden

WP 077
Identifying Prostate Cancer Biomarkers by Profiling Glycoproteins in Human Prostate Tissue; David Spiciarich1; Sophia L. Maund2; Sean Purcell3; Anthony T lavarone1; Donna M. Phee1; Carolyn R Bertozz2; 1University of California, Berkeley, CA; 2Stanford University School of Medicine, Palo Alto CA, USA; 3UC Berkeley, Berkeley, California; 4Stanford University, Stanford, CA; 5Howard Hughes Medical Institute, Chevy Chase, MD

WP 078
Mass Spectrometry-Based Proteomics of Human Breast Milk to Assess Breast Cancer Risk Using Different Protein Digestion procedures; Roshanak Aslebakh1; Kathleen F Arcaro2; Costel C. Darie1; 1Clarkson University, Potsdam, NY; 2University of Massachusetts Amherst, Amherst, MA

WP 079
Mass Spectrometric Analysis of Salivary Proteins from Medical Residents Performing Advanced Clinical Simulations Resulting in Acute Stress; Rachel Marvin1; Muncharie Brooke Saeppo1; Paul Rega1; Viviana Kazan1; Kenneth Hensley1; David Giovannucci1; Dragan Isailovic1; 1University of Toledo, Toledo, OH

WP 080
High Through-Put Quantitative Proteomics for the Discovery of Circulating Biomarkers in Cancer; Hong Wang1; Juan Chen1; Xiaojian Liu1; Clemente Aguilar Bonavides1; Ami Momim1; Hiroyuji Katayama1; Sam Hanashi1; 1MD Anderson Cancer Center, Houston, TX

WP 081
Proteomic Approach towards Early Diagnosis of Ventilator-Associated Pneumonia (VAP) in Critically Ill Patients; Khyaliben Pathak1; Marissa Saltzman2; Emmanuel BM Menashi1; Frederic Zenhausern1; Patrick Pirrotte1; 1Center for Proteomics, The Translational Genomics Research Institute, Phoenix, AZ; 2Center for Proteomics, Translational Genomics Research Institute, Phoenix, AZ; 3Laboratory for Genomics and Personalized Medicine, Honor Health Research Institute, Scottsdale, AZ; 4Center for Applied Nanobioscience and Medicine, University of Arizona, Phoenix, AZ

WP 082
Intact Protein Profiling of Proteoforms Moves toward the Clinic: Intact Protein Classification of Patients with Acute Rheumatic Fever; Giuseppe Infusini1; Laura Dagley2; Willy-John Martin3; Liam O'Connor1; Ian Wicks3; Andrew Webb4; 1Walter & Eliza Hall Institute, Parkville, VIC; 2Walter & Eliza Hall Institute, Parkville, Australia

WP 083
A SWATH-MS Method to Monitoring Oxidative Stress and Progression to Cell Death: From Secretome to Blood Diagnosis; Sandra Anjo1; Vera Mendes1; Mário Gráos1;2; Bruno Manjadas1; 1Center for Neurosciences and Cell Biology, Coimbra, Portugal; 2Biocant - Biotechnology Innovation Center, Cantanhede, Portugal

WP 084
Chronic Human African Trypanosomiasis Biomarker Discovery Using Quantitative Proteomics; Matthew Szuca1; Rushdy Ahmad1; Brett Eyford1; Terry Pearson2; Steven A Carr3; 1Broad Institute of MIT and Harvard, Cambridge, MA; 2University of Victoria, Victoria BC, Canada

WP 085
Application of Adductomics for Investigating Biomarkers Associated with Ovarian Cancer; Daniel Ladro1; William Funk1; 1Northwestern University, Chicago, IL; 2Northwestern University, Evanston, IL

WP 086
Serialised Nanoparticle-Mediated Enrichment and Profiling of the Saliva Proteome; Marissa Saltzman1; Kelsey Mitchell1; Kristine Tsantilas1; Khvatil Pathak1; Christophe Legendre1; Victoria David1; Matthew Rosenow1; Shane Caswell1; Lance Liotta2; Emmanuel Petricoin3; Patrick Pirrotte1; 1Translational Genomics Research Institute, Phoenix, AZ; 2Center for Applied Proteomics and Molecular Medicine, Manassas, VA; 3Sports Medicine Assessment and Testing (S.M.A.R.T.) Laboratory, Manassas, VA
BIOMARKERS: QUANTITATIVE ANALYSIS (PART 2)

WP 087  Identification of Serum Biomarker Candidates for Fatty Liver Disease through Depletion of Common High-Molecular-Weight Proteins; Sachin Sridharan1; Sobanana Jayakumar1; Keerthana Vinodh1; Adaikkalam Vellaichamy1; 1Anna University, Chennai, India

WP 088  Analysis of Possible Biomarkers for Complex Regional Pain Syndrome and Osteoporosis using nLC-MS; Johan Jackson1; Linus Svensberg1; Åsa Emmer1; 1KTH Royal Institute of Technology, Stockholm, Sweden

WP 089  Targeted Quantification of Mutant SPOP Proteins in Prostate Cancer; Hui Wang1; Christopher E. Barbieri2; Jintang He1; Yuqian Gao1; Chaochao Wu1; Athena A. Schepmoes1; Thomas L. Fillmore1; Tujin Shi1; Sung-Suk Chae2; Dennis Huang2; Juan Miguel Mosquera2; Wei-Jun Qian1; Richard D. Smith1; Sudhir Srivastava2; Jacob Kagan2; David Camp1; Karin D Rodland1; Mark A. Rubin2; Tao Liu1; 1Pacific Northwest National Laboratory, Richland, WA; 2Institute of Precision Medicine of Weill Cornell Medical College and New York Presbyterian Hospital, New York, NY; 3National Cancer Institute, Bethesda, MD

WP 090  Quantitative Tau Isoform Differentiation; Paul Auger1; Stephen Schauer2; W. Rodney Mathews1; Lee Honigberg1; Kristin R Wildsmith1; Genentech, South San Francisco, CA; 2Genentech Inc, South San Francisco, CA

WP 091  Developing LC-MS Assay for Pituitary Adenylate Cyclase-Activating Polypeptide; Ruina Li1; Yuzhong Deng1; Brian Dean1; Xiaorong Liang1; Genentech Inc, South San Francisco, CA

WP 092  Proteomic and Biochemical Analyses of EAM Rat; Jong Bok Seo1; Soo Jeong Park1; Seung Min Choi2; Jong Schepmoes1; Soo Jeong Park1; Seung Min Choi2; Jong

WP 093  Development of a Sensitive LC-MS/MS Method to Quantify Substance P Concentrations in Rat Cerebrospinal Fluid; Hanumanth Rao Pantangi1; Lakshmi Prasanna Rayapati1; Prathyusha Chunduru1; Saivishal Daripelli1; Ganesh Ayyanki1; Venkatesh Kamuju1; Ramakrishna Nirogi1; Suvun Life Sciences Ltd, Hyderabad, Telangana

WP 094  MRM-based Assay for Potential Protein Biomarker in Meningioma Patients; Shuvolma Mukhurjee1; Ajit Datar2; Rashid Kochhar2; Sanjeeva Srivastava3; Vedita Anand Singh1; Nikita Gahoi1; Saicharan Ghantasala1; Aliasgar Moyiadi1; Epari Shridhar1; Indian Institute of Technology Bombay, Mumbai, INDIA; 2Shimadzu Analytical (India) Pvt Ltd., Mumbai, INDIA; 3Tata Memorial Center, Mumbai, INDIA

WP 095  MRM Based Targeted Analysis of Serum Samples to Demonstrate Differentially Expressed Proteins in Severe Cases Of Falciparum Malaria; Vinod Kumar1; Shailesh Damale1; Ajit Datara1; Sanjeeva Srivastava1; Indian Institute of Technology Bombay, Mumbai, INDIA; Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India

WP 096  Development of MRM Assay for the Determination of Potential Biomarkers in Case of Severe Vivax Malaria; Sandip Patel1; Shailendra Rane1; Ajit Datara1; Swati Patankar1; Sanjeeva Srivastava1; Indian Institute of Technology Bombay, Mumbai, India; Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India

WP 097  Quantitative Profiling of Hypoxia-responsive Cellular Pathways Associated with Metastasis in Osteosarcoma by Parallel Reaction Monitoring Assay; Zifeng Song1; Liping Yang1; Luisa Zini1; Caleb Emmons2; Siva Kolluri1; Millan Shay1; Milan Milanovcance1; Claudia S Maier1; Oregon State University, Corvallis, OR; 2Proteome Software, Portland, OR

WP 098  Analysis of Glycosylation of Serum CD90 in Pancreatic Cancer by Mass Spectrometry; Jun Cap1; Jianhui Zhu1; Rui Yang1; Zhiqin Tan1; Mingui An1; David M. Lubman2; University of Michigan Medical Center, Ann Arbor, MI; 2Hanzhou Normal University, Hangzhou, China

WP 099  Quantification of the Unique eEF2 His715-Diphthamide post-translational Modification and Its Derivatives by Parallel Reaction Monitoring Mass Spectrometry; Axel Ducrot1; Sabine Kux van Geijtenbee1; Sebastian Stahl1; Ana Rita da Silva Mateus Seidi1; Sven Michel1; Gerhard Niederfellner1; Ruediger Rueger1; Ulrich Brinkmann1; Hoffmann-La Roche Ltd, Basel, Switzerland; 2Hoffmann-La Roche Ltd. Penzberg, Germany

WP 100  Analysis of Human Dried Blood Spots for Cotinine and trans-3'−Hydroxycotinine by Reversed Phase Ultra Performance Liquid Chromatography Tandem Mass Spectrometry; Alexandra L. Anstedt1, 2; Michael C. Stagl1; S. Alexandra Burt1; Matthew J Geiger1; Sara E Tomechko1; Michigan State University, East Lansing, MI; 2Department of Health & Human Services, Lansing, MI

WP 101  Novel Proteomics-Based Pipeline for Identifying Predictive Biomarkers of Taxane-Induced Neuropathy; Emily Chen1; Katherine D. Crew2, 3; Meghna Trivedi1; Danielle Awad1; Mathew Maurer2; Kevin Kalinsky4; Antonius Koller1; Purvi Patel1; Jenny Kim Kim1; 1Columbia University Medical Center, New York, NY; 2Department of Medicine, Columbia University Medical Center, New York, NY; 3Department of Epidemiology, Columbia University Medical Center, New York, NY; 4Herbert Irving Comprehensive Cancer Center, New York, NY

WP 102  Quantification of Lysosomal Storage Disease Specific Urinary Oligosaccharides for Potential Treatment Monitoring; Rongrong Huang1; Allison Cason1; Laura Pollard1; Tim Wood1; Greenwood Genetic Center, Greenwood, SC

WP 103  Evaluation of Stable Isotope Dimethyl Labeling and Spectra Counting for Protein Profiling in Mice with Nonalcoholic Steatohepatitis; Zicheng Jun1; Takhar Kasumov1; Northeast Ohio Medical University, Rootstown, OH; 2Northeast Ohio Medical University, Rootstown, OH

WP 104  Rapid Detection of a Low-Abundance Biomarker from Plasma Using Combined Capture and Digestion for Improved Sensitivity; John O’Grady1; Kevin Meyer1; Derrick Poe1; Perfinity Biosciences, Inc West Lafayette, IN

WP 105  Multiplexed Longitudinal Monitoring of Cancer Biomarkers in Dried Blood Spots using an Automated SISCAPA Workflow; Morteza Razavi1; Leigh Anderson1; Richard Yip1; Matthew E. Pope1; Terry W Pearson1; SISCAPA assay Technologies, Washington, DC

WP 106  Standardizing Targeted Mass Spectrometry

WP 107  Quantification of Dystrophin Toward Implementation in Clinical Trials; Kristy J Brown1; Meng Hsuan Han1; Mamta Gir1; Shivprasad Bhuvanendran1; Yoji Jaiswal1; Eric P Hoffman1; Yebrith Hathout1; Children’s National Healthy System, Washington DC, DC; 2Children’s National Medical Center, Washington, DC

WP 108  Rapid QQQ Screening and Quantification of Proteins from Complex Biological Matrices using Retention Time Predictor without Expensive Protein Standards; Rohana Liyanage1; Balamurugan Packialakshmi1; Jeremy Post1; Narayan C. Rath2; Jackson O. Lay, Jr2; University of Arkansas, Fayetteville, AR; 2University of Arkansas, Fayetteville, AR; Shimadzu Scientific Instruments, Columbia, MD - Maryland; 3PPPSRU, USDA, Agricultural Research Service, Fayetteville, AR
WP 108 Development of Peripheral Blood Mononuclear Cell (PBMC) Based Protein Biomarkers for Lung Cancer Diagnosis using DIA Mass Spectrometry; Shaohua Xu1; Chunlin Cai2; Feng Yao1; Qian Wu; Heng Zhao3; Wei Yan2; 1Shanghai Jiatong University, Shanghai, China; 2Shanghai Jiao Tong University, Shanghai, China; 3Shanghai Chest Hospital, Shanghai, China; 4Shanghai Center for Bioinformation Technology, Shanghai, China

WP 109 High Sensitivity and High Specificity LC-HRMS Method to Quantify the Corticosteroid Metabolome after Exposure to Inhaled Corticosteroids; Clementina A Mesaros1; Dominic Cicimaro2; 2Nathanial W Snyder2; 1University of Pennsylvania, Philadelphia, PA; 2Penn SRP Center and CEET, Philadelphia, PA

WP 110 Quantitative Evaluation towards the Glutathione S-Transferases in Human Plasma Using Affinity Coupling with LC-MS/MS; Fang Xi1; Beijing Institute of Genomics, CAS, Beijing, China

WP 111 Absolute Quantitation of Biomarkers Predictive of Recovery from Acute Kidney Injury after Liver Transplantation with nano-LC - Triple-Quadrupole Mass Spectrometry; Jacek W Sikora1; 1Paul M Thomas2; Joshua Levitsky3; Neil L Kelleher4; 1Proteomics Center of Excellence, Northwestern University, Evanston, IL; 2Proteomics Center of Excellence, Northwestern University, Evanston, IL; 3Comprehensive Transplant Center, Northwestern University Feinberg School of Medicine, Chicago, IL; 4Division of Gastroenterology and Hepatology, Northwestern University Feinberg School of Medicine, Chicago, IL

WP 112 Towards Routine Sub 100uL Serum/Plasma Analysis of Hepcidin-25 using LC/MS/MS; Joel Gummer1; 1Department of Environmental Chemistry Department Athens, GA; 2Rensselaer University, Boston, MA; 3Complex Carbohydrate Research Center & Department of Pharmacology, Columbia University Medical Center, New York, NY; 4Stanford University Mass Spectrometry, Stanford University, Stanford, CA; 5Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; 6Institute of Environmental Health Science, Wayne State University, Detroit, MI; 7Proteomics Core Facility, University of Maryland, College Park, MD; 8Center for Mass Spectrometry and Proteomics, University of Minnesota, St. Paul, MN

WP 113 Simultaneous Determination of Ceftazidime and Avibactam in Human Plasma by LC/MS; Xiaohua Li1; Xu Allan2; 1Keystone Bioanalytical, Inc. North Wales, PA

WP 114 Integrating Glycoproteomics in the Comprehensive Multi-Omics Profiling of Obesity-mediated Progression to Type II Diabetes; Christine Yeh1; Stanford, California

WP 115 An ABRF-PRG study; Identification of Low Abundance Proteins in a Highly Complex Protein Sample; Susan Van Ripper1; 1PREMIER Biosoft, Indore, India; 2Chen Emily; 3Allis Chien; 4Hennette Remmer; 5Paul M. Stemmer; 6Wang Yan; 7Pratik Jagtap; 8University of Minnesota Informatics Institute, University of Minnesota, Minneapolis, MN; 9Herbert Irving Comprehensive Cancer Center & Department of Pharmacology, Columbia University Medical Center, New York, NY; 10Stanford University Mass Spectrometry, Stanford University, Stanford, CA; 11Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; 12Institute of Environmental Health Science, Wayne State University, Detroit, MI; 13Proteomics Core Facility, University of Maryland, College Park, MD; 14Center for Mass Spectrometry and Proteomics, University of Minnesota, St. Paul, MN

WP 116 Particle-based N-linked Glycan Analysis of Selected Serum Proteins using Non-Glycosylated Binders as a Cancer Array Assay; Isabella Karlsson1; Anna Sroka-Bartnicka1; Alessandro Quaranta1; Lorena Ndreu1; Matthijs Pijnappel2; Gunnar Thorsén1; 1Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden

WP 117 Separation of Carbohydrate and Glycopeptide Isomers using Ion Mobility-Mass Spectrometry; Johanna Hofmann1; 1Heung Sik Hahn2; 2Weston B. Struve2; Hannes Hinneburg3; 3Daniel Kolarich3; 4Peter H Seeberger3; 5Kevin Page6; 6Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; 7Freie Universität Berlin, Berlin, Germany; 8Max Planck Institute of Colloids and Interfaces, Potsdam, Germany; 9Oxford University, Oxford, UK

WP 118 Non-Arbitrary Scoring Model for Structural Identification of Glycosaminoglycan Tandem MS; Jiana Duan1; 1Jon Amster1; 2University of Georgia, Athens, GA; 3University of Georgia, Chemistry Department Athens, GA

WP 119 In-depth Analysis of Non-arbitrarily Linked Glycans Using Ion Chromatography-Orbitrap Mass Spectrometry; Zoltan Szabo1; 1Junnan Wang2; Yury Agroskin3; Rosa Viner4; Julian Saba5; 1Thermo Fisher Scientific Japan, Yokohama, Japan; 2Thermo Fisher Scientific Inc, San Jose, CA; 3Thermo Fisher Scientific, San Jose, CA

WP 120 Hydrophilic Interaction Liquid Chromatography-Mass Spectrometric Imaging Platform for N-glycan Relative Quantitation using Stable-Isotope Labeled Hydrazide Reagents; Zhengwei Chen1; 1Xuefei Zhong; 1Tie Cai; 1Yatao Shi2; Xinxiang Zhang3; 3Lingjun Li2; 4University of Wisconsin Madison, Madison, WI; 5University of Wisconsin-Madison, Madison, US; 6Peking University, Beijing, China; 7Chinese Academy of Sciences, Shanghai, China

WP 121 A Comprehensive Mass Spectrometric Workflow to Investigate Glycosylation Impact on Viral Antigenic Sites; Edward Bodnar1; Lisa Parsons2; 2Yamnning An3; 3John F Cipollo2; 1Human and Health Services, U.S. Food and Drug Administration, Division of Bacterial, Parasitic and Allergenic Products, Laboratory of Bacterial Polysaccharides, Silver Spring, USA

WP 122 Mobilizing the Library: Using IMS-MS Data to Supplement GU Library Searching for Glycan Identification; William Alley1; 1Ying-Qing Yu1; 1Waters Corp., Milford, MA

WP 123 Glycosaminoglycan Peak Searching: A Novel GAG-Specific Method for Automated Tandem Mass Spectra Analysis; John D. Hogan1; 1Yu Huang2; Cheng Lin3; Joshua Klein1; Luis Carvalho4; Chengli Zong5; Geet-Jan Boons6; Joseph Zaia7; 1Program in Bioinformatics, Boston University, Boston, MA; 2Boston University School of Medicine, Boston, MA; 3Department of Mathematics & Statistics, Boston University, Boston, MA; 4Complex Carbohydrate Research Center UGA, Athens, GA

WP 124 Speeding up the High Throughput Searches for Glycan Analysis; Ningombam Sanjib Meltei1; 1Rupanjana Goswami1; 1Julian A Saba3; 2PREMIER Biosoft, Indore, India; 3PREMIER Biosoft, Palo Alto, CA; 4Thermo Fisher Scientific, San Jose, CA

WP 125 Comprehensive Assessment of Derivatization Strategies for LC-MS/MS Analysis of N-glycans; Shiyou Zhou1; 1Xue Dong1; 1Yehia Mechref1; 1Texas Tech University, Lubbock, TX

WP 126 Multiplex LC-MS Analysis of Isotopically Permethylated N-glycans Derived From Biological Samples; Xue Dong1; 2Shiyou Zhou1; 1Yehia Mechref1; 1Texas Tech University, Lubbock, Texas

WP 127 Capillary Electrophoresis Separation of Glycosaminoglycans Followed by Tandem Mass Spectrometry; Morgan Stickney1; 1Patience Sanderson1; 1Robert J Linhardt1; 2Jon Amster1; 1University of Georgia, Chemistry Department Athens, GA; 2Rensselaer Polytechnic Institute, Troy, NY
WP 132 Glyconote: A Software for the Automated Interpretation of Glycomics Data from Tandem Mass Spectrometry; Minjoo Liu1; Guy Treves2; Andres Guerrero2; Matthew Amicucci2; Jasmine Davis3; Lauren D Wu4; Pengyuan Yang3; Carillo B Lebrilla5; Fudan University, Shanghai, China; 2UC Davis Chemistry Department, Davis, CA

WP 129 Optimization of Dual Modifications Strategy for Simultaneous Characterization of Neutral and Sialylated N-Glycans by LC-MS/MS; Haiying Li1; Patricia Cho2; Stephen Kostel1; John Froehlich3; Richard Lee4; 1Boston Children’s Hospital, Harvard Medical School; Boston, MA; 2Department of Chemistry, Boston College; Dedham, MA; 3Duke University, Durham, NC; 4University of California, Irvine

WP 130 Semi-automated Glycan Screening and Quantitative Analysis of Longitudinal Plasma Samples; Elizabeth S. Hecht1; Alison Motsinger-Reif2; Brendan MacLean3; James N Petitte4; Michael J MacCoss5; David C Muddiman6; 1North Carolina State University, Raleigh, NC; 2University of Washington, Seattle, WA

WP 131 Sialyl Linkage-Specific Glycan Profiling using Solid-Phase SALSA: A Simple and Versatile Derivatization Approach; Takashi Nishikaze1; Hiroki Tsumoto2; Yuzo Yamazaki3; Shinichi Iwamoto1; Yuri Miura4; Koichi Tanaka5; 1Shimadzu Corporation, Kyoto, Japan; 2Tokyo Metropolitan Institute of Gerontology, Tokyo, Japan

WP 132 MS Based Method to Quantify Rheumatoid Arthritis Serum Glycosaminoglycans Using nano UPLC-ionkey MS/MS on a Xevo G2 Q TOF; Youjin Seo7; Arman Andaya8; Julie A Leary9; 1University of California Davis, Davis, CA

WP 133 Detailed Structure Elucidation of the N-linked Octasaccharide of the Archaeon Methanosarcina mazei by Mass Spectrometry; Deborah R. Leon1; Cheng Lin2; Yi Pu1; John R Haserick3; Rebecca S Glaskin4; Rachel R Ogorzalek Loo5; Joseph A Loo6; Robert Gunsalus7; Catherine E Costello8; 1Boston University School of Medicine, Boston, MA; 2UC, Los Angeles, CA

WP 134 Glyn: A New Tool for Glycan Structure Elucidation and Characterization; Eric Joyce1; Jinshan Gao2; 1Montclair State University, Montclair, NJ

WP 135 Developmental Profiles of Gangliosides in Prefrontal Cortex of Human Brain via Negative Ion Mode Nano-LC/MS and LC/MS/MS; Injung Ji1; Jae Yun Hwang2; Su Min Kim1; Dan Bi Park2; David Bradley3; Hyun Joo An4; 1Boston University, Boston, MA; 2Boston Children’s Hospital, Boston, MA; 3Duke University, Durham, NC; 4Northwestern University, Lake Forest, IL

WP 136 Tailoring Glycan Hydrazide Tagging Reagents for MS Functionality; James McCard1; David C Muddiman2; 1North Carolina State University, Raleigh, North Carolina

WP 137 Acid-Induced Fucose Migration; Yi Pu3; Yana Tang4; John Haserick1; Catherine E Costello2; Cheng Lin1; 1Boston University; Boston, MA; 2Boston University School of Medicine, Boston, MA

WP 138 Automated N-Glycan Sample Preparation with an Instant Glycan Labeling Dye for Mass Spectrometry; Ted Haxo1; Aled Jones; Michael J Kimzey1; Emily Dale1; Sergey vlasenko1; Steve mast1; 1ProZyme, Hayward, CA

DISEASE BIOMARKERS

WP 139 Identification of Novel Biomarker Candidates for Diagnosis of Follicular Carcinoma; Xianyin Lai1; Indiana University School of Medicine, Indianapolis, IN

WP 140 Identification of a CNS-specific Proteome Biomarker for Clinical Relapses and Progression of Multiple Sclerosis using a Systems-Biology Approach; Itay Raphael1; Carol A Hulzer1; Yanyan Qu2; Wendell P Griffith3; 1University of Texas at San Antonio, San Antonio, TX; 2Department of Chemistry, University of Texas at San Antonio, San Antonio, TX

WP 141 Biomarkers of Early Chronic Obstructive Pulmonary Disease (COPD) in Smokers and Former Smokers - A Comparison of Two Methods; Karin Barbara Sahlin1; Johan Malm1; Mikael Truedsson2; May Bugge3; Elisabet Wieslander4; Maria Yokaleva5; Magnus Dahlbäck6; Roger Appelqvist7; Thomas Fehninger8; György Marko-Varga9; 1Lund University, Lund, Sweden; 2Lund University, Lund, Sweden; 3Örebro University, Malmö, Sweden

WP 142 Large-Scale Analysis of Protein Conformational Changes for Biomarker Discovery; Fang Liu1; Michael C Fitzgerald2; 1Duke University, Durham, NC; 2University of California Davis, Davis, CA

WP 143 Study of Traumatic Brain Injury Biomarkers by Mass Spectrometry-Based Proteomics; Manasi Manaoanker1; Richard A Yost2; Kari Green1; 1University of Florida, Gainesville, FL

WP 144 Lipidomics Approach in Biliary Atresia for a Potential Diagnostic Method Based on Mass Spectrometry; Cibele Esteves1; Diogo Noin de Oliveira2; Carlos Fernando Odor Rodrigues Melo3; Luciana Di Paolo4; Gabriel Hessel5; Rodrigo Ramos Catharino6; 1University of Campinas, Campinas, Brazil; 2Institute of Gerontology, Tokyo, Japan

WP 145 Neonatal Neurodegeneration in 5XFAD Alzheimer’s Disease Transgenic Mouse Model; Aise Rumeysa Mazi1, 2; Aysegul Sumeyye Arzuman1, 2; Mehmet Ozansoy1, 2; Ahmet Tarik Baykal3; 1Regenerative and Restorative Medicine Research Center, REMER, Istanbul, Turkey; 2Institute of Health Science, Istanbul Medipol University, Istanbul, Turkey; 3Department of Physiology, International School of Medicine, Istanbul Medipol University, Istanbul, Turkey; 4Acibadem University, Atasehir-Istanbul

WP 146 A Proteomic Investigation of the Role of Neurotoxins Linked to Amyotrophic Lateral Sclerosis Disease Pathogenesis; Joshua Bert1; Michael S Bereman2; 1NC State University, Raleigh, NC

WP 147 Prediction of Response to Sorafenib in Hepatocellular Carcinoma: A Multimarker Panel of Potential Biomarkers by Multiple Reaction Monitoring-Mass Spectrometry; Hyunsoo Kim1; Injong Yeo1; Su Jong Yu1; Taesung Park1; Jung-Hwan Yoon2; Youngsoo Kim3; 1Department of Biomedical Engineering, Seoul National University College of Medicine, Seoul, Korea; 2Department of Internal Medicine and Liver Research Institute, Seoul National University College of Medicine, Seoul National University Hospital, Seoul, Korea; 3Department of Statistics, Seoul National University, Seoul, Korea

WP 148 Simultaneous Quantification of Tryptophan-Relatedmetabolitesas Biomarkers for Prediabetes; Nonhide Yokoi1; Ritsuko Hoshikawa2; Toshiya Matsubara2; Susumu Takei1; 1Regenerative and Restorative Medicine, Tokyo, Japan; 2Acibadem University, Ataşehir-Istanbul

WP 149 Comparison of Plasma Protein Profiles of Selected Cardiovascular Diseases by iTRAQ Quantification; Helenah Rehulkova1; Alena Myšlíková1; Alexey Lyashkov1; Pavel Rehulka2; Radek Pudil3; Jiří Stulík4; 1Faculty of Military Health Sciences, University of Defence, Hradec Králové, Czech Republic; 21st Department of Internal Medicine – Cardiangoiety, Faculty Hospital, Hradec Králové, Czech Republic

WP 150 Proteomics Analysis of Aged Healthy Human White Blood Cells; Cesereena Ubaidah-Mohien1; Alexey Lyashkov1; Arsun Bektas3; Robert Wersto1; Nan Ping Weng1; Ranjan Sen3; Luigi Ferrucci4; 1Intramural Research Program, National Institute on Aging, National Institutes of Health, Baltimore, MD – Maryland; 2Laboratory of Molecular Biology and Immunology, National Institute on Aging, Baltimore, MD

WP 151 Cardiovascular Disease - Metabolic Syndrome Induced Protein/PTM Changes; Mark E. McCorm1; Stephen A. Whelan1; Chunxiang Yao1; Jessica B. Behring1; Jean L. Spencer1; Christian F. Heckendorf1; Nancy M. Leymarie1; 1North Carolina State University, Raleigh, North Carolina
WP 152 An Adductomics Pipeline for Untargeted Analysis of Post Translational Modifications: Hasmik Grigoryan1; William Edmonds2; Sixin S Lu3; Yukiko Yano2; Anthony Iavarone2; Evan R Williams2; Stephen M Rappaport2; 1University Of California, Berkeley, CA; 2University of California, Berkeley, CA

WP 153 Localized Quantitative Proteomics on Amyloid Plaques Microdissected from Postmortem Tissue to Characterize Difference between Rapidly Progressive and Typical Alzheimer’s Disease: Shrutik Navak1; Steven Drummond1; Manor Askenazi1; Arline Faustin1; Geoffrey Pires1; Richard Hickman1; Jiri Safar1; Thomas Wisniewski1; Beatrix M Ueberheide1; NYULMC, New York, NY; 2Biomedical Hosting LLC, Arlington, MA; 3Case Western Reserve University, Cleveland, OH

WP 154 High Throughput Screening of Competitive Binders for Target Proteins using Rapid LC-MS Analysis: Kasun Imaduwa1; Eden P Go2; Heather Desaire1; 1University Of Kansas, Lawrence, KS; 2University Of Kansas, Lawrence, KS

WP 155 Implementation of Mass Spectrometry into High Throughput Screening Workflows to Improve Hit Quality: Gregory Adam1; Juncal Meng1; Adam Amoss1; Amita Patel1; Daniel Riley1; Victor Uebele1; Jeffrey Hermes1; Merck & Co., Inc., North Wales, PA; Merck & Co., North Wales, PA

WP 156 Application of High-Throughput Micro-Flow LC/MS to a Metabolic Stability Screening Workflow: Brendon Kapinos1; John S Janiszewski1; Mary Piotrowski1; Wayne Lootsma1; Steven Ainline1; William Schramm1; Hui Zhang1; Pfizer, Groton, CT; Sound Analytics, Niantic, CT

WP 157 Ultra High Throughput Drug Discovery Screening by MALDI-TOF Mass Spectrometry—Exceeding One Million Samples per Week: Peter S. Marshall1; Michelle Pemberton1; Carl Haslam1; Gabriella Clarke1; Jessica Chandler1; Adrian Dunn1; Neil Hardy1; Melanie Leveridge1; GlaxoSmithKline, Stevenage, UK

WP 158 High Throughput Screening-ADME; Transitioning from Triple Quadrupole to High Resolution Accurate Mass Spectrometry: Jason Causon1; Graeme Clark2; SCIEX, Warrington, UK; Cyprotech, Macclesfield, UK

WP 159 Utilizing High Resolution Accurate Mass Spectrometry for Quantification, MRMHR and SWATH® Acquisition Workflows: Jason Causon1; Lee Mendil1; Donna-Michelle Smith1; Neil Devineport1; Thomas Knapman1; Milla Neffling1; SCIEX, Warrington, UK; CRUK Cambridge Institute - University Of Cambridge, Cambridge, UK

WP 160 Simultaneous Analysis of Supernatant Components of Cell Culture using Triple Quadrupole LC/MS/MS: Qiaoxia Liu1; Hongyanu Hao1; Yuling Song2; Qiang Li2; Zhao Liu2; Taohong Huang2; Yuki Hashi1; Shimadzu, Shanghai, CHINA

WP 161 Assay Development of in vitro Blood-Brain Barrier Models for Drug Permeability Screening: Lie Min1; Jennifer L. Mantle1; Kelvin H. Lee1; 1Department of Chemical and Biomolecular Engineering and Delaware Biotechnology Institute, University of Delaware, Newark, DE

WP 162 Labeled Compound Detection Using Compound Discoverer Pattern Scoring From High Resolution Mass Spectrometry: Caroline Ding1; Tim J Stratton1; Martin Ströhalm2; Ji Ma3; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Bremen, DE; 3Amgen, Inc. South San Francisco, CA

WP 163 Evaluation of Ion Mobility Enabled Collisionless Cross Section Measurements for the Differentiation of Acyl and Phenolic Glucuronide Metabolites: Catherine Holdsworth1; Richard Clayton1; Daniel Weston2; Nick Tomczyk2; Martin Palmer1; Darren Hewitt3; Covance, Harrogate, UK; Waters, Wilmslow, UK

WP 164 Resolution and Characterisation of Co-eluting Isomeric Metabolites by Collision Cross Section Measurements using a Novel Geometry Travelling-Wave IMS-QToF Mass Spectrometer: Richard Clayton1; Catherine Holdsworth1; Daniel Weston2; Nick Tomczyk2; Martin Palmer1; Darren Hewitt3; Covance, Harrogate, UK; Waters, Wilmslow, UK

WP 165 Automatic Calculation and Layout of MS/MS Fragmentation Pathways: Ismael Zamora1; Blanca Serra2; Moretoni Luca1; Lead Molecular Design, S.L., Sant Cugat del Valles, Barcelona; 2Molecular Discovery, Ltd London, UK; 3Molecular Discovery, London, UK

WP 166 Drug Stability Study using Q Exactive Bench-Top Mass Spectrometer: Jie Ding1; Thomas Leitzinger1; Kate Comstock1; PPD Inc, Middleton, WI; Thermo Fisher Scientific, San Jose, CA

WP 167 Novel Drug Target Identification via Label Free Differential Mass Spectrometry and Thermal Stability Profiling: Harris Bell-Temin1; Steven J Mullett1; David Zaidins1; Andrey Bondarenko1; Mark E Schurda1; Andrew Michael Stern1; D. Lansing Taylor1; Nathan A Yates1; School of Medicine, University of Pittsburgh, Pittsburgh, PA; Drug Discovery Institute, University of Pittsburgh, Pittsburgh, PA; Infolinkia, Seattle, WA

WP 168 Quantitative Kinome Analysis as a Tool for Discovering Molecular Targets for Cancer Therapy: Weili Miao1; Yongsheng Xiao1; Yinsheng Wang1; University of California - Riverside, Riverside, CA; 2University of California, Riverside, CA

WP 169 Rapid Rank Ordering of Compounds in Mixtures by Orthogonal Affinity Selection – Mass Spectrometry: Christine L. Andrews1; Matthew P Richards1; Jacqueline Hicks1; John Caldwell1; Jared Cumming1; Andrew Stamford1; Corey Strickland1; Peter Dandliker1; Merck & Co, Kenilworth, NJ

WP 170 Platform Agnostic Data Processing Routine for Targeted and Untargeted Metabolite Identification in Drug Discovery: Richard Lee1; Vitaly Lashin3; Alexandr Sakarov2; ACD/Labs, Toronto, Canada; ACD/Labs, Moscow, Russia

WP 171 A MS Approach to Understand the Most Metabolically Labile Amide Bonds in Peptides: Ismael Zamora1; Tatiana Radchenko1; Elisabeth Ortega1; Lead Molecular Design S.L., Sant Cugat de Valles, Spain

WP 172 Identification of Active Herbal Ingredients by Affinity Selection Mass Spectrometry Coupled with Ultrafiltration: Yan Jin1; Fangzhou Xie1; Lei Fu1; Shanghai Jiao Tong University, Shanghai, China

WP 173 Glue Medicines Analysis by UHPLC Tandem Quadrupole-Time of Flight Mass Spectrometry: Hu Nan1; Zuo Shuai1; Du Wei1; Bo Tao1; Agilent Technologies (China) Limited, Beijing, China

WP 174 Rapid Determination of Protein Binding Affinity Using Solid Phase Micro Extraction: Emily Barrey1; Craig Aurand1; David Bell1; Sara Smith1; Sigma Aldrich, Bellefonte, PA

WP 175 Biochemical Assay Development Using Novel MALDI High-Throughput Screening System: Sergei Dikler1; Paul J Kowalski2; Bruker Daltonics, Billerica, MA; 2Bruker Daltonics, Inc., Billerica, MA

WP 176 Assessment of Chemical Probes for Identification of Cellular Targets of Small Molecules: Jeffrey Martin1; Mercedes Beyna1; Ceren Korkut1; Rajesh Prakash1; Jaqy Sherrer1; Kevin Guckian1; Erik Hett1; Peter Juhasz2; Biogen, Cambridge, MA
WP 180 Application of Molecular Dynamic Simulation to Improve the CCS Calculation Accuracy of Aromatic Compounds with Long Alkyl Chains; Aref Ahmed1; Dongwun Lim1; Hugh I. Kim1; Sunghwan Kim1;2; Kyungpook National University, Daegu, Republic of Korea; 1Korea University, Seoul, Republic of Korea; Green-Nano Materials Research Center, Daegu, Republic of Korea

WP 181 Characterization of a B-O-4 Trimeric Lignin Model Compound and Post Fenton Chemistry Products using HRAM Mass Spectrometry; Fan Huang1; Bert C Lynn1; 1University of Kentucky, Lexington, KY

WP 182 Investigating the Mechanism of Lipid Body Obesity in C. reinhardtii under Nitrogen Starvation Conditions using High Resolution Mass Spectrometry; Carter Lantz1; Ryan Rho1; Jeremy Sieker1; Matthew Brantley1; Alirea Abdolvahabi1; James Chang1; Sung-Joon Kim1; Tournaj Solouki1; Baylor University, Waco, TX

WP 183 Effect of Alkali Metals on Pyrolysis Kinetics of Carbohydrates Using dAPCI-TOF MS; Kristen O’Connor1; Carolyn Hutchinson1; Young Jin Lee1; Iowa State University, Ames, IA

WP 184 Characterization of Fast Pyrolysis Oil from Pine Feedstock; Ashley Wittrig1; Ross Mabon1; Boris Sheludko1; ExxonMobil, Annandale, NJ

WP 185 Exploring the Mechanisms of Fast Pyrolysis of Hemicellulose via Tandem Mass Spectrometry and Quantum Chemical Calculations: A Model Compound Study; Priva Murria1; John Degenstein1; Mckay Easton1; Hanyu Zhu1; John Nash1; Rakesh Agrawal1; Nicholas Delgass1; Fabio Ribeiro1; Kenttämaa Hilika1; Purdue University, West Lafayette, IN

WP 186 Chemical Reactions Causing Instability in Wood-Derived Bio-Oils: Enhanced Detection of Aldehydes using Peracetylation with Pyridine or DMAP; Elizabeth A. Stemmler1; Paige E. Speir1; Mason A. Bosse1; Matthew J. Rasmussen1; Bowdoin College, Brunswick, ME; Bowdoin College, Brunswick, ME

WP 187 Integrated Omics Reveals the Details of Metabolic Adaptation of Clostridium thermocellumATCC-27405 Grown on Switchgrass; Suresh Poudel1; 2; Richard J Giannone1; Miguel Rodriguez1; Babu Raman1; Madhavi Z Martin1; Nancy L Egle1; Nookaew Intawat1; Steven D Brown1; Timothy J Tschaplinski1; David Ussery1; Hettich L Robert1; Oak Ridge National Laboratory, Oak Ridge, TN; University of Tennessee, Knoxville, TN; Dow AgroSciences, Indianapolis, IN

WP 188 Large scale Identification of Polymorphic Peptides via Cross-Species Spectral Networks in Microbial Proteomics; Seungjin Na1; Sam Payne2; Nuno Bandeira3; 1University of California San Diego, La Jolla, CA; 2Pacific Northwest National Lab, Richland, WA

WP 189 Development of GeLC-MRM Approach to Study Carbon Concentrating Mechanism during Nitrogen Starvation in Chlorella sp ITO FC2; Vineeta Rai1; Deepali Bhandarkar1; Ajit Datar1; Sanjeeva Srivastava1; Indian Institute of Technology Bombay, Mumbai, India; 2Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India

ENVIRONMENTAL ANALYSIS: WATER QUALITY
WP 190 Development of Method for Quantification of Iodoacetic Acids in Drinking Water Using GC/EI-MS/MS; Hannah Liberatore1; Amy A. Cuthbertson1; Susan D Richardson1; University of South Carolina, Columbia, SC

WP 191 Water Quality Growth and Change, Advanced Technology Method Change to Prescribe a Desirable Future to US EPA Method 521, (2004); Andrew Eaton1; Konjit Tadigo1; Charles Grady1; Ron Homfeld1; Eurofins Eaton Analytical Inc, Monrovia, CA; 2Agilent Technologies, Prescott, AZ

WP 192 A New Approach for Identification of Unknown Disinfection Byproducts in Drinking Water using Multiplex Solid Phase Extraction /HPLC-tandem Mass Spectrometry; Xing-Fang Li1; Yanan Tang1; Guang Huang1; Lindsay Jsmall1; Ian Vander Meulen1; University of Alberta, Edmonton, AB; University of Alberta, Edmonton, Canada

WP 193 Direct Analysis of PFAAs in Water using Different Mobility Spectrometry-Mass Spectrometry: Matthew Noestheden1; KC Hyland1; Simon Roberts1; Chris Higgins1; SCIEX, Concord, ON; SCIEX, Redwood City, CA; Colorado School of Mines, Golden, CO

WP 194 Significantly Improved Detection in Volatile Organic Analysis (VOA) of Water using Static Headspace and GCMS with a High Efficiency Source; Harry Prest1; Melissa Churely1; Peter Gastachi1; Agilent Technologies, Santa Clara, CA; Agilent Technologies, Santa Clara, CA; Agilent Technologies Sales & Services GmbH, Waldbronn, Deutschland

WP 195 Increased Capabilities for the Analysis of Hormones in Drinking and Waste Water using SPE and LC/MS/MS; Xianrong (Jenny) Wei1; Sean Orlowicz1; Phenomenex, Torrance, CA; Phenomenex, Torrance, CA

WP 196 Analysis and “Fingerprinting” of Non-Ionic Surfactants in Hydraulic Fracturing Waters by Ion Mobility Mass Spectrometry; E. Michael Thurman1; Imma Ferrer1; Jerry Zweigenbaum1; Aaron Boice1; John Fieldsted; University of Colorado, Boulder; Colorado; Agilent Technologies, Little Falls, DE; Agilent Technologies, Santa Clara, CA

WP 197 Cloud-based Analysis of Complex Sample Systems for Outlier and Trend Analysis in the Context of Water Monitoring; Ralf Tautenhahn; Tim J Stratton1; Dipankar Ghosh1; Thermo Fisher Scientific, San Jose, CA

WP 198 Two Birds with One Stone: Simultaneous GC/MS Analysis of Volatile and Semivolatile Water Pollutants; Olga V Polvakova1; Dmitry Mazur1; Vitaly Artaev2; Albert T. Lebedev3; Moscow State University, Moscow, Russia; LECOR Corporation, St Joseph, MI; Moscow State University, Moscow, Moscow

WP 199 Unknown Profiling of Drinking Water Using High Resolution LC-MS/MS and New Software; Caroline DING1; Anastasia Kalli1; Charles Yang1; Tim J Stratton1; Thermo Fisher Scientific, San Jose, CA

WP 200 Environmental Screening of Water Samples utilizing Ion Mobility Enable High Resolution Mass Spectrometry: Lauren Mullin1; Douglas Stevens1; Gareth Cleland1; Adam Ladak1; Waters, Milford, MA

WP 201 Using Mass Spectrometry to Detect Silanol Compounds in Water from the International Space Station; Jeffrey A. Rutz1; C.K. Mike Kuo1; James T. Alverson1; William T. Wallace1; Daniel B. Gazda1; Wyle Science, Technology, and Engineering Group, Houston, TX; NASA Johnson Space Center, Houston, TX
FOOD SAFETY: OTHER CONTAMINANTS (PART 1)

WP 207 Characterization of the Volatile Degradation Products of Soybean Oil after Frying Process by HS-SPME-GC-MS; Ya-Ting Tsaí; Maw-Rong Lee; Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; 2National Chung-Hsing University, Taichung, Taichung

WP 208 Non-targeted Analysis Approach for Distinguishing of Various Vegetable Oils and Adulterated Oils using HS-SPME-GC-MS; Yu-Hao Chen; Maw-Rong Lee; Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; 2National Chung-Hsing University, Taichung, Taichung

WP 209 Significant Robustness Improvements of PAHs Analysis in Palm Oil using the Self-Cleaning Ion Source (SCIS) in a GC/MS/MS System; Michel Lesieur1; Elizabeth Almasi2; Terry Sheehan; 4Agilent Technologies, Les Ulis, France; 2Agilent Technologies, Santa Clara, CA

WP 210 Analysis of Fish Oil for Contaminants by LC Time-of-Flight Mass Spectrometry with All Ions Confirmation; Sue Dantonio; Joan Stevens; 4Agilent Technologies, Flatonia, TX; 2Agilent Technologies, Wilmington, DE

WP 211 Quality Control of Cooking Oils by Metabolic Profiling and Spectral Fingerprinting; Chi Yuen Cheung; HKUST, Hong Kong

WP 212 Direct Analysis of Brominated Vegetable Oil in Commercial Soft Drinks by LC-MS; Priyanka Chitranshi; Goncalo Gamboa Da Costa; 1US FDA NCTR, Jefferson, AR

WP 213 Determination of Phthalates in Vegetables by GC–GCMS; Zhang Xi; SHIMADZU (CHINA) CO., LTD.; Beijing Branch, Beijing, China

WP 214 Representative, Two-Gram Incurred Food Samples using mini-QuEChERS, Cryomilling and GC/MS/MS Analysis with a High Efficiency Ion Source; Joan Stevens; Melissa Churley; 4Agilent Technologies, Wilmington, DE; 2Agilent Technologies, Santa Clara, CA

WP 215 Identification of Contaminants in Powdered Beverages by Direct Extraction Thermal Desorption GC/MS; Ronald Shomo; Christopher W Baker; John Manura; 3Scientific Instrument Services, Ringoes, NJ

WP 216 Simultaneous Separation and Determination of Fifteen Organic UV Filters in Sunscreen Cosmetics by HPLC-EI-MS/MS; Qiang Ma; Xianhuang Meng; Guansheng Xi; 'Chinese Academy of Inspection and Quarantine, Beijing, China

WP 217 Determination of Chlorinated Compounds Arising from the Thermal Degradation of Sucralose; Diogo Noin de Oliveira; Maico Menezes; Rodrigo Ramos Catharino; 1Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil

WP 218 A High Throughput, Low Cost and Green Approach to Automated Extraction, Clean Up, and Concentration for Same Day POPs Analysis; Tom Haji; Ruud Addink; 2Fluid Management Systems, Watertown, MA

WP 219 Total Residue Analysis of Glyphosate and Three Metabolites in Soy and Milk-Based Nutritional Ingredients by Liquid Chromatography – Mass Spectrometry; Stefano Fata; Todine Reddy; 1Abbott Nutrition, Columbia, OH

WP 220 Infant Formula and Milk: Chlorinated Dioxins and Furans Analysis Using Automated Extraction and Column Chromatography; Alek Shapabay; Rudolf Addink; 1Toxic Report, Watertown, MA

WP 221 Simultaneous Determination of Total vitamins B1, B2, B3, B5, and B6 and Total Folate in Infant Formula and Related Nutritional; Nicholas Cellar; Todine Reddy; 1Abbott Nutrition, Columbia, OH

WP 222 Simultaneous Determination of Choline, Carnitine, and Myo-inositol by LC-MS/MS; Jonathan Drahner; Nicholas A Cellar; Todine Reddy; 1Abbott Nutrition, Columbia, OH; 2Abbott Nutrition, Columbia, PA

WP 223 Multi-residue Antibiotic Analysis of Dairy Products using UHPLC-MS/MS with a Heated Laminar Flow Interface and a Modified QuEChERS Method; Avinash Dalima; Sharanya Reddy; Thomas P White; Tong Chen; Wilhad Reuter; David Welkie; Lisa Cousins; Joshua Ye; Reza Javahery; 1PerkinElmer Health Sciences, Inc., Shelton, CT; 2IONICS Mass Spectrometry, Bolton, Canada

WP 224 Rapid Determination of Lactulose in Heat Treated Milk using Ultra-performance Convergence Chromatography Coupled with Mass Spectrometry; Feng Wen; Yao Tian; Yongwei Xu; Nan Zheng; Qiongling Sun; Songli Li; Jiaqi Wang; 1Ministry of Agriculture Laboratory of Quality & Safety Risk Assessment for Dairy Products (Beijing), Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China; 2Ministry of Agriculture - Milk and Dairy Product Inspection Center (Beijing), Beijing, China; 3Waters Corporation, Shanghai, China

WP 225 Mass Barcode-Based Signal Amplification for Highly Sensitive Multiplex Diagnosis of Allergy; Xiaojing Zhong; Liang Qiao; Natalia Giansiov; H Girault; 1Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; 2Fudan university, Shanghai, China

WP 226 Multi-Allergen Quantitation in Thermally Processed Foods by Liquid Chromatography Tandem Mass Spectrometry; Chelsea M. Coffey; Christine H. Parker; Timothy R Crollie; 1US Food and Drug Administration, College Park, MD

WP 227 Ultra-Fast Analysis of Allergens using Capillary Electrophoresis Coupled to Mass Spectrometry and Ultraviolet Photodissociation; Chien-Hsien Chen;
WP 228 Chlorinated Dioxins, Furans and Biphenyls Analysis in Beverages Using Automated Extraction and Reduced Solvent Volume Column Chromatography; Matt Falkenstein1; Rudolf Addink1; "Toxic Report, Watertown, MA"

WP 229 Rapid Analysis of Key Aflatoxins in Rice by Microwave Plasma Torch Mass Spectrometry; Tao Jiang1; Runzhi Zhou1; Zhiqiang Zhu1; Huanwen Chen1; "East China Institute of Technology, Nanchang, China; East China University of Technology, Nanchang, Mainland"

WP 230 A High Sensitivity LC/MS/MS Method with QuEChERS Sample Pre-treatment for Determination of Aflatoxins in Milk Powders; Yin Ling Chew1; Jie Xing2; Guan Seng Leonard Lim3; Zhaoqi Zhan1; "Shimadzu (Asia Pacific) Pte Ltd, Singapore; Shimadzu (Asia Pacific) Pte Ltd, Singapore"

WP 231 Development of Automated Screening and Quantitation Method on a Novel On-line SFE-SFC-MS/MS Platform – (II) For Aflatoxins in Powdered Food; Jie Xing1; Yin Ling Chew1; Jun Xiang Lee1; Li Wen Tung1; Zhaoqi Zhan1; "Shimadzu (Asia Pacific) Pte Ltd, Singapore"

WP 232 Simultaneous Analysis of 23 Mycotoxins using Ultra-High Speed LC-MS/MS with a Pentfluorophenyl Column; Matsumoto Keiko1; Jun Watanabe3; Mochizuki Naoki2; Shimadzu Corporation, Kyoto, Japan; Shimadzu Corporation, Kyoto; "Asahi Group Holdings, Limited Moriya, Japan"

WP 233 LC-MS Analysis of Graviola and Other Neurotoxic Fruits; Kevin Tran1; Pushkar Shejwalkar2; Kenji Hara3; Ingrid de Moraes1; "US FDA, Lenexa, KS; Tokyo University of Technology, Tokyo, JP; State University of Campinas, Campinas, Brazil"

WP 234 Rapid Development of Quantitative Method for Determination of Plant Growth Regulators and Streptomyacin in Fruits using LC/MS/MS; Anant Lohar1; Shailendra Rane1; Ashutosh Shelar1; Purushottam Satuar1; Shailesh Damale1; Deepti Bhandarkar1; Rashi Kochhar1; "Shimadzu Corporation, Kyoto, Japan; Shimadzu Corporation, Kyoto; "Asahi Group Holdings, Limited Moriya, Japan"

WP 235 A Streamlined Processing Method for High Resolution Mass Spectrometric Data to Compare Food-Grade Glycerin with Crude-Glycerins to Screen for Jatropha Toxins; Kithsiri B Herath1; Lauren Girard1; Renate Reimschuessel1; Hiranthi Jayasuriya1; "Center for Veterinary Medicine/FDA, Laurel, MD"

WP 236 Determination of Relative Amounts of iso- and n-Alpha Acids in Beer without Prior Separation via Chemometric Analysis of MS/MS Data; Kevin D. Clark1; Joshua Driver1; Jon Amster2; "Innovare, Dept. of Chem & Biochem Norman, OK"

WP 237 SPME and Liquid-Liquid Extraction, Complimentary Methods for Analysis of Coffee Flavor Components by GCMS?; Emily P Erdman1; Stephanie I Allred1; Steven B Foster1; Ronald L Halterman1; "University of Oklahoma, Dept. of Chem & Biochem Norman, OK"

WP 238 New Analytical and Statistical Tools to Study the Flavor-formation during the Roasting Process of Coffee Beans, Cacao Beans and Nuts; Sven Ehlert1; Hendryk Czech1; Jessalin Howell1; Romy Hertz-Schuenemann1; Chahan Yeretzian1; Thorsten Streibel1; Ralf Zimmermann1; University of Rostock, Rostock, Germany; "JM Smucker Inc., Orrville, Ohio; ZAHW, Zuerich, Switzerland; University of Rostock, Rostock; Helmholtz Zentrum Muenchen, Oberschleissheim, Germany"

WP 239 Understanding the Role of Origin, Roasting & Storage on Flavor Components in Coffee Employing Gas Chromatography Mass Spectrometry; Steven B Foster1; Emily P Erdman1; Melissa M Henniger1; Jessica R McConahey1; Gabrielle C Thng1; Ronald L Halterman1; "University of Oklahoma, Dept. of Chem & Biochem Norman, OK"

WP 240 New Approach Analyzing Food Functionality using MALDI-MS-based Metabolic Profiling Technique: Evaluation of Green Tea Extracts; Chihiro Kawano1; Yoshinori Fujimura1; Ayaka Maeda-Murayama1; Eisuke Hayakawa1; Taketoshi Ishii1; Hiroyuki Wariishi1; Dai Suisuke Miura1; ICMMR, Kyushu University, Fukuoka, Japan; "Faculty of Arts and Science, Kyushu University, Fukuoka, Japan"

WP 241 Non-Targeted Modification-Specific Metabolomics Investigation of Glycosylated Metabolites in Tea (Camellia sinensis L.) by Liquid Chromatography-High Resolution Mass Spectrometry; Weidong Dai1; Meiling Lu1; Zhi Lin2; Shan Zhou1; Junxi Cao1; "Tea Research Institute, Guangdong Academy of Agricultural Sciences, Hangzhou, China; Agilent Technologies (China) Limited, Beijing, China"

WP 242 Study of the Aroma Variation in Oolong Tea Processing by Solid-Phase Micro-Extraction and Gas Chromatography-Mass Spectrometry; Chengying Ma1; Shan Zhou1; Aiqing Miao1; Wenwen Wang1; Junxi Cao1; "Tea Research Institute, Guangdong Academy of Agricultural Sciences, Hangzhou, China; Agilent Technologies Company Ltd, Beijing, China"

WP 243 Analysis of Catechins in Brewed Tea by LC-TOF Mass Spectrometry; Robert J. Seward1; Jason Weisenseel2; Craig Young1; Wilhad M. Reuter1; "PerkinElmer, Waltham, MA"

WP 244 Determination of Catechins in Tea by using in-situ Derivatization with a Direct Analysis in Real Time Source Equipped Mass Spectrometer; Robert Googuen1; Brian D. Musselman2; JonSense, Inc, Saugus, MA; "JonSense, Inc., Saugus, MA"

WP 245 Foodomic Profiling of Vinegars in China with Metabolomics Workflow by Agilent 6545 UHPLC-ESI/QTOF; Shaozhen Wang1; Shan-An Chang1; "Agilent Technology, Inc., Shanghai, China; Agilent Technology, Inc., Shanghai, China"

WP 246 High Sensitive LC-MS Analysis of Stevia Sweeteners Using a Polymer-Based Amino Column; Junji Sasuga1; Tomokazu Umekawa1; Leah Block1; Shouha Denko K.K., Kawasaki, Japan; "Shodex, Shouha Denko America, Inc., New York, NY"

WP 247 Differences in the Composition of Milk during Lactation using High-Resolution Mass Spectrometry; Tatiane Melina Guerreiro1; Rodrigo Ramos Catharino1; "Innovare Biomarkers Laboratory - UNICAMP, Campinas, Brazil"

WP 248 Analysis of Water Soluble Vitamins in Infant Formula using UHPLC with Tandem Mass Spectrometry and a Heated Laminar Flow Interface; Wilhad Reuter1; Sharanya Reddy1; Avinash Dalma1; Tong Chen1; Thomas White1; Lisa Cousins1; Joshua Ye1; "PerkinElmer, Shelton, CT; "IONICS Mass Spectrometry, Bolton, Canada"

WP 249 Preliminary Investigation of Canadian Wheat Varieties Low Molecular Weight Glutenin Subunits Relative to Functional Gluten Strength; Dave Hatcher1; Bin Xiao Fu1; Ray Bacala1; "Grain Research Laboratory, Canadian Grain Commission, Winnipeg, Canada"
WP 250 - Direct Separation and Quantitation of Amino Acids in Commercial Supplements and Nutraceuticals using LC-MS and HILIC Chromatography: Kimberly Dunn-Meynell; Patricia Atkins; 'Spx Cetriprep, Metuchen, NJ

WP 251 - Reductive Amination Assistance to Quantitate Garlic Components in Isotope Dilution Analysis: Shih-Shin Liang; Kaohsiung

WP 252 - A Metabolomics Approach to Characterize Raw, Pasteurized and Ultra-High Temperature Milk using UPLC-QTOF-MS and Multivariate Data Analysis: Yangdong Zhang; Chinese Academy of Agricultural Sciences, Beijing, China

FORENSICS (PART 2) 253 - 278

WP 253 - Mass Spectrometry by Paper Spray Ionization (PS-MS) – A Swiss Army Knife in Forensic Chemistry: Elollision Domingos; Heloia Santos; Lilian V Tose; Radigaya M Correia; Flávia Tosato; Thays C. Carvalho; Christopher Thompson; Paulo R Filgueiras; Boniek G Vaz; Wanderson Romão; UFES, Vitória, Brazil; 'UFES, Vitória, Brazil; 'UFES, Vila Velha, Brazil; 'UFG, Goiânia, Brazil

WP 254 - Quantification of Cocaine and Its Adulterants by Paper Chromatography Revealed by Dragendorff Reagent and Paper Spray Ionization Mass Spectrometry: Heloia Santos; Flavia Tosato; Aryanne Souza Lima; Elollision Domingos; Boniek G Vaz; Wanderson Romão; UFES, Vitória, Brazil; 'UFES, Vila Velha, Brazil; 'UFG, Goiânia, Brazil

WP 255 - Detection of NBOMe Designer Drugs on Blotter Paper using Ambient Ionization High Resolution Time-of-Flight Mass Spectrometry: A Forensic Case Study: Jamie Foss; David Barajas; Saha Botch-Jones; Frank Kero; Craig Young; Jason Weisenseel; 'Maine Health & Environmental Testing Lab, Augusta, ME; 'Boston University School of Medicine, Boston, MA; 'PerkinElmer, Shelton, CT

WP 256 - Evaluating an All-Ions Method for the Identification of NBOMEs on Seized Blotter Papers using Q-TOF LC/MS: Andrea Chaves1; Boniek G Vaz3; Wanderson Romão1; UFES, Vitória, Brazil; 'UFES, Vitória, Brazil; 'UFES, Vila Velha, ES; 'PerkinElmer, Shelton, CT

WP 257 - Forensic Applications of Probe Electrospray Ionization Mass Spectrometry (PESI-MS) using a Needle Coated with Polypyrrole: Carla S. de Freitas1; Ricardo Alves Bernardo1; Gessica Adriana Vasconcelos1; Veronica Vale Cavalo1; Thays Colletes Cavalo1; Wanderson Romão1; Andrea Chaves1; Boniek G Vaz1; 'Federal University of Goias, Goiania, GO; 'Federal University of Espirito Santo, Vitória, Brazil

WP 258 - Rapid Detection of Drugs-of-abuse in Body Fluid by Mass Spectrometry: Tsai-Tsun Yu1; Pui-Kin So1; Bin Hu1; Zhong-Ping Yao1; 'Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hong Kong SAR, China

WP 259 - Classification of Synthetic Cathinones Using Neutral Losses by Direct Analysis in Real Time Mass Spectrometry (DART-MS): Kristien Fowble1; Jason Shepard1; Rabi A. Musah1; 'University at Albany-SUNY, Albany, NY

WP 260 - Solid-phase Microextraction Combined with a Laminar Flow LC-MS/MS for High-Throughput and High Sensitive Analysis of Drugs in Oral Fluids: Vincent Bessonnette1; Janusz Pawliszyn1; 'University of Waterloo, Waterloo, Canada; 'University of Waterloo, Waterloo ON, Canada

WP 261 - Magnetic Graphene Framework as Adsorbent for the Enrichment of Flunitrazepam from Beverage Samples Prior to Its Determination by Mass Spectrometry: Qihua Wu1; Si Cheng2; Zhi Li1; Hao Chen1; 'Ohio University, Athens, OH; 'Ohio, Athens, OH

WP 262 - LC-MS/MS Analysis of Drugs of Abuse Using Biocompatible Solid Phase Micro Extraction: Sara Smith1; Emily Barrey1; Craig Aurand1; David Bell1; Candace Price1; 'MilliporeSigma, Bellefonte, PA

WP 263 - Evaluation of Solid Phase Micro Extraction Sample Preparation for LC-MS Analysis of Drugs in Urine and Plasma for Forensics: Marta Kozak1; Nathaly Reyes Garcés1; German Augusto Gomez-Rios1; Cornelia Boesert1; Sarracino David1; 'Thermo Fisher Scientific, San Jose, CA; 'University of Waterloo, Waterloo, Ontario (ON); 'University of Waterloo, Waterloo ON, Canada; 'Thermo Fisher Scientific, San Jose, CA

WP 264 - The Development of a Two-Dimensional Liquid Chromatography-Tandem Mass Spectrometry Method for the Analysis of Designer Drugs in Urine: Holly Castellano; Duquesne University, Pittsburgh, PA

WP 265 - Drugs of Abuse Extraction from Whole Blood using Supported Liquid Extraction (SLE) Prior to GC/MS Analysis: Katie-Jo Teehan1; Rhys Jones1; Lee Williams2; Paul Roberts1; Helen Lodder1; Adam Senior1; Alan Edgington1; Geoff Davies1; Steve Jordan1; Claire Desbrow1; Victor Vandelli1; Dan Menasco1; 'Biotage GB Limited, Cardiff, UK; 'Biotage GB Limited, Cardiff, 'Biotage LLC, Charlotte, NC

WP 266 - Illegal Drugs Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time- Mass Spectrometry (TDP/DART-MS): Hiroko Abe1; Chikako Takei1; Yasuo Shida1; Motoshi Sakakura1; Teruhisa Shiotani1; Kayako Suga1; Daichi Yajima1; Hiroto Iwase1; 'University of Chiba, Chiba, Japan; 'Biochromato, Inc. Fujisawa, Japan; 'University of Yamanashi, Kofu, Japan; 'AMR Inc., Meguro-Ku, Japan; 'AB SCIEX, Tokyo, Japan; 'University of Tokyo, Tokyo, Japan

WP 267 - Development of an LC-MS/MS Screening Method for 101 Targeted Compounds in Whole Blood, Using Library Searching on a QTRAP MS: Heather Singletary1; Amanda Sweet1; 'Metro Nashville PD-Crime Lab, Madison, TN

WP 268 - Fast and Reliable Quantitation of Z-drug Hypnotics and Benzodiazepines in Serum using UHPLC-QTOF Mass Spectrometry: Sebastian Goetz1; Karin Wendt1; Tony Drury1; Matt Willetts2; Carsten Bessmann1; 'Baker Daltonik GmbH, Bremen, Germany; 'Baker Daltonics, Coventry, UK; 'Baker Daltonik, Billerica, MA

WP 269 - Urine and Serum Ultra-Rapid Analysis of Flakka (alpha-PVP) in 9 Seconds per Sample by Laser Diode Thermal Desorption Mass Spectrometry: Jonathan Rochon1; Annie-Claude Bolduc1; Réal Paquin1; Alex Birsan2; Serge Auger1; Jean Lacoursiere1; Pierre Picard1; 'Université Laval, Québec, Canada; 'Phytormix Technologies, Inc. Quebec, Canada

WP 270 - SWATH Data Used for Data Mining: What kind of Adulterants, Diluents and Other Toxic Compounds are Consumed Together with Cocaine?: Stefan Körös1; Thomas Würtsch1; Marie Martin2; Werner Bernhard3; Wolfgang Weinmann2; Susanne Nussbäumer2; 'Institut für Rechtsmedizin, Universität Bern, Bern, Switzerland; 'Institut für Rechtsmedizin, Bern, Switzerland

WP 271 - Quantitative Multi Target Screening (MTS) using Liquid Chromatography-Tandem Mass Spectrometry with MS/MS Library Based Forensic Toxicology: Alan Barnes1; Tiphaine Robin1; Simon Ashton1; Neil Loftus1; Pierre Marquet2; Sylvain Dulaurent2; Franck Saint-Marcoux2; 'Shimadzu, Manchester, UK; 'CHU Limoges, Limoges, France

WP 272 - Comprehensive and Sensitive Quantitation of More Than 100 Synthetic Cannabinoids in Serum by LC-MS/MS: Laura M. Huppertz1; Rafaela Martin1; Markus Meyer1; Ronja Peter2; Juergen Kempf1; 'Institute of Forensic Medicine Freiburg, Freiburg, Germany; 'Baker Daltonik
WP 273
Rapid Update of Screening Methods for the Detection of Synthetic Cannabinoid Use in Human Urine by Software Assisted Metabolite Identification; Bioern Moosmann1; Laura M. Huppertz2; Florian Franz1; Sebastian Götz2; Volker Auwärter1; Institute of Forensic Medicine Freiburg, Freiburg, Germany; Bruker Daltonik GmbH, Bremen, Germany

WP 274
Strategies for Classification and Annotation of Novel Synthetic Designer Drugs; Fanny Chu1; A. Daniel Jones2; Ruth Waddell Smith1; Forensic Science Program, School of Criminal Justice, Michigan State University, East Lansing, MI; Department of Chemistry, Michigan State University, East Lansing, MI; Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI

WP 275
Comprehensive Detection and Identification of Prescription Analgesics and Illicit Opioids in Post-Mortem Specimens using Ion Trap LC-MSms; Elsa N. Shoff1; Georgia W. Hine2; Carmen Haessmann2; Diane M. Boland1; Miami Dade Medical Examiner Dept., Miami, FL; Bruker Daltonik GmbH, Bremen, Germany

WP 276
CE-MS Analysis of Controlled Substances with Optical Isomer Resolution in a about a Minute; Mehdi Moin1; Christopher Rollman1; George Washington University, Washington, DC

WP 277
Screening Procedure to Detect Peptide Hormones Prohibited in Sports. CESI-MS vs LC-ESI-MS; Monica Mazzarino1; Xavier de la Torre1; Francesco Botrè1; Antidoping laboratory of Rome, Rome, Italy; Antidoping laboratory of Rome, FMSI Rome, Italy

WP 278
Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry (HLIC-MS/MS) Method for the Quantitation of gamma-Aminobutyric Acid (GABA) in Equine Plasma; Rong Yi1; Sarah Zhao1; Noel Kong1; Julia Zhang1; Devan Loganathan1; Sandrine Merette1; Barbara Morrissey1; MAXXAM, Burnaby, Canada

WP 279
Development of a Multi-Turn TOF Mass Spectrometer with a Cold Trap “iniTOF-CT” for Trace Gas Analysis; Hirofumi Nagao1; Shinichi Miki1; Ikunori Kannoh1; Zhejiang University of Technology, Hangzhou, China

WP 280
GC-MS with Cold EI and Its Unexpected Benefits; Aviv Amirav1; Alexander B. Fialkov2; Volker Auwärter1; Institute of Forensic Medicine Freiburg, Freiburg, Germany; Bruker Daltonik GmbH, Bremen, Germany

WP 281
Evaluation of Organometallic Compounds using GC/O-TOF with a Novel High Efficiency Source; David Kao1; Jennifer Sanderson1; Sofia Nieto1; Agilent Technologies, Santa Clara, CA

WP 282
On-Line Coupling of Microscale Distillation with GC-MS for Analysis of Complex Samples; Ya-Ru Tang1; Pawel Lukasz Urban1; National Chiao Tung University, Hsinchu, Taiwan; Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.)

WP 283
Fast Analysis Workflow with No Sample Preparation for Forensic Applications using Open Probe FastGC/MS: Unit and High Resolution Mass Spectrometers; Luis Cuadra-Rodríguez1; Jennifer Sanderson1; Bjorn Flatt1; Bill Russ1; Agilent Technologies, Santa Clara, CA

WP 284
Vacuum Ultraviolet (VUV) Spectroscopy – an Alternative to Mass Spectrometry for Gas Chromatography Detection; Changling Gliu1; Allegra Leghissa1; Jonathan Smuts1; Kevin A Schug1; University of Texas at Arlington, Arlington, TX; VUV Analytics, Inc., Cedar Park, TX

WP 285
Gas Chromatography Electrospray Ionization Mass Spectrometry Analysis of Trimethylsilyl Derivatives; Ren-Yu Hsu1; Jian-Hong Liao1; Hsin Wen Tien1; Guor-Rong He1; National Taiwan University, Taipei, Taiwan

WP 286
Characterization of lignans of Schisandra sphenanthera Fruit by Flash Evaporation-Gas Chromatography/ Mass Spectrometry; Huijuan Lu1; Yilei Huang1; Zhongping Huang1; Yutian Chen1; Lili Wang1; Zhejiang University of Technology, Hangzhou, China

WP 287
Interfacing Gas and Liquid Chromatography with High Temperature Plasma Mass Spectrometry, Synchyi Cheng1; Jentia Sheia1; National Sun Yat-Sen University, Kaohsiung, Taiwan

WP 288
EPA Method 325B, Novel Thermal Desorption Instrument Modification to Improve Sensitivity; Ronald Shomo1; John Manura1; Christopher W Baker1; Scientific Instrument Services, Ringoes, NJ

WP 289
Trace Elemental Quantification of Carbon via the Production of Cyanide Anions in Plasma Assisted Reaction Chemical Ionization Mass Spectrometry (PARCI-MS); Peter Hafer1; Haopeng Wang1; Kaveh Jarobchi1; Georgetown University, Washington, DC

WP 290
How We Can Improve Number of Compounds Found by Deconvolution in One Essential Oil Sample with GCMS?; Celso Blatt1; Romao Beserra1; Agilent Technologies Brasil Ltda, Sao Paulo, Sao Paulo

WP 291
Raising the Identification Confidence in Non-Target Analysis of House Dust by Combining Classic and Soft Electron Ionization GC-HRMS; Peter Haglund1; Sofia Nieto1; Vadin Kalmyer1; Nathan Eno1; Jennifer Sanderson1; Umea University, Umea; Agilent Technologies, Santa Clara, CA

WP 292
GCxGC with Simultaneous Mass Spectrometry/Flame Ionization Detection for Routine Petrochemical Analyses; Laura McGregor1; Nick P Bukowski1; Matthew Edwards1; Pete Grosshands1; Chris Hall1; Massimo Santoro1; Markes International, Cardiff, UK; Markes International Inc, Cincinnati, OH

WP 293
A High Efficiency Ion Source for GC/MS; Jeffrey Kerman1; Agilent Technologies, Santa Clara, CA

GLYCOPROTEINS (TANDEM MS, SEPARATIONS, AND AUTOMATION/SOFTWARE)

WP 294
Extending the Energy-resolved Collision-Induced Dissociation Method for Structural Characterization of Sialylated N-Glycopeptides; Venkata Kolli1; Katherine N Schumacher1; Eric D Dodds1; University of Nebraska - Lincoln, Lincoln, NE

WP 295
Detailed Characterization of Glycans and Glycopeptides by Collisional and Electron Activated Dissociation; Kshilji Khatri1; Yi Pu1; Joshua Klein1; Cheng Lin1; Joseph Zaia1; Boston University, Boston, MA

WP 296
Glycopeptide Analysis Using Parallel Data-Dependent Acquisition at Varied Normalized Collision Energies; Crystal Daniels1; Joseph Otto1; Jana Rocker1; Lindsay Schambeau1; Mitchell Cancer Institute, Mobile, AL

WP 297
Comparative Effectiveness and Specificity of Glycopeptide Enrichment Strategies for Qualitative LC-MS/MS Analysis of Depleted Human Plasma; Sarah Michelle Totten1; Majlinda Kullolli1; Chrisita Faeley1; Sharon J Pitter1; Stanford University School of Medicine, Palo Alto, CA
CA; 1Stanford University School of Medicine, Palo Alto CA; 2Thermo Fisher Scientific, Palm Beach, FL

WP 299 Online Cotton HILIC: An Easily Accessible and Affordable Enrichment of Glycopeptides; Jingfu Zhao1; Ehwang Song1; Yehia Mechref1; 2Texas Tech University, Lubbock, Texas

WP 300 Affinity-capture Based Methods for N-glycan Analysis of Specific Serum Proteins; Gunnar Thorssén1; Alessandro Quaranta2; Isabella Karlsson2; Anna Sroka-Bartnicka3; Matthijs Pijnappel4; Lorena Ndreu5; 1Stockholm University, Stockholm, Sweden; 2Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, SE

WP 301 Separation and Detection of PSA-derived Sialic Acid Attachment Isoforms Using a Heated PGC Column and LC-MS/MS; Yifan Huang1; Shiyue Zhou1; Yehia Mechref1; 1Texas Tech University, Lubbock, TX

WP 302 N-glycosylation Analysis of Specific Serum Proteins using an Automated Microfluidic Platform and MALDI-MS: Alessandro Quaranta1; Anna Sroka-Bartnicka1; Isabella Karlsson2; Lorena Ndreu3; Matthijs Pijnappel4; Thorsén Gunnar1; 1Stockholm University, Stockholm, Sweden; 2Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, SE

WP 303 Identification and Separation of N-glycans by HILIC/MS; ZsuZsanna Lakos1; Elena Drmena1; Robert Carney1; John L. Snyder1; 1Eurofins Lancaster Laboratories, Lancaster, PA

WP 304 Silk-Based Glyco-Enrichment Tip for Purification and Enrichment of Glycans and Glycopeptides; Haci Mehmet Kayili2; Mehmet Atakay1; Bekir Salim2; 1Hacettepe University, Department of Chemistry, Ankara, Turkey; 2Cankırı Karatekin University, Department of Chemistry, Çankırı, Turkey

WP 305 N-linked Glycosylation Analysis of Seasonal Influenza Vaccine Hemagglutinins; Yanming An1; Lisa Parsons1; John F. Cipollo1; 1FDA/CBER, Silver Spring, MD

WP 306 Assisting the Identification of Isoformic Glycoforms with a Hydrophilic Interaction Liquid Chromatography Retention Time Model for Procanimamide Tagged N-linked Glycans; Emily Betchy1; Barry Boyes2; Ron Orlando3; 1CCRC, University of Georgia Athens, GA; 2Advanced Materials Technology, Wilmington, DE

WP 307 Glycopeptidomics with Ion Mobility Spectrometry for Elucidating Glycan Structures; Miklos Guttman1; Kelly Lee1; 1University of Washington, Seattle, WA

WP 308 Automated Processing of LC-MS/MS Data for Quantitative Analysis of the Human-like N-glycosylation of Glycoproteins Produced by a Glyco-optimization Cell Platform; Robert Wilmanowski1; Catherine Evans1; Anja Resemann1; Peter Hufnagel1; Rainer Pape1; Detlev Suckau1; Wolfgang Jabs1; Sven Bahre2; Keven Lohret1; Andrea Hahn2; 1Glycotope GmbH, Berlin, Germany; 2Bruker Ltd, Coventry, UK; 3Bruker Daltonics GmbH, Bremen, Germany

WP 309 N-glycan Analysis using GIG-automation on Sialylglycansferase Knock-in CHO Cell Line; Shuang Yang1; Qiong Wang2; Lijun Chen3; Boijia Yin2; Li Shuwei1; Michael Benetanha4; Hui Zhang1; 1John Hopkins Dept. of Pathology, Baltimore, MD; 2Johns Hopkins University, Baltimore, MD; 3Johns Hopkins School of Medicine, Baltimore, MD; 4University of Maryland, College Park, MD

WP 310 GPQuest: A Free Software for Identification of Glycans and Intact Glycopeptides; Yongwei Hu1; Shadi Toghi Eshghi1; Weiming Yang1; Punil Shah1; Shisheng Sun1; Shuang Yang1; Lingquan Deng1; Xingde Li2; Hui Zhang1; 1Department of Pathology, School of Medicine, Johns Hopkins University, Baltimore, MD; 2Department of Biomedical Engineering, School of Medicine, Johns Hopkins University, Baltimore, MD

WP 311 Scalable Computational Tool for Identifying Intact Glycopeptides in Complex Samples Using Mass Spectrometry; Lei Wang1; Chuan-Yih Yu1; Anoop M Mayamunaparithi1; Rui Zhui1; Ehwang Song2; Yehia Mechref1; Haixu Tang1; 1Indiana University, Bloomington, IN; 2Texas Tech University, Lubbock, Texas

WP 312 GLYMS: A Tool to Automatically Assign Glycopeptides from MSData; Lisa Parsons1; Yanming An1; John F. Cipollo1; 1FDA/CBER, Silver Spring, MD

WP 313 Confident, Automated N-glycoproteomics Profiling in Unenriched and Glycopeptide-Enriched Cancer Cell Samples; Shadab Ahmad1; Amol Prakash1; Sergei I Snovida1; Scott M Peterman1; Chu-Wei Kuo2; Kay-Hooi Kho3; Gauri Muradia3; Jeremy P Kunke3; Jessie L Ravoie3; Nina Soltero1; Julian A Saba4; 1Optys Tech Corporation, Brighton, MA; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Scientific BRIMS, Cambridge, MA; 4Academia Sinica, Taipei, Taiwan; 5Health Canada, Ottawa, Canada

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY

WP 314 The Development of a Fully Customized HDX-MS Platform with Exceptional Performance on Back-Exchange, Robustness and Reproducibility; Chengjie Ji1; Jeff Zhu1; Qian Li1; Yankun Li1; 1Novabioassays LLC, Woburn, MA

WP 315 MALDI Compatible Protease Chips - A Novel Platform For Protein H/D Exchange; Michal Rosulek1; 2; Petra Darebna1; 2; Daniel Kavan1; 2; Petr Jan1; 2; Michael Volny1; 2; Petr Pompa1; 2; Petr Novak1; 2; 1Institute of Microbiology CAS, Prague, Czech Republic; 2Faculty of Science, Charles University in Prague, Prague, Czech Republic; 3AffiPro, s.r.o, Mráten, Czech Republic

WP 316 Protease Type XVIII Columns for Enhanced Digestion Efficiency and Sequence Resolution for Protein HDX Monitored by Q Exactive MS; Chengjie Ji1; Qian Li1; Yankun Li1; 1Novabioassays LLC, Woburn, MA

WP 317 Improvements to HDX Workbench Software for Analysis and Interpretation of HDX MS Data; Bruce D. Pascal1; Venkatathasaraman Dharmarajan1; Scott Novick1; Jie Zheng1; Vinh Lam1; 1The Scripps Research Institute, Jupiter, Florida

WP 318 In-source Column Cooling for nanoHDX-MS on Complex Druggable Protein Scaffolds; Joey Sheff1; David Schriemer1; 1University of Calgary, Calgary, Canada

WP 319 Post-column Hydrogen-deuterium Exchange Method for the Identification of Organic Compounds; Emmanuel Evsier1; Xavier Belleros1; Jean-Michel Lavoie1; Pedro A Segura1; 1Université de Sherbrooke, Sherbrooke, QC

WP 320 How Precise are HDX-MS Measurements? Results from the NIST HDX-MS Interlaboratory Comparison Project; Jeffrey W. Hudgens1; Elyssia S Gallagher1; 2; Ioannis Karageorgos2; 2; National Institute of Standards and Technology, Rockville, MD; 3Institute for Bioscience and Biotechnology Research, Rockville, MD

WP 321 Phospho-2-Specific Characterization of Protein Conformational Changes Induced by Multisite Phosphorylation; Jingji Pan1; Albert Cho2; Supting Zhang1; Christoph H. Borchers1; 2; University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3MRM Proteomics Inc, Victoria, BC, Canada; 4Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

WP 322 Top-Down Analysis of ‘On-the-Fly’ HDX of NativeProtein Ions; Ken Chanhamont1; 2; Nawanporn Sanguantrakran2; 3; Michael L Gross3; 4; Washington University in St Louis, St Louis, MO; 2Saint Louis College of Pharmacy, St. Louis, MO; 3Washington University in St. Louis, Saint Louis, MO
WP 323 HDXMS Studies of Membrane Proteins (GPCR) 
Expressed in Virus like Particles (VLP); Deepa 
Balasubramaniam1; Carrie A Shipley2; Beata A Zamlynnyn;
Margarita Garcia-Calvo1; Payal Sheth1; Michael Kavana1;
David G McLaren1; Merck Research Labs, Kenilworth, NJ

WP 324 HX-MS Reveals a Loss of Helical Structure in an 
Intrinsically Disordered Protein under Highly Crowded 
Conditions; Farai Rusingw, University of Kansas, Lawrence, KS

WP 325 Observation of H/D Exchange at Non-labile C-H Sites 
Capable by an Increase in Desolvation Temperature in 
ESI-source; Alexander Zherebker1, 2; Yury Kostyukovich3, 4, 5; Alexey S Kontonikhin4, 5; Vitaliy Roznyatovsky4; Igor A Popov4, 5; Yuri K. Grishin1; Irina V Perminova1; Eugene 
Wilson1; Madhurima Das2; Xiaohu Mei2; John R Engen1; Lars Konermann1; John R Engen1; Northeastern 
University, Boston, MA; 2University of Pittsburgh School of 
Medicine, Pittsburgh, PA

WP 326 Towards a High Throughput Binding-Site Specific 
Drug Screening by HDX MS: ROMAN ZUBAREV1, 2; Juan Astorga-Wells1, 2; 3, 4 Thorleif Lavold1; Karolinska 
Institutet, Stockholm, Sweden; Karolinska Institutet, Solna, Sweden; 4Biomol AB, Stockholm, Sweden; 5HDXperts AB, 
Stockholm, Sweden

WP 327 Negative Ion Electron Capture Dissociation (niECD) of 
Deuterated Peptides; Qingyi Wang1; Kristina Håkansson1;
1University of Michigan Department of Chemistry, Ann Arbor, MI

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION (PART 1) 328 - 336

WP 328 Utilizing Hydrogen Exchange Mass Spectrometry to 
Interrogate KRas Binding to SOS1 at Two Distinct 
Sites; Rane A Harrison1; Andreas Zoepfel1; Klaus Rumpel1;
John R Engen1; 1Department of Chemistry and Chemical 
Biology, Northeastern University, Boston, MA; 2Department of Medicinal Chemistry, Boehringer Ingelheim RCV GmbH 
& Co KG, Vienna, Austria; 3Department of New Therapeutic 
Concept Discovery, Boehringer Ingelheim RCV GmbH & Co KG, Vienna, Austria

WP 329 Local Dynamics in Lipid-Associated Apolipoprotein 
A-I and Effects of Disease-Causing Mutations Probed 
by Hydrogen-Deuterium Exchange MS; Christopher Jay 
Wilson1; Madhumita Das1; Xiaohu Mei1; John R Engen1; 
Olga Gursky2; 2Department of Chemistry and Chemical 
Biology, Northeastern University, Boston, MA; 3Department of Physiology and Biophysics, Boston University School of 
Medicine, Boston, MA

WP 330 Integrating XL-MS and HX-MS2 Data to Develop a Model 
of DNA Binding to DNAPKcs; Morgan Henburn1; Daniel 
Saltzberg2; Yapping Yu1; Susan Lees-Miller1; Andrej Sali2; 
David Schiemer1; 1University of Calgary, Calgary, Canada; 2University of California, San Francisco, CA

WP 331 Identification of a Structural Conduit for Thermal 
Energy Transfer from Solvent to Enzyme Active 
Site using Hydrogen/Deuterium Exchange Mass 
Spectrometry; Anthony T laronde1; Adam R Offenbacher1; 
Judith P Kliman1; UC Berkeley, Berkeley, CA

WP 332 Examining the Importance of Conformational Dynamics 
for the Function of Pyruvate Kinase: Insights from HDX-
MS; Courtney S Fast1; Siavash Vahidi1; Stanley D Dunn1; 
Lars Konermann1; 1Western University, London, Canada

WP 333 Analysis of HIV Nef Dimerization and Binding 
Partner Interactions by Hydrogen Exchange Mass 
Spectrometry; Jamie Moroco1; John Jeff Alvarado1; 
Thomas E Smithgal1; John R Engen1; Northeastern 
University, Boston, MA; 2University of Pittsburgh School of 
Medicine, Pittsburgh, PA

WP 334 Pre-Amyloid Oligomer Dissociation Kinetics Studied 
by Hydrogen/Deuterium Exchange Mass Spectrometry; 
Zhe Zhang1; Richard W Vachet1; 1University of 
Massachusetts Amherst, Amherst, MA

WP 335 Gas-Phase H/D Exchange Monitored by MS Reveals a 
Dense Network of Side-Chain Interactions Stabilizing 
Oligomers of Alzheimer’s Disease Aβ Peptide; Kasia 
Przygonska1; Kinga Fituch1; Ewa Sitkiewicz1; Kasper D 
Rand2; Michal Dadlez2; 2Institute of Biochemistry and 
Biophysics, Polish Academy of Science, Warsaw, Poland; 3Department of Pharmacy, University of Copenhagen 
Kopenhagen, Denmark

WP 336 Effect of Protein Structure on Antibody Deamidation 
Rates: A Combination of Peptide Mapping, 3D 
Modeling, and Hydrogen/Deuterium Exchange Mass 
Spectrometry; Paul Mawson; Ridgefield, CT

ICP AND ISOTOPE RATIO MS: ELEMENTAL 337 - 341

WP 337 Measurement of the Molar Mass of 28Si-enriched 
Silicon Crystal with High Resolution Inductively 
Coupled Plasma Mass Spectrometer; Tongxian Ren1; Jun Wang2; Tao Zhou2; Hai Liu3; 1National Institute of 
Metrology, Beijing, Chaoyang; 3National Institute of 
Metrology, Beijing, China

WP 338 Selenium Accumulation and Speciation in 
Supplemented Aquaponic Systems Using Reverse 
Phase HPLC and ICP-QQQ; Skylar Smith1; Julio A. 
Landero-Figueroa2; Megan Schmale3; 1University of 
Cincinnati, Cincinnati, OH

WP 339 Environmental Source Determination Using Stable 
Lead Isotope Ratios in American Woodcock (Scolopax 
minor) Feathers and Bone; Amanda D. French1; Warren 
C Conway1; Daniel S Sullins2; David Klein3; 1Texas Tech 
University, Lubbock, Texas; 2Kansas State University, 
Manhattan, KS; 3Texas Tech University, Lubbock, TX

WP 340 Rapid Determination of Calcium in Water by Spray 
Microwave Plasma Torch Mass Spectrometry; Meiling, 
Yang1; Xincheng Wang1; Tao Zhong1; Huanwen Chen1; 1East 
China Institute of Technology, Nanchang, China; 2East 
China Institute of Technology, Nanchang, Mainland 
China; 3Determination of Absolute Isotopic Composition of 
Mo by MC-ICP-MS using Synthetic Isotope Mixtures 
and Uncertainty Evaluation; Panshu Song1; Jun Wang1;
1National Institute of Metrology, Beijing, China

IMAGING MS: METHOD DEVELOPMENT (DESI/SIMS/MISC) 342 - 364

WP 341 Determination of Absolute Isotopic Composition of 
Mo by MC-ICP-MS using Synthetic Isotope Mixtures 
and Uncertainty Evaluation; Panshu Song1; Jun Wang1;
1National Institute of Metrology, Beijing, China

WP 342 A Novel Quantitative Imaging Strategy of Elements in 
Biological Tissue by Isotope Dilution Laser Ablation 
ICP-MS; Liuxing Feng; National Metrology Institute, China, 
Beijing, Beijing

WP 343 Differential Protein Profiling using Virtual 2D Gel-Mass 
Spectrometry; Neil R Quebbemann1; Joseph A Loo2; 
Rachel R. Ogorzalek Loo1; 1University of California, Los 
Angeles, Los Angeles, CA

WP 344 Targeted DESI Mass Spectrometry Imaging in Ovarian 
Cancer; Nicola Doria1; James McKenzie1; Anna Mroz1; 
Abigail Speller1; Francesca Rosini1; David Phelps1; Emrys 
Jones1; Renata Soares1; Kirill Veselkov1; Sadaf Ghaem-
Maghami1; Zoltan Takats1; Imperial College, London, UK; 
1Waters, Manchester, UK

WP 345 Tissue Imaging with Specificity for Unsaturated Lipid 
Isoomers Using Mass Spectrometry with Photochemical 
Reactions; Chengu Guo1; Xiaoxiao Ma1; Yuan Su2; 
Ran Tian3; Ruiy Shi2; Fei Tang1; Yu Xia2; Zheng Ouyang2; 
1Tsinghua University, Beijing, China; 2Purdue University, 
West Lafayette, IN
WP 346 Methodology for Drug Delivery Quantitation in Single Cells using TOF-SIMS; Anthony Castellanos1; Quentin Vanbellingen2; Francisco Fernandez-Lima3.1; Florida International University, Miami, FL; 2Biomolecular Science Institute, Miami, FL

WP 347 Single Cell Analysis using nano-DESI Mass Spectrometry: Hilde-Marlène Bergman1; Ingela Lanekoff2; Uppsala University, Uppsala, Sweden

WP 348 Region- and Enzyme-Specific Bioconversion of Dynorphin Neuropeptide Detected by in situ Histochemistry and MALDI Imaging Mass Spectrometry: Erik Biv Hed2; Stromovall Robert1; Malin Andersson1; Uppsala University, Uppsala, Sweden

WP 349 Combining SRS Microscopy and MS Imaging: Elizabeth C. Randall1; Alasdair Rae2; Alan M. Race3; Helen J. Cooper4; Josephine Bunch1; University of Birmingham, Birmingham, UK; 2National Physical Laboratory, Teddington, UK

WP 350 Tissue Classification using Mass Spectrometry and Membrane Microarrays: Jone Garate1; Roberto Fernandez2; Tarson Tolentino-Cortez2; Sergio Lage3; Gabriel Barreda-Gómez4; Egozt Astigarraga5; Jose A Fernandez1; University of Basque Country, UPV/EHU Leioa Basque Country, Spain; 2IMM Pharma Biotech, Zamudio, Spain

WP 351 Ambient Ionization Mass Spectrometry for Preoperative Diagnosis of Indeterminate Thyroid Nodules: Jialing Zhang1; Wendong Yu2; Clara I Feidert3; Jerry Buentello4; Robert Tibshirani1; James W Sullivan2; 4Stanford University, Stanford, CA

WP 352 Mass Spectrometry Imaging of the Human Pancreas Lipidome: Grant Barry1; Daniel Cavazos2; Igor Veryovkin3; Manami Hara4; Graeme Bell5; Luke Hanley6; 1University of Illinois at Chicago, Chicago, IL; 2University of Chicago, Chicago, IL

WP 353 Simultaneous Detection and Imaging of Drugs and Delivery Vehicles using LDI-MS: Bo Zhao1; Mine Canakci1; Sankanar Thayumanavan1; Richard W Vachet2; 1University of Massachusetts Amherst, Amherst, MA

WP 354 Polarity Switching and Quantitative Mass Spectrometry Imaging of Healthy and Cancerous Hen Ovarian Tissue Sections using IR-MALDESI: Milad Nazari1; Mark T Bokhart2; Kenneth P Garrard3; 1North Carolina State University, Raleigh, NC

WP 355 Rapid Detection and Imaging of Fire- retardant- Cylodextrin-Inclusion Complexes on fibers and films by using IR-MALDESI Mass Spectrometry; Yufei Chen1; Nanshan Zhang1; Milad Nazari1; Mark Bokhart1; Maans Ekeloef2; David C Muddiman3; Nelson R Vinuexa4; North Carolina State University, Raleigh, NC

WP 356 Metabolomic Imaging of Biofilm and Other Biological Materials for Studying Metabolic Heterogeneity: Tomasz Ruman1; Joanna Niziol1; Vincent Bonifay1; 1University of Alberta, Edmonton, Canada

WP 357 Matrix-free Analysis of Resveratrol in Intact Rat Retina Tissue Using REDChip: Amanda Martinez1; Andrea Kelley1; Madeline Colley1; Stephanie Bach1; University of Texas at San Antonio, San Antonio, TX

WP 358 Lanthanide Labeled Antibody Detection by SIMS nano-TOF II of Human Intestinal Injury Markers; Keeley Pierczlaski1; Maastricht, Limburg

WP 359 Mass Spectrometric and FT-IR Spectroscopic Imaging to Probe Organic Ligands and Their Binding Schemes on Nanocrystals: Tae Lee1; Jin Gyeong Son2; Jeong Hee Moon1; Sang Woo Han1; 1KRIS, Daejeon; 2KAIST, Daejeon, Republic of Korea; 3KRRIB, Daejeon, Republic of Korea

WP 360 Analysis of Medical Devices in 2D and 3D by Secondary Ion Mass Spectrometry: Adam Taylor1; Felicia Green1; Bonnie Tyler1; Josephine Bunch2; 1National Physical Laboratory, Teddington, UK

WP 361 Multiplex Proteins and Lipids SIMS Imaging of Mouse Hippocampus Tissues: Eunseok Seo1; Sun young Lee2; Young-ho Park3; Eunsook Choi4; Eunjo Kim5; Dong Kwon Lim6; Su II In7; DaeWon Moon1; 1DGIST, Daegu, Korea; 2Korea University, Seoul, Korea

WP 362 Imaging Mass Spectrometry as a Novel Approach to Synapse Zinc: Masoumeh Dowlatshahi Pour1; 2Lin Ren1; Andrew G Ewing1; 3Per Malmberg1; 4Chalmers University of Technology, Gothenburg, Sweden; 5National Center for Imaging Mass Spectrometry, Gothenburg, Sweden

WP 363 Precursor Ion Selector Scan for Discovery of Analyte Specific Fragments in MALDI-TOF/TOF-MS/MS; Stanislav Rubakhin1; Jonathan V Sreedeer1; Beckman Institute, UIUC, Urbana, IL; 2University of Illinois at Urbana- Champaign, Urbana, IL

WP 364 MS Imaging to Aid in the Transition from Early Goal-Directed Phase to Late Habitation Phase of Spatial Learning in Mice: Geert Baagden1; 2Jeroen Aerts3; Laurens Minerva4; Dirk Valkenberg1, 2, 4; Aneilles Lahermans3; D’hooge Rudi5; Kurt Boonen6; Lutgarde Arcens1; 1Flemish Institute for Technological Research (VITO), Mol, Belgium; 2University of Antwerp, Antwerp, Belgium; 3KU Leuven, Leuven, Belgium; 4Hasselt University, Diepenbeek, Belgium

INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES

WP 365 A Processing Pipeline for Dramatically Increased Statistical Power in Label-Free Quantitative Proteomics: Michael J Sweredoski1; 2Annie Moradian1; Tanya R Porras-Yakushi1; Sonja Hess1; Caltech, Pasadena, CA

WP 366 Missing Value Prediction in Metabolite-Intensity Matrix of a Quantitative Metabolomic Dataset Generated by Chemical Isotope Labeling Liquid Chromatography Mass Spectrometry: Yung Song1; Tao Huan1; Liang Li2; 1University of Alberta, Edmonton, Canada

WP 367 Improved Qualitative and Quantitative Analysis of the Human Mitochondrial Proteome by Hybrid Acquisition; Maurizio Ronci1; Enrico Cilio2; Steven Ciavarini2; Curt Devlin2; Brad Williams3; Scott Geromans3; Chris Hughes1; Johannes Vissers1; Andrea Urbani1; 1University of Rome Tor Vergata, Rome, Italy; 2Waters, Milford, MA; 3Waters, Wilmslow, UK; 4Waters Corporation, Wilmslow, Greater Manchester

WP 368 Development of MSn Spectral Database and the Search Algorithm using Multiple MSn Spectra: Yohhei Yamada1; Akemi Suzuki1; Umemura Yoshikatsu1; Hirokui Yasuda1; Yutaro Yamamura1; Hideshi Fujiwaka1; Kageyama Tettsuya1; 1Shimadzu Corporation, Kyoto, Japan; 2Tokoh Pharmaceutical University, Miyagi, Japan

WP 369 Analysis of Polarity-Switched DESI Images of Colorectal Tissue Samples: James Stuart McKenzie1; Anna K Mróz2; Renata Filipe-Soares1; Zoltan Takats1; Imperial College, London, UK

WP 370 Mass Graptolite-Based Proteofrom Identification by Top-Down Mass Spectrometry: Qiang Kou1; Si Wu1; Nikola Tollic1; Lijilana Pasa-To1; Xiaowen Liu3, 4; 1Indiana University-Purdue University, Indianapolis, IN; 2University of Oklahoma, Dept. of Chem & Biochem Norman, OK; 3Pacific Northwest National Laboratory, Richland, WA; 4Indiana University-Purdue University Indianapolis, Indianapolis, IN; 5Indiana University School of Medicine, Indianapolis, IN
WP 371 A Very Fast Bayesian Engine for Truly unified MS1- and MS2-based Protein Inference; Julianus Pfueffler; Xiao Liang; Knut Reiner; Oliver Kohlbacher; Oliver Serang; Eberhard Karls Universität Tübingen, Tübingen, BW, Deutschland; Freie Universität Berlin, Berlin, Germany; Freie Universität Berlin, Berlin

WP 372 An Adjusted-Median Approach to Missing Values in Label Free Quantitation; Seth Just; Luisa Zini; Nick Vincent-Malone; Brian C Searle; Proteome Software, Portland, OR; University of Washington, Seattle, WA

WP 373 Machine Learning Algorithms for Advanced Identification of Tumor Tissue and Tumor Borders; Evgeny Zhvansky; Igor A Popov; Anatoly Sorokin; Nikita Levin; Vsevolod Shurkhay; Denis Bormotov; Maria Indyekina; Alexey S Konolinikhin; Yury Kostykuevich; Evgeny Kukaev; Alexander Potapov; Eugene Nikolaev; Moscow Institute of Physics and Technology, Moscow, Russia; Institute for Energy Problems of Chemical Physics, Moscow, Russia; Burdenko Neurosurgical Institute, Moscow, Russia; Institute of Problems of Chemical Physics, Moscow, Russia; Moscow Institute of Physics and Technology, Moscow, Russia; National Physical Laboratory, Teddington, UK

WP 374 Making the Most of Multi-Modality Imaging: Exploring Fusion of Mass Spectrometry Imaging with Stimulated Raman Spectroscopy; Alan Race; Alasdair Ras; Jean-Luc Vorni; Roy Steven; Josephine Bunch; Ian Gilmore; National Physical Laboratory, Teddington, Middlesex; National Physical Laboratory, Teddington, UK

WP 375 Automated Tumor Typing of Tissue Sections Based on Characteristic Spectral Patterns Extracted from MALDI Mass Spectrometry Imaging Data; Tobias Boskamp; Delf Lachmund; Nicolas Jathe; Christian Ettmann; Janina Oetjen; Rita Casadonte; Jan Hendrik Kobarg; Dennis Trede; Jörg Kriegsmann; Peter Maas; University of Bremen, Bremen, Germany; SciLS GmbH, Bremen, Germany; Proteopath GmbH, Trier, Germany; Center for Histology, Cytology and Molecular Diagnostic, Trier, Germany

WP 376 Virtual Lock Masses: An Algorithmic Method to Enable Mass Spectra Comparison in Untargeted Studies; Francis Brochu; Pier-Luc Plante; Alexandre Drouin; Louis-Émile Robilaille; François Laviolle; Mario Marchand; Jacques Corbeil; Université Laval, Québec, Canada; Centre de Recherche du CHU de Québec, Québec, Canada

WP 377 Isotopic Tree: Fast Calculation of Fine and Coarse Isotopic Envelopes up to a Predefined Margin of Error; Dmitry Avtonomov; Alexey I Nesvizhskii; University of Michigan, Ann Arbor, MI

WP 378 DISCO - Data Independent Signal Correlator; David Shtryenberg; Samuel L Bader; Andrew Keller; Michael Hoopmann; Luis Mendoza; Eric Deutsch; Robert L Moritz; Institute for Systems Biology, Seattle, WA

WP 379 A Parameterized Averaging Model Improves Feature Detection of Oligonucleotides and Increases Wider Applicability of Feature Finding Algorithm; Samuel Wein; Benjamin A Garcia; University of Pennsylvania, Philadelphia, PA; University of Pennsylvania, Philadelphia, PA

WP 380 MassTodon - Electron Transfer driven Fragmentation Analyzer and Automatic Spectrum Calibrator; Mateusz Krzysztof Laci; Frederik Lemty; Michal Startek; Dirk Valkenborg; Frank Sobott; Anna Gambini; University of Warsaw, Warszawa, Mazowieckie; Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; Biomolecular & Analytical Mass Spectrometry group, University of Antwerp, Antwerpen, Belgium; UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; VITO, Mol, Belgium

WP 381 IsoSpec - a Hyperfast Algorithm for Fine Isotopic Structure Peaks with Preset Total Probability; Mateusz Krzysztof Laci; Michal Startek; Dirk Valkenborg; Anna Gambini; Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; UA-VITO Center for Proteomics, University of Antwerp, Antwerpen, Belgium; Interuniversity Institute for Biostatistics and Statistical Bioinformatics, Hasselt University, Hasselt, Belgium; VITO, Mol, Belgium

WP 382 Robust Algorithms for Denoising, Eliminating Dispersion Similar to Phasing in 1D FT-MS Spectra and Reconstructing Non Uniformly Sampled 2D FT-ICR Data; Lionel Chiron; Fabrice Bray; Christian Rolando; Marc-André Delisc; CASC4DE, Strasbourg, France; Université de Lille, Villeneuve d’Ascq, France; Univ. de Lille 1, Sciences et Technologies, Villeneuve d’Ascq; Université de Strasbourg, Strasbourg, France

WP 383 Finding the Peaks: Performance Enhancement of Portable MS using a Bayesian Approach; Simon Maher; Simon Maskell; Sarfaraz Syed; Fred Junju; Stephen Taylor; Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK; Maastricht University, Maastricht, NL

WP 384 Integrated GlycoProteome Analyzer (i-GPA) for Automatic Identification and Quantitation of Site-Specific N-Glycosylation; Gun Wook Park; Jin Young Kim; Heeyoun Hwang; Ju Yeon Lee; Young Hee Ahn; Hyun Kyong Lee; Eun Sun Ji; Hoi Keun Jeong; Ki Na Yur; Yong-Sam Kim; Jeong-Heon Ko; Hyun Joo Ar; Jae Han Kim; Young-Ki Paik; Jong Shin Yoo; Chungnam National University, Cheongju, Chungbuk; Korea Basic Science Institute, Cheongju-Si, Republic of Korea; Cheongju University, Cheongju-Si, Republic of Korea; Korea Research Institute of Bioscience and Biotechnology, Daejeon, Republic of Korea; Chungnam National University, Daejeon, Republic of Korea; Yonsei University, Seoul, South Korea

WP 385 Identification of N-glycopeptides using Open Spectral Library Search; Chiu Wai Au; Qingbo Shu; Hao Lv; Jianjun Yu; Fuquan Yang; Yan Fu; Chinese Academy of Sciences, Beijing, Beijing

WP 386 Extending MS Interpreter: A Freely-Available Tool for Structure/Spectrum Self-Consistency of High Resolution Tandem Mass Spectra; Alexey V. Mayrovoy; Yuri Mirokhin; Dmitriy Tkhekovskoi; University of Massachusetts, Amherst, MA

WP 387 Machine Learning-Driven Validation Platform for Mass Spectrometry Imaging using Tandem Mass Spectra and Chemical Structure Databases; Ivan Lapponogov; Emilie J L Cauet; James McKenzie; Robert C Glen; Zoltan Takats; Kirill Veselkov; Imperial College London, London, London; Imperial College, London, UK

WP 388 Improving LC-MS Coverage through New Charge State and Monoisotopic m/z Assignment Algorithms; Graeme McAlister; Derek Bailey; Romain Huguet; Michael Senko; Thermo Fisher Scientific, San Jose, CA

WP 389 SAINToq: Robust Screening of Protein-Protein Interactions in Quantitative AP-SWATH Experiments; Guozi Teo; Hiromi WL Koh; Damian Fermin; James Knight; Hiromi WL Koh; Carmen Ferrin; James-Philippe Lambert; Thermo Fisher Scientific, San Jose, CA

WP 390 Portable MS using a Bayesian Approach; Simon Maher; Simon Maskell; Sarfaraz Syed; Fred Junju; Stephen Taylor; Department of Electrical Engineering and Electronics University Of Liverpool, Liverpool, UK; Maastricht University, Maastricht, NL

64TH ASMS CONFERENCE ON MASS SPECTROMETRY PAGE 145
INFORMATICS: WORKFLOW AND DATA MANAGEMENT

WP 390 Galaxy-P: Recent Developments and Emerging Applications: Pratik Jagtap1;2; James Johnson2; Thomas McGowan3; Innocent Onsongo3; Benjamin Lynch4; Candace Guerrero5; Kevin Murray5; Lloyd M Smith5; Michael R Shortreed6; Anthony J Cesnik6; Lennart Martens6; Adrian Hegeman6; Timothy Griffin7;8; University of Minnesota, Minneapolis, MN; 2Center for Mass Spectrometry and Proteomics, UMN St.Paul, MN; 3University of Minnesota Supercomputing Institute, Minneapolis, MN; 4University of Wisconsin Madison, Madison, Wisconsin; 5Ghent University, Ghent, Belgium; 6VIB, Ghent, Belgium

WP 391 Optide-Hunter: Informatics Solutions for Optimized Peptide Drug Development through the Integration of Heterogeneous Data and Adaptation of Various LC-MS Technologies: Mi-Youn Bruinjadi1; Emily Girard3; Bernard Lee3; Chris Mehlin3; Yuki Ogata3; Phillip Galffen6; Hector Ramos2; Jim Olson2; Fred Hutchinson Cancer Research Center, Seattle, WA; 2LabKey Software, Seattle, WA

WP 392 APOSTL: An interactive Galaxy Pipeline For Reproducible Analysis of Affinity Proteomics Data: Brent Kuenzi1; Adam Borge1; Jiannong Li2; Uwe Rix2; Paul Stewart3; Eric Haura1; 1H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL

WP 393 Enabling Collaborative Discovery in Big Data Visual Analytics: Joon-Yong Lee1; Ryan Wilson1; Grant M Fujimoto1; Gary R Kiebel1; Richard D Smith1; Nick Cramer4; Samuel H Payne1; 1Pacific Northwest National Lab, Richland, WA

WP 394 Scientific Workflows for Data Analysis and Visualization in Quantitative Proteomics: Arzu Turge Guler1; Dmitri Travin2; Yassene Mohammed2; Magnus Palmblad2; Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands; 2Faculty of Bioengineering and Bioinformatics, Lomonosov Moscow State University, Moscow, Russia

WP 395 Integration of Peptide-Centric Searching of Data Independent Acquisition Data without an MS/MS Spectrum Library with Data in the Chorus Project: Michael J. MacCoss1; Brian C Searle1; Sonia Ying Ting1; Jarrett Egerton1; Christine C Wu1; Andrii Lobada1; Oleksii Tymchenko1; Andrey Bondarenko1; 1Univ of Washington, Seattle, WA; 2Stratus Biosciences, Seattle, WA; 3Infoclinika, LLC, Seattle, WA

WP 396 High Performance Computing at the National Resource for Translational and Developmental Proteomics: Ryan T Fellers1; Richard D LeDuc2; Bryan P Early1; Joseph B Greer1; Alexandra J Van Nispen1; Paul M Thomas1; Neil L Kelleher1; 1Northwestern University, Evanston, IL

WP 397 The Massive Repository for Interactive Annotation of Proteomics Big Data: Jeremy Carver1; Mingxun Wang1; Nuno Bandeira1; 1UCSD, La Jolla, CA

WP 398 The Potential of Functional Annotation of Mass Spectrometry Tools: Magnus Palmblad1; Arzu Turge Guler1; Kristian Davidsen1; Jon Ison1; Veit Schwämmle1; Leiden University Medical Center, Leiden, the Netherlands; 1Technical University of Denmark, Copenhagen, Denmark; 2University of Southern Denmark, Odense, Denmark

WP 399 Recent Developments in ProteomicsDB: From FDR Estimates to Proteomic Assays and More: Mathias Wilhelm1; Daniel Paul Zolig1; Hans-Christian Ehrlich2; Stephan Aiche2; Mohammed AbuJarour2; David Weese2; Judith Schlegi2; Tobias Schmidt1; Wilhelm Becker2; Lars Rücker2; Jan Huenges2; Susan Klaeger1;4; Stephanie Heinzlmeir1;4; Hannes Hahne1; Bernhard Kuster1;4; Chair of Proteomics and Bioinformatics, Technical University of Munich, Freising, Germany; 1Innovation Center Potsdam, SAP SE, Potsdam, Germany; 2SAP SE, Walldorf, Germany; "German Cancer Consortium (DKTK), Muenchen, Germany; 2German Cancer Research Center, Heidelberg, Germany; 3OmicScouts GmbH, Freising, Germany

WP 400 Dredging the Mass Spectrometry Data Lake for Hidden Information with Teradata Database and Business Intelligence Software: Alan Dickson1; Tony Ly1; Vackar Afzal2; Dalila Bensaddek1; Jens Hukelmann1; Angus Lamond2; Centre for Gene Regulation and Expression, Dundee, UK

WP 401 Comparison of Data Processing Strategies for Optimal Detection of Protein-Protein Interactions: Gerhard Overbergen1; Florian Staneck1; Johannes Dobalmann1; Zuzana Demianova1; Karl Mechtler2; 1GMI - Gregor Mendel Institute of Molecular Plant Biology, Vienna, Austria; 2IMP - Research Institute of Molecular Pathology, Vienna, Vienna; 3IMP - Research Institute of Molecular Pathology, Vienna, Austria

WP 402 Proteomics in Perl: A Streamlined Approach: Jeremy D. Volkening1; Michael R Sussman1; 1University of Wisconsin-Madison, Madison, WI

WP 403 RAId GUI: A Graphical User Interface for RAId Tandem Mass-Spectrometry Database Search Tool: Danny Lee1; Aleskay Oourtsoy1; Gelo Alves2; Yi-Kuo Yu3; National Center for Biotechnology Information, NLM, NIH, Bethesda, MD

WP 404 Xcalibur Workbench: A Lua Based Data Browser: Michael W. Senko1; Graeme C McAlister1; Derek Bailey1; 1Thermo Fisher Scientific, San Jose, CA

WP 405 CHORUS is Innovative and User Friendly Platform for Third Party Mass Spectrometry Software Integration: Andrey Bondarenko1; Andrii Lobada1; Oleksii Tymchenko1; Vladimir Moiseiev2; Nathan Yates3; Mai Sun4; Michael J MacCoss5; Brendan Maclean5; Christine Wu6; Brian C Searle6; Sonia Ying Ting1; Jimmy K Eng1; Nick Shulman1; Juergen H Cox1; Chris Becker1; Infoclinika, Bellevue, WA; 2TeamDev, Kharkiv, Ukraine; 3University of Pittsburgh, Pittsburgh, PA; 4University of Washington, Seattle, WA; 5Max Planck Institute for Biochemistry, Martinsried, Germany; 6Protein Metrics Inc., San Carlos, CA

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS

WP 406 Fingerprinting of Falsified Artemisinin Combination Therapies (ACTs) via DART Ionization Coupled to a Compact Single Quadrupole Mass Spectrometer: Matthew Bernier1; Frederick Li1; Joseph LaPointe2; Brian D Musselman3; Paul Newton4; Facundo M Fernandez4; Georgia Institute of Technology, Atlanta, GA; 1IonSense, Inc. Saugus, MA; 2Lao-Oxford-Mahosot Hospital Wellcome Trust Research Unit (LOMWRU), Vientiane, Laos; 3Centre for Tropical Medicine and Global Health, University of Oxford, Oxford, UK

WP 407 Explosive Detection Using a Portable Benchtop Cylindrical Ion Trap-Mass Spectrometer: Stephen Davila1; Corey Stedwell1; Daniel DeBord1; 11st Detect Corporation, Webster, TX

WP 408 Establishing a Baseline for a Portable Stable Carbon Isotope Detection System: Brian Thomas1; Steve Taylor1; Tim Clary2; Dave McIntosh3; University of Liverpool, Liverpool, UK; 1The King's University, Southlake, TX

WP 409 Micro Mass Spectrometer Approach for Cometary Exploration: Ashish Chaudhary1; Friso van Amerom1; Tim Short1; Emily Barrentine2; Yun Zheng2; Daniel Glavin3; William Brinckerhoff4; Paul Mahaffy4; 1SRF International, St. Petersburg, FL; 2NASA GSFC, Greenbelt, MD

WP 410 Development of Compact Laser Desorption/Ionization Time-of-Flight Mass Spectrometer for Planetary Missions: Xiang Li1; Stephanie Getty2; Andrej Grubic3; Kyle Ucket1; William Brinckerhoff4; Timothy J Cornish1;
WP 411 Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer: Performance Testing in GC-MS and LD-MS Modes of Operation; Veronica Pinnick1; Ryan Danelli2; Friso van Amerom1; Samuel Larson1; Arnaud Buch1; Cyril Szopa1; Xiang Li1; Andrej Grubisic1; Ricardo Arevalo3; Stephanie Getty4; William Brinckerhoff1; Paul Mahaffy1; Francois Raulin5; Fred Goessmann1; University of Maryland, Baltimore County, Greenbelt, MD; Danell Consulting, Inc. Winterville, NC; NASA GSFC, Greenbelt, MD; Ecole Centrale, Paris, France; Laboratoire Atmosphères, Paris, France; University of Maryland, College Park, Park College, Park College, MD; C&E Research, Inc, Columbia, MD

WP 412 Characterization of the Mars Organic Molecule Analyzer Mass Spectrometer Intrinsic Dynamic Range; Friso H.W. Van Amerom1; Xiang Li1; Ryan Danelli2; Veronica T Pinnick2; Stephanie Getty4; Ricardo Arevalo3; Andrej Grubisic1; Lars Hovmand1; William Brinckerhoff1; Paul Mahaffy1; Fred Goessmann1; Mini-Mass Consulting, Inc, Hyattsville, MD; University of Maryland, Baltimore County Greenbelt, MD; Danell Consulting, Winterville, NC; NASA GSFC, Greenbelt, MD; University of Maryland, College Park, Park College, Park College, MD; Max Planck Institut für Sonnensystemforschung, Göttingen, Germany

WP 413 The Europa Mass Spectrometer for Planetary Exploration (MASPEX). A High-Resolution Multi-Pass Time-of-Flight Mass Spectrometer; Gregory P. Miller1; Jack Hunter Waite, Jr.; Tim Brockwell1; John Roberts1; Keith S Pickens2; Ryan C Blase1; Paul Wilson V; Southwest Research Institute, San Antonio, TX; Southwest Research Institute, San Antonio, TX

WP 414 Silence is Golden: Detector Radiation Shielding at Europa for MAss Spectrometer for Planetary Exploration (MASPEX); Ryan C Blase1; Roland R Benke2; Keith S Pickens1; Gregory P Miller1; Tim Brockwell1; John Roberts1; Paul Wilson V; J H Waite, Jr.; Southwest Research Institute, San Antonio, TX; Atom Consulting LLC / Consultant to SwRI, Austin, TX

WP 415 Development of an Integrated LC-MS Prototype for an in situ Mission to an Icy Body in the Solar System; Adrian Souther1; Stephanie Getty2; Jerome P Ferrance3; Brian N Stamos4; Jamie E Elsila2; Manuel A Balvin2; Daniel P Glavin1; Daniel S Stewart1; Brandon J Colon-Curiel5; John Roberts1; Keith S Pickens2; Ryan C Blase1; Paul Wilson V; Southwest Research Institute, San Antonio, TX; University of Puerto Rico Mayaguez, Mayaguez, PR

WP 416 Towards Remote Chemical Sensing Using an Aerodynamic Assisted Portable Mass Spectrometer; Yanbing Zhai1; Ting Jiang2; Wei Xu1; Beijing Institute of Technology, Beijing, China

WP 417 Portable Multiple Ionization Sources Biological Mass Spectrometer; Jung-Lee Lin1; Ming-Lee Chu1; Chung-Hsuan Chen1; Academia Sinica, Taipei, Taiwan

WP 418 Low Temperature Co-fired Ceramic (LTCC)-Packaged MEMS Micro-ion Source for Miniature Mass Spectrometry Applications; Charles B Parker1; Erich J Radauensch1; Kristin H Gilchri1; Shane DiDonna3; Zachary E Russell4; Stephen D Hall5; James B Carlton6; Sonia Greg7; Steven J Edwards8; Roger P Sperrine8; M. Bonner Denton3; Ryan R Stoner1; Jeffrey T Glass1; Daniel Austin1; Jessica Higgs1; Kit White1; Yuan Tian1; Brigham Young University, Provo, UT

WP 419 Handheld and Portable DAPCI Source for Point and Shoot Applications: Towards Onsite in-situ Explosives Analysis; Fred Paul Mark Jjunju1; Simon Maher2; Stephen Taylor2; Graham R Cooks3; Department of Electrical Engineering and Electronics University of Liverpool, Liverpool, UK; University of Liverpool, Liverpool, UK; Q-Technologies Ltd, Liverpool, UK; Department of Chemistry, University of Arizona, Tucson, AZ

WP 420 Improving the Selectivity of a High Pressure Mass Spectrometer; Andrew Hampton1; UNC - Chapel Hill, Chapel Hill, NC

WP 421 Improving the Selectivity of a High Pressure Mass Spectrometer: Andrew Hampton1; UNC - Chapel Hill, Chapel Hill, NC

WP 422 Failing Through the Cracks: High Resolution Quadrupole Mass Spectrometer; Dave McIntosh1; Mariya Antony-Joseph3; Simon Maher1; John Ray Gibson1; Stephen Taylor1; University of Liverpool, Liverpool, UK

WP 423 Utilizing Silicon on Insulator Materials to Fabricate Miniature Ion Traps for High Pressure Mass Spectrometry; Zachary Dyer1; Craig Cavanaugh3; Kenion Blakeman2; Tina Stacy1; Michael J Ramsey1; UNC Ramsey Group, Chapel Hill, NC; University of North Carolina at Chapel Hill, Chapel Hill, NC

WP 424 Miniaturized Toroidal Ion Trap using Cylindrical Electrodes; Daniel Austin1; Jessica Higgs1; Kit White1; Yuan Tian1; Brigham Young University, Provo, UT

WP 425 Overcoming the Tradeoff between Resolution and Sensitivity in Miniature Mass Spectrometry using Spatially Coded Apertures; Zachary E Russell1; 2; Evan X Chen1; Shane T DiDonna1; Jason A Jamsden1; Charles B Parker1; Scott D Wolter3; Ryan M Danell1; Brian R Stoner1; Gottfried Kibela1; Michael E Gehm1; David W Brady1; Jeffrey T Glass1; University of Durham, NC; Stanford University, Stanford, CA; Elion University, Elon, NC; Danell Consulting, Inc, Winterville, NC; RTI International, Raleigh, NC; XYLEM/OI Analytical, College Station, TX

WP 426 Coupling Thin-Layer Chromatography with Matrix Assisted Inlet Ionization for Small Molecule Analysis; Khoo Hoang1; Charles N McEwen1; 2; MStm, philadelphia, pa; University of the Sciences in Philadelphia, Philadelphia, PA; MSTM, LLC, Hockessin, DE

WP 427 Interfacing UPLC to Mass Spectrometry via a Liquid-junction, Secondary Ultrasonic API Source; Steve Bajic1; David S Douce1; Gordon A Jones1; Waters Corporation, Manchester, England

WP 428 Development and Optimization of an Inlet System for Desorption Atmospheric Pressure Photoionization – Mass Spectrometry (DAPPI-MS); Kai Kroll1; Christine Polaczek1; Tiina Kaupilla1; Anu Vaikkinen1; Hendrik Kersten1; Thorsten Benter1; University of Wuppertal, Wuppertal, Germany; University of Helsinki, Helsinki, Finland

WP 429 Glove Box MS Interface for the Measurement of Reaction Kinetics of Airsensitive Compounds; Alan T. Taylor1; Ruth Dooley2; Mark Baumert2; Clive Aldcroft2; Mark Allen3; C. Logan Mackay2; Guy Lloyd-Jones1; University of Edinburgh, Edinburgh, Lothian, School of Chemistry, The University of Edinburgh, Edinburgh, UK; Advison UK Ltd, Essex, UK
WP 430 Volatile Terpene Analysis in Cannabis, Spices and Fresh Produce by Tandem Mass Spectrometry Fitted with a Modified Plasma Source: Frank Kero; Craig Young; Heather Gamble; Joshua Ye; Lisa Cousins; Chuck Jollife; Chai Yuan-Cheng; Lin Jing-Chao; PerkinElmer, Downsview, IL; 2Ionics, Bolton, Canada; 3PerkinElmer, Shanghai, China

WP 431 A New Interface Design for Coupling a Liquid Stream to an Electron Ionization Source: Alexander Lekkas; Dimitris Papanastasiou; Emmanuel Raptaakis; Francesca Rigano; Danilo Sciarrone; Luigi Mondello; 1Fasmatelch, Athens, Greece; 2Chromatront s.r.l., Messina, Italy; 3Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Messina, Italy

WP 432 LC-MS with Cold EI – The New System and Recent Applications: Svetlana Tsizin; Avir Amirav; Alexander B Fialkov; Tal Alon; Tel-Aviv University, Tel-Aviv, Israel; Tel-Aviv University, Tel-Aviv

WP 433 Study of Vaporization Surfaces in Liquid Chromatography – Electron Ionization Mass-Spectrometry: Federica Bianchi; Laura Magrini; Nicolò Riboni; Maria Careri; Achille Cappiello; 1University of Parma, Parma, Italy; 2University of Urbino, Urbino, Italy

WP 434 DEI vs. LEI: A Novel, Advanced System for Interfacing Liquid Chromatography and Electron Ionization Mass Spectrometry: Achille Cappiello; Maurizio Pieriggiovanni; Giorgio Famiglini; Veronica Temporoli; Pierangela Palma; 1University of Urbino, Urbino, Italy

WP 435 Evaluation of an Induction-Based Fluidics System for Delivery of Low Volume (nL) Samples: Kelly Hanssen Smith; Susan M Schulz; Bryce F Dozorzi; Ernest H Braue; Irwin Koplovitz; Kathleen Housman; Lee I Roberts; Jonathan Oyler; 1USAMRICD, Aberdeen Proving Ground, MD

WP 436 AP-to-vacuum inlet with New Features – Optimization of Desolvation Conditions in Liquid AP-MALDI MS: Jeff Brown; Pavel Ryumin; Michael Morris; Rainer Cramer; 1University of Reading, Reading, UK; 2Waters, Wilmslow, UK

WP 437 Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Time of Flight Mass Spectrometry (GC-TOF-MS) for Identification and Quantification of Halogenated Compounds: Kunyu Zheng; Hamid Badiei; Kaveh Jorabchi; 1Georgetown University, Washington, DC; 2PerkinElmer, Woodbridge, ON

WP 438 A Novel Method for Online Analysis of Electronic Cigarette Aerosol: Christian Lindinger; Alfons Jordan; Philipp Sulzer; Kostianyi Breiv; Kerstin M.M. Burseg; Grant O’Connell; Eugen Hartungen; Stefan S. Biel; Xavier Cahours; Stephane Colard; Frank Kero; Craig Young; Daniel Chaplin; Ash Buck; Keith Richardson; Jeff Brown; Kevin Giles; Zoltan Takats; Bangor University, Bangor, UK; Waters, Wilmslow, UK; Imperial College, London

WP 439 Collision Cross Section (CCS) Measurements for Small Molecular Mixture by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Hu Miang; Zhang Linzlhui; Xu Chunming; Quan Shi; 1China University of Petroleum, Beijing, China; 2State Key Laboratory of Heavy Oil Processing, Changqing, Beijing

WP 440 Assessment of using Projection Superposition Approximation (PSA) with Molecular Modeling to Compute Collision Cross Sections For Ion Mobility Spectrometry: Glenn Spangler; Technispan LLC, Lutherville, MD

WP 441 Predicting Theoretical Collision-cross Sections for Peptides and Peptide Fragments: Bela Paizai; Oscar Hernandez; Daniel Chaplin; Ash Buck; Keith Richardson; Jeff Brown; Kevin Giles; Zoltan Takats; Bangor University, Bangor, UK; Waters, Wilmslow, UK; Imperial College, London

WP 442 Evaluation of Collision Cross Section Measurements Obtained by Uniform Field Drift Tube IM-MS: Insight into Instrument Settings and Theoretical Calculations: Sarah Bow; Jody C. May; James N Dodd; Andrzei Balinski; Emma E Rennie; Ruwan T Kurulgama; John Fildes; John A McLean; 1Vanderbilt University, Nashville, TN; 2Agilent Technologies, Santa Clara, CA

WP 443 Hide-and -Seek: The effect of Localisation of Partial Charged Ions on Their Calculated CCS Values: Lukasz Grzegorz Migas; Eleanor Sinclair; Christopher Gray; Sabine Flitsch; Perdita Barran; University of Manchester, Manchester, UK

WP 444 On the Structural Denaturation of Biological Analytes in Trapped Ion Mobility Spectrometry - Mass Spectrometry: Fanny Caroline Liu; Samuel R. Kirk; Christian Bleiholder; Florida State University, Tallahassee, FL

WP 445 Collision Cross Section Accuracy of Common MS Calibrants Across a Large Number of Measurements in Positive and Negative Ion Modes: Jody C. May; Ruwan T Kurulgama; George C Stafford; John C Fildes; John A McLean; 1Vanderbilt University, Nashville, TN; 2Agilent Technologies, Santa Clara, CA

WP 446 Elucidating the Structural Heterogeneity of Biomolecules in the Gas Phase using Traveling Wave Ion Mobility Arrival Time Distributions: Suyovan Dixit; Brandon T Ruotolo; University of Michigan, Ann Arbor, MI

WP 447 Towards using Trapped IMS in Structural Biology Applications: Christian Bleiholder; Fanny C Liu; Samuel R Kirk; Meggie Young; Mengqi Chai; Florida State University, Tallahassee, FL; Florida State University, Tallahassee, FL

WP 448 Characterizing Instrumental Parameters in Trapped Ion Mobility Spectrometry (TIMS) for Transmission and Preservation of Native Analyte Structures and Their Complexes: Samuel Kirk; Christian Bleiholder; Florida State University, Tallahassee, FL

WP 449 Fundamentals of Trapped Ion Mobility Spectrometry: Fluid Dynamics: Melvin A. Park; Karsten Michelmann; Mark E Ridgeway; Joshua Silveira; Bruker Daltonics, Inc., Billerica, MA; Bruker Daltonic GmbH, Bremen, Germany

WP 450 Decomposition Pathways during Explosive Analysis Using TIMS-MS and Molecular Dynamics: Alan McKenzie; Mark E Ridgeway; Melvin Park; Francisco Alberto Fernandez Lima; Florida Int’l University, Miami, FL; Bruker Daltonic, Billerica, MA; Florida International University, Miami, FL

WP 451 Improving Ion Mobility – Mass Scan for the High Performance Ion Mobility Spectrometry – Mass Spectrometry: Jianglin Wu; Adam M Graichen; Mark Osgood; China Wu; Excellims Corporation, Acton, MA

WP 452 Structures for Lossless Ion Manipulations (SLIM) using Multilevel Traveling Wave Ion Escalators for Obtaining Ultrahigh Resolution Ion Mobility Separations: Ahmed M Hamid; Yehia M Ibrahim; Sandilya V. B Garimella; Ian K Webb; Liulin Deng; Gordon A Anderson; Spencer A Prost; Jeremy A Sandoval; Randolph V Norheim; Erin S Baker; Richard D Smith; Pacific Northwest National Laboratory, Richland, WA

WP 453 Development and Evaluation of Long Serpentine Path Traveling Wave SLIM Modules for High Resolution Ion Mobility Separations: Liulin Deng; Yehia M Ibrahim; Ahmed M Hamid; Sandilya Garimella; Ian Webb; Xing Zhang; Tsung-Chi Chen; Xueyun Zheng; Erin Baker;
WP 454  Comparing Ion Multiplexing Techniques: Tangible Enhancement for Ion Mobility-Mass Spectrometry; Brian H. Clowers 1; Austen L. Davis 2; Kelsey A Morrison 3; 1Washington State University, Pullman, WA

WP 455  A Comparative Study of nanoESI and ESI on an Atmospheric Pressure High Performance Ion Mobility Spectrometer; Mark Osgood 1; Adam M Graichen 2; Ching Wu 3; 1Excellima Corporation, Acton, MA

WP 456  Modeling Space Charge Effects on the Performance of Transversal Modulation Ion Mobility Spectrometry: A Numerical Approach; Cesar Barrios 1; Guillermo Vidal-de-Miguel 2; 1SEADM, Boeicillo, Spain; 2Fossil Ion Technology S.L., Madrid, Spain

WP 457  Coupling of High-Resolution Atmospheric Pressure Drift Tube Ion Mobility Spectrometry with High-Resolution Accurate Mass Orbitrap Mass Spectrometry; Joel D. Keefer 1; Anyin Li 2; Brian H Clowers 3; Facundo M Fernandez 4; 1Georgia Institute of Technology, Atlanta, GA; 2Washington State University, Pullman, WA

WP 458  Peak Width Analysis for Automated Detection of Unresolved Isomers in Ion Mobility; Matthew Brantley 1; Michael Pettit 1; Brett Harper 1; Brooke Brown 1; Touradi Solouki 1; 1Baylor University, Waco, TX

WP 459  Altering the Mobility-Time Continuum: Methods for Targeted, Yet Lossless, High Resolution Trapped Ion Mobility-Mass Spectrometry; Joshua Adam Silveria 1; William Danielsen 2; Jacob Meier 2; Mark E Ridgeway 2; Melvin Park 2; 1Texas A&M University, College Station, Texas; 2University of the Pacific, Stockton, CA

WP 460  Comprehensive Electric Field Analysis of Resistive Glass Drift Tubes, Reflectrons, and Other Electro-Optical elements; Robert Jackson 1; Matthew Breuer 2; Paula Holmes 3; Jeffrey DeFazio 4; 1Instrumental Design Physics, LLC, Littleton, MA; 2Photonis USA, Sturbridge, MA; 3PHOTONIS USA, Lancaster, PA

WP 461  Ion Mobility Coupled to Extended Mass Range Orbitrap for Structural Analysis of Large Proteins and Protein Complexes: Michael Potholm 1; Kyle Fort 2; David H Russell 3; 1Texas A&M University, College Station, Texas; 2Utrecht University, Utrecht, The Netherlands; 3Texas A&M University, College Station, TX

WP 462  Multistage Transversal Modulation IMS Coupled with IonMax Electrospray and Ion Trap MS to Provide a Modular ESI-IMS-MS Solution; Guillermo Vital-de-Miguel 1; Miriam Macia 2; Gonzalo Arranz 2; Alberto Tejero 2; 1Fossil Ion Technology S.L., Madrid, Spain; 2SEADM, Boecillo, Spain

WP 463  Development of a Drift Tube Mass Spectrometer Associated with Plasma Microjets; Joel Lemaire 1; Bessem Brahim 1; Michel Henninger 2; Essyfli Louam 3; Helene Mestdagh 4; Gerard Bauville 5; Nicole Blin Simiand 6; Et-Touhami Es-Sebar 7; Michel Fleury 8; Stephane Pasquier 9; Joao Santos Sousa 10; Elsa Bauchard 11; Julien Leprovost 12; 1LCP, UMR8000, CNRS-Universite Paris Sud, Universite Paris Saclay, Orsay, France; 2LPSP, UMR8578, CNRS-Universite Paris Sud, Universite Paris Saclay, Orsay, France; 3AlyXan, Jvisusy sur Orge, France

ION STRUCTURE/ENERGETICS

WP 464  Gas Phase Conformation of the Complex of Cyclodextrins with Amino Acids Revealed by Ion Mobility-Mass Spectrometry and Molecular Dynamics Calculation; Yinyin Chen 1; ZhiCheng Zuo 1; XinHua Dai 2; Wenning Wang 3; Chuanfan Ding 2; Fudan University, Shanghai, China; 1National Institute of Metrology, Beijing, China; 2Fudan University, Shanghai, CN

WP 465  Fragmentation of Nickel Nitrate Anions; Daniel Goebbert 1; 1The University of Alabama, Tuscaloosa, AL

WP 466  Effects of Solvent Systems and Source Conditions on Protonation Site: The Case of p-Aminobenzoic Acid; Amanda L Patrick 1; Nicolas C Polfer 2; 1University of Florida, Gainesville, FL

WP 467  How Does Zinc Do It? Transformations of Alcohols by Gas-Phase Zinc Cation Complexes; Evan Perez 1; Cassandra Hanley 2; Theodore A Corcoviolas 3; John K Gibson 4; Jonathan Martens 5; Jos Oomsens 5; 1Washington State University, Pullman, WA; 2Lawrence Berkeley National Lab, Berkeley, CA; 3Radboud University Nijmegen, Nijmegen, Netherlands; 4University of Amsterdam, Amsterdam, The Netherlands

WP 468  Synthesis and Study of Metal Oxide Cores through Sequential Fragmentation of Co(NO3)3; Thomas Hester 1; Daniel J. Goebbert 2; 1The University of Alabama, Tuscaloosa, AL

WP 469  Effects of D-amino Acids on the Gas Phase Acidity of Oligopeptides; Zachary Buen 1; Jianhua Ren 2; 1University of Toronto, Toronto, ON; 2University of Alberta, Edmonton, AB

WP 470  Fragmentation Mechanisms of Metal-yersiniabactin Complexes by Low-Energy Collision-induced Dissociation Tandem Mass Spectrometry: An Empirical and Theoretical Study; Daryl Giblin 1; Eun-Ik Koh 2; Jan R Crowley 3; Michael L Gross 4; Jeffrey P Henderson 5; 1Washington University in St. Louis, St. Louis, MO; 2Washington University in St. Louis, Saint Louis, MO

WP 471  A Study of Diaryl Iodonium Complexes with Crown Ethers in the Gas Phase; Dmitri Zagorevski 1; Michael F Aldersley 1; Rensselaer Polytechnic Institute, Troy, NY

WP 472  Underwater: A Computational Examination of the Gas-phase Basicity Scale Weaker than 700 kJ/mol; John Bartmess 1; University of Tennessee, Knoxville, TN

WP 473  Potential Energy Surface of the Gd+ Reaction with O2 Mapped with GIBMS and Theory; Maria Demireva 1; Peter B Armentrout 2; 1Department of Chemistry, University of Utah, Salt Lake City, UT

WP 474  The Spider versus the Fly: Cationized Carbohydrate Gas-phase Fragmentation Chemistry informs Saccharide Sequence Elucidation; Maha T Abutokah 1; Ashley R Wagener 2; Benjamin J Bythell 3; 1University of Missouri-StLouis, St. Louis, MO

WP 475  Structure, Thermochromy, and Reactivity Studies of Gas-Phase Aikali Metal Ion-Coordinated ProLeu and LeuPro; Yasaman Jamilelahmad 1; Travis D Fridgen 2; 1Memorial Univ of NL-Canada, St. John’s, NL; 2Memorial University of NL, St. John’s, Canada

WP 476  Studies of Dihalogen Radical Anion Formation from Maleic Acid-Acene Compounds by Negative Chemical Ionization (NCI) and Time-of-Flight Mass Spectrometry (TOFMS); Daryl Giblin 1; Jonathan P Hopwood 2; Brittni A Qualizza 3; 1Washington University, St. Louis, MO; 2Loyola University, Chicago, IL

WP 477  Solution pH Can Affect Electrosprayed Metal-Ion Binding Patterns: IRMPD Structures of Metal-Ion Tripeptide Complexes; Robert C. Dunbar 1; Jonathan Marins 2; Giel Berden 3; Jos Oomsens 4; 1Case Western Reserve Univ, Cleveland, OH; 2Radboud University Nijmegen, Nijmegen, Netherlands; 3Radboud University, Nijmegen, Netherlands

WP 478  Prediction of CID/HCD Spectra by First-Principle Molecular Dynamics for Aimed Routine Compound ID; Michal Raab 1; Robert Mistrik 2; 1HighChem, Bratislava, Slovakia; 2HighChem, Bratislava, SK

WP 479  Unimolecular Dissociation and Structures of Gaseous Self-Assembled [Ca(Uracil)4,5,6]2+ Complexes; Ruodi Cheng 1; Travis Fridgen 2; 1Memorial University of NL, St. John’s, Canada; 2Memorial University of NL, St. John’s, NL

64TH ASMS CONFERENCE ON MASS SPECTROMETRY

PAGE 149
WP 480  Ligand Binding Energies and Structural Isomerism Accompanying Phosphine Exchange on the Cationic Gold Clusters; Marshall Ligare1; Jose Ulises Reveles2; Grant E Johnson1; Erin Baker1; Julia Laskin1; 1Pacific Northwest National Lab, Richland, WA; 2Virginia Commonwealth University, Richmond, VA

WP 481  Metal Ion Adducts of Cysteine and Cysteine-Containing Peptide Radicals: Structure and Reactivity; Victor Ryzhov1; Michael Lesslie1; John Lawler1; Kai-Chi Justin Lau2; Alan C Hopkinson2; 1Northern Illinois University, DeKalb, IL; 2York University, Toronto, Canada

WP 482  Mass Spectrometric and Computational Investigation of the Protonated Carnosine–Carboxylatin Complex Fragmentation; Idi Ritacco1; Emilia Sicilia1; Tamer Shoeib2; 3Mohamed Korany2; Nino Russo2; 1Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Calabria, Italy; 2Department of Chemistry, The American University in Cairo, New Cairo, Egypt; 3Centre for Analytical Science, Department of Chemistry, Loughborough University, Loughborough, UK

LC-MS: SAMPLE PREPARATION (PART 1) 483 - 504

WP 483  Improved Recovery, Reproducibility and Matrix Effects with an Advanced Technology in Solid Phase Extraction (SPE) – Oasis PRiME HLB; Xin Zhang1; Jonathan Danaceau2; Erin Chambers1; 1Waters, Milford, MA

WP 484  Comprehensive Analysis of Protein Glycosylation using NGAG Method; Shisheng Sun1; 1University of Oklahoma, Norman, OK

WP 485  Methylmalonic Acid: Evaluation of Sample Preparation and Simplicity of Method Implementation using Automated Sample Preparation Prior to LC-MS/MS Analysis; Rhyos Jones1; Helen Ladder1; Lee Williams2; Geoff Davies3; 1Axel Semrau GmbH; 2University at Buffalo, Buffalo, NY; 3Shimadzu Corporation

WP 486  Integration of Steroids Analysis in Serum using LC-MS/MS with Full-Automated Sample Preparation; Tohkiazu Minohata1; Kawakami Daisuke1; 1Shimadzu Corporation, Kyoto, Japan

WP 487  Determination of Pharmaceuticals in Wastewater using Online SPE Coupled to Liquid Chromatography Mass Spectrometry; Andreas Bruchmann1; Claudia vom Eyser2; Thorsten Teutenberg3; Jochen Tuerk1; Axel Semrau GmbH & Co.KG, Sprockhoevel; 1IUTA, Duisburg, Germany

WP 488  Applying a Tangential Flow Filtration Approach for Low Concentration Proteomics Sample Preparation; Woodard Toni1; Zhe Wang1; Ma Hongsyan1; Saurav Mallia1; Si Wu1; 1University of Oklahoma, Norman, OK

WP 489  SPE Method Optimization and Transfer to an Automated Sample Preparation Platform for Low Level Catecholamine Analysis using LC-MS/MS; Alan Edgington1; Adam Senior1; Lee Williams1; 1University of Massachusetts Amherst, Amherst, MA

WP 490  Dual Immobilized Enzyme Reactors for Peptide, Glycan, and Glycopeptide online LC-MS/MS Analysis; Kerry Wooding1; Rui Zhu1; Yehia Mechref1; 1Texas Tech University, Lubbock, TX

WP 491  Handy Devices for Quantitative Capillary Blood Microsampling; Shinobu Kudoh1; Ipei Takeuchi2; 1Shimadzu Techno-Research, Inc., Ohta-Ku, Tokyo; 2Shimadzu Corp, Kyoto, Japan

WP 492  Rapid, Efficient and Reproducible Sample Preparation for Quantitative Proteomics by a Surfactant-Aided Precipitation/Ont-Pellet Digestion Strategy; Shichun Shen1; Bo An2; Jun Li1; Xiaoming Shen1; Chengjian Tu1; Jun Qu1; 1University at Buffalo, Buffalo, NY

WP 493  A Quantitative LC-MS Method to Determine Lutein Levels in Whole Human Blood Using Dried Blood Spot Analysis (DBS); Carl Norren1; Todime Reddy2; Stefan Ehling1; 1Abbott Nutrition, Columbus, OH

WP 494  Fully Automated Extraction of Dextrorphan Experimental Procedure by DBS In-Tips, analyzed with RT-LC-MS/MS; Sylvain R Letarte1; SERGE AUGER2; Pierre Picard1; 1Phytronix Instruments, Boisbriand, Canada; 2Phytronix Technologies, Quebec, QC

WP 495  In-depth Proteomic Quantification of Cell Secretome in Serum-Containing Conditioned Medium; Yejing Weng1; 1Korea Basic Science Institute, Chungbuk, South Korea; 2Chungnam National University, Daejeon, South Korea; 3Cheongju University, Cheongju, South Korea

WP 496  A Multiwell Magnetic Mixer for Automated Sample Preparation: Chang Liu; Don W Arnold2; Thomas R Covey1; 1SCIEX, Concord, ON; 2SCIEX, Redwood City, CA

WP 497  Quantitative Analysis of low-Abundance Serological Proteins with Peptide Affinity-Based Enrichment and Pseudo-Multiple Reaction Monitoring by Hybrid Quadrupole Time-Of-Flight Mass Spectrometry; Kwang Hoe Kim1; 1Shimadzu Techno-Research, Inc., Ohta-Ku, Tokyo; 2Shimadzu Corporation, Kyoto, Japan

WP 498  Advancing the MStern Blotting – PVDF Membrane-Based Peptide Fractionation in a 96 Well Format; Sebastian Berger1; 1Biorad; Saima Ahmed2; Michaela Helmel3; Hanno Steen4; 1Boston Children’s Hospital, Boston, MA; 2Harvard Medical School, Boston, MA; 3Boston Children’s Hospital, Harvard Medical School, Boston, MA

WP 499  Quantification of Celecoxib in Rat Skin using LC-MS/MS Method after Collagenase Digestion and Bead Lysis; Raghunath Aleli1; Ilayaraja Kalaikadhan1; Sallakshmi Chennupati1; Devender Reddy Ajal1; Ramakrishna Nirgi1; 1Suven Life Sciences Ltd, Hyderabad, Telangana

WP 500  Basic Reverse Phase Fractionation on OasisHLB-eElution Plates as a Fast Sample Preparation Technique for LC/MS Analysis of Low Protein Amounts; Robert N O’Meally1; Tatiana N. Boronina1; Maximilian Konig2; Felipe Andrade1; Robert N Cole1; 1Johns Hopkins University School of Medicine, Baltimore, MD

WP 501  LC/MS/MS Analysis with On-line Cartridge for Removal of Phospholipids from Protein Precipitation Biological Fluid Samples; David S. Bell1; Xiaoning Lu1; Hillel K. Brandes1; Craig R Aurand1; Sarah Smith1; Carmen T. Santasania1; 1MilliporeSigma, Bellefonte, PA

WP 502  Different Approach for Improvement of Low Recovery Dried Blood Spot Storage Sample and Its Application in Bioanalytical Assay; Dawei Zhou1; John Ma1; Mohamed Osman1; Xinping Fang1; 1Wuxi AppTec Co., Plainsboro, NJ

WP 503  Simultaneous Quantitation of Five Leachables in Lipid Emulsions by LC-MS/MS Using 2,2-Dimethoxypropane; Yousheng Hu1; Jim Story1; Pelfeng Hu1; 1Baxter Healthcare, Round Lake, IL

WP 504  A Conventional Procedure to Reduce Asn Deamidation Artifacts during Trypsin Peptide Mapping; Yekaterina Kori1; 1University of Massachusetts Amherst, Amherst, MA; 2Alexion Pharmaceuticals, Cheshire, CT

WP 505  A Conventional Procedure to Reduce Asn Deamidation Artifacts during Trypsin Peptide Mapping; Yekaterina Kori1; 1University of Massachusetts Amherst, Amherst, MA; 2Alexion Pharmaceuticals, Cheshire, CT
WP 505 Optimization of Female Sex Hormone Extraction for
Semi-Quantitative Analysis in Human Plasma by
UHPLC/MS/MS. Juan Aristizabal Henao1; Richard W Smith1; Ken D Stark1; 1University of Waterloo, Waterloo ON, Canada

WP 506 Lipidic Profiling of Biological Samples using
Off-Line Two-Dimensional High-Performance Liquid
Chromatography-High Resolution Mass Spectrometry;
Monica Narvaez-Rivas1; Qibin Zhang2; 1University of North Carolina at Greensboro, Karlanna, NC; 2University of North Carolina Greensboro, Greensboro, NC

WP 507 UHPLC Combined with Ultra-high Resolution QTof-MS
for Rapid Lipidomic Profiling of Serum for Discovery of
Lipid Biomarkers of Parkinson’s Disease; Jaspal Tatlay1;
Dorothea Mung1; Richard Camicioli1; Liang Li1; 1University of Alberta, Edmonton, Canada; 2Neuroscience and Mental Health Institute, Department of Medicine, Edmonton, AB, Canada

WP 508 Environmental Lipidomics: Examining the Case of
Pansteatitis in Mozambique Tilapia, John Bowden1; Jeremy Koelmel1; Stephen E Somerville1; Timothy J Garrett1; Richard A Yost2; Robert Chapman3; Louis Guillette1; 1NIST, Charleston, SC; 2University of Florida, Gainesville, FL; 3Medical University of South Carolina, Charleston, SC; 4South Carolina Department of Natural Resources, Charleston, SC

WP 509 Comprehensive Lipid and Protein Analysis of Size
Fractionated Serum Lipoproteins in Normal versus
Dyslipidemic Subjects; Michael Gardner1; Zsusanna Kuklenyik1; David M Schieltz1; Jon Rees1; Lisa G McWilliams2; Yulanda Williamson1; Christopher Toth1; Jeffrey Jones1; Michael Andrews1; John R Barr1; 1Centers for Disease Control and Prevention, Atlanta, GA

WP 510 Reverse Phase LC-ESI-QTOF Methodology for the
Analysis of Lipids in Whole Blood; Ralph Hindle1; Ken D Stark1; Juan J Aristizabal Henao1; Richard W Smith1; Sheher Mohsini1; 1Vogon Laboratory Services, Alberta, Cochrane, Canada; 2Department of Kinesiology, University of Waterloo, Waterloo ON, Canada; 3University of Waterloo Mass Spectrometry Facility, Waterloo, Ontario ON, Canada

WP 511 The Application of Lipidomics to the Study of
Hepatocellular Carcinoma (HCC) Induced by Low Dose, High-Energy, High Charge Ions (HZE); Brooke L Barnette1; Jeremy Koelmel1; Stephen E Somerville1; Timothy J Garrett1; Richard A Yost2; Robert Chapman3; Louis Guillette1; 1NIST, Charleston, SC; 2University of Florida, Gainesville, FL; 3Medical University of South Carolina, Charleston, SC; 4South Carolina Department of Natural Resources, Charleston, SC

WP 512 Analysis of Lipids in Spinal Cords of Experimental
Autoimmune Encephalomyelitis (EAE) Mice using On-Line Photochemical Derivatization and Tandem Mass Spectrometry; Leelyn Chong1; Xiaoxiao Ma1; Yu Xia1; Zheng Ouyang1; 1Purdue University, West Lafayette, IN

WP 513 Lipid Peroxidation Profiles in Acute Hepatic Ischaemia-
Reperfusion Injury; Michael Dunn1; Aimen Amer1; Margaret Knight1; Claire Roper1; Peter Blair1; Matthew Wright1; 1Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK; 2Institute of Cellular Medicine, Newcastle University, Newcastle upon Tyne, UK

WP 514 The Comparison of Glycosphingolipids in an Epithelial
Ovarian Cancer Cell Line and a Nontumorigenic
Epithelial Ovarian Cell Line using MALDI-MS; Krishani Kumari Rajanayake1; William Taylor1; Dragan Isailovic1; 1The University of Toledo, Toledo, OH

WP 515 Fatty Acid Re-Esterification in Adipose Tissue -
Beneficial Fettle Metabolite Cycling; Ondrei Kuda1; Martina Rombolová1; Jan Kopecký1; 1Institute of Physiology, CAS, Prague, Czech Republic

WP 516 Analysis of Phospholipids, Lipid A and Sterols from
Outer Membrane Vesicles Shed by Acinetobacter baumanniiDU202; Geul Bang1; Semin Park1; Sung-Ho Yun1; Seung Il Kim1; Man Ho Choi1; Yun-Gon Kim1; Young Hwan Kim1; 1Korea Basic Science Institute, Cheongiu, Korea; 2Korea Basic Science Institute, Daejeon, Korea; 3Korea Institute of Science and Technology, Seoul, Korea; 4Soongsil University, Seoul, Korea

WP 517 Differing Effects of Red-tide Exposure on the Lipidome
of Phytoplankton Competitors; Scott Hogan1; Remington Poulin1; Julia Kubanek1; Facundo M Fernandez1; 1Georgia Institute of Technology, Atlanta, GA

WP 518 Fusarum oxyssporum f. spubense Aggressiveness
Investigated by MALDI-TOF-MS Lipid Profile; Daniele F. O. Rocha1; Cristiane M. S. Cunha2; Katia R. A. Belaz1; Fabio N. dos Santos1; Robert H. Hinz2; Adriana Pereira1; Alexandre Visconti1; Ester Wicket1; Lidiane Maria de Andrade1; Claudio A. O. Nascimento1; Nogueira Marcos Eberlin1; 1Thomson Mass Spectrometry Laboratory-UNICAMP, Campinas, Brazil; 2Flora Biotecnologia Ltda, Itajai, Brazil; 3Empresa de Pesquisa Agropecuária e Extensão Rural de Santa Catarina- EPAGRI, Itajai, Brazil; 4Chemical Engineering Department of Polytechnic School of University of São Paulo, São Paulo, Brazil

WP 519 Direct Analysis of Phospholipids in Biological Tissues
Using Internal Extractive Electrospray Ionization Mass
Spectrometry; Haiyan Lu1; Jianyong Zhang1; Wei Zhou1; Yiping Wei1; Huanwen Chen1; 1East china university of Technology, Nanchang, China; 2Second Affiliated Hospital of Nanchang University, Nanchang, China; 3East China Institute of Technology, Nanchang, China; 4East China University of Technology, Nanchang, Mainland

WP 520 Ambient Ionization Methods and Liquid
Chromatography – Mass Spectrometry Analysis of
Human Melanoma Biopsies; Louis Searcy1; Candice Ulmer2; Matthew Kazaleh2; Michael Costanzo2; Nikolaus Gravenstein1; Richard A Yost1; 1University of Florida, Gainesville, FL; 2University of Florida, Gainesville, FL

WP 521 In-situ and in-vitro Regional Analysis of Lipids in
Mammalian Vitreous Humor using MALDI-MS; Abby Schnepf1; M. Cecilia Yappert2; Douglas Borchman1; 1Georgia Institute of Technology, Atlanta, GA; 2Waters, Wilmslow, UK; 3Imperial College, London, UK

WP 522 Analysis of Phospholipids, Lipid A and Sterols from
Outer Membrane Vesicles Shed by Acinetobacter baumanniiDU202; Geul Bang1; Semin Park1; Sung-Ho Yun1; Seung Il Kim1; Man Ho Choi1; Yun-Gon Kim1; Young Hwan Kim1; 1Korea Basic Science Institute, Cheongiu, Korea; 2Korea Basic Science Institute, Daejeon, Korea; 3Korea Institute of Science and Technology, Seoul, Korea; 4Soongsil University, Seoul, Korea

WP 523 Detection of Altered Brain Lipids by LC-MS and Imaging
Mass Spectrometry in Demyelinating, Remyelinating and Dysmyelinating Mouse Models; Xiaoping L. Hronowski1; Raj Maganti1; Robert Dunstan1; Peter Juhasz1; 1Biogen Inc., Cambridge, MA

WP 524 A General Normal Phase HPLC Separation Hyphenated
with HR-AM – Tandem Mass Spectrometric Method for
Whole Lipidomics Profiling; Qifeng Zhang1; Michael J.O. Wakelam1; 1Babraham Institute, Cambridge, UK

WP 525 Comprehensive Profiling of Lipids in Chicken Skin
by High Resolution Mass Spectrometry with Online
Information Dependent Acquisition Workflow; Yushi Pan1; Kevin zhang2; Huaidong Yu3; Yong Fang4; 1Pan YS, Nanjing, China; 2Beijing, Beijing; 3Yu HD, Beijing, China; 4Fang Y, Nanjing, China

WP 526 Comprehensive Profiling of Lipids in Chicken Skin
by High Resolution Mass Spectrometry with Online
Information Dependent Acquisition Workflow; Yushi Pan1; Kevin zhang2; Huaidong Yu3; Yong Fang4; 1Pan YS, Nanjing, China; 2Beijing, Beijing; 3Yu HD, Beijing, China; 4Fang Y, Nanjing, China

WP 527 Comprehensive Profiling of Lipids in Chicken Skin
by High Resolution Mass Spectrometry with Online
Information Dependent Acquisition Workflow; Yushi Pan1; Kevin zhang2; Huaidong Yu3; Yong Fang4; 1Pan YS, Nanjing, China; 2Beijing, Beijing; 3Yu HD, Beijing, China; 4Fang Y, Nanjing, China
WP 526 Phospholipid Profiling by Two Distinct MRMs Measures to Identify Phospholipid's Class and Fatty Acid Composition, Tsuyoshi Nakanishi1; Masaki Yamada1; Suzumi Tokouka1; Yoshihiro Kita2; Takao Shimizu2; 1Shimadzu Corporation, Kyoto, Japan; 2University of Tokyo, Tokyo, Japan; 3National Center for Global Health and Medicine, Tokyo, Japan

WP 527 Lipid Profiling of Madin-Darby Canine Kidney Cells and Its Lipid Changes Induced by Aristolochic Acid(I) using Two-Dimensional LC-MS, Hongqiang Nie1; Liu Ranran2; Yang Youyou3; Liu Huwei1; Bai Yu1; 1Peking University, Beijing, China; 2Chinese Oil & Foodstuffs Corporation (COFCO) Nutrition and Health Research Institute, Beijing, China

WP 528 High-Throughput Lipidomics Workflow for Identification and Quantification of >1000 Lipids in 13 Different Lipid Classes, Richard John Robinson1; Fred Hubbard1; Philip Michael Charpia2; Alexanderia Conner2; Anne Evans1; Luke Miller2; Steve Watkins1; Don Hanavan1; 1Metabolon, Inc., Durham, NC; 2Metabolon, Inc., Durham, NC

WP 529 Lipidomic Analysis of Cultured Cells Lines, Finnur Freyr Eiriksson1; Manuela Magnusdottir2; Halldorsson Skarphedinsdottir2; Otta Rolfsson2; Helga M. Ogmundsdottir2; Margrét Thorsteinsdottir2; 1ArcticMass, Reykjavik, Iceland; 2University of Iceland, Reykjavik, Iceland

WP 530 Profiling Lipids in Plants Using Infusion and Chromatography Based High Resolution Mass Spectrometry Methods with Automated Data Processing, Yelena A. Adelidinskaya1; Daniel J J Gachotte1; Jeffrey R Gilbert2; Jesse L Balcer2; Laura L Wayne1; 1Dow AgroSciences, Indianapolis, IN

WP 531 Lipid and Fatty Acid Analysis in Grape Seeds and Grape Seed Oil with High Resolution Mass Spectrometry, Zareen Khan1; Akanksha Singh2; Ahammed Shabeeb T.P.1; Manoj Pillai3; Kaushik Banerjee1; 1National Referral Project and Prediction of Survival in Bladder Cancer: A Linkage to Cancer Genome Atlas Project and Prediction of Survival, Nagireddy Putluri1; 1Bayor College of Medicine, Houston, TX; 2Agilent Technologies, Wilmington, DE

WP 532 Methods to Analyze Beneath the Surface of Oil Seeds using Mass Spectrometry, Suresh Annangudi1; Callee Walsh2; Trust T Razungzwa2; Jeffrey R Gilbert1; 1Dow AgroSciences, Indianapolis, IN; 2Protea Biosciences, Inc. Morgantown, WV

WP 533 Accelerating Lipid Profiling Acquisition Strategies using Differential Mobility Spectrometry and SWATH® Data Collection, Eva Duchoslav1; Brad T Patterson2; Larry J Campbell1; Yves J C LeBlanc1; 1SCIEX, Concord ON, Canada; 2SCIEX, Gurgaon, Haryana

WP 534 A Simple, Flexible, and Automated Infusion System for Lipidomic Analysis using Mass Spectrometry, Jeff McDonald1; Steve Stiller2; 1UT Southwestern Medical Center, Dallas, TX; 2LEAP Technologies, Carrboro, NC

WP 535 The Rapid Evaporative Ionisation Mass Spectrometry (REIMS) iKnife Identifies Gynaecological Tissue with Excellent Accuracy in the ex-vivo and in-vivo Setting, David L Phelps1; Julia Baldog2; Louise Gildea1; Mona El-Bahrawy1; Abigail Speller1; Robert Brown1; Sadaf Gharem-Maghami2; Zoltan Takats3; 1Imperial College, London, UK; 2Waters Corporation, Budapest, Hungary; 3Imperial College London, South Kensington Campus London, UK

WP 536 REIMS has the Potential to Improve Diagnostic of Hepatocellular Carcinoma Liver – Perspectives towards Intraoperative Molecular Diagnostics, Tiffany Porta1; Julia Baldog2; Flora Olivier1; Pierre-Maxence Vaysse3; Ulf P. Neumann1; Steven W.M. Olde Damink2; Thorsten Cramer3; Ron M.A. Heeren1; 1M4 Institute - Maastricht University, Maastricht, The Netherlands; 2Waters Corporation, Wilmlow, UK; 3RWTH Aachen, Aachen, Germany; 4Maastricht University Medical Center +, Maastricht, The Netherlands

WP 537 Identifying “Sweet-spots” of Preeclamptic Urine Metabolomics with High Resolution and Accurate Mass Measurements, Hongwu Jing1; Yu Cao1; Arpad Somogyi1; Guomao Zhao2; Michelle Axe2; Catalin S Buhimschi3; Irina A Buhimschi3; Vicki H Wysocki4; 1The Ohio State University, Columbus, OH; 2Nationwide Children’s Hospital, Columbus, OH

WP 538 Integrative Pathway Analysis of Metabolic Signature in Bladder Cancer: A Linkage to Cancer Genome Atlas Project and Prediction of Survival, Nagireddy Putluri1; 1Bayor College of Medicine, Houston, TX; 2Agilent Technologies, Wilmington, DE

WP 539 Development of Highly Sensitive Quantification Method for Testosterone Human Serum by Liquid Chromatography–Tandem Mass Spectrometry, Vasanta Pulturi1; Srijayma Donepudi1; Feng Jin1; Andre Szczensiowski1; Vaidaraja B Bhat2; J Peter Cook3; Dolores J Lamb1; Arun Sreekumar1; Nagireddy Pulturi1; 1Bayor College of Medicine, Houston, TX; 2Agilent Technologies, Wilmington, DE

WP 540 Targeted Metabolomics of Liver Donor Allografts: A Clinical Application, Jeffrey A Culver1; Andrew V Zelenin1; Christopher Petucci1; Stephen J Gardell1; John B Seals1; Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; 2Southeast Center For Integrated Metabolomics, Gainesville, FL; 3Ochsner Medical Center, New Orleans, LA

WP 541 Metabolomics and Flux Analysis Informed on the Mechanism of Response of AML to IACS-10759, a Potent and Selective OXPHOS Inhibitor, Pietro Morlacchi1; UT MD Anderson Cancer Center (IACS/CCCT), Houston, TX

WP 542 Use of a Novel C18-Based Stationary Phase for Human Urine Metabolite Profiling By UHPLC-High Resolution Accurate Mass Spectrometry (HRAM), Alan P McKeown1; Catherine Oort2; Geoffrey Faden3; 1Advanced Chromatography Technologies Ltd, Aberdeen; 2The School of Pharmacy, University of Nottingham, Nottingham, UK; 3MACMOD Analytical Inc., Chadds Ford, PA

WP 543 Discriminatory Ability of Ambient Ionisation Mass Spectrometry in Analysing Skin Secretions: A Non-Discriminatory Ability of Ambient Ionisation Mass Spectrometry in Analysing Skin Secretions, Tsuyoshi Nakanishi1; Akanksha Singh2; Ahammed Shabeeb T.P.1; Manoj Pillai3; Kaushik Banerjee1; 1National Referral Project and Prediction of Survival in Bladder Cancer: A Linkage to Cancer Genome Atlas Project and Prediction of Survival, Nagireddy Putluri1; 1Bayor College of Medicine, Houston, TX; 2Agilent Technologies, Wilmington, DE

WP 544 Comprehensive Cerebrospinal Fluid Metabolomic Profiling for Mechanism Study of Idiopathic Intracranial Hypertension, Liang Zhao1; Xiali Zhong2; Abhay Moghekar3; Thomas Hartung4; 1Johns Hopkins University, Baltimore, MD

WP 545 Isotope-based Metabolomic Analysis of Human Samples, Kevin Y Cho1; Ying-Jr Amanda Chen1; Nathaniel G Mahieu1; Gary Patti1; 1Washington University School of Medicine, St. Louis, MO

WP 546 Integrative Metabolomic and Proteomic Analysis Reveals Biomarkers Related to Oxidative Stress in Traumatic Brain Injury, Veerana Venkata Ratnam Bandaru1; Sartaj Ahmad Mir1; Frederick Kerley1; Robert D Stevens1; Akihilesh Pandey1; 1Johns Hopkins University School of Medicine, Baltimore, MD

WP 547 Bioaccessible Phytochemicals from Black Raspberries after Interaction with Saliva – Determining Exposure in the Oral Cavity Using a Metabolomics Approach, Ken M Riedl1; Jennifer Ahr-Jarvis1; Matthew Teegarden1; Thomas Knobloch1; Christopher Weghorst2; Pumima Kumar1; Steven Clinton3; Yael Vodovoz2; Steven J Schwartz2; 1The Ohio State University, Columbus, OH
METABOLICOMICS: UNTARGETED METABOLITE PROFILING (ANIMAL/HUMAN/OTHER)

WP 550 - 574

WP 550 Drosophila as a Model System for Microbiome Research - a GCMS Based Metabolomics Approach: Bhavapriya Vaithesevaran1; John McMullen2; Anthony Macherone3; Angela E Douglas2; Justin R Cross1; 1Oregon State University, Corvallis, OR; 2Oregon Health & Science University, Portland, OR; 3Oregon State University, USA

WP 551 Lipidome and Metabolome Analyses of Mouse Hippocampus in Response to Low-dose X-ray Irradiation using Liquid Chromatography-Mass Spectrometry: Fereshteh Zandkarimi1; Jeffrey Morris1; Jacob Raber1; Claudia S Maier1; 1Oregon State University, Department of Chemistry Corvallis, OR; 2OHSU, Dep. Behavioral Neuroscience, Neurology, & Radiation Medicine, ONPRC, Portland, OR

WP 552 Comparative High Resolution Metabolomics of Metastatic vs. Non-Metastatic Tumors in a Murine Medulloblastoma Model: Danning Huang1; Martin R L Paine1; Jingbo Liu2; Sophie Bantos1; Shuzhao Li1; Tobey MacDonald1; Facundo M Fernández1; 1Georgia Institute of Technology, Atlanta, GA; 2Emory University School of Medicine, Atlanta, GA

WP 553 Caloric Restriction Improves Diabetes-Induced Nonalcoholic Fatty Liver Diseases by Changing Metabolism: Youngae Jung1; Geum-Sook Hwang1; 1Western Seoul Center, Korea Basic Science Institute, Seoul, Republic of Korea; 2Department of Life Science, Ewha Womans University, Seoul, Republic of Korea

WP 554 Comprehensive HPLC-MS Metabolomics Analysis of Brain Tissue Reveals Age, Region, and Gender-Specific Effects of Centenaria asatica: Parram Lark1; Nora Gray2; Luisa Zini1; Phillip Seitzer1; Christopher Harris2; Joseph Quinn2; 1Oregon State University, Corvallis, OR; 2Oregon Health and Sciences University, Portland, OR; 3Proteome Software, Portland, OR; 4PADRECC, Portland, OR; 5Portland Veterans Affairs Medical Center, Portland, OR

WP 555 Global Lipid Profiling in Aging Mouse Model associated with Osteoporosis: Eun-Hwa Kim1; Geum-Sook Hwang1; 1KBSI Western Seoul Center, Seoul, Republic of Korea

WP 556 Metabolomics Approach for Mice Serum Associated with Epidermal Growth Factor Receptor and BaP-induced Mouse Lung Tumor Genesis using Liquid Chroma: Hui Ling Lee1; Fu Jen Catholic University, New Taipei, TAIWAN

WP 557 Global Metabolomic Profile Differentially Segregates with Calcium Supplementation in Mice Fed a High-Fat Western Style Diet: Muhammad Aslam1; Li Zhang1; Christine Bassis1; Maureen Kachman2; Charles Burant2; Ingrid Bergin1; James Varani1; 1Department of Pathology, Internal Medicine, Medical of School, University of Michigan, Ann Arbor, MI; 2Michigan Regional Comprehensive Metabolomics Resource Center; University of Michigan, Ann Arbor, MI; 3Unit for Laboratory Animal Medicine, University of Michigan, Ann Arbor, MI

WP 558 LC-MS/MS Based Metabolomic Analysis of the Effect of Biogenic Amines in A LPS-induced Sepsis Mouse Model: Yu-Min Liu1; Soo-Ray Wang2; Maw-Rong Lee1; 1National Chung-Hsing University, Taichung, Taiwan (R.O.C.); 2Chung Shan Medical University, Taichung, Taiwan (R.O.C.)

WP 559 Diabetes Markers: Using Orbitrap HRAM and a New Workflow for Differential Analysis of Zucker Rat Plasma Metabolome: Junhwa Wang1; Maciej P Bromirski2; Ralf Tautenhahn2; David Peake2; Kyomin Reiko2; Tina Settineri2; Ken Miller2; 1Thermo Fisher Scientific Inc, San Jose, CA; 2Thermo Fisher Scientific, Bremen, DE; 3Thermo Fisher Scientific, San Jose, CA; 4Thermo Fisher, San Jose, CA

WP 560 Effects of Dietary Different Coppers and High Fructose Feeding on Rat Fecal Metabolome: Blyun Shi1; 2; Ming Song2; Xiaoai Wei1; 2; Ximmin Yin1; 2; Dale Schuschte1; Imhoi Koo1; 2; Craig McClain3; 3; Xiang Zhang1; 3; 1Department of Chemistry, University of Louisville, Louisville, KY; 2Center for Regulatory and Environmental Analytical Metabolomics, University of Louisville, Louisville, KY; 3Department of Medicine, University of Louisville, Louisville, KY; 4Department of Physiology and Biophysics, University of Louisville, Louisville, KY; 5Department of Pharmacology and Toxicology, University of Louisville, Louisville, KY

WP 561 Optimization of Tissue Extraction for GCMS Metabolomic Analysis Reveals Altered Metabolism of Barbiturates in a Polycystic Kidney Disease Model: Hayley Abbiss1; 2, 3; Garth L Maker2; 4; Gabrielle C Musk5; 6; Catherine Rawlinson3; 4; Joel P.A. Gummer3; 4; Patricia A. Fleming3; Jacqueline K. Phillips3; Mary C. Boyce4; John Moncur5; Robert D. Trengove4; 6; Murdoch University, Perth, Western Australia; 7Curtin University, Perth, Australia; 8Macquarie University, Sydney, Australia; 9Edith Cowan University, Perth, Australia

WP 562 Spatial-temporal Analysis of Metabolite Expression in Xenopus laevisembryos during Early Development: Jennifer Arceo1; Nicole M Schiavone1; Danielle A Boley1; Norman J Devon1; 1University of Notre Dame, Notre Dame, IN; 2University of Notre Dame, Notre Dame, IN

WP 563 Capillary Zone Electrophoresis-Electrospray Ionization-Mass Spectrometry for Xenopus laevismetabolomic Analysis: Nicole Schiavone1; Jennifer Arceo1; Danielle A Boley1; Norman J Devon1; 1University of Notre Dame, Notre Dame, IN

WP 564 Evaluating the Metabolic Impact of Feeding Baboons a High Fat, High Caloric Diet using an Accurate Mass GC/QTOF: Mark Libardi1; Matthew Curtis2; Stephan Baumann3; 1Southwest Research Institute, San Antonio, TX; 2Agilent Technologies, Santa Clara, CA

WP 565 Profiling and Quantitative Analysis of Small Molecule Metabolites and Neurotransmitters in Crustacean Hemolymph/Neuronal Tissues Using Reversed-Phase and Mix-Mode LC-MS/MS: Qinjiewen Cai1; Chuanzi OuYang1; Xuefei Zhong1; Lingjun Li2; 1University of
An Untargeted Metabolomics Approach for Determining Biomarkers Involved in Spontaneous Pre-Term Birth (sp-PTB) Delivery, using a Label-Free LC-DIA-MS Approach; Shirish Yakindii; Lee Gethingsii; James Langridgeii; Louise Kennyii; iii; Cork University Maternity Hospital, Cork; ivWaters, Wilmslow, UK; vCork University Maternity Hospital, Cork, Ireland; viUniversity College Cork, Cork, Ireland

Global Metabolomics and Lipidomics of Non-Alcoholic Fatty Liver Disease and Non-Alcoholic Steatohepatitis in Human Plasma by LC-HRMS; Allison J Levyi; Rainey E Pattersoni; Jeremy P Koelmeli; Srilakshmi Kalavalapalli; Nishanth Sunnyii; Fernando Brilli; Kenneth Cusi; Timothy J Garrett; Richard A Yost; iii; Chemistry Department, University of Florida, Gainesville, FL; ivDepartment of Medicine, University of Florida, Gainesville, FL; vDepartment of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL; viUniversity of Alabama, Birmingham, AL; viiUniversity of California, Davis, CA

Evaluation of Ion Mobility/TOF Mass Spectrometry with Multiple LC Method Parameters for Enhanced Detectionin Metabolomic Profiling; Paul Rainvillei; David Heywoodii; Langridge Jamesii; Robert Plumb; Jose Castro-Perezii; vWaters, Milford, MA; viWaters, Manchester, UK

Profiling the Gut Microbiota Metabolome using HPLC coupled to Ion Mobility-Mass Spectrometry to Study Obesity; James Polandi; Alexandra C Schirme-Rutledgei; Charles Robb Flynnii; John A McLean; iVanderbilt Dept. of Chemistry, Nashville, TN; viVanderbilt University, Nashville TN USA Nashville, TN

Identification of Eicosanoids Mediating Thromboresistance using an Untargeted Metabolomics and Informatics Approach; Patrizia B Stadleri; Shunyao Mi; Philip Selitzer; Christopher M Colangeli; Jeffrey J Radei; Scott A Shafferi; University of Massachusetts Medical School, Worcester, MA; iiProteome Software, Portland, OR; iiiPrimary Ion, Old Lyme, CT

Untargeted Profiling using GC-QTOF MS and Parallel El and Cl analysis to identify Biomarker Panels to Stratify Patients to Treatment; Robert Trenqovi; 1, 2, 3; Tom Dignani; 4; Ben Hunterii; 4; Garth Makeri; 4; Hayley Abbissi; 4, 5; Joel Guimeri; 4, 5; Murdoch University, Murdoch, WA; iiSchool of Veterinary and Life Sciences, Murdoch University, Murdoch, Australia; iiiMetabolomics Australia, WA Node, Murdoch, Australia; ivSchool of Veterinary and Life Sciences, Murdoch University, Murdoch, Australia; vUniversity of Florida, Gainesville, FL

Metabolomic Analysis of Melanoma Skin Tissues by Liquid Chromatography – Mass Spectrometry; Matthew Kazalehi; Candice Ulmer; Louis Searcyy; Michael Costanzo; Nikolaus Gravenstein; Richard A Yost; University of Florida, Gainesville, FL

Segmented Flow Sampling with Push-Pull Theta Pipettes for Electrospray Ionization Mass Spectrometry; Anumita Saha-Shahi; Curtis M Greeni; David H Abrahamii; Lane A Baker; iiiIndiana University Dept. Chemistry, Bloomington, IN

Development of a Microfluidic Platform for High Throughput Validation of Candidate Disease Biomarkers; iHisuan Chen; iiNing Bao; iiiWeiguo Andy Tao; ivPurdue University, West Lafayette, IN; viUniversity of Texas, Arlington, TX; viiChina Medical University, Shenyang, China

Ionic Liquid Matrices for MALDI Analysis and CE Separation; Leila Josefsso; 1; Johan Jacksen; ii; Åsa Emmeri; KTH Royal Institute of Technology, Stockholm, Sweden

Sensitivity Gains using Microflow LC/MS for Oligonucleotide Analysis; Michael Doneani; 1; James P Murphy; iiWaters, Milford, MA

Study of Ionization Efficiency on Silicon-Based, Micro-Fabricated Electrospray Nozzles for Micro Flow LC-ESI-MS Applications; Christine Wang; Simon J Prosseri; 1; Joel Gummer; iiJoan Crowther; iii; Louis Kenny; ivUniversity College Cork, Cork, Ireland

Decreasing Cycle Time While Maintaining Analytical Sensitivity in Microflow LC/MS utilizing a Novel Valve Switching Algorithm; Jay S. Johnsoni; James P Murphyi; Water Corporation, Milford, MA; iiWaters Corporation, Milford, MA

Increasing Operable Flow Range of a Nano-spray Source for High-Performance Microspray on a Curtain Gas Equipped Triple – Quadrupole API-MS; Amanda Berg; iiHelena Svobodovi; iiiGary A Valaskoviciv; New Objective, Inc., Woburn, MA; ivNew Objective, Woburn, MA

Picodroplet Mass Spectrometry for Miniaturized High Throughput Analysis of Synthetic Biology Clones; Xin Li; Murray J Brown; Clive A Smith; vWaters, Milton, MA

High-throughput Enzymatic Characterization by Integration of Nanostructure-Initiator Mass Spectrometry and Droplet to Digital (D2D) Microfluidics; Joshua Vance Heinemanni; Kai Deng; ii; Steve C.C. Shih; iiiJian Gao; ivMarkus de Raad; vBenjamin P Boweni; viPaul D Adams; viiAnup K. Singhi; viiiTrent Northen; ixLawrence Berkeley Nat’l Lab, Berkeley, CA; xSandia National Laboratories, Albuquerque, NM; xiJoint BioEnergy Institute, Berkeley, CA

A Novel Targeted Metabolic Profiling Workflow for Simultaneous Reverse Phase and HILIC microflow LC/MS/MS Analysis; Daniel M Warren; iJeffery D Miller; 1; SCIX, Redwood City, CA

An Affordable and Simple-To-Use Snap-Chip-iMALDI Technology for Measuring Plasma Rennin Activity; Hueyan Li; 1, 2; Anva Tavakoli; 1; Robert Popp; 1; Christoph H Borchers; 1, 2; David Juncker; 1, 2; University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 1Biomedical Engineering Department, McGill University, Montreal, QC, Canada; 2McGill University and Genome Quebec Innovation Centre, Montreal, QC, Canada; 3University of Victoria - Genome BC Proteomics Centre, Victoria, BC; 4Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada
PLANT ‘OMICs’ 587 - 613

WP 587 Quantitative Analysis of Crosslinked Protein Complexes: A Novel Interactive Approach to Assess Pathogen-Triggered Unconventional Secretion in Arabidopsis; Tricia Ho1; Kevin Blackburn1; John D Williamson1; Michael B Goshe1; 1North Carolina State University, Raleigh, NC

WP 588 Identification of Direct Substrates of MAP Kinases Activated by Environmental Stresses in Arabidopsis Thaliana through Protein Kinase Assay Linked-Phosphoproteomics; Chuan-Chih Hsu1; Pengcheng Wang2; Chunhao Zhao2; Jiankang Zhu2; Weiguo Andy Tao2; 1Purdue University, West Lafayette, IN; 2Purdue University, West Lafayette, IN

WP 589 Chloroplast Protein Maturation, Regulation and Degradation; Elden E. Rowland1; Jitae Kim1; Klaas J. van Wijk1; 1Cornell University, Ithaca, NY

WP 590 Emerging Role of Sirtuins and Lysine Acylation in the Regulation of Plant Metabolism; Dana M Freund1; Jerry D Cohen1; Adrian D. Hegeman1; 1University of Minnesota at Twin Cities, Saint Paul, MN

WP 591 Label-free Quantitative Mass Spectrometry-Based Proteomic Approach for Comprehensive Analysis of Protein Complexes and Protein-Protein Interactions in Plants; Uma Arv1; Zachary McBride2; Donglai Chen2; Jun Xie1; Daniel Szynski1; 1Purdue Proteomics Facility, West Lafayette, IN; 2Purdue University, West Lafayette, IN

WP 592 Plant Proteomes Aplenty: Quantitative and Phylogenetic Analysis of Five Angiosperms, a Gymnosperm and a Bryophyte; Harold Mary1; Alicia L. Richards1; Dhileepkumar Jayaraman2; Jean-Michel Ané3; Joshua J Coon4; 1University of Wisconsin-Madison, Madison, WI

WP 593 Investigating the Expressed Kinome in C. reinhardtii; Emily Werth1; T.S. Karim Gilbert1; Lee M Graves2; Leslie M Hicks1; 1UNC Chapel Hill, Department of Chemistry Chapel Hill, NC; 2UNC Chapel Hill, School of Medicine Chapel Hill, NC

WP 594 Quantitative Proteomics of Phaeodactylum tricornutum Phosphate Limited Environment; Shiang-Yu Tsai1; Pang-Hung Hsu2; 1Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan

WP 595 UHPLC-HRMS Analysis of Herbal Plant Extracts to Screen for Small Molecule Drugs with Antibacterial Activity; Gaganpreet Monga1; Anima Ghosal1; Dl Ramanathan1; 1Keen University, Union, NJ

WP 596 Comparative Protein Analysis of Oil Palm Mesocarp from Elaeis Guineensis and Elaeis oleifera to Investigate Acidification Process.; Jessica K. A. Macêdo1; Jorge C. Rodrigues-Neto1; 1Department of Biochemistry and Molecular Biology, University of Minas Gerais, Belo Horizonte, Brazil

WP 597 MALDI-Mass Spectrometric Imaging of Endogenous Peptides and Proteins in Medicago truncatula: Caitlin Keller1; Erin Gempertline1; Junko Maeda1; Dhileepkumar Jayaraman1; Michael R Sussman1; Jean-Michel Ané2; Lingjun Li1; 1University of Wisconsin-Madison, Madison, WI

WP 598 iTRAQ 8-plex Labeling-Based Proteomics Analysis Reveals Difference of Protein Expression from Sorghum Root which was Treated by Aluminum; Yong Yang1; 1USDA-ARS at Cornell University, Ithaca, NY

WP 599 Extracellular Proteomic Response of Thermally Stressed Symbiondium: Implications for Symbiosis Breakdown during Bleaching; Contessa Ricardo1; Bren Ledbetter1; Yam Nguyen1; Saffiul M Chowdhury1; Laura Mydlarz1; 1University of Texas at Arlington, Arlington, TX

WP 600 Deep Proteome Analysis of Gerontoplasts from the Inner Integument of Developing Seeds of Jatropha curcas; Mohibullah Shahn1; Emanuela L. Soares1; Magda alberto fernandez lima1; Camila B. Pinheiro1; Arlete A. Soares1; Gilberto B Domont1; Fabio CS Noqueira1; 1Federal University of Ceará, Fortaleza, Brazil; 2Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

WP 601 Quantitative Proteomics of Phaeodactylum tricornutum Acidified Environment; Tai-Yi Jiang1; Pang-Hung Hsu1; 1Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung, Taiwan

WP 602 Standard-flow UHPLC Coupled with TripleQuad MS is a Versatile Platform for Both Targeted Metabolomics and Proteomics; Daniel Vi1; Meike Burow2; Barbara Ann Halkier2; 1University of Copenhagen, Frederiksberg C, Denmark; 2University of Copenhagen, Copenhagen, Denmark

WP 603 Stable Isotopic Labeling of intact Plants for Molecular Turnover Measurement by HRMS: New Labeling Apparatus and Data Processing Approaches; Calvin P Peters1; Dana M Freund1; Aaron K Rendahl1; Jerry D Cohen1; Adrian D. Hegeman1; 1University of Minnesota at Twin Cities, Saint Paul, MN

WP 604 Multi-OMICs Investigation of the Lignin Deposition Altering Enzyme Family of Arogenate Dehydratases in Arabidopsis and Poplar Tree; Kim K. Hixson1; Washington State University, Richland, WA

WP 605 Qualification and Quantification of Cannabinoids and Terpenes in Extracts of Cannabis sativaby Gas Chromatography – Mass Spectrometry; Aliegra Leghissa1; Zacariah L. Hildenbrand1; Sean Jun1; Aaron L Hicks2; Kevin A Schug3; 1The University of Texas at Arlington, Arlington, TX; 2Inform Environmental, LLC, Dallas, TX; 3C4 Laboratories, LLC, Mesa, AZ

WP 606 Systemic Defense Induction and Post-Ingestive Rearrangement of Plant Toxins in Insects– a Metabolomics Approach Driven by Automated Compound Identification; Sven Heiling1; Aiko Barsch2; Heiko Neuweger1; Emmanuuel Gaquerel1; 1Purdue University, West Lafayatte, IN; 2Purdue Proteomics Facility, West Lafayette, IN

WP 607 Metabolic Profiling of Stilbenes by LC-MS for Genetic Analysis in an F2 Interspecific Grapevine Hybrid Family; Soon Li Teh1; Bety Rostandy1; Mani Awale1; Shanshan Yang2; Jonathan Fresnedo-Ramirez3; Qi Sun4; Matthew D. Clark1; Anne Y. Fennell2; James J. Luby1; Adrian D. Hegeman1; 1University of Minnesota at Twin Cities, Saint Paul, MN; 2South Dakota State University, Brookings, SD; 3Cornell University, Ithaca, NY

WP 608 Comparative Analysis of Tropical Flower Secondary Metabolites; Elena Stashenko1; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

WP 609 Accounting for Complexity: A Procedure for the Targeted Analysis Of Primary- and Secondary-Metabolites, and Phytohormones from a Single Plant Extract; Martin Schäfer1; Christoph Brütting1; Mario Kallenbach1; Gordon van ’t Slot2; Paul Speir3; Ian T Baldwin1; 1Max Planck Institute for Chemical Ecology, Jena, DE

WP 610 Depth Profiling of Whole Soybean Nodules using Laser Ablation Electrospray Ionization Mass Spectrometry; Christopher Anderton1; Sylwia A Stopka1; Beverly J Agtuca1; 1University of Minnesota at Twin Cities, Saint Paul, MN; 2Purdue University, West Lafayette, IN; 3University of Missouri, Columbia, MO

64TH ASMS CONFERENCE ON MASS SPECTROMETRY PAGE 155
WP 611
Identification of Metabolites Involved in the Color Reversion Process in Blackberry Fruit using LC-ESI-QTOF; Victor Manuel Mondragon Olguin; Georgina Alejandro Pérez Pérez; Edmundo M. Mercado Silva; Gelasio Perez; 1Agilent Technologies Mexico, Mexico, DF; 2Universidad Autonoma de Queretaro, Queretaro, QRO

WP 612
REIMS (Rapid Evaporative Ionization Mass Spectrometry) and Multi-Variant Statistics, Two Tools in Support of Weed Grass Speciation and Phenotype Characterization; Sasa Stead; 1Jackson Pong; 2Robert Edwards; 3Melissa Brazier-Hicks; Catherine Tetard-Jones; 4Zoltan Takats; 5Waters corp., Manchester, Lanc; 6Waters, Wilmslow, UK; 7University of Newcastle, Newcastle upon Tyne, UK; 8Imperial College, London, UK

WP 613
DESI-MS Imaging with Ion Mobility and Multivariate Analysis for the Determination of Weed Grass Species and Surface Level Characteristics; Philippa Jayne Hart; Sara Stead; 1EmmanuelClaude; 2HernandoOlivos; 3Melissa Brazier-Hicks; Catherine Tetard-Jones; 4Robert Edwards; 5Waters Corporation, Wilmslow, UK; 6Waters Corporation, Beverly, Massachusetts; 7Newcastle University, Newcastle upon Tyne, UK

WP 614
Method Development of an Automated Hybrid LBA-LC/MS Assay for the Quantitative Bioanalysis of the Biotherapeutic Teraparatide in Human Plasma; Jean-Nicholas Mess; 1Daniel Villeneuve; 2Georges Koudssi; 3Anahita Keyhani; 1Algorithmic Pharma Inc., Laval, Canada

WP 615
Improving the Sensitivity for an Immunocapture LC-MS Assay of Influenza in Rat Plasma Using Trap-and-Elute MicroLC-MS; Remco van Soest; 1Lei Xiong; 2SCIEX, Redwood City, CA

WP 616
Development and Validation of an LC-MS/MS Method for the Quantification of Linker-extended Cynovarin-N in Rat Plasma; Hui Hong; 1Wenzhong Liang; 2Xin Zhang; 3Xiping Fang; 4WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China

WP 617
Quantitation of Insulin Giargine and Major Metabolites in Human Plasma Using Hybrid LBA-LC/MS with Automated Magnetic Particle Processing; Kevork Mekhsissian; 1Jean-Nicholas Mess; 2Anahita Keyhani; 1Algorithmic Pharma Inc., Laval, Canada

WP 618
Quantitation of a Modified Insulin in Rat Plasma Using Triple Quad 6500 LC-MS/MS; Rong Huang; 1Gunchun Zhou; 2Joshua Froning; 3Yong-Xi Li; 4Medpace Bioanalytical Laboratories, Cincinnati, OH

WP 619
Automated Biotherapeutic Quantitation from Tissue: Kristin Geddes; 1Lisa A Vasicek; 2Daniel S Spellman; 3Kevin P Bateman; 4Merck and Co, Inc, West Point, PA; 5Merck & Co., Inc., West Point, PA

WP 620
Quantitative Bioanalysis of Rituximab and Reditux for Biosimilarity Assessment Comparing Triple Quadrupole and Hybrid Time-of-Flight Platforms; Richard Lavalée; 1Daniel Villeneuve; 2Kevork Mekhsissian; 3Jean-Nicholas Mess; 4Anahita Keyhani; 1Algorithmic Pharma Inc., Laval, Canada

WP 621
Using a Tandem Protein Precipitation/Immunooaffinity Purification Extraction to Resolve Specificity and Sensitivity Roadblocks: Bioanalysis of a PEGylated Human Protein Analog; Jonathan R Sti-Germain; 1Luca Genovesi; 2Jean-Nicholas Mess; 3Anthony T Murphy; 4Selina Estwick; 5Patricia L Brown-Augsburger; 6Anahita Keyhani; 1Algorithmic Pharma Inc., Laval, Canada; 2ElI Lilly and Company, Indianapolis, IN

WP 622
Comparison of Bottom-Up and Top-Down Analytical Methodologies for the Quantitative Bioanalysis of Large Therapeutic Peptides in Biological Matrix; Georges Koudssi; 1Jean-Nicholas Mess; 2Anahita Keyhani; 1Algorithmic Pharma Inc., Laval, Canada

WP 623
Generic Quantitative LC-MS/MS Assay for Analysis of hlgG1 Based Therapeutic Proteins in Cynomolgus Monkey Serum Using Immunocapture with MSIA™. D.A.R.T.’S™; Christian Lanshoefit; 1Oliver Heudi; 2Sarah Cianfariani; 3Eric Niederkofler; 4Ravindra Chaudhari; 5Andrew Paul Warren; 6Franck Picard; 7Olivier Kretz; 8Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; 9Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; 10Thermo Fisher Scientific, Tempe, AZ

WP 624
Applying Rapid Trypsin Digestion for Targeted Protein Quantification in Rat Plasma by Liquid Chromatography/ Tandem Mass Spectrometry: Moucun Yuan; 1Morse Faria; 1Jinlin Shen; 2Song Zhao; 3Eric Ma; 4Elizabeth Dompkowsk; 5Michael Waldron; 6Bruce Hidy; 7William R. Mylott Jr.; 8Rand Jenkins; 9PPD, Richmond, VA

WP 625
Absolute Quantitation of Glycan and Site-Specific Glycoforms on Commercial mAbs using Multiple Reaction Monitoring; 1Nari Seo; 2Ungyum Kim; 3Hyun Joo An; 4GRAST&AGRS, Chungnam National University, Daejeon, Republic of Korea; 5Asia-Pacific Glycomics Reference Site (AGRS), Daejeon, Republic of Korea

WP 626
Improved Reagents and Software for Comparing Biosimilar and Originator Therapeutic Proteins: Accurate Analysis of Deamidation and Disulfide Bond Scrambling; Wilfred H Tang; 1Marshall Bern; 2John St Skilton; 3Eric Carlson; 4Michael J Ford; 5Karthik Pispatui; 6Anna Schwendeman; 7Chris Hosfield; 8Sergei Saveliev; 9Michael M Rosenblatt; 10Marjeta Uhr; 11Chris Becker; 12Protein Metrics Inc., San Carlos, CA; 13MS Bioworks, LLC

WP 627
The Use of Generic Surrogate Peptides for the Quantitative Analysis of hlgG1 in Pre-Clinical Studies with High-Resolution Mass Spectrometry: Christian Lanshoefit; 1Thierry Wolf; 2Oliver Heudi; 3Sarah Cianfariani; 4Samuel Barteau; 5Markus Walles; 6Kelly B Doering; 7Guillaume Bechade; 8Franck Picard; 9Olivier Kretz; 10Novartis Institutes for Biomedical Research, Drug Metabolism and Pharmacokinetics, Basel, Switzerland; 11Université de Strasbourg, Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien, Strasbourg, France; 12Waters, Milford, MA; 13Waters AG, Baden-Daettwil, Switzerland

WP 628
Host Cell Protein Analysis by microflow-LC High Resolution SWATH-MS of Vaccine Samples under Development; 1Seren Heissel; 2Milla Neffling; 3Rikke Raen Lund; 4Thomas Kofod; 5Marie Grimsstrup; 6Nick Morrice; 7Anne Fich Holmbjerg; 8Max Per Kristiansen; 9Ingrid Kromann; 10Peter Højrup; 11Eivind Mærtz; 12Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; 13SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; 14Aphalyse A/S, Odense M, DK; 15Statens Serum Institut, Copenhagen, Denmark

WP 629
Highly Sensitivitiy and Reproducible MRM Based Quantitation of Follicle Stimulating Hormones (FSH) in Human Plasma using QUATRPTM 6500; Faraz Rashid; 1Rahul Baghla; 2Prashant Kale; 3Manoj Shukla; 4Milan Shah; 5Dipankar Malakar; 6Anoop Kumar; 7Manoj Pillai; 8SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India; 9SCIex Gurgaon, Gurgaon, India; 10Lambda Therapeutic Research Ltd, Ahmedabad, India
WP 630 Streamlining the Complete Sequence Variant Analysis Workflow for Biotherapeutics: Andrew Dadyw1; Michelle English2; Melissa Ly3; Andrew Saalif; Lisa A Marszilii; Olga Friese2; Jason C Rouse2; Yong J Kil3; Marshall Bern3; Eric Carlson2; Chris Becker3; Pfizer, Inc. Chesterfield, MO; Pfizer, Inc. Andover, MA; Protein Metrics Inc., San Carlos, CA

WP 631 Comparison of First Dimension Fractionation Strategies for Directed MS Analysis of Host Cell Proteins: Jody Hsiang1; Te-Wei Chu2; Gregory O Staples1; Oscar Potter1; Hongfeng Yin1; Kevin Killeen1; Agilent Technologies, Santa Clara, CA

WP 632 Determination of Total Recombinant Human α-Galatosidase A in Plasma Samples by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS); Richard Hamler1; Kees Bronsma2; Peter Pruium2; Peter Buils2; Deborah Hilliard3; Russell Gotschall1; Franklin K Johnson2; Hung Do1; Kenneth Valenzano1; Nico van de Merbel1; Elfrida R Benjamin1; Amicus Therapeutics, Cranbury, NJ; PRA Health Sciences, Assen, The Netherlands

WP 633 Herceptin Quantitation Using Universal and Signature Peptides by Hybrid LBA/LCMS Method: Xi Qiu1; Daniell Rowes1; Susan Zondio1; John Kolman1; Zamas Lam1; QPS, Newark, DE

WP 634 Quantitative Analysis of Adalimumab using nano-Surface and Molecular-Orientation Limited (nSMOL) proteolysis and LC/MS/MS; Deepthi Bhandarkar1; Ravi Krovdi1; Rash I Kochhar1; Shailendra Rane1; Shailesh Damale1; Purushotham Sutar1; Anain Lohan1; Ashutosh Shelar1; Jitendra Kelkar1; Ajit Datar1; Pratap Rasam1; Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; Lambda Therapeutic Research, Ahmedabad, India

WP 635 SSPQa: A Subtractive Method for the Parallel Quantification of the Degree of Modification at Every Possible Site of a Protein: Guillaume Gabant1; Alain Boyer1; Martina Cadene1; CBM CNRS UPR4301, Orleans, France

WP 636 Quantification of the Antibody Drug Conjugate, Trastuzumab Emtansine and the Monoclonal Antibody, Trastuzumab in Plasma Using a Generic Kit-Based Approach: Hua Yang1; Mary E Lame1; Erin E Chambers1; Sherri Naughton1; Waters Technologies Corporation, Milford, MA

WP 637 Applying a Standardized, Kit-based Approach to Achieve 10 ng/mL Inflximab from 35 µL Plasma: Mary E Lame1; Hua Yang1; Erin E Chambers1; Sherri Naughton1; Waters, Milford, MA

WP 638 Quantification of Host Cell Proteins in Biotherapeutics using Stable Isotope Labeled Chinese Hamster Ovary Proteins (SIL-CHOP) as an Internal Standard: Parag R Jall1; Zhiyun Cao1; Kevin Ray1; Rong-Rong Zhu2; 1Agilent Technologies, Santa Clara, CA; 2Protein Metrics Inc., San Carlos, CA

WP 639 Host Cell Protein Analysis of Biotherapeutics using Automatic Offline Fractionation and LC/MS: Alex Zhu1; Jing Chen2; Steve Murphy2; Jordy Hsiao2; Agilent Technologies, Wilmington, DE; Agilent Technologies, Inc. Madison, WI; Agilent Technologies, Santa Clara, CA

WP 640 Exploiting His-tags in Recombinant Protein Therapeutics to Introduce Metal Tracers for Tracking Biodistribution of Biotherapeutics in vivo: Chenqfeng Ren1; Grégoire Bonvin1; Cedric Bobst1; Igor A Kaltashov2; University of Massachusetts Amherst, Amherst, Massachusetts

WP 641 Analysis of N-Glycans Released from Monoclonal Antibodies using an ESI-MS-friendly Fluorescent Tag: Oscar Potter1; Gregory O Staples1; Hongfeng Yin1; Kevin Killeen1; Agilent Technologies, Santa Clara, CA

WP 642 Evaluation of Transferrin Metal Tracers using Native ESI-MS and in-vitro Model for Tracking Its Biodistribution with ICP-MS: Grégoire Bonvin1; Cedric Bobst2; Igor A Kaltashov1; University of Massachusetts Amherst, Amherst, Massachusetts; University of Massachusetts-Amherst, Amherst, Massachusetts

WP 643 Comprehensive HCP Profiling by Targeted and Untargeted Analysis of DIA Mass Spectrometry Data with PRM qualification: Simion Kreimer1; Yuanwei Gao1; Mi Jin2; Nesredin Mussa2; Alexander R. Ivanov1; Barry L. Karger1; Barnett Institute and Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; Bristol-Myers Squibb, Devens, MA

WP 644 A Promising Alternative to SRM-very-high-resolution selected-ion- Monitoring (vHR-SIM@500k) Enables Ultra-sensitive and Selective Biotherapeutics Quantification: Yang Qu1; Bo An1; Ming Zhang; Xiaoming Shen; Shichen Shen; Jun Li; Jun Qu; SUNy at Buffalo, Buffalo, NY

WP 645 Significant Throughput Increase in Peptide Mapping/ Wagner 1; Alexander C. Segura2; Rasha Jalili1; Zhiyun Cao1; Kevin Ray1; Rong-Rong Zhu2; 1Lambda Therapeutic Research, Ahmedabad, India; 2Protein Metrics Inc., San Carlos, CA

WP 646 Sulfur-based Characterization of Protein Standards using Isotope Dilution Inductively Coupled Plasma Mass Spectrometry: Hyun-Seok Lee1; Sook Heun Kim2; Ji-Seon Jeong1,2; Yong-Moon Lee1; Yong-Hyeon Yim1,2; KRiSS, Daejeon, Republic of Korea; College of Pharmacy, Chungbuk National University, Cheongju, Korea; Department of Analytical Sciences for Biology, University of Science and Technology (UST), Daejeon, Korea

WP 647 Bioanalysis of Radiolabeled Payload by Isotopic Pattern Deconvolution and LC-MS/MS to Investigate Tissue Distribution of Protein Drug Conjugates: Wei-Chi Chen1; Wenyung Li1; Jinping Gan1; Bristol-Myers Squibb Co., Princeton, NJ

WP 648 Site-Specific Glycosylation Quantitation of Bioengineered Recombinant Therapeutic Glycoproteins: Muchena J. Kailemia1; Wanghui Wei1; Kalimuthu Karuppanan2; Jasmine M. Corbin1; Yanhong Li1; Li My Phu1; Abhaiya Dandekar1; Xi Chen1; Somen Nandi1; Karen McDonal1; Carlito Lebrilla1; University of California, Davis, Davis, CA

WP 649 Large-scale and Ultra-Sensitive Investigation of Biotherapeutics by A Novel Antibody-Free, Dual-Mechanism Enrichment Strategy: Ming Zhang1; Bo An1; Yang Qu1; Shichen Shen1; Jun Qu1; SUNy at Buffalo, Buffalo, NY

WP 650 Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic: Wei Fu1; Bo An1; Ming Zhang1; Yang Qu1; Jun Qu1; SUNy at Buffalo, Buffalo, NY

PROTEOMICS: NEW APPROACHES (GLOBAL) 651 - 674

WP 651 ProteomeTools: Large Libraries of Synthetic Peptides, Spectra and Software for Facilitating Human Proteome Research: Daniel Paul Zolg1; Mathias Wilhelm1; Peng Yu1; Karsten Schnatbaum2; Johannes Zerweck1; Tobias Knautse1; Ulf Reimer1; Holger Wenschuh2; Bernhard Delanghe1; Thomas Moehring1; Andreas Huhmer2; Gina Tan1; Mohammed Abujaour1; Siegfried Gessulat1; Stephan Aiche1; Hans-Christian Ehrlich1; Bernhard Kuster1,2; Chair

WP 652 JPT Peptide Technologies GmbH, Berlin, Germany; Thermo Fisher Scientific, Bremen, DE; Thermo Fisher Scientific, San Jose, CA; SAP SE, Innovation Center Potsdam Potsdam, Germany; Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany
WP 652 Comprehensive Draft of the HeLa Proteome to a Depth of More than 13,000 Proteins; Christian Dahl Keistrup1; Dorte B Bekker-Jensen1; Tanveer S Batth1; Sara C Larsen1; Michael L Nielsen1; Jesper V Olsen1; CPR, University of Copenhagen, Copenhagen, Denmark

WP 653 Subtilisin for Large Scale (phospho)proteinomics – the Beginning of a Wonderful Love Story?; Humberto Goncazarovas-Jorxe1, 2; Stefan Loroch1; Margherita Dell’Aia1; René Zahedi1; ISAS, Dortmund, Germany; 1CAPES Foundation, Ministry of Education of Brazil, Brasilia-Brazil; 2ISAS, Dortmund

WP 654 A New Approach to the Analysis of Intact Major Urinary Proteins (MUPs) from Mouse Urine by CESI-MS; Stephen J. Lock1; Robert J. Beynon2; Guadalupe Gomez-Baena2; Edna Betgovarzev2; 1SCIXE, Warrington, Cheshire; 2Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, UK; 3SCIXE, Concord ON, Canada

WP 655 Proteogenomics of HEK293 Cell Line: Identification of Variant Peptides using Deep Proteome Data from the Inter-Laboratory Studies; Anna Lobas1, 2; Dmitriy Karpov1; Arthur Kopylov2; Elizaveta Solovyeva1; 1Mark Ivanov1, 2; Irina Ilina1; Vassily Lazarev2; Ksenia Kuznetsova3; Timpe2; Bruce Macher2; University, Atlanta, GA; 2Emory University School of Medicine, Atlanta, GA; 3Institute for Energy Problems of the Inter-Laboratory Studies of Variant Peptides using Deep Proteome Data from the Inter-Laboratory Studies of Key Secretome Proteins from Human Lung Spheroid Cells; Dipul Paudel1, Phuong-Luyen Dinh2; Jhon Cores3; 1NCSU, Raleigh, NC; 2North Carolina State University, Raleigh, NC; 3North Carolina State University, Raleigh, NC

WP 656 Novel Approaches in de novo Peptide Sequencing and Proteogenomics as Tools to Explore Uncharted Organisms; Bernhard Blank-Landeshammer1; Karsten Biß1; Laxmikanth Kolippara1; Vera Rieder2; Marleen Stuhrt3; Tilman Schell4; René P Zahedi1; Markus Pfenninger4; Jörg Rahnenführer1; Hildegard Westphal3; Albert Sickmann1; 1Institute for Energy Problems of the Inter-Laboratory Studies; 2Centre for Proteome Research, Institute of Integrative Biology, University of Liverpool, UK; 3SCIXE, Concord ON, Canada

WP 657 Proteomic Study of Rhizopus Microsorus Fungus Growing in Presence of Copper; Meriellen Dias1; Lidiane Maria de Andrade1; Enrique Eduardo Rozas1; Mariana de Paula Eduardo1; Maria Ana Mendes1; 1University of São Paulo, São Paulo, SP

WP 658 Identification of Methylation and Phosphorylation in Arginine/Serine-Rich Domains by Electron Transfer Dissociation Mass Spectrometry; Isaac Bishop1; Duc M. Duong2; Eric B. Dammer2; Nicholas T. Seyfried2; 1Emory University, Atlanta, GA; 2Emory University School of Medicine, Atlanta, GA

WP 659 Capturing Protein Binders to Yeast Ribosome Biogenesis and Stress Response Genes Using Multiplexed HyCCAPP; Yuxiang Dai1; Julia Kennedy-Daring1; Mark Scalf1; Audrey Gasch1; Lloyd M Smith1; 1San Francisco State University, San Francisco, CA; 2San Francisco State University, San Francisco, CA

WP 660 Elucidation of Dynamic Cell Surface Protein-Protein Interactions using Chemoproteomic Technologies; Damaris Bausch-Fluck1; Maria P Pavlou1; Bernd Wollschel1; 1Institute of Molecular Systems Biology, Dep. of Health Sciences and Technology, ETH Zürich, Zürich, Switzerland

WP 661 Development of an On-Slide-Digestion, MS Assay from Formalin-Fixed Paraffin Embedded (FFPE) Breast Tissue; Ten-Yang Yen1; Moe Thein1; Roger Yen1; Leslie Timpe1; Bruce Macher1; 1San Francisco State University,
WP 675 Development of Dimethyl Pyrimidinyl Ornithines (DiPyRO) as Mass Defect-Based Tags for Quantitative Proteomics; Amanda Rae Buchberger; Dustin Frost; Lingjun Li; 1University of Wisconsin-Madison, Madison, WI

WP 676 Examining pH Specificity of Peptide N-terminal Amine Tagging Reagents for cPlOET Analysis; Lindsay Osentoski; Yaphet Geadion; Joseph Dudenhoeffer; Christina King; Renä A.S. Robinson; 1University of Pittsburgh, Pittsburgh, PA

WP 677 Information of SuperQuant to Obtain Quantitative Investigation of the Glioblastoma Proteome: Thiago Verano-Braga; Vladimir Gorshkov; Sune Munthe; Mia Dahl Soerenesen; Bjare Winther Kristensen; Frank Kjeldsen; 1Department of Biochemistry and Molecular Biology, University of Southern Denmark Odense, Denmark; 2Odense University Hospital, Odense, DK; 3BMM, Odense M

WP 678 Combining of iTRAQ Labeled Peptides from HPLC Fractions: Where is the Limit for Peptides/Proteins Detected and Quantified?; Trong Khoa Pham; Kirsty Richards; Jo Roobol; Colin Robinson; Phillip C. Wright; 1Department of Chemical and Biological Engineering, The University of Sheffield, Sheffield, UK; 2School of Biosciences, University of Kent, Canterbury, UK; 3Faculty of Science, Agriculture and Engineering, Newcastle University, Newcastle upon Tyne, UK

WP 679 Increasing Protein Quantification in 6-plex TMT Experiments; Jane Liu; Michael Sweredoski; Sonja Hess; 1Pomona College, Claremont, CA; 2California Institute of Technology, Pasadena, CA

WP 680 Evaluation of a Pulsed SILAC-TMT Multiplexing Strategy for Measurement of Proteome Dynamics; Jana Zecha; Chen Meng; Mathias Wilhelm; Susan Klaeger; Bernhard Kuster; 1Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; 2Bavarian Biomolecular Mass Spectrometry Center, Technical University of Munich, Freising, Germany

WP 681 Extended Mass Range QQQ for Routine Analysis of Large, Low-Charge State Peptide Ions; Linfeng Wu; Christine A Miller; 1Aglent Technologies, Santa Clara, CA

WP 682 Pseudo-isobaric Fragment Ions Provide Accurate and Precise Proteome Quantification Results; Yuan Zhou; Jianhui Liu; Zhigang Sui; Lihua Zhang; Yukui Zhang; 1Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

WP 683 Investigation of Q-TOF Instruments Advantages for label-free Proteome Analysis; Stephanie Kaspar-Schoenefeld; Markus Lubeck; Annette Michalski; Pierre-Olivier Schmitt; 1Bruker Daltonik GmbH, Bremen, Germany; 2Bruker Daltonique S.A., Wissembourg, France

WP 684 Stable-isotope Maleic Anhydride Labeling-based Approach for Quantitative Proteomics; Kai Zhang; Shuzhen Zheng; Shanshan Tian; Zhenchang Guo; Guijin Zhai; 1Tianjin Medical University, Tianjin, Tianjin; 2Nankai University, Tianjin, China; 3Tianjin Medical University, Tianjin, China

WP 685 Intact Protein Quantitation up to a 1000-fold Using Protein Universal Pseudo-isobaric Dimethylation; Zhixin Tian; Houjin Fang; Kaijia Xiao; 1Department of Chemistry, Tongji University, Shanghai, Shanghai

WP 686 Evaluation of a Novel Tandem Quadrupole Mass Spectrometer for the Quantitative Analysis of Peptides using a Multi-Point Internal Calibration Method; Billy Molly; Donald JL Jones; 1University of Wisconsin-Madison, Madison, WI; 2University of Pittsburgh, Pittsburgh, PA

WP 687 Comparison of Label-Free and TMT Quantification for Global Phosphoproteome Analysis of Apoptotic Cells; Emmanuelle Lefrançais; Christoph Schmutz; Simon Josef Ittig; Erik Ahmeh; Alexander Schmidt; 1Biozentrum, University of Basel, Basel, Switzerland

WP 688 Examining Protein Transfer and Ion Scattering for Intact Proteins in a Triple Quadrupole Mass Spectrometer; Evelyn H Wang; Dananjaya Kalu Appulage; Erin A. McAllister; Kevin A Schurg; 1University of Texas at Arlington, Arlington, TX; 2Shimadzu Scientific Instruments, Columbia, MD

WP 689 α- and β-tubulin isotype Repertoire Quantification by LC-SRM in Blood Platelet and HeLa Cells; Agnes Hovasse; Magda Magiera; Catherine Strasselli; Alain Van Dorsseelaer; Carsten Janke; Francois Lanza; Christine Schaeffer-Reiss; 1Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, Alsace; 2Institut Curie, Orsay, France; 3UMR_S 949 Inserm, EFS-Alsace, Université de Strasbourg, Strasbourg, France; 4Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR7178, Centre National de la Recherche Scientifique, Université de Strasbourg, Strasbourg, France

WP 690 Combination of Ultrasonic Sample Preparation and NHS-chemistry Enables Sensitive Quantitative of Lysine Acetylation and Large Proteome Coverage; Christian Frese; Ozge Karayel; Joren Krigsveld; 1DKFZ German Cancer Research Center, Heidelberg, Germany

WP 691 Combining Ion Mobility Enhanced DDA and DIA Workflows for Label-Free Quantitative Phosphoproteomics; Ute Distler; Pedro Navarro; Jennifer Hahlbrock; Kuharev Jörg; Stefan Tenzer; 1Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany; 2Focus Program Translational Neuroscience (FTN), University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany

WP 692 Comprehensive Relative Quantification of the Cytochromes P450 by micro-LC and SWATH® Acquisition and Data Processing using Cloud Computing; Rosalind E. Jenkins; Sibylle Heidelberger; Thomas Knapman; Francesco Brancia; Neil Kittingham; Kevin B Park; 1Mark Carfazzo; 2MRC Centre for Drug Safety Science, Liverpool, UK; 3SCIEX, Phoenix House Lakeside Drive Warrington Cheshire UK; 4Sciex, Redwood Shores, CA

WP 693 Interference-free Multiplexed Quantification with Complement Reporter Ions: Technological Advances and Application to Nucleocytoplasmic Partitioning; Martin Wuehr; Graeme C McAllister; Thomas Güttler; Brian K. Erickson; Matthew Sonnett; Ramin R. Rad; Keisuke Ishihara; Leonid Peshkin; Aaron C. Groen; Marc McAllister; Kevin A Schurg; 1Massachusetts General Hospital, Boston, MA; 2Thermo Fisher Scientific, San Jose, CA; 3Massachusetts General Hospital, Boston, MA

WP 694 Veracity or Serendipity? Contradicting Conjectures in Protein Quantification; Russell P Grant; Christopher M Shuford; Patricia L Holland; 1Laboratory of Comparative Medicine, Boston, MA; 2Johns Hopkins University, Baltimore, MD; 3Laboratory of Comparative Medicine, Boston, MA; 4Harvard Medical School, Boston, MA; 5Brookhaven National Laboratory, Upton, NY; 6New York Medical College, Valhalla, NY

WP 695 A New and Easy Approach for End-User Driven Quantification of SIL Peptide Solutions in Targeted Proteomics; Markus Schnatbaum; Lars Hornberger; Johannes Zerweck; Tobias Knaut; Lawrence Eckler; Ulf
WP 699  Highly Multiplexed MRM-based Peptide Quantitation in Human Plasma Using Two Different Stable Isotope Labeled Peptides for Calibration; André LeBlanc1; Sarah Michaud2; Andrew Percy1; Darryl B Hardie1; Juncong Yang1; Nicholas Sinclair1; Jillaine Proudfoot1; Adam Pistikwa1; Derek S Smith1; Christopher J Petzold1; Jillaine Proudfoot1; Larry Zarnon1; Stephen P Gygi1; "Harvard Medical School, Boston, MA; "University of Victoria, Victoria, BC, Canada; "University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; "Washington University School of Medicine, Saint Louis, MO.

WP 700  Second Generation Combinatorial Mass Tag (CMT) Isobaric Reagents with Improved Quantitative Precision; Craig Braut1; Brian Erickson1; Gregory Bird2; Steven P Gygi1; "Harvard Medical School, Boston, MA; "Dana Farber Cancer Institute, Boston, MA.

WP 701  Utilizing Synthetic Peptides and Skyline for Validating Quantitative Changes in Biological Proteomics; Chia-Fang Lee1; Chen-Hsun Tsai1; Lydia M. Contreras1; Maria D. Person1; "University of Texas at Austin, Austin, TX.

WP 702  A Peptide-Retrieval Strategy Enables Significant Improvement of Quantitative Performance Without Compromising Confidence of Identification; Chengjian Tu1; Chichen Shen1; Quanhui Sheng1; Yu Shyr1; Jun Qu1; "University at Buffalo, Buffalo, NY; "Vanderbilt University, Nashville, TN.

WP 703  Multiplexing Quantification of Proteins by Single-Cell CE-μESI-HRMS Finds Translational Cell Heterogeneity in the 16-cell Frog (Xenopus) Embryo; Camille Lombard-Banek1; Sally A Moody1; Peter Nemes1; Sushma Reddy1; "The George Washington University, Washington, DC; "Florida Atlantic University, Boca Raton, FL; "University of Victoria, Victoria, BC, Canada; "MedImmune, Gaithersburg, MD.

SMALL MOLECULES: QUANTITATIVE ANALYSIS (PART 1)

WP 705  Dilute and Shoot FI-MS/MS BC Quantification of Glycocalyx Acid in Human Bile Using Standard Addition Method; Raghavi Kakarla1; Ramakrishna reddy Voggu1; Janet R Donaldson1; Baochuan Guo1; "Cleveland State University, Cleveland, OH; "Mississippi State University, Starkville, MS.

WP 706  Development of Cost-Effective Liquid Chromatography-Tandem Mass Spectrometry Method for Polar Drugs and Metabolites; Xiaodong Zhu1; Jingguo Hou1; Jerry Gardella1; Melvin Tan1; Tom Lloyd1; Edward Wells1; "Worldwide Clinical Trials Drug Development Solution, Austin, TX; "Washington University School of Medicine, Saint Louis, MO.

WP 707  Development and Validation of an Ultra Sensitive and Automated LC-MS/MS Method for the Measurement of Naloxone, Buprenorphine and Norbuprenorphine; Nick Peng1; Ben Gaboury1; Nichole Boice2; Dan Pederson1; Ardeshr ardeshr khakang1; "Axis Clinicals, Dilworth, MN.

WP 708  Development and Validation of a Simple, Rugged and Automated LC-MS/MS Method for the Determination of Mesalazine in Human Plasma; Nick Peng1; Ben Gaboury1; Sarah Maasjo1; Ardeshr Khadang1; "Axis Clinicals, Dilworth, MN.

WP 709  Simultaneous Determination of Tamsulosin and Solifenacin in Human Plasma by Ultra-High Performance Liquid Chromatography with Tandem Mass Spectrometry; Jin Sun Woo1; Hwa Suk Kim1; Seo Hyun Yoon1; Joo-Youn Cho1; "Seoul National University College of Medicine, Seoul, South Korea.

WP 710  Applications of Improved GCMS Method for Fatty Acid Analysis in Samples from Bariatric Patients and Mice Fed Omega-3 Fatty Acids; Kazimierz Surowiec1; Nadeeja N. Wijayatunga1; Latha Ramalingam1; Valerie G. Sams1; Gregory J. Marchini2; Matthew L. Mancini1; Yehia Mchref2; "Dana Farber Cancer Institute, Boston, MA; "University of Victoria, Victoria, BC, Canada; "Washington University School of Medicine, Saint Louis, MO.

WP 711  A Two-dimensional Liquid Chromatography (2D-LC) to Separate an Interference Peak from Norfentanyl for Its Successful Bioanalysis; Moo-Young Kim1; Brendan Laing1; Fumin Li1; "PPD, Middleton, WI.

WP 712  Development and Validation of a LC-MS/MS Method for the Simultaneous Quantitation of Carboplatin and Etoposide in Human Plasma and Ultrafiltrate; Jessica Sima1; Ganesh S Moorthy1; Athena Zuppa1; Elizabeth Fox1; "Children’s Hospital of Philadelphia, Philadelphia, PA; "Children’s Hospital of Philadelphia, Philadelphia, PA.

WP 713  Highly Accurate Sample Collection, Handling and LCMSBS Bioanalysis of Liposomal Amphotericin B Plasma Samples; Jason Bilodeau1; François Viel1; Nadine Boudreau1; Clark Williard1; "inVentiv Health, Quebec, Canada.

WP 714  Determination of Unconjugated Naloxone, Conjugated Naloxone and Total Naloxone in Human Plasma by LC-MSMS; Louis-Charles Boisvert1; Nicolas Jean1; Guy Havard1; Philippe Belanger1; Marie-Josée Marcoux1; Sylvain Lachance1; Nadine Boudreau1; Clark Williard1; "inVentiv Health, Quebec, Canada.

WP 715  Trace Level Quantitative Determination of Phthalates from High Risk Dosage Pharmaceutical Formulations using LC/MS/MS; Purushotham Sutar1; Rashi Kochhar1; Deepti Bhandarkar1; Shailendra Rane1; Shailesh Damale1; Anant Lohar1; Ashutosh Shelar1; Jitendra Kelkar1; Pratap Rasam1; Ajit Datar1; "Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India.

WP 716  Highly Sensitive Multiplexed Analysis of Levosulbutamol from Plasma using LC/MS/MS; Ashutosh Shelar1; Shailesh Damale1; Shailendra Rane1; Purushotham Sutar1; Anant Lohar1; Deepti Bhandarkar1; Rashi Kochhar1; Pratap Rasam1; Jitendra Kelkar1; Ajit Datar1; "Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India.

WP 717  Robust, Sensitive and Accurate Determination of Different Opioids in Human Plasma by LCMSMS; Genevieve Emmond1; Marc Fournier1; Marie-Claude Théberte1; Nathalie Pelletier1; Marie-Josée Marcoux1; Sylvain Lachance1; Nadine Boudreau1; Clark Williard1; "inVentiv Health, Quebec, Canada.

WP 718  Simultaneous Assay of Multiple Synthetic Contraceptive Hormones in Human Serum by LCMSMS; Steven W Blue1; Rachel Lieberman2; David W Erikson1; Christopher Gilles1; "Oregon National Primate Research Center, Beaverton, OR; "Shimadzu Scientific Instruments, Columbia, MD.
WP 719  Highly Sensitive Automated Assay for the Determination of Oxytocin in Human Plasma by LC-MS/MS; Nicolas Jean1; Philippe Bélanger2; Carine Lévesque1; Marie-Claude Théberge1; Nadine Boudreau1; Clark Williard1; Hermes Licea-Perez2; Jonathan Kehler2; Thomas Mencken2; 1inVentiv Health, Québec, Canada; 2GlaxoSmithKline, Upper Merion, PA

WP 720  Quantification of Tenofovir and Emtricitabine in Human Plasma using High Throughput LDTD-MS/MS; Jean Lacoursiere1; Annie-Claude Bolduc2; Alex Birsan1; Serge Auger1; Pierre Picard1; Phytronix Technologies, Inc. Quebec, Canada; 2Université Laval, Québec, Canada

WP 721  A Sensitive LC-MS/MS Method for Quantitation of Naltrexone and 6β-Naltrexol in Human Plasma (1 pg/mL); Dawei Zhou1; Shaoting Zhang1; Mohamed Osman1; Xinping Fang1; WuXi AppTec Co., Plainsboro, NJ

WP 722  Quantification of N-Hydroxy Riluzole Metabolite in Human Plasma: The Investigation of the Stability of the Analyte; Luc Bouchard1; Nathalie Pelletier1; Sylvain Lachance1; Nadine Boudreau1; Clark Williard1; inVentiv Health, Québec, Canada

WP 723  Ultra-Sensitive LCMSMS Determination of Teriparatide in Human Plasma; Philippe Bélanger1; Marie-Josée Marcoux1; Nadine Boudreau1; Clark Williard1; inVentiv Health, Québec, Canada

WP 724  Development of an Ultrasensitive Assay for Quantification of Free Ticagrelor in Plasma using Equilibrium Dialysis and LC-MS/MS; Ann-Sofie Sandinge1; Annika Janefeldt1; AstraZeneca R&D, Gothenburg, Sweden

WP 725  Bioanalytical LC/MS/MS Method for the Determination of a Vitamin E analog in Human Plasma; Jeff Jeppson1; Elizabeth Dibbern1; Ridha Nachi1; Celerion, Lincoln, NE

WP 726  Comparison of the Quantitation of Bile Acids using Full Scan and Targeted SIM Mode on using UPLC/HRAM MS; Brandon Wilcock1; Lijuan Fu1; Nan Zhao1; Cassidy Hatch1; Nidhi Jaiswal1; Min Meng1; Troy Voelker1; Scott Reuschel1; Covance, Salt Lake City, UT

WP 727  A Selective and Ultra-Sensitive LC-MS/MS Method for Simultaneous Quantitation of Norgestrel and Norgestimate in Human Plasma; Shuyu Hou1; Sheth Raj1; Hongkun Liang1; Yuan-Shek Chen1; Hsu Ben1; QPS, LLC, Newark, DE

WP 728  Rapid Analysis of Ceftriaxone in Human Intestinal Chyme, Human Plasma, and Dog Plasma by HPLC/MS/MS; Todd Lusk1; John F Kokai-Kun2; Michael Schlosser3; Stacey Zeman1; Sara Brady1; Daniel 1 Mulvana4; Thad Yousey5; Q2 Solutions Bioanalytical and ADME Labs, Ithaca, NY; 2Synthetic Biologics, Inc., Rockville, MD; 3MSR Pharma Services, Inc., Lincolnshire, IL; 4Q2 Lab Solutions Bioanalytical and ADME Labs, Ithaca, NY; 5Quintiles, Ithaca, NY
THURSDAY POSTERS

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

Ambient ionization: Fundamentals and Instrumentation
(DART/Plasma, Laser, SAWN) ................................... 001 - 030
Biomarkers: Discovery (Part 2) ................................. 031 - 068
Biomarkers: Quantitative Analysis (Small Molecules &
Metabolites) ....................................................... 059 - 089
Drug Metabolism: Quantitative Analysis ....................... 090 - 107
Food Safety: Other Contaminants (Part 2) ..................... 108 - 141
GC/MS: Instrumentation and Applications (Applications) 142 - 171
H/D Exchange: Protein Structure/Function (Part 2) .......... 172 - 195
Imaging MS: Method Development (MALDI) ................. 196 - 215
Imaging MS: Small Molecules .................................... 216 - 247
Informatics: General, SRT, and Dia ............................. 248 - 269
Informatics: Protein ID and Quantification ..................... 270 - 281
Instrumentation: New Developments in Ionization and Sampling (Ionization) .................................... 282 - 308
Ionization Mechanisms .......................................... 309 - 323
LC-MS: Sample Preparation (Part 2) ........................... 324 - 345
Lipids: Quantitative Analysis ..................................... 346 - 375
MALDI: Sample Preparation ..................................... 376 - 401
Metabolomics: Identification of Unknown Metabolites ....... 402 - 425
Metabolomics: Quantitative Analysis ......................... 426 - 446
Natural and Nanomaterials ....................................... 447 - 455
Peptides: Fragmentation Mechanisms ......................... 456 - 470
Peptides: Quantitative Analysis .................................. 471 - 504
Peptides: Sequence Analysis ..................................... 505 - 518
Peptidomics ......................................................... 519 - 530
Protein Therapeutics: Structural Characterization .......... 531 - 566
Proteins: Conformation Analysis and Structural Biology .... 567 - 585
Proteins: PTMs (Part 2) .......................................... 586 - 605
Proteomics: New Approaches (Other) ......................... 606 - 625
Proteomics: Quantitative (Pre-MS and Platforms/Informatics/
MultiOms/Dynamics) ........................................... 626 - 649
Prometabolites: Tissue ............................................. 650 - 675
Small Molecules: Quantitative Analysis (Part 2) ............. 676 - 698
Systems Biology (Protein Modifications and Cells) .......... 699 - 719
Toxicology ......................................................... 720 - 748

THP 006 Direct Quantification Technique for Natural Moisturizing Factor (NMF) in Stratum Corneum by Direct Analysis in Real Time Mass Spectrometry (DART-MS); Katsuyuki Maeno1; Yasuo Shida2; Haruo Shimada3; Shisheido Global Innovation Center, Yokohama, Japan; University of Yamanashi, Kofu, Japan

THP 007 Accurate Quantification of Urinary Creatinine by Stable Isotope Dilution and DART Coupled to Quadrupole Time-of-Flight Mass Spectrometry; Ning Zhang1;2; Yuanyuan Song1; Meiling Lu1; Weibing Zhang2; HaiLin Wang1; Xiaokun Duan1; Charles C. Liu1; Research Center for Eco-Environmental Sciences, Beijing, China; East China University of Science and Technology, Shanghai, China; Agilent Technologies (China) Limited, Beijing, China; ASPEC Technologies LTD, Beijing, China

THP 008 Research of Real-Time Monitoring Method for Volatiles in Chinese Liquor (Baijiu) Tasting; Ming Liu1; Zijing Xu2; Jianghao Lu1; Yi Zhang1; Qiding Zhong1; Xiaomei Yuan1; Zhenghe Xiong1; Xiaokun Duan1; Kai Liu1; China National Research Institute of Food & Fermentation Industries, Beijing, China; Sichuan Jiannanchun Group Co. Ltd, MianZhu, Sichuan; ASPEC Technologies LTD, Beijing, China

THP 009 Screening Analysis of Primary Aromatic Amines in Textiles using DART-MS; Yamamura Yuutoro1; Maeda Ken’go2; Jun Watanabe3; Sakakura Motoshi4; Shiota Teruhisa4; Shimadzu Corporation, Kyoto, Japan; Shimadzu Co., Kyoto, Japan; Shimadzu Corporation, Kyoto, AMR Inc., Tokyo, Japan

THP 010 A Study of DART® as a Technique for Ambient Surface Analysis of Polymers; Dana Reedi1; Katri Huikko2; Steven Pachuta; Ali Rafali3; 3M Corporation, St. Paul, MN

THP 011 On-line Coupling of Surface Plasma Resonance to Ambient Mass Spectrometry; Huwei Liu1; Yiding Zhang1; Yu Bai1; Peking University, Beijing; Peking University, Beijing, China

THP 012 An Interface for Online Coupling Surface Plasma Resonance with Mass Spectrometry using Dielectric Barrier Discharge Ionization; Yiding Zhang1; Yu Bai1; Huwei Liu1; Peking University, Beijing, China

THP 013 Determination of Peroxide Explosives and Related Compounds by Dielectric Barrier Discharge Ionization-Mass Spectrometry (DBDI-MS); Sebastian Hagenhoff1; Heiko Hayen1; University of Muenster, Munster, Deutschland

THP 014 Surface Erosion and Analysis of Polymer Sample via Micro Dielectric Barrier Plasma Jet Mass Spectrometry; Songyu Shi1; Xiaoxia Gong2; Xinyue Liang2; Gerardo Gamez3; Texas Tech University, Lubbock, TX

THP 015 Low Temperature Plasma Desorption/Ionization Mass Spectrometry for Quantitative Analysis of Exhaled Breath Collected on Filter Substrates; Xiaoxia Gong1; Songyu Shi1; Xinyue Liang1; Mohammad Choudhury1; Gerardo Gamez2; Texas Tech University, Lubbock, TX

THP 016 Effects of Molecular Gas Addition on a Helium Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Desorption/Ionization (ADI) Source; Suniti Barad1; Jacob T. Shelley1; Department of Chemistry and Biochemistry, Kent State University, Kent, OH

THP 017 Reactive Ambient Mass Spectrometry with Flowing Atmospheric Pressure Afterglow; Gerardo Gamez1; Xiaoxia Gong1; Xinyue Liang1; Songyu Shi1; Mohammad Choudhury1; Texas Tech University, Lubbock, TX

THP 018 A Microwave Plasma for Simultaneous Molecular and Atomic Ambient Ionization of Solids; Kenyon Evans-
**ThP 019**

**Automatic Analyte Ion Recognition and Background Removal for Ambient Mass Spectrometry Data Based on Cross Correlation**

Yi You1; Sunil P. Badal1; Jacob T. Shelley2; Department of Chemistry and Biochemistry, Kent State University, Kent, OH

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**ThP 020**

**Characterization of Chemical Noise in AP MALDI using LTQ and Orbitrap Mass Spectrometry**

John Moskovets1; Vladimir M Doroshenko2; Shelley N Jackson2; Amina S Woods1; MassTech Inc, Columbus, MD; 3NIDA-IRP, NIH Baltimore, MD

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**ThP 021**

**Magnetic-Field-Assisted Laser-Ablation Ambient Mass Spectrometry**

Yao Lu1; Yun Shen Zhou1; Lei Liu1; Xi Huang1; Yongfeng Lu1; Dept of Electrical and Computer Engineering, University of Nebraska-Lincoln, Lincoln, NE

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**ThP 022**

**Sensitivity Improvement of Infrared Laser Atmospheric Pressure Ionization Mass Spectrometry by Synchronizing a Q-TOF Mass Spectrometer and the Laser Pulse**

Hashiya Homang1; Iguchi Yasunari1; Hazama Hisaanao; Awazu Kunio3; Osaka University, Saita; Osaka University, Saita, Japan

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**ThP 023**

**Coaxial Gas Flow Enhances Sample Plume Transfer Efficiency for Remote Laser Ablation Electrospray Ionization Mass Spectrometry**

Jarod Fincher1; Brent Reschke2; Nicholas Morris3; Akos Vertes3; The George Washington University, Washington, DC; 3Protea Biosciences, Inc. Morgantown, WV

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**ThP 024**

**Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Identify Microorganisms at Species Level from Pure and Mixed Cultures**

Simon Cameron1; Frankie Bolt1; Adam Burke1; Zsolt Bodai2; Alvaro Perdones-Montero1; Julia Balog1; Tamas Karancsi2; Daniel Ory1; Jean Schaffer1; Daniel Pavanish Kumar6; Bhairav Paleja6; Amit Singhal6; Gennaro De Libero6; Markus R Wenk4; Xi Huang1; Yongfeng Lu1; Larry J Campbell2; Sung Hwan Yoon2; Tao Liang2; David P A Kilgour3; Anne K Bendt4; Cynthia Chee5; Yee Tang Wang5; Thomas Schneider2; Sung Hwan Yoon2; Tao Liang2; David R Goodlett2; Facundo M Torta4; Stephen Zambrzycki1; Matthew C Bernier2; Joel Keelor2; Huipeng Neo1, 2, 3; Shanshan Ji4; Federico Derivatives

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**ThP 025**

**Surface Acoustic Wave Nebulization Sample Introduction for Vacuum-Assisted Plasma Ionization**

Thomas Zambrycki1; Matthew C Bernier2; Joel Keelor2; Sung Hwan Yoon2; David R Goodlett2; Facundo M Torta4; Stephen Zambrzycki1; Matthew C Bernier2; Joel Keelor2; Huipeng Neo1, 2, 3; Shanshan Ji4; Frederico Derivatives

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**ThP 026**

**Surface Acoustic Wave Nebulization – Mass Spectrometry: A Tool for Rapid Analysis of Food Products**

Gloria S Yen1; Thomas Schneider2; Benjamin L Oyler3; Sung Hwan Yoon2; David R Goodlett4; 1University of Maryland School of Pharmacy, Baltimore, MD; 2University of Maryland School of Pharmacy, Baltimore, MD; 3School of Chemistry, The University of Edinburgh, Edinburgh, UK; 4Deurion LLC, Seattle, WA

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**ThP 027**

**Performance Characterization of Surface Acoustic Wave Nebulization for Lipid A Mass Spectrometric Analysis**

Tao Liang2; Thomas Schneider2; Sung Hwan Yoon2; Benjamin L Oyler3; Andrew Dennison1; Gloria S Yen1; Yue Huang1; Adam A Stokes2; Anthony J Walton2; Robert K Ernst2; Erik Nilsson4; David R Goodlett5; 1University of Maryland School of Pharmacy, Baltimore, MD; 2School of Pharmacy, University of Maryland Baltimore, MD; 3School of Chemistry, The University of Edinburgh, Edinburgh, UK; 4Deurion LLC, Seattle, WA; 5School of Engineering The University of Edinburgh, Edinburgh, UK

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**ThP 028**

**Surface Acoustic Wave Nebulization – Mass Spectrometry on a TripleTOF Mass Spectrometer**

Thomas Schneider2; Benjamin L Oyler3; Larry J Campbell2; Yves J C LeBlanc1; Tom Covey1; Gloria S Yen1; Erik Nilsson4; David R Goodlett5; 1University of Maryland School of Pharmacy, Baltimore, MD; 2AB SCIEX, Concord, Canada; 3AB SCIEX, Concord ON, Canada; 4Deurion LLC, Seattle, WA

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**BIOMARKERS: DISCOVERY (PART 2)**

**ThP 031**

**Non-Target Urinary and Serum Metabolomic Study of Radix Astragali Treated on Rheumatoid Arthritis Rats Using UPLC-Q-TOF-HDMS**

Zhiqian Li1; Bengde Xu1; Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, CN

**ThP 032**

**Potential Diagnostic Biomarkers and Pathway Analysis of Ovarian Cancer by Lipidomics**

Yangyang Zhang; Institute of Chemistry, Chinese Academy of Sciences, Beijing, China

**ThP 033**

**Death Domain Associated Protein DAXX May Regulate a Distinct Lipid Metabolism Signature in Breast Cancer**

Iqbal Mahmud1; Timothy J Garrett1; Daqing Liao1; University of Florida, Gainesville, FL

**ThP 034**

**Identification of Unusual Bile Acids as Biomarkers for Niemann-Pick C Disease Using Charge-Remote Fragmentation of N-(4-Aminomethylphenyl)Pyridinium Derivatives**

Xuntian Jiang1; Laurel Mydock1; Fong-Fu Hsu1; Douglas Covey1; David E Scherrer1; Rohini Sidhu1; Forbes D Porter3; Nicole M Yanjanin1; Dennis J Dietzen1; Jean Schaffer1; Daniel Ory1; Washington University in St. Louis, St. Louis, MO; 2Washington University in St. Louis, St Louis, MO; 3NIH/NIAD, Bethesda, MD

**ThP 035**

**Human Plasma Lipidome Variations in Active Tuberculosis**

Hui Peng1,2,3; Shan Shanshan J1; Federico Derivatives

**ThP 036**

**Mass Spectrometry-Based Metabolomics for Biomarker Discovery after Angioplasty**

Yatao Shi1; Bowen Wang1; Xudong Shi1; Liang-Wang Guo1; K. Craig Kent1; Lingjun Li1; University of Wisconsin-Madison, Madison, WI

**ThP 037**

**Lysophosphatidylinositol: A Novel Biomarker of Ischemia and a Potential Prognostic Indicator of Cardiac Arrest**

Koichiro Shinozaki1; Tai Yin1; Junhwan Kim1; T The Feinstein Institute for Medical Research, Manhasset, NY

**ThP 038**

**Following Biomarkers of Central Metabolism in Muscles from Diabetic Mouse Model: Metabolic Pathway Imaging**

Juliette Masure1; Gregory Hamm1; Philippe Delataille1; Corinne Foucart1; David Bonnell1;
Carole Belanger; Raphael Darteil; Jonathan Stauber; "imaBiotech, MS Imaging Dept. LOOS, France; "Genfit, Loos, France

ThP 039 Analysis of Volatile Organic Compounds in Pleural Effusions by HS-SPME-cryo-trap-SC/MS: Zhongping Huang; Jie Zhang; Huijun Liu; Lili Wang; Zhejiang University of Technology, Hangzhou, China

ThP 040 Controlling the Misuse of Anabolic Steroids by Steroidal Biomarkers Profiling: Kin-Sing Wong; George H.M. Chan; Emmie N.M. Ho; Terence S.M. Wan; "Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, China

ThP 041 Serum Total Fatty Acids as Potential Biomarkers for Differentiate Benign Lung Diseases from Lung Cancer; Junling Ren; Zhili Li; "Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, CN; 1BMS, CAMS& PUMC, Beijing

ThP 042 Modeling the Exosome Paradigm: Exposure Analysis of the Western Honey Bee; Chloe Wang; Malia Wenny; Robert L Broadnup; Christopher Mayack; Anthony Macherone; 4; Haverford College, Haverford, PA; 5Swarthmore College, Swarthmore, PA; 6Aglent Technologies, Wilmington, DE; 7Johns Hopkins University School of Medicine, Baltimore, MD

ThP 043 Proteomics of Human Plasma in Heart Failure with Preserved Ejection Fraction (HFpEF) using Novel Chemical Affinity, Mixed Mode Matrix (M3); Richard Mbausu; Donald DL Jones; Lisa M Heaney; Leong L Ng; Sandhu K Jatinderpal; Paulene Quinn; Daniel C Chan; University of Leicester, Leicester, Leicesterhire; 2University of Leicester, Leicester, UK

ThP 044 Mass Spectrometry Based Proteomics to Investigate and Characterize the Jumping Translocation Breakpoint (JTB) Protein using Cancer Cell Lines; Devika Channavveerapag; Kangling Li; Costel C. Darie; "Clarkson University, Potsdam, NY

ThP 045 Label-free Shotgun Proteomics Identifies Markers of Inflammation from Fetal Fibroblasts; Owen E Branson; Brian C Wulff; Miranda L Gardner; Traci A Wilgus; Michael A. Freitas; Ohio State University, Columbus, OH

ThP 046 Mass Spectrometry Based Proteomic Investigation of Plasma Samples from Children with Autism Spectrum Disorder (ASD) and Matched Controls; Kelly Wormwood; Megan M Borland; Emalyn J Dupree; Alisa G Woods; Blythe Corbett; Costel C. Darie; "Clarkson University, Potsdam, NY; 2Vanderbilt University, Nashville, TN

ThP 047 Using LC-MS/MS and Stable Isotope Tracers to Explore Circulating Biomarkers for the Kinetics of Liver Fibrosis; Hsinhong Zhou; Yangqing Kan; Ying Chen; Ye Tian; Yongchong Huang; Yonghua Zhu; Taro Akiyama; David Kelley; Stephen Previs; Shiry Pinto; Merck & Co., Inc., Kenilworth, NJ; 2Merck & Co, Kenilworth, NJ

ThP 048 Quantitative Proteomic Analysis of Serum Exosomes from Patients with Pancreatic Cancer Reveals the Differentially Expressed Proteins after Chemo-/Radio-Treatment; Mingrui An; Zhijing Tan; Jianhua Zhu; Jing Wu; Jun Cao; Rui Yang; Xiucang Pei; David M. Lubman; 1University of Michigan, Ann Arbor, MI; 2University of Michigan Medical Center, Ann Arbor, MI

ThP 049 Development of an Integrated and Effective Pipeline for Profiling Microbial Proteins from Mouse Fecal Samples by LC-MS/MS; Jing Wu; Jianhua Zhu; Haidi Yin; Mingrui An; Nicholas Pudlo; Eric Martens; Grace Chen; David M Lubman; 1University of Michigan Medical Center, Ann Arbor, MI; 2University of Michigan Medical School, Ann Arbor, MI

ThP 050 CD90 Expression is Associated with Pancreatic Intraepithelial Neoplasias; Xiucang Pei; Jianhua Zhu; Rui Yang; Jiaqi Shi; Zhijing Tan; Mingrui An; David M Lubman; 1University of Michigan Medical Center, Ann Arbor, MI; 2University of Michigan Medical School, Ann Arbor, MI

ThP 051 Facilitate Biomarker Discovery using Integrated “Omics” Differential Analysis with High Resolution Accurate LC/MS Approach: Reiko Kiyonami; Julian A Saba; Sergei I Snovida; David Peake; Devin Drew; Andreas Huhmer; Ken Miller; "ThermoFisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, San Jose, CA; 3Thermo Fisher Scientific, Rockford, IL

ThP 052 Proteomic Analysis of Minute Amount of Colonic Biopsy Samples from Patients by Enteroscopy for Biomarker Discovery; Xing Lu; Zhou Hu; Xu Yanli; Chinese Academy of Sciences, Shanghai, China; "Fuyang People’s Hospital, Fuyang, China

ThP 053 Early Diagnostic Biomarkers for Acute Liver Transplantation Rejection; Su Jung Kim; Ji Hyun Kim; Na Young Kim; Shin Hwang; Hyun Ju Yoo; 1Asan Institute for Life Sci, Asan Medical Center Seoul, South Korea; 2Dep. Liver Transplantation and Hepotobiliary Surgery, Asan Medical Center, Seoul, Republic of Korea; 3Biomedical Research Center, Asan Institute for Life Sciences, Asan Medical Center, Seoul

ThP 054 The Identification of Biomarkers of Normobaric Hypoxia and Recovery via Exhaled Breath; Sean Harshman; Brian Geier; Leslie Drummond; Laura Flory; Maomian Fan; Jeffrey Phillips; Darrin Ott; Claude Grigsby; "UES Inc, Air Force Research Laboratory, WPAFB, OH; 1UES, WPAFB, OH; 2Naval Medical Research Unit-Dayton, WPAFB, OH; 1Air Force Research Laboratory, WPAFB, OH; 2US AF School of Aerospace Medicine, WPAFB, OH

ThP 055 Integration of Tissue and Urine Proteomes for Biomarker Discovery and Verification of Renal Cell Carcinoma; Yi-Ting Chen; Chien-Lun Chen; Jau-Song Yu; Pei-Chia Wang; Hsiao-Wei Chen; Ying-Hsuo Chang; Yu-Sun Chang; Ting Chung; Tsung-Shih Lin; 1Department of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; 2Molecular Medicine Research Center, College of Medicine, Chang Gung University, Taoyuan, Taiwan; 3Graduate Institute of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; 4Graduate Institute of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; 5Graduate Institute of Biomedical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan; 6Division of Urology, Department of Surgery; LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan; 7Graduate Institute of Clinical Medical Sciences, College of Medicine, Chang Gung University, Taoyuan, Taiwan

ThP 056 N-terminal Endogeneous Fragments of Tau in Human Cerebrospinal Fluid; Gunnar Brinkmalm; Claudia Cocognola; Erik Portelius; Henrik Zetterberg; Kaj Blennow; Kina Höglund; "University of Gothenburg, Mölndal, Sweden; 2UCL Institute of Neurology, London, UK; 3Karolinska Institutet, Huddinge, Sweden

ThP 057 Developing a Lysosomals Panel for Biomarker Discovery in Neurodegenerative Diseases using PRM; Simon Sjödin; Gunnar Brinkmalm; Annika Öhrfelt; Henrik Zetterberg; Kaj Blennow; "University of Gothenburg, Mölndal, Sweden; 2UCL Institute of Neurology, London, UK

ThP 058 Longitudinal Profiling of Type 1 Diabetes Human Plasma Using TMT10-based Quantitative Proteomics Approach: Chih-Wei Liu; Lisa Bramer; Bobbie-Jo Webb-Robertson; Kathleen Waugh; Marian J Rewers; Qing Zhang; "University of North Carolina at Greensboro, Greensboro, NC; 2Pacific Northwest National Laboratory, Richland, WA; 3University of Colorado School of Medicine, Aurora, CO
**BIOMARKERS: QUANTITATIVE ANALYSIS**

**SMALL MOLECULES & METABOLITES**

**ThP 068**

Profiling of Medium-to-Long Chain acyl-CoAcs Converted from Metabolism of Exogenous Fatty Acids in Mammalian Cells using LC-MS/MS: Xiangkun Yang; University of Georgia, Athens, GA

**ThP 062**

A Validated Multiplex Assay for the Quantification of Tryptophan and Four of Its Catabolites in Human Plasma and Cerebrospinal Fluid: Joachim Hoke1; Andre Liesener2; Stefan Blech1; ‘Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany; ‘Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany

**ThP 064**

In vivo Metabolic Profiling of the TCA Cycle: Stephanie Dale1; Sheerin Shahidi-Latham2; E. Ellen Jones3; Cristine Quisain; ‘Genentech Inc, South San Francisco, CA

**ThP 060**

Comprehensive Profiling of Neuropeptides in Cerebrospinal Fluid by LC-MS/MS: Kanta Horie1; Yoshiaki Sato1; Takashi Kosasa1; Takeyasu Tomioka1; Motohiro Shiotani1; Makoto Ogo1; Yoshiya Oda2; ‘Eisai Co. Ltd., Tsukuba, Japan; ‘Eisai Inc, Woodcliff Lake, NJ

**ThP 066**

A Simultaneous Quantification Method Offrmacroxylic Acid Cycle Precursors and Intermediate: Paul Rainville1; Robert Plumb2; Jose Castro-Perez3; James Langridge4

**ThP 065**

Development of a Quantitative LC-MS Assay to Evaluate Depletion of Wall Teichoic Acid in Staphylococcus Aureus: Olga Berejinaia; Merck & Co., Inc., Rahway, NJ

**ThP 067**

Challenges in Development of LC-MS Methods for Highly Polar, Low Molecular Weight Compounds: A Quantitative Assay for Quinolinic Acid: Regina Oliveira1; Asoka Ranasinghe2; Joelle M Onorato1; Celia D’Arienzo1

**ThP 068**

Development and Validation of a Method for the Determination of Total Plasma Cholesterol Levels to Hydroxyprogesterone (17-OHP) in Human Plasma: Keegan J Nicodemus1; Dana Freeman1; Justin Lamar Brown2; Li Zhang1; Lanning Wang; ‘Centers for Disease Control and Prevention, Atlanta, GA; ‘ORISE Centers for Disease Control and Prevention, Atlanta, GA; ‘Battelle Memorial Institute, Atlanta, GA

**ThP 069**

A Simple, Robust Method for Quantitative Analysis of Bile Acid Biomarkers in Human, Monkey, Dog, Mouse, and Rat Plasma Samples: Angela Q. Shen1; Alyssa Kabat1; Wenin Yuan1; Ritika Kuran2; Brittany Perley1; Steven Wiltshire1; ‘Agilux Laboratories, Worcester, MA; ‘Boehringer Ingelheim Pharma GmbH & Co KG, Biberach, Germany; ‘Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach an der Riss, Germany

**ThP 070**

Simultaneous Determination of Dehydroepiandrosterone (DHEA) and 17-Hydroxyprogesterone (17-OHP) in Human Plasma using LC-MS/MS: Guangnong Zhang1; Gaungchun Zhou1; Feng Yin1; Morgan Byrd1; Tian-Sheng Lu1; Yong-Xi Li1; Medpace Bioanalytical Laboratories, Cincinnati, OH

**ThP 071**

Quantitative Analysis of Serum 2-Hydroxyglutarate using Gas Chromatography-Mass Spectrometry: Sall Kaur Bhowmk1; S. Nagreddy Puttur1,2; Arun Sreekumar1,2; ‘Dept. of Molecular and Cell Biology, Baylor College of Medicine, Houston, TX; ‘Aikek Center for Molecular Discovery, Baylor College of Medicine, Houston, TX; ‘Advanced Technology Care, Baylor College of Medicine, Houston, TX; ‘Verna and Marrs McLean Department of Biochemistry, Baylor College of Medicine, Houston, TX

**ThP 072**

Scaling Up: Improving Automated, High Throughput Measurement of Tobacco-Specific Nitrosamines in Urine by Liquid Chromatography-Atmospheric Pressure Ionization Tandem Mass Spectrometry: Baoyun Xia1; Christina R Brosius2; Yang Xia1; Tonya Guilt1; John Lee1; Keegan J Nicodemus1; Dana Freeman1; Justin Lamar Brown2; Li Zhang1; Lanning Wang; ‘Centers for Disease Control and Prevention, Atlanta, GA; ‘ORISE Centers for Disease Control and Prevention, Atlanta, GA; ‘Battelle Memorial Institute, Atlanta, GA

**ThP 073**

Rapid Quantitative Analysis of 15 Major Bile Acids in Human Serum by UPLC-Tandem Mass Spectrometry: Tian-Sheng Lu1; Aiping Zhu1; Wanqing Lu1; Emily Epure1; Christopher Dietz1; Emily Anstadt2; Robert Clark2; Michael Smith1; Frank Nichols2; Xudong Yao1; Feng Yin1; Morgan Byrd1; Tian-Sheng Lu1; Yong-Xi Li1; Medpace Bioanalytical Laboratories, Cincinnati, OH

**ThP 076**

Quantification of the Organic Acid Biomarkers Pyruvate and Lactate in Biological Matrices: Dylan Bennett1; Allysen Meymaris1; Vikki Tsefriskas1; ‘Agilux Laboratories, Worcester, MA

**ThP 077**

Quantitative Analysis of Short Chain Fatty Acids and Ketone Bodies in Plasma and Tissues as Oximes Derivatives by LC-MS/MS: Huachuan Marc Cao1; Mingfei Zeng1; ‘Eli Lilly and Company, Shanghai, China

**ThP 078**

Quantitation of (C22:6)-bis(monoacylglycerol) phosphate and Profiling of Additional BMPS in Rat Urine as Markers of Phospholipidosis: Joelle Onorato1; Petia Shipkova1; Mike Reilly1; Yan He1; David Nelson2; Lois Lehman-McKeeman1; ‘Bristol-Myers Squibb Co., Princeton, NJ; ‘Bristol-Myers Squibb Co., Princeton, NJ; ‘Bristol Myers Squibb, Princeton, NJ

**ThP 080**

Quantitative Analysis of D-Alanine in Cerebral Spinal Fluid Using a Chiral HPLC Coupled with High Resolution Mass Spectrometry: Brendan Tierney1; Christopher Holliman1; Hangying Gao2; ‘Pfizer, Inc., Groton, CT

**ThP 081**

High Throughput UPLC-MS/MS Method for the Profiling of 11 Hydrosoluble Vitamins in Human Plasma: Oksana Lavrynenko1; Serge Rezzi2; ‘NIHS, Molecular Nutrition Group, Lausanne, CH

**ThP 082**

Detection of Aromatic Amines in Human Urine at ppt Level: a Semi-Automated Hamilton STAR/GC/MS/MS Method: Tiffany Seyler1; Elizabeth Cowan1; Susan Pyatt2; Aaron Danberry3; Kyle Emer1; ‘CDC, Atlanta, GA; ‘Former Associate Fellow, Atlanta, GA; ‘Former ORISE Fellow, Atlanta, GA

**ThP 083**

LC-MS/MS Quantitative Analysis of the Biomarkers Tryptophan, Kynurenic, and Kynurenic Acid in Mouse and Rat Plasma and Brain: Alyssa Kabat1; Brittany Perley1; Steven Wiltshire1; ‘Agilux Laboratories, Worcester, MA
ThP 084 Bioactivation of Heterocyclic Aromatic Amines by UDP Glucuronosyltransferases; Tingting Cai1; Lihua Yao1
Robert Turesky2; 1University of Minnesota at Twin Cities, Minneapolis, MN

ThP 085 Urine Steroid Metabolite Profiling Using LC-HRMS for Diagnosing Adrenal Cortical Carcinoma; Jolaine Hines1; Irina Banocs2; Robert L Taylor3; Raman Deep Singh4; Aditya V Avula5; Stefan K Grebe6; Ravinder J Singh7; 1Mayo Clinic, Rochester, MN

ThP 086 Quantification of Lathosterol in Human Plasma Using UPLC-MS/MS System; Guangchun Zhou1; Tian-Sheng Liu2; Nicole Green3; Yong-Xi Liu4; 1Medpace Bioanalytical Laboratories, Cincinnati, OH

ThP 087 Determination of Amino Acids and Biogenic Amines in Plasma and Urine in Cri Du Chat Disease by Mass Spectrometry; Danielle Zildeana Furtado1; Leticia Dias Lima Jedlicka1; Heron Domingues Silva1; Nilson Antonio Assuncao1,2; 1UNIFESP, São Paulo, Brasil; 2The Scripps Research Institute, La Jolla, CA

ThP 088 Multiplex Quantitative Localized Analysis of Metal-Tagged Antibodies using Event-By-Event Cluster Secondary Ion Mass Spectrometry; Dmitry Verkhotorov1; Kyungin Son2; Stanislav V Verkhotorov3; Michael J Eller4; Alexander Revzin5; Emile A Schweikert6; 1University of Miami, College Station, TX; 2University of California-Davis, Davis, CA

ThP 089 Improvements in LFQ for Reproducible Quantification of Proteomic Experiments: How DDA Outperforms DIA; Ignacio Ortea1; Michael Blank2; Romain Huguet2; David M Horn3; Daniel Lopez Ferrer3; Andreas Huhmer2; 1Keystone Bioanalytical Inc, North Wales, PA; 2Amgen, Inc. South San Francisco, CA

DRUG METABOLISM: QUANTITATIVE ANALYSIS 090 - 107

ThP 090 Anti-Cancer Drug Detection at the Single Cell Level; Shawna Standke1; Ning Pan2; Naga Rama Kothapalli3; Zhibo Yang1; Anthony W. Burgrett1; 1University of Oklahoma, Dept. of Chem & Biochem Norman, OK

ThP 091 Comparative Studies on Intrinsic Clearance Prediction of Low Turnover Compounds Using the Regular and Relay Cryopreserved Hepatocyte Methods; Min Jiang1; Zhicai Wang2; Dan Rock3; 1Amgen, South San Francisco, CA; 2Amgen, Inc. South San Francisco, CA

ThP 092 Evaluation of QTOF HRMS Platform for Highly Sensitive Analysis of Raltegravir in Plasma in Support of Human Microdosing; Li Sun1; Kevin Bateman2; Sukhdev Bangar3; Yun W Aleyunias4; Mark Wrone5; Sheila Breidinger6; Eric Woolf7; 1Merck & Co., Inc., West Point, PA; 2Waters Corporation, Beverly, MA; 3Waters, Milford, MA

ThP 093 Characterization of Ketamine Metabolism in Liver S9 Fractions from Aging Sprague Dawley Rats by Liquid Chromatography Tandem Mass Spectrometry; Raphael Santamaria1; Marie-Chantal Giroix2; Pascal Vachon3; Francis Beaudry1; 1Université de Montréal, St-Hyacinthe, QC

ThP 094 Methods for Analysis of Hydroxywarfarin Regio- and Stereoisomers in Bioanalytical Samples; Karm Keller1; Laura Drake1; Crystal D Sergent2; Edward Wells3; Steve E Unger4; 1Worldwide Clinical Trials, Austin, TX

ThP 095 Determination of Cariprazine and Metabolites in Human Plasma by LC-MS/MS; Jing Ke1; Guiyan Chen2; Allan Xu3; 1Keystone Bioanalytical Inc, North Wales, PA

ThP 096 Characterization of clozapine-N-oxide using LC-MS/MS; Jeffery F Kuhn1; Yu-wei Chen1; Patricia Jensen1; Leesa Deterding1; 1NIEHS, RTP, NC

ThP 097 Development and Validation of a Novel Enzyme Inhibition Assay for Determination of Statin Acid in Human Plasma using LC-MS/MS; Yanjun Hu1; Huafang Jiang1; Junxian Zhao2; Wanhui Liu3; Xinping Fang1; Xin Zhang4; Wenzhong Liang5; 1WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China; 2Lyue Pharma Group Co., Ltd, Yantai, China; 3WuXi AppTec (Shanghai) Co. Ltd., Shanghai, Shanghai

ThP 098 Development and Validation of the Determination of Total CRS3123 in Human Urine by High Performance Liquid Chromatography Tandem Mass Spectrometry; X. Steven Yan1; Marsha L. Luna1; ChenYu Chung2; Julie Showalter3; Yansheng Liu4; Matthew E Hinz5; 1KCAS Bioanalytical & Biomarker Services, Shawnee, KS; 2DynPort Vaccine Company, Frederick, MD

ThP 099 LC-MS/MS Method for the Quantification of Fingolimod and Fingolimod Phosphate in Rat blood with Storage Stability; Rajesh Kumar Boggavarapu1; Nagasurya Prakash Padala1; Praveen kunduru1; Devender Reddy Ajala1; Ramakrishna Nirogi1; 1Suven Life Sciences Ltd, Hyderabad, Telangana

ThP 100 Testing the Ability of UBP-310 to Diffuse into Mouse Brain via LC-MS/MS (QQQ) Quantification; Sandy Stayle1; Russel Pickford2; Justin Nash3; Bryce Vissel1; 1Garvan Institute, Sydney, Australia; 2University of New South Wales, Sydney, Australia

ThP 101 Solving the Enigma of Nitrate Tolerance with a Stable Isotope-Assisted, Multi-Platform Work Flow; Elizabeth Axton1; Eleonoro Cristobal2; Fred Stevens1; 1Oregon State University, Corvallis, OR

ThP 102 Using Triplicate Calibration Curves and Weighted Least Squares Regression to Reduce Experimental Error; Kenneth Anderson1; Kevin P Bateman2; 1Merck & Co., Inc., West Point, PA; 2Merck & Co., Inc., West Point, PA

ThP 103 Systematic Investigation of the Failure of One Analyte during Method Transfer and Cross Check of a 4-in-1 LC-MS/MS Method; Biao Qian1; Daniel Neddermann2; Lihua Qiao3; Yixin Yang1; Xian Zhang4; 1WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China, 2Novartis Pharma AG, Basel, Switzerland

ThP 104 Ionization Efficiency of Oligopeptides and Small Hydrophilic Molecules in ESI/MS; Piia Lissang1; Karl Kaupmees2; Anneli Kruve3; 1University of Tartu, Institute of Chemistry, Tartu, Estonia

ThP 105 In-vitro Metabolic Stability and Profiling of Ponatinib, Vandetanib and Masitinib using Liquid Chromatography Tandem Mass Spectrometry; Sawssan M Amer1; Adnan A. Kadi2; Hany W Darwish3; Mohamed W. Atwa4; 1College of Pharmacy, Cairo University Cairo, Egypt, 2College of Pharmacy, King Saud University Riyadh, Saudi Arabia

ThP 106 Unusual Matrix Effects Observed during Quantitative LC-MS/MS Methods Development; Yuyong Ke1; Nicki Hughes1; Fernand Labrie1; 1Bioanalytical Laboratory Services, a Division of LifeLabs LP, Toronto, Ontario; 2EndoCeutics, Quebec City, QC

ThP 107 Evolution, Development, and Application of a Dynamic, High-Throughput, Enterprise-Level Autosampler for High-Performance LC/MS/MS Bioanalysis; Brendon Kapinos1; John S Janiszewski1; Hui Zhang2; Mary Piotrowski1; Jianhua Liu3; Wayne Lutomski4; Steven Ainley4; 1Pfizer, Groton, CT; 2Sound Analytics, Niantic, CT

FOOD SAFETY: OTHER CONTAMINANTS (PART 2) 108 - 141

ThP 108 Food Safety Detection of Targeted and Unknown Compounds Using OrbitrapTMLC-MS/MS System; Charles T. Yang1; Dipankar Ghosh1; Jamie Humphries2; Nick Duczak2; Caroline Ding1; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Austin, TX

ThP 109 A Multi-Residue Liquid Chromatography/Tandem Mass Spectrometry Method for the Analysis of Macrolides in Food Matrices; Pavel Metalnikov1; Iliya Bato1; Renat
ThP 110
Determination of Wilfordine and Wilforine in Honey using Liquid Chromatography with Tandem Mass Spectrometry; Chen Jianli; Shimadzu, Wuhan, China

ThP 111
Determination and Quantification of Perchlorate in a Fruit Matrix Using Accelerated Solvent Extraction and IC-MS; Kyle Renfew; Amanda Hartman; Nicholas Santiago; Thermo Fisher Scientific, Austin, TX

ThP 112
Determination of Papaverine and Other Alkaloids in Hot Pot Condiment by Direct Analysis in Real Time Mass Spectrometry; Yi Li; Weixia Wang; Xiaohui Xiang; Jiehui Hu; Charles C. Liu; Nanjing Tech University, Nanjing, Jiangsu; ASPEC Technologies Limited, Beijing, Beijing

ThP 113
Use of Ambient Ionization Mass Spectrometry for the Rapid Authentication of Food and Dietary Supplements; Kari Organtini; Gareth Cleland; Beth Loecken; Adam Ladak; Waters, Milford, MA

ThP 114
Accessible and Efficient Screening of Multiclass Contaminants in Food; Eimear McCaill; Ramesh Rao; Adam Ladak; Jennifer Burgess; Waters, Wilmslow, UK; Waters, Milford, MA

ThP 115
Authentication and Chemical Standardization of Licorice Dietary Supplements Using UHPLC-MS/MS; Guannan Li; Charlotte Simm ler; Dejan Nikolic; Shao-Nong Chen; Guido F. Pauli; Richard B. van Bremen; UIC/NHIN Center for Botanical Dietary Supplements Research, Chicago, IL; Department of Medicinal Chemistry and Pharmacognosy, University of Illinois College of Pharmacy, Chicago, IL

ThP 116
Analysis of Phosphodiesterase Type 5 Inhibitors Extracted from Herbal Preparations by DSA-TOF MS; Robert J. Seward; Jason Weisenseel; Craig Young; Wilhad M. Reuter; PerkinElmer, Waltham, MA

ThP 117
Simultaneous Determination of Multiple Plant Growth Regulators in Bean Sprouts using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry; Cheng Zheng; Qiao Yuan Cheng; Weifang Ni; Chengyuan Cai; Jingchao Lin; Yongming Xie; Zhejiang Institute of Food and Drug Control, Hangzhou, China; PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China

ThP 118
High Sensitive Analysis of Peanut Allergen in Cumin and Spice Mix; Clifford Robert; Tairo Ogura; Shimadzu Scientific Instruments, Columbia, MD

ThP 119
Simultaneous Determination of Hormones in Edible Bird’s Nest using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry; Dunning Xu; Leping Zhong; Sannie Zeng; Lihong Yang; Chengyuan Cai; Jingchao Lin; Yongming Xie; Xiamen Entry-Exit Inspection and Quarantine Bureau, Xiamen, China; PerkinElmer Management (Shanghai) Co., Ltd, Shanghai, China

ThP 120
Mass Spectrometry Based Methods to Detect the BoNTE in Catfish Specimen; Tibor Pechan; Olga Pechanova; Jennifer Arnold; Mississippi State University, Mississippi State, MS; Mississippi State University, Starkville, MS; Edward Via College of Osteopathic Medicine - Carolinas Department of Biomedical Science, Spartanburg, SC

ThP 121
Rapid Screening and Quantification of Domoic Acid in Shellfish Homogenates using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS); Pamela S. Cantrell; Callee M. Walsh; Haddan E. Goodman; Pearse McCarron; Kelley Reeves; Wade A. Rourke; Sinead O’Brien; Daniel G. Beach; Protea Biosciences, Morgantown, WV; Protea Biosciences, Inc. Morgantown, WV; National Research Council Canada, Halifax, Nova Scotia, Canada; Canadian Food Inspection Agency, Dartmouth, Nova Scotia, Canada; Marine Institute, Galway, Ireland

ThP 122
Analysis of Diarrhetic Shellfish Poisoning and Azaspiracid Shellfish Poisoning Toxins by Liquid Chromatography-Tandem Mass Spectrometry; Li Yang; Randy Self; James Stuart; Theodore Lapainis; Daniel Rice; Wen-Hsin Wu; James Hungerford; Food and Drug Administration, Bothell, WA

ThP 123
Multi-analyte Investigation in Relation to the Illicit Treatment of Fish Food with Hydrogen Peroxide; Claudio Mediana; Riccardo Aigotti; Federica Dal Bello; Valentina Santoro; Claudio Balocchi; University of Turin, Torino, Italy

ThP 124
Origin Determination of Eastern Oyster (Crassostrea virginica) by Combination of Heavy Metal Concentrations, Whole-Body Bulk and Compound Specific Isotope Analyses; Mayara P. V. Matos; Marc E Engel; Glen P Jackson; Department of Biology, West Virginia University, Morgantown, WV; Florida Department of Agriculture and Consumer Service, Tallahassee, FL; Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV

ThP 125
Quantitative Determination of Veterinary Drug Residues in Eggs by UPLC-MS/MS Using a Simple, Rapid and Effective Cleanup Approach; Sujie XIA; Dimple Shah; Corey C. Shin; Michael S Young; Adam Ladak; Laura Suaholdnik; Shanghai Institute for Food and Drug Control, Shanghai, China; Waters, Milford, MA

ThP 126
Targeted Veterinary Drugs Screening in Food Matrix using EMR QuEChERS and Newly Developed Triple Quadrupole Mass Spectrometer; Yanan Yang; Dan-Hui Yang; Agilent Technologies, Inc, Santa Clara, CA; Agilent Technologies, Santa Clara, CA

ThP 127
Development of Multi-Class, Multi-Residue UHPLC MS/MS Method for Screening/Quantification of Veterinary Drugs in Complex Food Matrices and Related Products; Azeem Hasan; Hui Zhao; John Zulkoski; Barb Mitchell; Thomas Vennard; Katerina Mastovska; Covance, Madison, WI

ThP 128
Extending the Linear Dynamic Range for Measurements Targeting Veterinary Drug Residues in Animal Feed by UPLC-laminar Flow HSID-MS/MS; JASON Kong; Frank Ker o; Joshua Ye; Lisa Cousins; Craig Young; Sharanya Reddy; Ohio Department of Agriculture, Reynoldsburg, OH; PerkinElmer, Shelton, CT; Ionics Mass Spectrometry Group, Bolton, Canada

ThP 129
Mass Spectrometry Reveals Distinct Extracellular Proteins of Food-Borne Escherichia coli O157:H7 and O104:H4; Nazul Islam; Attila Nagy; Garrett M. Wesley; Xiangwu Nou; Bret Cooper; Dan Shelton; University of Maryland, College, College Park, MD; Environmental Microbial and Food Safety Laboratory, USDA-ARS, Beltsville, MD; Animal Biosciences and Biotechnology Laboratory, USDA-ARS, Beltsville, MD; Soybean Genomics and Improvement Laboratory, USDA-ARS, Beltsville, MD

ThP 130
Meat Species Identification by Protein Profiling and Spectral Fingerprinting using MALDI-TOF-MS; Man On So; The Hong Kong University of Science and Technology, Hong Kong SAR, HK

ThP 131
Dispersive Liquid Liquid Microextraction of Beta-agonist Residues from Bovine Muscle and Their Determination using ESI-LC-MS/MS; Phomolo Kgotli; Simiso Dube; Mathew Mzi Nindi; Botswana National Veterinary Laboratory, Gaborone, Botswana, Gaborone, Botswana; University of South Africa, Florida Park, Roodepoort, Gauteng; University of South Africa, Department of Chemistry, College of Science Engineering and Technology, Unisa Science Campus, Florida Park, Roodepoort, South Africa
ThP 132  Quantification of Brominated Fatty Acids in Rat Tissues and Serum using Isotope Dilution UPLC/ESI/MS/MS; Kellie Woodling1; Priyanka Chitranshi1; Goncalo Gamboa da Costa2; 1FDA/NCTR, Jefferson, AR

ThP 133  Matrix-Standardization and Post-Extraction Addition of Internal Standard to Overcome Challenges during LC/MS/MS Quantification of Neomycin and Oxytetracycline in Rabbit Tissues; Aimin Tan1; Xuan Susan Gu1; Molly Wong2; Gordon Bolger2; Albert Licollari3; John C Fanaras3; 1Nucro-Technics, Scarborough, ON; 2Nucro-Technics, Scarborough ON, Canada

ThP 134  Determination of Meat Authenticity using a Comprehensive Proteome Strategy, Data-Independent Acquisition and High-Resolution Mass Spectrometry; Alberto Ruiz Orduna1; Erik Husbys2; Claudia P. Martins2; Dipankar Ghosh3; Francis Beaudry4; 1Université de Montréal, St-Hyacinthe, QC; 2Thermo Fisher Scientific, San Jose, CA

ThP 135  A Green Sample Preparation Method for the Determination of Chloramphenicol and its Metabolite Residues in Meat and Milk using ESI-LCMS/MS; Ompelege E Kemborgatla1; Simiso Dube2; Mathew Muzi Nindi1; 1Botsswana National Veterinary Laboratory, Gaborone, Botswana; 2Gaborone, Gaborone, Botswana; 3University of South Africa, , Florida Park, Roodepoort, Gauteng; 4Department of Chemistry, College of Science and Technology, Unisa Science Campus, Florida, Roodepoort , Republic of South Africa, Florida Park, Roodepoort, South Africa

ThP 136  Direct Quantitative Analysis of Lean Meat Essence in Pork Tissues using Internal Extractive Electrospray Ionization Mass Spectrometry; Yipo Xiao1; Halyan Lu1; Jianyong Zhang2; Yiping Wei1; Huawei Chen1; 1East China Institute of Technology, Nanchang, China; 2Department of Cardiothoracic Surgery to Second Affiliated Hospital of Nanchang University, Nanchang, China; 3East China University of Technology, Nanchang, Mainland

ThP 137  DART-HRMS and MS/MS of Spectra of Sweeteners for Screening Beverages; Luke K Ackerman1; Romina Shah1; 1FDA/CFSAN, College Park, MD

ThP 138  Direct Determination of Four Pyrazole Fungicides in Grape Wines by Paper Spray Mass Spectrometry; Han Chao1; Fan Pu1; Wenpeng Zhang2; Zheng Ouyang3; 1Wenzhou Entry-Exit Inspection and Quarantine Bureau, Wenzhou, China; 2Weldon School of Biomedical Engineering, Purdue University, West Lafayette, IN; 3Purdue University-Department of Chemistry, West Lafayette, IN

ThP 139  Assay of Resveratrol in Red Wine by Paper Spray Tandem Mass Spectrometry and Isotope Dilution; Fabio Mazzotti1; Domenico Taverna1; Leonardo Di Donna2; Lucia Bartella2; Anna Napoli1; Giovanni Sindona1; 1Dipartimento di Chimica e Tecnologie Chimiche Università della Calabria, Rende, Italy; 2Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Rende, Italy

ThP 140  Rapid Assay of Multi-Class Antimicrobials Residues in Food of Animal Origin by Paper Spray Mass Spectrometry; Yuan Su1; Zheng Ouyang1; 1Purdue University, West Lafayette, IN

ThP 141  Weight-loss Herbal Medicine Control Quality and Authenticity by Paper Spray Ionization Mass Spectrometry; Gésica A Vasconcelos1; Verónica Carvalho1; Carla Freitas1; Igor da Silva1; Ricardo Borges2; Wanderson Romão1; 1Bionavicio Gentilio Vaz1; 2Federal University of Goiás, Goiânia, Brazil; 3Federal University of Espirito Santo, Vitória, Brazil; 4Federal University of Goiás, Goiânia, GO

ThP 142  Determination of Pesticide Residues in Traditional Chinese Medicinal Materials Milkvetch Root; Xizhi Wang1; Shiheng Luo1; Feifei Tian1; Guixiang Yang1; Jun Fan2; Taohong Huang2; Shin-ichi Kawano2; Yuki Hashi2; 1Shimadzu (China) Co., Beijing, China; 2Shimadzu (China) Co., Shanghai, China

ThP 143  Efficient Headspace Extraction of Plasticizers from Aqueous and Ethanolic Extracts; Douglas Doster; Aspen Research Corporation, New Germany, MN

ThP 144  Analysis of Isomeric Metabolites by GC-EI/PI/PI-MS; Takeshi Furushashi1; Koji Okuda2; Akihiko Kusai2; Takemichi Nakamura2; Ryukyu University, Okinawa, Japan; 1JEOL Ltd., Akishima, Japan; 2RIKEN, Wako, Japan

ThP 145  Determination of Tobacco-Specific N-nitrosamines in Mainstream Cigarette Smoke using in-pipette-tip Solid-Phase Extraction; Yan-bo Luo1; Xiao-Jing Chen1; Hong-Fei Zhang1; Xing-Yi Jiang1; Xue Li2; Xiang-Yu Li1; Feng-Peng Zhu1; Yong-Qiang Pang1; Hong-Wei Hou1; 1China National Tobacco Quality Supervision and Test Center, Zhongzhou, China

ThP 146  Substance Characterization of Polyphenyelene by EI GC/MS. O. David Sparkman1; Kirill Ttreyakov2; Patrick Batoon1; Isuko Iwai Iwa1; Terry L. Ramus1; 1University of the Pacific, Antioch, CA; 2Dakota Consulting Inc., Silver Springs, MD; 3University of the Pacific, Stockton, CA; 4Diablo Analytical, Antioch, CA

ThP 147  Multi Pesticides Residue Analysis in Ayurvedic Cough Syrup by GCMS/IMS using QuEChERS’ Extraction Method; Durvesh Sawant1; Ankush Bhone1; Dheeraj Ramus4; 1Shimadzu Analytical (India) Pvt. Ltd., Navi Mumbai, India; 2Dakota Consulting Inc., Silver Springs, MD; 3University of the Pacific, Stockton, CA; 4Diablo Analytical, Antioch, CA

ThP 148  Study of the Electron Ionization Fragmentation Patterns of 1-Alkoxyalkylohydroxenes; Kreg theorem

ThP 149  Identification of Leachable Impurities from Pharmaceutical Container Closure Materials using Orbitrap Based GC-MS; Andrew Feilden1; Richard Barlow2; Jason Cole2; Paul Silcock2; Kyle D’Silva1; Alexander Semenyov1; 1Thermo Fisher Scientific, Runcorn, UK; 2Smithers Rapra, Shawbury, UK; 3Thermo Fisher Scientific, Austin, TX; 4Thermo Fisher Scientific, Austin, TX

ThP 150  Determination of Ceramides using GC/Q-TOF with a Novel High Efficiency Source, Jennifer Sanderson1; Viorica Lopez-Avila1; Sofia Nieto1; 1Agilent Technologies, Santa Clara, CA

ThP 151  Differentiation between Type of Dialkyl Phthalates Based on their EI Mass Spectra; O. David Sparkman1; Jianhua Ren Ren2; Patrickhenny Batoon2; Sven Hackbush2; Andreas H Franz1; 1University of the Pacific, Antioch, CA; 2University of the Pacific, Stockton, CA

ThP 152  Quantitative Determination of Dioxins in Drinking Water by Isotope Dilution Triple Quadrupole GC-MS/MS; Jackie Jackie1; Chong Chiew Mei1; Yeong Hui Xian Crystal1; Lahey Cynthia Melanie1; Lou Sai Chin1; Shimadzu (Asia Pacific) Pte Ltd, Singapore

ThP 153  GC/MS Metabolomics: Metabolic Mapping of Prostate Cancer Cell Lines; Jan Crowley1; 2; Kristopher Kirmess2; Jeffrey Arnett1; Kevin Yarasheski1; 3; Joseph Ippolito1; 1Washington University, St Louis, MO; 2Department of Medicine, Washington University St. Louis, MO; 3Washington University in St Louis, St Louis, MO
ThP 154  Characterization of Little Cigar Smoke Tar by GC-MS; Steven Reaber1; Arunava Ghosh1; Robert Taran1; Gary L. Glish1; 1The University of North Carolina at Chapel Hill, Chapel Hill, NC

ThP 155  Development and Validation of an Analytical Method to Quantitate Sulfonyl in Rodent Plasma by GC/MS; veronica Robinson1; Teruyo Uneoyama2; Brenda Fletcher2; Stephen Cooper2; Melanie R. Rehder Silinsky3; Reshan Fernandez4; Suramyia Waidyanatha2; 1NI/EHS/NIH, RTP, NC; 2RTI International, RTI Int Research Triangle Park, NC

ThP 156  Fast and Accurate Analysis of Fluorotolene Alcohols and Acrylates using Triple Quadrupole GC/MS; Cynthia Melanie Lahey1; Guo Wei Elgin Ting2; Hui Xian Crystal Yeong3; Jackie Jackie4; Chiew Mei Chong5; Lai Chin Loo6; 1Shimadzu Analytical (India) Pvt. Ltd, Singapore; 2Nanyang Technological University, Division of Chemistry and Mathematical Biology, School of Physical and Mathematical Sciences, Singapore

ThP 157  Evolved Hydrogen Gas Analysis from the Industrial Materials using a Quadrupole Mass Spectrometer; Masahiro Hashimoto1; Koji Okuda1; Makoto Okano2; Tetsuo Higuchi2; Akishko Kusai3; 1JEOL Ltd., Akishima, Japan; 2Bilkent University, Bilkent University 06800 Bilkent Ankara, Turkey

ThP 158  Qualitative Determination of Aromatic Amines Formed from Azo Dyes in Textile using GC/MS/MS; Ankush Bhone1; Durvesh Sawant1; Dheeraj Handique1; Prashant Hase1; Sanket Chiplunkar1; Ajit Datar1; Jitendra Kelkar1; Pratap Rasam1; 1Shimadzu Analytical (India) Pvt. Ltd, Mumbai, INDIA

ThP 159  Chemical Profiling of Whiskies using Orbitrap GC-MS; Roberts Dominic1; Jana Hajslova1; Michal Stupak1; Jana Pulkrobova1; Jason Cole2; Paul Silcock2; 1Thermo Fisher Scientific, Runcorn, UK; 2Institute of Chemical Technology, Prague, Czech Republic; 3Thermo Fisher Scientific, Austin, TX

ThP 160  Analysis of Volatile Organic Compounds in Crude Oil using High Resolution Orbitrap GC/MS; Aikaterini Kondyl1; Wolfgang Schrader1; 1Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany

ThP 161  Metabolic Profiling of Arabidopsis Tissue Extract using GC-MS/MS Technology; Pratap Rasam1; Sue E Fenton1; Leesa J Deterding1; Fred Bjorn Lih1; Deirdre K Outten2; Patrick Frantom1; 1University of North Carolina at Chapel Hill, Chapel Hill, NC; 2The Scripps Research Institute, Jupiter, FL

ThP 162  Insights into Dynamics of SufBC2D Fe-S Scaffold of AIMP3 (aminoacyl-tRNA Synthetases-Interacting Multifunctional Proteins) Revealed by H/D Exchange Mass Spectrometry; Shiri Guan1; Guanchao Dong2; Wayne Outten2; Patrick Frantom1; 1University of Alabama, Tuscaloosa, AL; 2University of South Carolina, Columbia, SC

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION (PART 2) 172 - 195

ThP 163  Chemical ionization Mass Spectrometry of Variations of a Peptide Probe: Azido-TRPTK; Remy Souza1; Douglas Papenmeier1; Steven C. Weddle1; 1University of Western Ontario, London, ON; 2University of Western Ontario, London, ON (UK)

ThP 164  Determining Toxic Byproducts from Pyrolytic Reactions via Pyrolysis/Gas Chromatography/Mass Spectrometry Techniques; Douglas Papenmeier2; Steven C. Weddle3; Eric J. Miklaszewski1; Caroline K. Wilharm1; Matthew A. Neiswinger1; Jonathan M. Dilger1; 1Special Warfare and Expedi- tionary Systems Department, Naval Surface Warfare Center, Crane Division, Crane, IN; 2Spectrum Warfare Systems Department, Naval Surface Warfare Center, Crane Division, Crane, IN; 3Science Applications International Corporation (SAIC), Crane, IN

ThP 165  A Novel Ladder Approach for the Characterization of Disononyl Phthalate using GC-MS; Ian W. Shaffer1; Josh Allen Willhite2; William R. LaCourse2; 1University of Maryland, Baltimore County Baltimore, MD; 2Transition Metal Catalyzed Lignin Hydrotreatment and Determination of Products by GC-MS and Thermal Carbon Analysis; Honna Bilek; University of North Dakota, Grand Forks, ND

ThP 166  Rapid On Site Analysis of BTEX Aromatics with a Miniaturized Field Portable Gas Chromatograph-Mass Spectrometer; Alan Gallasy1; Frank Kero1; 1PerkinElmer, Oak Brook, IL; 2PerkinElmer, Wallaam, MA

ThP 167  Comparison of Headspace Methods for GC/MS Analysis of Foods; Adam J. Patkin1; Sharanaya Reddy2; David Scott1; Leeman Bennington1; Lee Marotta1; 1PerkinElmer, Shelton, CT

ThP 168  Unambiguous Identification of Reaction Products from Conversion of Nitric Oxide over Novel Photocatalyst Surfaces; Ian G. M. Anthony1; Matthew R Brantley1; Adam R Floyd1; Abayomi D. Olaitan1; Deniz A Erdogan1; Emrah Özensoy1; Tourajd Solouki1; 1Baylor University, Waco, TX; 2Bilkent University, Bilkent University 06800 Bilkent Ankara, Turkey

ThP 169  Development and Validation of an Analytical Method to Quantitate Sulfolane in Rodent Plasma by GC/MS; Min Guo2; Alan Gallaspy1; Frank Kero2; 1PerkinElmer, Shelton, CT; 2Spectrum Warfare Systems Department, Naval Surface Warfare Center, Crane Division, Crane, IN; 3University of North Carolina at Chapel Hill, Chapel Hill, NC

ThP 170  Probing the Structural Dynamics of the Prokaryotic Amino Acid Transporter LeuT by Hydrogen/Deuterium Exchange Mass Spectrometry; Patrick Sascha Merkle1; Kamil Golfrty2; Uli Gethér2; Claus Juul Løland2; Kasper Dyrberg Rand1; 1Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; 2Department of Neuroscience and Pharmacology, University of Copenhagen, Copenhagen, Denmark

ThP 171  pH Modulation of Myristate Exposure in the Human Immunodeficiency Virus Type-1 Matrix Protein: A Hydrogen Deuterium Exchange Mass Spectrometry Study; Yiming Xiao1; Gary S. Shaw2; Lars Konemann2; 1University of Western Ontario, London, ON; 2University of Western Ontario, London, ON (UK)
**ThP 178**

**Gas-phase Hydrogen Deuterium Exchange as a Structural Probe: Assessing Similarities in Gas- and Solution-Phase Peptide Structures**

Mahdiar Khakinejad1; Samaneh Ghasabai-Kondaladj1; Stephen J Valentine1; West Virginia University, Morgantown, WV

**ThP 179**

**HDX-MS to Map the Allosteric Site for Efavirenz, a Drug that Stimulates Cholesterol-Metabolizing P450 CYP46A1 Activity**

Kyle W Anderson1,2; Natalia Mast1; Jeffrey W Hudgens1,2; Joseph Lin1; Iliarion V Turko1; Irina A Pikuleva1; National Institute of Standards and Technology, Gaithersburg, MD; Institute for Bioscience and Biotechnology Research, Rockville, MD; Case Western Reserve University, Cleveland, OH

**ThP 180**

**Characterization of Conformation of Therapeutic Antibody Aggregation with Optimized Hydrogen/Deuterium Exchange Mass Spectrometry**

Shanhua Lin1; Terry Zhang2; David M Horn2; Stephane Houel2; Xiaodong Liu2; Jonathan L Josephs1; Thermo Fisher Scientific, Sunnyvale, CA; Thermo Fisher Scientific, San Jose, CA

**ThP 181**

**Rapid Mapping of Antigen-Antibody Binding Sites utilizing Oxidative Footprinting and New Software**

Yining Huang1; Ke Sherry Li1; Manolo D. Plasencia1; Henry Liu1; Jonathan L Josephs2; Braden Sweeting3; Marcy Taylor3; Mark Reed3; Derek J. Wilson2; Esben Trabjerg1,2; Fredrik Kartberg2; Søren Domer; Lundbeck A/S, Brøndby, Denmark

**ThP 182**

**Conformational Characterization of Nerve Growth Factor-b and the Impact of its Regulatory Pro-Part Domain**

Ebens Traerberg1; Fredrik Karlberg2; Søren Christensen1; Kasper D. Rand1, Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; Lundbeck A/S, Valby, Denmark

**ThP 183**

**Time-Resolved Hydrogen Deuterium Exchange Reveals the Structural Basis of Amyloidogenesis Inhibition by Alzheimer’s Drug Candidates**

Shaoalong Zhu1; Bin Deng2; Braden Sweeting1; Marcy Taylor1; Mark Reed1; Derek J. Wilson2; York University, Toronto, Ontario; York University, Toronto, Canada; Treventis Corporation, Toronto, Canada

**ThP 184**

**Equilibrated and Kinetic Epitope Mapping for Therapeutic Antibodies by Time-Resolved ElectroSpray Ionization Hydrogen Deuterium Exchange (TRESI-HDX) Mass Spectrometry**

Bin N/A Deng1; Shaoalong N/A Zhu1; Cristina N/A Lento1; Derek J. Wilson1; York University, Toronto, Canada

**ThP 185**

**Conformational Changes in the Regulatory Domains of the Tec-family Tyrosine Kinase Btk upon Lipid Interaction**

Thomas E Waile1; Ragi E. E Joseph2; Amy H. Andretto1; John R. R Engen1; Northeastern University, Boston, MA; Iowa State University, Ames, IA

**ThP 186**

**Probing Protein Surface Chemistry and Unfolding Pathways by Coupling Gas-Phase HDX and Native MS**

Shane A Chandler1; Todd H Milze1; Michael R Morris2; Justin L. P. Benesch1; Oxford University, Oxford, UK; Waters, Wilmotkow, UK

**ThP 187**

**Deprotection by Interaction in HXMS: A Glimpse into a Highly Dynamic Cellulolytic System**

Alan Kadek1; 2; Daniel Kavan1; 2; Roland Ludwig1; Petr Halada1; Petr Man1; 2; Institute of Microbiology CAS, Prague, Czech Republic; Faculty of Science, Charles University in Prague, Prague, Czech Republic; University of Natural Resources and Applied Life Sciences (BOKU), Vienna, Austria

**ThP 188**

**HDX/MS of the E. coli Replicative DNA Polymerase Identifies Stabilizing Interactions between the DNA Sliding Clamp, Exonuclease and Clamp Loaders**

Rafael Fernandez Leiro1; Sarah Louise Maslen1; Meindert H Lamers1; Mark Skehel1; MRC Laboratory of Molecular Biology, Cambridge, UK; Medical Research Council, Cambridge, Cambridgehire

**ThP 189**

**Protein Footprinting and Mass Spectrometry Map the Interface of Marburg virus VP24 interacting with Keap1**

Jing Li1; Britney Johnson2; Daisy W Leung3; Christopher F Basler1; Gaya K Amarasinghe1; Michael L Gross1; Washington University in St. Louis, St. Louis, MO; Washington University School of Medicine, St. Louis, MO; Mount Sinai School of Medicine, New York, NY

**ThP 190**

**HDX-MS Characterization of Selective Modulators for Retinoic-acid Receptor-related Orphan Receptor RORγT in Protective Immune Therapy**

Venkat Dharmarajan1; Scott Novick2; Mi Ra Chang2; Christelle Doebelin2; Ruben Garcia-Ordonez2; Ted Kamenecka2; Pat Griffin2; Scripps Research Institute, Jupiter, Florida, Jupiter, FL; The Scripps Research Institute, Jupiter, FL

**ThP 191**

**Probing Cadherin Adhesive Interactions by Hydrogen/Deuterium Exchange with Positive Electrospray 14.5 T FT-ICR Mass Spectrometry**

Pellu Li1; Samantha Davila2; Susan Diane Pedigo1; Alan G Marshall1,2; National High Magnetic Field Lab, Tallahassee, Florida; Department of Chemistry and Biochemistry, University of Mississippi, University, MS; National High Magnetic Field Laboratory, Tallahassee, FL; Florida State University, Tallahassee, FL

**ThP 192**

**Conformation-specific Interactions with Tomm34 Move Footprint 70 Folding and ATPase Activities**

Jiri Haunser1;2; Michal Durech1; Filip Troka2; Dominika Coufalova2; Daniel Kavan1 2; Petra Dvorakova4; Lenka Hrenychova4; Elizabeth A. Blackburn4; Petr Man1 2; Petr Muller3; Borivoj Vojtisek2; Institute of Microbiology CAS, Prague, Czech Republic; Faculty of Science, Charles University in Prague, Prague, Czech Republic; RECAMO, Masaryk Memorial Cancer Institute, Brno, Czech Republic; Edinburgh Centre for Chemical Biology, University of Edinburgh, Edinburgh, UK

**ThP 193**

**Beyond Structure Characterization: Structure Dynamics (Hydrogen deuterium exchange) Guided Biocatalyst Improv**

Susie Dai; Office of the Texas State Chemist, Department of V, College Station, TX

**ThP 194**

**Structure and Dynamics of RNA Binding to the Non-Canonical RNA Recognition Motif (RRM2) in Human La Protein**

Kerene Brown1; Mark Bayfield1; Derek Wilson1; York University, Toronto, Ontario; York University, Toronto, Canada

**ThP 195**

**Determination of Site-specific Protein-Ligand Binding Affinities using Protein Ligand Interaction Mass Spectrometry Titration and Hydrogen Deuterium Exchange (PLIMSTEX) Strategy**

Jagat Adhikari1; Don L. Rempel1; Michael L Gross2; Washington University in St. Louis, St Louis, MO; Washington University in St. Louis, St Louis, MO

**IMAGING MS: METHOD DEVELOPMENT (MALDI)**

**ThP 196**

**Regional Analysis of Anacardic Acids on the Surface of Pelargonium xhortorum (Geranium) Leaves using MALDI-MSI with a New Stable Matrix**

Marta Yapner1; Bryan Wessel1; David Schultz2; Department of Chemistry, University of Louisville, Louisville, KY; Department of Biology, University of Louisville, Louisville, KY

**ThP 197**

**Method Development for Imaging Mass Spectrometry on Dense Mineralized Tissue of Mouse Incisors**

Madeline Colley1; Yong-Hee Patricia Chun2; Stephan BH Bach1; University of Texas at San Antonio, San Antonio, TX; UT Health Science Center at San Antonio, San Antonio, TX

**ThP 198**

**MALDI-MSI for the Study of Flow-Cell and Agar Bound Microbial Biofilms**

Bin Li1; Sage Dunham2; Tong Si2; Ning Yang3; Clint Arnett3; Sweedler Jonathan2; University of Illinois at Urbana-Champaign, Urbana, IL; University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; Engineer Research and Development Center-Construction Engineering Research Laboratory (ERDC-CERL), Champaign, IL
THURSDAY POSTERS

ThP 199 Microscopic MALDI-imaging Mass Spectrometry in Intestinal Tumors of Apc Mutant Mice using Two-Step Matrix Application; Shuichi Shimma1; Satoko Osawa2; 3; Masahiro Aoki3; 4; Yasushi Kojima3; 4; Tomoyoshi Soga3; 4; 1Osaka University, Suita, Osaka; 2AMED-CREST, Tokyo, Japan; 3Osaka University, Suita, Japan; 4Aichi Cancer Center, Nagoya, Japan; 5Keio University, Tsukuba, Japan Imaging of Lipids using 2,6 Dihydroxyacetophenone Matrix with an AP-MALDI Source; Ludovic Muller; Shelley N Johnson; Aurelie Roux; Berk Oktem; Vladimir M Doroshenko; Amina S Woods; 1NIH/NIDA-IRP, Baltimore, MD; 2All Children’s Hospital Johns Hopkins Medicine, Saint Petersburgh, FL; 3MassTech, Inc, Columbus, MD

ThP 200 Enhanced On-Tissue Analyte Derivatization with Electrospray Deposition of Reagents for MALDI MS Imaging of Neurotransmitters; Qian Wu1; Stanislav S. Rubakhin1; Troy J. Comi1; Jonathan V. Sweedler1; 1University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

ThP 201 MALDI FTICR-IMS of a Mouse Lung for 3D Imaging and Reconstruction; E. Ellen Jones1; Stephanie Dale1; Katherine A Kellersberger2; Christian Berg; Cristine Quaison; Sheerin Shahidi-Latham3; 1Genentech Inc, South San Francisco, CA; 2Bruker Daltonic, Billerica, MA

ThP 202 From 2D to 3D MALDI Imaging Mass Spectrometry - A Reconstruction of a Multidimensional Image Epididymis; Regis Lavigne1; Blanilde Guevel1; Michael Becker2; Janine Beckmann1; Dennis Trede1; Herbert Thiele1; Melanie Lagarrigue2; Charles Pineau1; 1Protim, Rennes, France; 2Bruker Daltonic GmbH, Bremen, Germany; 3SCiLS GmbH, Bremen, Germany; 4Fraunhofer MEVIS Project Group Image Registration, Luebeck, Germany

ThP 203 Quantitative MALDI-MS Imaging of Tumour Spheroids; Rebecca Day1; Laura Cole1; Ieva Palubeckaite1; David Smith1; Neil Cross2; Malcolm R Clerch1; 1Sheffield Hallam University, Sheffield, UK

ThP 204 MALDI Directed – Infrared Laser Ablation Sample Transfer for Spatially Resolved Biomolecule Analysis; Kailin Wang1; Fabrizio Donnarumma1; Kermit K Murray1; 1Louisiana State University, Baton Rouge, LA

ThP 205 In-parallel MS and MS/MS MALDI Imaging without Having to Sacrifice Spatial Resolution; Rebecca Hansen1; 2; Young Jin Lee1; 2; 1Iowa State University, Ames, IA; 2Iowa State University-US DOE, Ames, Iowa

ThP 206 MALDI Imaging-Driven Microproteomics Workflow for Biomarker Discovery Assays; Deborah Alberts1; Rémi Longuespée1; Charles Pottier2; Nicolas Smaragdoss1; Gabriele Mazuccelli1; Dominique Balivair1; Philippe Delvenne3; Fabien Pamelard1; Gaël Picard de Muller1; Edwin De Pauw1; 1Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 2Proteoglypha GmbH, Trier, Germany; 3Department of pathology, University of Liége Liege, BELGIUM; 4Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 5Mass Spectrometry Laboratory, University of Liege, Liege, Belgium; 6GIGA Proteomics Facility, University of Liege, Liege, Belgium; 7imaBiotech, Lille, France

ThP 207 Method Development on a MALDI Orbitrap Platform to Achieve High Throughput in situ DDA Analysis via Multiplex Mass Spectrometric Imaging; Chuanzi OuYang1; Bingming Chen1; Lingjui Li1; 1University of Wisconsin Madison, Madison, WI

ThP 208 A Rapid, Cell Culture-Based Method for Biomarker Discovery and Drug Screening by MALDI-MSI; Courtney E Chandler1; Alison J Scott1; George A. Belov1; David R Goodlett1; Shane Ellis1; Robert K Ernst1; 1University of Maryland Baltimore, Baltimore, MD; 2University of Maryland, College Park College Park, MD; 3Maastricht University, Maastricht, NL

ThP 209 Microscopic MALDI-imaging Mass Spectrometry in Intestinal Tumors of Apc Mutant Mice using Two-Step Matrix Application; Shuichi Shimma1; Satoko Osawa2; 3; Masahiro Aoki3; 4; Yasushi Kojima3; 4; Tomoyoshi Soga3; 4; 1Osaka University, Suita, Osaka; 2AMED-CREST, Tokyo, Japan; 3Osaka University, Suita, Japan; 4Aichi Cancer Center, Nagoya, Japan; 5Keio University, Tsukuba, Japan Imaging of Lipids using 2,6 Dihydroxyacetophenone Matrix with an AP-MALDI Source; Ludovic Muller; Shelley N Johnson; Aurelie Roux; Berk Oktem; Vladimir M Doroshenko; Amina S Woods; 1NIH/NIDA-IRP, Baltimore, MD; 2All Children’s Hospital Johns Hopkins Medicine, Saint Petersburgh, FL; 3MassTech, Inc, Columbus, MD

ThP 210 History-Directed Lipid Identification: Advanced Imaging Mass Spectrometry and Liquid Extraction Technologies Enable Spatially Specific Tandem Mass Spectrometry; Daniel Ryan1; Boone Prentice1; Raf Van de Plass2; Jeffrey Spraggins3; Richard M Caprioli4; 1Vanderbilt University, Nashville, TN; 2Delft University of Technology, Delft, Netherlands

ThP 211 Bottom-up Imaging of Prostate-Cancer Protein Biomarkers by MCAEF (Matrix Coating Assisted by an Electric Field)-LDI/FTMS; Teesha C Baker1; Jun Han2; Darryl B Hardie3; Christopher H Borchers4; 1Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada; 2University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3University of Victoria - Genome BC Proteomics Centre, Victoria, BC

ThP 212 MALDI Imaging for the Quantification of Small Molecules and the Understanding of Toxicity Mechanisms; Melanie Lagarrigue; Régis Lavigne; Andrew Palmer; Charles Pineau; 1; 2Protim, Rennes, Brittany; 2Protim - Inset Inserm U 1085, Rennes, France; EMBL, Heidelberg, Germany; 2Protim, IRSEE, Germany; 1Protim - Erset Inserm U 1085, Rennes, France; 2University Rennes 1, Rennes, France

ThP 213 An Investigation of MALDI Imaging with Higher Speed Sample Stage “Rastering” from an Ion Mobility Enabled Q-TOF Mass Spectrometer; Towers Mark1; Paul Murray1; Migas Lukasz2; Claude Emmanuelle1; Hoyes Emmy1; Chapman Richard1; 1Waters, Wilmslow, UK; 2University of Manchester, Manchester, UK

ThP 214 High-Throughput Single Cell Analysis using High Spatial Resolution and High Sensitivity Imaging Mass Spectrometry; Bo Yang1; Jeffrey M Spraggins2; Richard M Caprioli3; Jeremy L Norris3; 1Vanderbilt University MSRC, Nashville, TN

ThP 215 Lobolly Pine Seedling Imaging Analysis by DESI-MS and MALDI-MS; Michelle Reid1; Gary F Peter2; Richard A Yost1; 1University of Florida, Gainesville, FL

IMAGING MS: SMALL MOLECULES 216 - 247

ThP 216 Exploring the Chemical Ecology of Fungi via Secondary Metabolite Distribution; Vincent Siria1; Huzefa Raja1; Cedric Pearce3; Nicholas H Oberlies1; 1UNC - Greensboro, Greensboro, NC; 2MycoSynthetix, Hillsborough, NC

ThP 217 Microbial Metabolite and Lipid Analysis by Imaging Laser Desorption Ionization Mass Spectrometry on Silicon Nanopost Array Platforms; Rachelle Jacobs1; Akos Vertes1; 1George Washington University, Washington, District of Columbia

ThP 218 Optimizing the Production of Fungal Epipolythiodioxopiperazinol Alkaloids Facilitated by Rapid Analysis via the droplet-LMJ-SSP Coupled with UPLC-PDA-HRMSMS/MS; Soumia Amrine1; Huzefa Raja1; Cedric Pearce3; Nicholas Oberlies1; 1UNC Greensboro, Greensboro, NC; 2MycoSynthetix, Hillsborough, NC

ThP 219 Profiling Secondary Metabolites from a Culture Evaluation of Penicillium restrictum with Droplet-Liquid Microjunction Surface-Sampling Probe; Diana Kao1; 1University of North Carolina at Greensboro, Greensboro, NC

ThP 220 MALDI-FTMS Imaging Reveals Secondary Metabolites Produced during Interaction of Micro-Organisms with Higher Organisms: Dirk Wunderlich1; Jens Fuchser2; Stephanie Grond1; Florian Zubeli; Dorothee Wiesbrod1; 1Bruker Daltonics, Bremen, Germany; 2Protim - Irset Inserm U 1085, Rennes, France; 3University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 4University of Victoria - Genome BC Proteomics Centre, Victoria, BC

ThP 221 Mass Spectrometry Imaging of Curtobacteriumsp. ER1/6, an Endophytic Bacterium with Potential Biocontrol against Citrus-Variegated Chlorosis; Francisca D. S. Araujo1; Dainene S. Santos2; Welington L.
THURSDAY POSTERS

ThP 222 Imaging Mass Spectrometry of S-containing Metabolites in Asparagus officinalis: Ryo Nakabayashi1; Tetsuya Mori1; Hiroshi Sudo1; Kuminori Toyooka1; Kazuki Saito1, 2; RIKEN Center for Sustainable Resource Science, Yokohama, Japan; 3; Hoshi University, Shinagawa, Japan; 4; Chiba University, Chiba, Japan

ThP 223 MALDI Imaging Mass Spectrometry Revealed the Different Distribution Patterns of Anthocyanin Species in Strawberry: Hirofumi Enomoto1; Ryosuke Sato1; Hisakazu Yamane1; Fumiaki Yoshizawa1; Teikyo University, Utsunomiya, Japan; 2; Utsunomiya University, Utsunomiya, Japan

ThP 224 Three-dimensional Visualization of Membrane Phospholipid Heterogeneity in Arabidopsis thaliana seeds by MALDI-MS Imaging: Drew Sturtevant1; Maria Dueñas1; Young Jin Lee1; Kent D. Chapman1; University of North Texas, Denton, TX; 2; Center for Plant Lipid Research, Denton, TX; 3; Iowa State University, Ames, IA; 4; Ames Laboratory-US DOE, Ames, IA

ThP 225 Spatial Distribution of Lipids in Coffee Leaves (Coffea arabica) using MALDI Imaging Mass Spectrometry: Karen T. Henández-Osorio1; Jeferson A. Valencia-Dávila1; Cristian Blanco-Tirado1; Marianny Y. Combariza1; 1; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

ThP 226 Localization of the Salvinorin A diterpenoid Pathway in Savia divinorum by MALDI-FTICR-MS Imaging: Jeong Jin Park1; Xiaoyue Chen1; Anna Berin1; Jing Wang1; David R. Gang1; Washington State University, Pullman, WA

ThP 227 Imaging Non-uniform Spatial Distribution of Energy Dense Metabolites for Efficient Capture and Chemical Storage of Solar Energy by Plants: Bo Xie1; Liza Alexander1; Jennifer Chmielowski1; 1; Ames Laboratory-US DOE, Ames, IA; 2; Iowa State University, Ames, IA

ThP 228 Imaging Mass Spectrometry Revealed Distributions of Anthocyanin Species in Haskap: Takahiro Hayasaka1; Miwako Sugawara2; Masafumi Kudo2; Hitoshi Chiba2; 1; University of Saito, Saito, Japan; 2; Hoshi University, Shinagawa, Japan; 3; Teikyo University, Utsunomiya, Japan

ThP 229 Maldi Imaging of Alkaloids in Catharanthus roseus Leaves: Lorenzo Caputi1; Gerhard Saalbach1; Sarah E. O’Connor1; John Innes Centre, Norwich, UK

ThP 230 Development of Laser Ablation Direct Analysis in Real Time Imaging Mass Spectrometry (LADI-MS): Rabi Musah1; Kristen L. Fowble1; University at Albany-SUNY, Albany, NY

ThP 231 Mass Spectrometry Imaging Enhances Biochemical Pathway Elucidation: David Gang1; Park Jeong-Jin1; Willis Mark1; Jing Wang1; Washington State University, Pullman, WA

ThP 232 Matrix Assisted Laser Desorption Ionization Mass Spectrometry Imaging of Glycosphingolipids in Rat Eye Tissue: Method Development and Optimization: Gargey B. Yagnik1; Mandy Crowrell1; Alexander Brezzi1; Kelly Keefe1; Mark Bree1; Dinesh Bangari1; Petra Oliva1; Thomas O'Shea1; Hanlan Liu1; Drug Metabolism and Pharmacokinetics, Sanofi, Waltham, MA; Rare Disease Pharmacology, Sanofi, Waltham, MA; Preclinical Toxicology, Sanofi, Waltham, MA; Pathology, Sanofi, Framingham, MA; Biological Mass Spectrometry, Sanofi, Framingham, MA

ThP 233 Sub Micrometric 3D Analysis of Mosquito Ovaries using TOF-SIMS Imaging: Quentin Vanbellingen1; Anthony Castellanos1; Marcela Nuzzoza2; Fernando G. Noriega1; Francisco Fernandez-Lima1; 1; Florida International University, Miami, FL; 2; Universidad de los Andes, Bogota, Colombia

ThP 234 Three Dimensional MALDI-MS Imaging of a Single Cell Zebrashield Embryo: Maria Emilia Duenas1; Adam Feenstra1; Jeffrey Essner1; Young Jin Lee1; Iowa State University, Ames, IA; Ames Laboratory-USDOE, Ames, IA

ThP 235 The Embryome: Molecules in Space and Time During the Early Stage Development: Laszlo Mark1; Janos Homoki1; 2; Department of Analytical Biochemistry, Institute of Biochemistry and Medical Chemistry, Medical School, University of Pecs, Pecs, Hungary; 3; PTE-MTA Human Reproduction Research Group, Pecs, Hungary; 4; Imaging Center for Life and Material Sciences, University of Gothenburg, Gothenburg, Sweden

ThP 236 Optimisation of Matrix Condition for the Analysis of the Antifungal Agent (Terbinafine hydrochloride) in a Living Skin Equivalent Model: CristinaRuss1; Malcolm R Clench1; Neil Brickebank2; Catherine Duckett1; Stephen Mellor3; Stephen Rumblow4; 1; Sheffield Hallam University, Sheffield; 2; Sheffield Hallam University, BMRC Sheffield, UK; 3; Croda Europe Ltd, Snaith, UK; 4; Croda Inc, New Castle, DE

ThP 237 Benchmarking New GCIB-SIMS Technology against MALDI and Applying GCIB-SIMS to Study Myocardial Infarction: Amir Saied Mohammadi1; Sanna Sämfors1; Andrew G Ewing2; John Fletcher3; Chalmers University of Technology, Gothenburg, Sweden; 1; University of Gothenburg, Gothenburg, Sweden

ThP 238 Mass Spectrometric Imaging of a Three-Dimensional Osteosarcoma Model: Ieva Palubeczkal1; Neil Cross1; Malcolm R Clench1; Christine Le Maitre1; Sheffield Hallam University, Sheffield, UK

ThP 239 The Effects of Diets on rat Brain Regional Lipid Composition using GCIB-SIMS: Amir Saied Mohammadi1; Alastair Ross1; John S Fletcher2; Andrew G Ewing1; Chalmers University of Technology, Gothenburg, Sweden; 1; University of Gothenburg, Gothenburg, Sweden

ThP 240 Specific Isotopic Pattern of Brominated Pyrylium Salts Facilitates Mass Spectrometry Imaging and Identification of Derivatized Small Molecule Neuroactive Compounds: Mohammadreza Shariatgorji1; Anna Nilsson1; Per E Andren1; Upsalla University, Upsalla, Sweden

ThP 241 MALDI Imaging with High Spatial Resolution for the Direct Analysis of Phospholipids in Rat Brain Tissue: Simona Salivo1; Yuzo Yamazaki2; Omar Belgacem2; Peter Quinto Tranchida2; Luigi Mondello3; University of Messina, Messina, Italy; 1; Shimadzu Corporation, Kyoto, Japan; 2; Shimadzu, Kratos Manchester, UK

ThP 242 MALDI-TOF Imaging Mass Spectrometry Reveals a Massive Loss of Polysaturated Cardiolipins after Traumatic Brain Injury: L. J. Sparvero1; Andrew A Amoscano2; Arthur B. Fink3; Tamil Anthonymuthu2; Simon Watkins2; Valerian E. Kagan1; Hulya Bayir3; University of Pittsburgh, Pittsburgh, PA; 1; University of Pittsburgh, Pittsburgh, PA

ThP 243 Compounds Screening in Dosed Human Skins by Quantitative Mass Spectrometry Imaging: David Bonnel1; Sylvain Ghilini1; Raphael Legouffe1; Claude Verrier1; Gael Picard-de Muller2; Marie-Jose Cuadrador2; Fabien Pamelard1; Gregory Hamm1; Jonathan Stauber1; ImaBiotec, MS Imaging Dept. Loos, France; 1; Galdemar, Sophia-Antipolis, France; 2; Shimadzu, Kratos Manchester, UK

ThP 244 Imaging of Drugs and Lipids in Living Skin Equivalents by MALDI MS and SIMS: Josephine Bunch1; Rory Steven1; Alan Race1; National Physical Laboratory, Teddington, UK

ThP 245 Adjustable Hydrophobic GUMBOS Matrices for MALDI Mass Spectral Imaging: Tia Vergas1; Kermit K Murray1; Isiah M Warner1; Tia Vargas1; Kermit K Murray1; 1; Louisiana State University, Baton Rouge, LA

ThP 246 Evaluating DESI imaging and High Resolution Mass Spectrometry to Improve an Industrial Component Cleaning Process: Peter Hancock1; Jonathan Jones1;
Scout-MRM: Extended Portability of Large Multiplexed TOF-SIMS Parallel Imaging MS/MS; John Hammond1; Zaia2; Andrew Percy1; Andrew G Chambers1; Andrea Palmer4; BC Proteomics Centre, Victoria, BC; 2Department of Technology, Gaithersburg, MD; 2NIST, Rockville, MD

Identification and the Relation between Low-Quality Experiments and Experiments by Multivariate Quality Control Metrics; Automatic Quality Assessment of Mass Spectrometry Technology, Chanhassen, MN

A Glycan Structure MS/MS Search Platform in Python; Joshua Klein1; Kashitl Khatri1; Yi Pu2; Lin Cheng3; Joseph Zaia1; Boston University Program for Bioinformatics, Boston, MA; 2Boston University, Boston, MA

Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics and the Relation between Low-Quality Experiments and Identifications; Wout Bittremieux1; Pieter Meysman1; Lennart Martens2; Dirk Valkenborg3; Kris Laakens1; 1University of Antwerp, Antwerp, Belgium; 2Ghent University, Ghent, Belgium; 3VITO, Mol, Belgium

Spectrum Acquisition for Building the NIST Tandem MS Library; Yuxue Liang1; Pedersen Neta1; KU Leuven, Leuven, Belgium; 1National Institute of Standards and Technology, Gaithersburg, MD; 2NIST, Rockville, MD

DIAProbe – Implementation of a Statistical Tool for Data Independent Acquisition in Skyline for SWATH Analysis; Alexandros DSouza1; Birgit Schilling1; Bradford W Gibson1; 1Buck Institute for Research on Aging, Novato, CA

Automated Design of Optimal SRM & PRM Assays using Empirical Modular Models; Jerome Renaux1; Alexandros Sarafianos, Kurt De Grave; Jan Ramon1; KU Leuven, Leuven, Belgium; 1National Institute of Standards and Technology, Gaithersburg, MD; 2NIST, Rockville, MD

PTM-Annotation: A Python Library for Annotation of Post-Translation Modification from Proteomic Mass Spectrometry Analysis; Amin Momin1; Hailey E Haut1; Michela Capello1; Juan Chen1; Hong Wang1; Samir M Hanash1; 1MD Anderson Cancer Center, Houston, TX

Proteomic Sequencing and Resurrection of a Monoclonal Antibody; Natalie Castellana1; Kenin Huang1; Hua Tu1; 1Digital Proteomics, LLC, San Diego, CA; 2LakePharma, Inc., Fremont, CA

MADpipe – An MRM Assay Design PIPEline for Multiplexed Multiple and Parallel Reaction Monitoring (MRM and PRM) Experiments; Yassene Mohammed1, 2; Derek S Smith1; Dominik Domanski1, 2, 3; Angela M Jackson1; Andrew Percy1; Andrew G Chambers1; Andrea Palmer1; Suping Zhang1; Christoph H. Borchers4, 5, 6; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, The Netherlands; 3Segal Cancer Proteomics Center, Lady Davis Institute, Mc Gill University, Montreal, QC, Canada; 4MRM Proteomics, Inc., Victoria, BC, Canada; 5University of Victoria - Genome BC Proteomics Centre, Victoria, BC; 6Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

Scout-MRM: Extended Portability of Large Multiplexed Peptide Assay; Blandine Rougemont1; Romain Carriere1; Sophie Aycirix1; Jean Marie Lacroix2; David Cox3; Yves J C LeBlanc1;入学 Institut des Sciences Analytiques, UMR 5280 CNRS, Université de Lyon, Villeurbanne, France; 2UGSF UMR Lille1-CNRS 8576, Villeneuve d’ascq Cedex, France; 3SCIX, Concord, ON

EasyCont: Identify Contaminants On-Line for Free on ms.cheminfo.org; Daniel Ortz1; LAURE MENIN1; Luc Patiny1; 1EPFL, Lausanne, Switzerland

BioDocker: An Open Source and Community-Driven Framework for Software Standardization in Proteomics; Felippe de Veiga Leprevost1; Saulo Alves Affitos2; Björn Grüning1; Hannes Roest1; Harald Barsnes1; Rafael Jimenez3; Henning Hermjakob4; Alexander I. Nesvizhskii1; Yassar Perez-Riverol5; 1University of Michigan, Ann Arbor, MI; 2Wageningen University, Wageningen, The Netherlands; 3University of Freiburg, Freiburg, Germany; 4Stanford University School of Medicine, Palo Alto CA, USA; 5University of Bergen, Bergen, Norway; 6EMBL-EBI, Hinxton, UK

CRAPome 2.0: A Comprehensive Resource for Affinity Purification Mass Spectrometry Data; Dattatreya Meilacherruy2; Zachary Wright1; Anne-Claude Gingras3; Alexey I Nesvizhskii1; 1University of Michigan, Ann Arbor, MI; 2Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON

Without Sacrificing Dwell Time, Achieving 1/N Smaller SWATH Windows (N = Number of MS Samples) to Quantify Low-Abudance Ions; GAUTAM SAXENA; Vidya Venkatraman1; Sarah Parker1; Ronald Holewinski2; Jennifer E Van Eyk3; 1Deep Search, Bethesda, MD; 2Cedars-Sinai Medical Center, Los Angeles, CA - California

Analysis of Independent Acquisition Mass Spectrometry Data with DIA-Umpire 2; Chih-Chiang Tsou1; Chia-Feng Tsai2; Yu-Ju Chen1; Guo Te2; 1Claude- Gingras; Alexey Nesvizhskii1; 1University of Michigan, Ann Arbor, MI; 2Academia Sinica, Taipei, Taiwan; 3Lunenfeld-Tanenbaum Research Institute, Toronto, Canada

Proteomics for Ricin Bioforensics: Protein Content of Castor Seed Extracts and Related Informatics Approaches; Eric Merkley1; Alaine M. Garrett1; Kristin H Jamaran1; Owen P Leiser2; Jennifer A Arce1; Kristin D Victory1; Angela M Melville1; David S Wunschel1; Stephen R. Cendorowski1; Karen L Wahl1; 1Chemical and Biological Signature Sciences Group, Pacific Northwest National Laboratory, Richland, WA; 2National Biodefense Analysis and Countermeasures Center, Fort Detrick, MD; 3Applied Statistics and Mathematics Group, Pacific Northwest National Laboratory, Richland, WA

Simulations Reveal the Pertinent Factors for High Quality Mass Spectrometry Based Microorganism Identification; Jan Eriksson1; David Fenyö2; Sabina Ko3; Tomasz Niedziela; 1Swedish University of Agricultural Sciences, Uppsala; 2Laboratory of Computational Proteomics, Center for Health Informatics and Bioinformatics, New York University School of Medicine, New York, NY; 3Institute of Immunology & Experimental Therapy PAN, Wroclaw, Poland

Top-down MSMS Data Analysis: Software and Algorithms for Protein Identification and Fragment Ion Assignment; Christian F. Heckendorf1; Roger Theberge1; Deborah R. Leon1; Kashitl Khatri1; Jean L Spencer1; Catherine E. Costello1; Mark E. McComb1; 1Boston University School of Medicine, Boston, MA

Process Analytical Technology (PAT) Applications of Mass Spectrometry: Real-time Monitoring of Drying Process; Heewon Lee; Boehringer Ingelheim Pharma, Ridgefield, CT

New Developments in MSStats: Statistical Process Control, LoDiLoQ, and Relative Protein Quantification with Split Plot Approach; Meena Choi1; Eralp Dogu2; Cyril Galitzine1; Olga Vitek; 1Purdue University, West Lafayette, IN; 2National Biodefense Analysis and Countermeasures Center, Fort Detrick, MD; 3Laboratory of Computational Proteomics, Center for Health Informatics and Bioinformatics, New York University School of Medicine, New York, NY; 4Institute of Immunology & Experimental Therapy PAN, Wroclaw, Poland

Combinatorial Use of Multiple Spectral Libraries Drastically Improves the Number, Breadth, and Confidence of Identified Proteins in a Murine Model; Mark A. Winger1; Troy H Patience1; Avedis A. Kazanjian1; Jessica L. Slack1; Vivek S. Ramachandran1; Elizabeth H. Yohannes1; Andrew S. Thagard2; 1Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, WA; 2Maternal Fetal Medicine, Madigan Army Medical Center, Tacoma, WA
INFORMATICS: PROTEIN ID AND QUANTIFICATION

ThP 270	Evaluation and Improvement of Quantification Accuracy in Isobaric Mass Tag Based Protein Quantification Experiments; Erik Ahlm1; Timo Glatter1; Cristina Viganò1; Conrad von Schubert1; Erich A. Nigg1; Alexander Schmidt2; Robin Hillen1; Duygu Erdogdu1; Klaus Brockmann1; Hendrik Kersten1; Thorsten Benter1; University of Wuppertal, Wuppertal, Germany

ThP 271	Analysis Workflow for Quantitative Proteomics, Employing Triplex Dimethyl Labelling and Ion Mobility Assisted Data Independent Acquisition; Andrew Paul Collins1; 2; Antony McCabe1; 3; Ian Moms3; Chris J Hughes3; Johannes PC Vissers3; Andrew Robert Jones1; 2; University of Liverpool, Liverpool, UK; 3OMIC Analytics, Liverpool, UK; 2Nonlinear Dynamics Limited, Newcastle upon Tyne, UK; 1Waters Corporation, Waltham, MA

ThP 272	De novo Profiling Strategies to Examine Divergent Mutation of Influenza Vaccines; Ryan D. Leib1; Louis Jacob1; Allis Chien1; Emmanuelle Mignot1; Christopher M Adams1; 1Stanford University, Stanford, CA; 2Descartes University, Paris, France

ThP 273	Diffacto: Robust Quantification for Large Sample Size Shotgun Proteomics; Bo Zhang1; Mohammad Pirmoradian1; Roman A Zubarev1; Lukas Käll1; 1Karolinska Institutet, Solna, Sweden; 2KTH Royal Institute of Technology, Stockholm, Sweden

ThP 274	Fast and Accurate Protein False Discovery Rates on Human Proteome Study Scale with Percolator 3.0; Matthew The1; 2; Michael J. MacCoss2; William S. Noble2; Lukas Käll2; 1KTH - Royal Institute of Technology, Stockholm, Sweden; 2University of Washington, Seattle, WA

ThP 275	New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data; Luis Mendoza1; David Stetzenberg1; Joseph Slager1; Michael Hoopmann1; Jason Winget1; Henry Lam1; Jimmy K Eng1; Eric Deutsch2; Robert L Mortiz2; 1Institute For Systems Biology, Seattle, WA; 2Institute for Systems Biology, Seattle, WA; 2Hong Kong University of Science and Technology, Hong Kong, China; 3University of Washington, Seattle, WA

ThP 276	Quantification with MultiNotch MS3 across Multiple LC-MS Runs with PEAKS Q; Lei Xin1; Hao Lin1; Baozhen Shan1; 1Bioinformatics Solutions Inc., Waterloo, Canada; 2Bioinformatics Solutions Inc., Waterloo, ON

ThP 277	False Discovery Rate Estimation in Large Scale Proteomic Datasets; Avinash Sharanmugam1; Alexey I Nesvizhskii1; 1University of Michigan, Ann Arbor, MI

ThP 278	A Proteogenomic Approach to Identify Sample-Specific Variant Proteins in a Myeloid Cell Line; Hossein Fazelinia1; Kian Huit Lim1; Hua Ding1; Tina Glisovic-Aplenc1; Richard Aplenc1; Saar Gill1; Sarah Tasiian1; Steven H. Seeholzer1; 1Children’s Hospital of Philadelphia, Philadelphia, PA; 2University of Pennsylvania School of Medicine, Philadelphia, PA; 3Children’s Hospital of Philadelphia, Philadelphia, PA

ThP 279	Proteogenomic Approaches to Improve the Identification of Proteins in Non-Human Primate Tissue Samples; Avinash Jadhav1; Michael J Proffitt2; Jeremy Glenn3; Anthony Cesnik2; Michael R Shortreed3; Kavangah Kyle4; Laura Cox1; Michael Olivier1; 1Texas Biomedical Research Institute, San Antonio, TX; 2UW-Madison, Madison, U.S.A; 3Wake Forest University School of Medicine, Winston-Salem, NC

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING (IONIZATION)

ThP 282	Development of a Novel Ion Source for µ-plasma Induced Proton Transfer Reaction Mass Spectrometry; David Mueller1; Yessica Brachthäuser1; Nele Hartmann2; Robin Hillen1; Duygu Erdogdu4; Klaus Brockmann1; Hendrik Kersten1; Thorsten Benter1; University of Wuppertal, Wuppertal, Germany

ThP 283	CNT Functionalized Corona Pin Sampling of Benzo(j)fluoranthene; Keaton Nahans1; Anne Vonderheide1; Vesselin Shanov1; Julio Landerio Figueroa2; 1University of Cincinnati, Cincinnati, OH; 2University of Cincinnati, Cincinnati, Ohio

ThP 284	Formation of Protonated and Metal-Adducted Organic and Biological Compound Ions by High Temperature Plasma/Mass Spectrometry; Jentia Sheen1; S-Y-Chyi Cheng1; 1National Sun Yat-Sen University, Kaohsiung, Taiwan; 2National Sun Yat-Sen Univ., Kaohsiung, Taiwan

ThP 285	Seconds Per Sample with Echo-DART-MS: Acoustic Loading of a Mass Spectrometer for High-Throughput Label-Free Screening; Eric Hall1; Martin Bachmann1; Ian Sinclair1; Jonathan Wingfield1; Lars Majlov1; Musselmann Brian1; Sammy Datwani1; Luke Ghislain1; 1Labcyte, Sunnyvale, CA; 2AstraZeneca, Macclesfield, UK; 3AstraZeneca, Cambridge, UK; 4IonSense, Inc. Saugus, MA

ThP 286	Utility of an Off-Axis Vapor Sampler with Direct Analysis in Real Time source equipped Mass Spectrometer; Brian D. Musselman1; Joseph Tice1; Robert Goguen2; Frederick Li2; 1IonSense, Inc., Saugus, MA; 2IonSense, Inc. Saugus, MA

ThP 287	Molecular Ionization Desorption Analysis Source (MIDAS) for Mass Spectrometry: A Flexible Ambient Platform; Greg Winter1; Joshua Wilhide1; William LaCourse1; 1UMBC Department of Chemistry and Biochemistry, Baltimore, MD

ThP 288	Ionization and Tunable Fragmentation of Biopolymers at Atmospheric Pressure with a Direct-Sampling Solution-Cathode Glow Discharge; Jake Shelley1; Andrew J Schwartz2; Kelsey L Williams1; 1University of Kentucky, Lexington, KY; 2Indiana University, Bloomington, IN

ThP 289	Solution-Cathode Glow Discharge: A Versatile Ion Source for Atomic and Molecular Mass Spectrometry; Andrew Schwartz1; Kelsey Williams1; 1University of Kentucky, Lexington, KY; 2Indiana University, Bloomington, IN; 3Kent State University, Kent, OH
**THURSDAY POSTERS**

**ThP 291**  
*On-The-Spot* Analysis using Liquid Extraction Probes;  
G. J. Van Berkel;  
Vilmos Kertesz;  
Oak Ridge National Laboratory, Oak Ridge, TN;  
Oak Ridge National Laboratory, Oak Ridge, TN

**ThP 292**  
Monitoring of Chemical Reactions in Real Time by Polarization Induced Electrospray Ionization Mass Spectrometry;  
Anil Kumar Meher;  
National Chiao Tung University, Hsinchu, Taiwan

**ThP 293**  
Paired-Ion Sonic-Spray Ionization Mass Spectrometry (PSI-SSI-MS) for the Analysis of Anionic Ions: Progress towards Even Lower Limits of Detection;  
Emmanouil Mavrikas;  
Leonidas Mavroudakis;  
Spiros Pergantis;  
University of Crete, Heraklion, Greece

**ThP 294**  
Ultrasoundation-spray Ionization Based Micro-reactors for On-line Monitoring of Chemical Reactions and Desalting;  
Te-Yu Chen;  
Yu-Chie Chen;  
National Chiao Tung University, Hsinchu, Taiwan

**ThP 295**  
The SIERRA Particle Amplification Method  
An Electrospray Ionization Based Approach for Spectrometry, Bolton, Canada  
Sarah M Matt1; Jiexun Bu1; Scott A McLuckey1;  
Washington University, Washington DC

**ThP 296**  
Ion Sampling and Cluster Formation in Nanospray Pulsed-Field Atmospheric-Pressure Ion Mobility MS;  
William McMahon1;  
Kaveh Jobarchi1;  
Georgetown University, Washington, DC

**ThP 299**  
Development of a Disposable Cartridge with Integrated Antibody for Protein Detection by Paper Spray Mass Spectrometry;  
Chengsen Zhang1; Nicholas E Manicke1;  
IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN

**ThP 300**  
Next-Generation Multinozzle Emitters for Interfacing Microflow LC and NanoESI-MS;  
Pan Mao1;  
Geuncheol Gil1; Dajiong Wang1;  
Newomics Inc, Emeryville, CA

**ThP 301**  
An Electrospray Ionization Based Approach for Detecting Circulating Tumor Cells (CTCs) using the SIERRA Particle Amplification Method;  
Adam Hollerbach;  
Stephen Ayrton;  
Zane Baird1;  
Valentina Piro1;  
Cathleen Hanau1;  
Karen Marfurt1;  
Michael Pugia1;  
Graham Cooks1;  
Purdue University, West Lafayette, IN;  
Siemens Healthineers Healthcare Diagnostics, Elkhart, IN

**ThP 302**  
Further Development of an Integrated Acoustic Electrospray Source for High-Throughput Label-Free Mass Spectrometry Biochemical Screening;  
Ian Sinclair1;  
Jonathan Wingfield1;  
Bachman Martin1;  
Steven D Pringle1;  
Hall Eric1;  
Lucien Ghislain1;  
Lars Majdof1;  
Stearns Rick1;  
Sammy Daltwain1;  
AstraZeneca, Macclesfield, UK;  
AstraZeneca, Cambridge, UK;  
Waters, Wimslows, UK;  
Labcyte, Inc., Sunnyvale, CA - California;  
Labcyte Inc, Sunnyvale, CA

**ThP 303**  
ThermoFisher Scientific, San Jose, CA

**ThP 304**  
Performance Evaluation of a Pneumatically Assisted Electrospray Ionization Source in the Microflow Regime;  
Harikrishnan Sukumar1;  
Eloy R Wouters1;  
Lee Earley1;  
Mark E Hardman1;  
Jean-Jacques Dyunych1;  
Thermo Fisher Scientific, San Jose, CA

**ThP 305**  
Droplets: IBF Mass Spectroscopy and Analytical Chemistry;  
Drew Sauter1;  
Andrew D Sauter2;  
Gary Groenewold3;  
Robert Ross4;  
Patrick A Limbach4;  
Nonoliter, LLC, Henderson, NV;  
Nonoliter LLC, Henderson, NV;  
Idaho National Laboratory, Idaho Falls, ID;  
University of Cincinnati, Cincinnati, OH

**ThP 306**  
Thread Spray Mass Spectrometry for Direct Analysis of Capsaicinoids in Evidentiary Garments;  
Patricia Capone1;  
Abraham Badu-Tawiah1;  
The Ohio State University, Columbus, Ohio

**ThP 307**  
Exploring the REIMS Interface Using the DSCM Method and Particle Tracking in Realistic Low Pressure Gas Flows;  
Athanasios Zacharos1;  
Julia Abda2;  
Alexander Lekkas1;  
Dimitris Papastassios1;  
Emmanuel Raptakis1;  
Tamas Karancsi2;  
Zoltan Takats2;  
Fasmatech, Athens, Greece;  
Imperial College, London, UK;  
Waters Research Centre, Budapest, Hungary

**ThP 308**  
Optimization of Matrix assisted Rapid Evaporative Ionisation Mass Spectrometry (MAREI-MS) System;  
Daniel Simon1;  
Tamas Karancsi2;  
Julia Balog1;  
Emrys A Jones1;  
Steven Pringle1;  
Zoltan Takats1;  
Waters Research Center Ltd., Budapest, Hungary;  
Waters, Wimslows, UK;  
Imperial College, London, UK

**IONIZATION MECHANISMS**

**ThP 309**  
Impact of ChemicalModifiers on the Cluster Chemistry during Electrospray Ionization;  
Marco Thinius1;  
Markus Langner1;  
Thorsten Benter1;  
University of Wuppertal, Wuppertal, Germany

**ThP 310**  
Examination of Droplet Size Dependence of Charge Reduction Methodologies;  
Ashley Marie Moon1;  
Bojana Opacic1;  
Peter Ta Reilly1;  
Washington State University, Pullman, WA

**ThP 311**  
Water Phase pH Effects on Electrospray Ionization Efficiency;  
Jaanus Ligand1;  
Asko Laaniste1;  
Anneli Kruve1;  
University of Tartu, Institute of Chemistry, Tartu, Estonia

**ThP 312**  
Novel Method for the Detection of Ionization Suppression;  
Richard King1;  
Carmen Fernandez-Metzler1;  
PharmaCadence Analytical Services, LLC, Shaftt, PA;  
PharmaCadence Analytical Services, Hatfield, PA

**ThP 313**  
Incorporating Cations and Anions into Molecular Dynamics Simulations of the Electrospray Process and the Resemblance to a “Salting-Out” Process;  
DoYong Kim1;  
Nicole D. Wagner1;  
David H Russell1;  
Texas A&M College Station, TX

**ThP 314**  
Application of Chemical Supercharging Electrospray Ionization to Small Organic Molecules;  
Andrew T. Ball1;  
Anthony W T Bristow1;  
Martin Sims1;  
Mike Morris1;  
Jackie Mosely1;  
Durham University, Durham, UK;  
AstraZeneca, Macclesfield, UK;  
Waters, Wimslows, UK

**ThP 315**  
Theoretical Investigation of Low Detection Sensitivity of Carbohydrates in ESI and MALDI;  
Jien-Liang Chen;  
Academia Sinica, Taipei, TAIWAN (R.O.C.)

**ThP 316**  
Protonation sites in multifunctional compounds upon positive mode ESI and APCI in a linear quadrupole ion-trap;  
Rashmi Kumar1;  
Ravikiran Kerabolu1;  
John Y Kong1;  
Chungang (Chuck) Gu1;  
Hilka I Konttamaa1;  
Purdue University-Department of Chemistry, West Lafayette, Indiana;  
Purdue University-Department of Chemistry, West Lafayette, IN;  
AstraZeneca, Boston, MA

**ThP 317**  
Ab initio Studies on the Mechanisms of ipso-Substitution Observed in DA-APPI;  
Alexander Haack1;  
Claire Markert1;  
Tiina Kauppila2;  
Hendrik Kersten1;  
Thorsten Benter1;  
University of Wuppertal, Wuppertal, Germany;  
University of Helsinki, Helsinki, Finland

**ThP 318**  
Combined Study of Ionic Processes on Surfaces: Photoelectric and Photocatalytic Effects;  
Christine Polaczek1;  
Valerie Derpmann1;  
Hendrik Kersten1;  
Thorsten
ThP 319  
Production of NH3 in N2-Corona Discharges and 63Ni Sources: Unequivocal Identification and Quantification; Nele Hartmann1; Sonja Klée1; Marco Thinis1; Sarah Peters1; Joerg Kleffmann3; Thorsten Benter1; *University of Wuppertal, Wuppertal, Germany

ThP 320  
Importance of Solvent Clusters in the Mechanism of Atmospheric Pressure Photo Ionization Evidenced by Theoretical Calculation and Experimental Results; Sung-Hwan Kim1; Arif Ahmed1; *Chemistry Department, Kyungpook National University, Daegu, Asia; Kyungpook National University, Daegu, Republic of Korea

ThP 321  
Interaction of keV Fullerene Ions with Molecules Supported on Free Standing Graphene: Mechanism of Molecule Ejection and ionization; Stanislav Verkhovturov1; Mikolaj Golunski1; Sheng Geng1; Dmitry S Verkhovturov1; Michael J Eller1; Zbigniew Postawa1; Emile A Schweidert1; *Texas A&M University, College Station, TX; *Department of Physics of Nanostructures and Nanotechnology, Institute of Physics, Jagiellonian University, Krakow, Poland

ThP 322  
Effects of Nanoelectrospray Emitter Size on Protein Desalting in Native Mass Spectrometry; Anna Susa1; Zijie Xia1; Evan R Williams1; *UC Berkeley, Berkeley, CA

ThP 323  
Flow Rate Measurements on a nano-ESI Source by Digital Image Analysis; Alejandro Cohen1; Axel J Soto1; *Dalhousie University, Halifax, NS

LC-MS: SAMPLE PREPARATION (PART 2)  
324 - 345

ThP 324  
IST: Sample Preparation for High Throughput Clinical Proteomics; Garwin Pichler1; Nils A. Kulah1; *PreOmincs GmbH, Gauting, Germany

ThP 325  
Automated Desorption, SPE Extraction, and LC/MS/MS Analysis of Dried Blood Spots; Fredrick Foster1; John Stoff1; Edward Pfannkoch1; *Gerstel, Inc. Linthicum, MD

ThP 326  
Fast Quantitation of Target Compounds Present in Small Volume of Complex Matrices by Miniaturized Solid Phase Microextraction Device; Hamed Piris-Rios1; Barbara Bojko1; Janusz Pawliszyn1; *University of Waterloo, Waterloo ON, Canada

ThP 327  
Developing Methods for Analyzing Proteins from Sperm Cells; Cheylene Tanimoto1; Mark Flory1; Parag Mallick1; Kevin Wang1; Sharon J Pitter1; *Stanford University, Stanford, CA; *Stanford University School of Medicine, Palo Alto CA

ThP 328  
A Rapid Clean-up with Cleannet HMF-F for The Analysis of 25-OH-Vitamin-D in Human Plasma by LC-MS/MS; Wan Wang1; Ruiy Wang1; *Bonna-Agela Technologies, Tianjin, China

ThP 329  
Electrospray Ionization Analysis of Dextran and Carboxymethylated Dextran, Jesus Tapia1; Karolien Denef1; Claudia M Boot1; Melissa M Reynolds1; *Colorado State University, Fort Collins, CO

ThP 330  
All Roads Lead to Robots: Automation of Customized, Effective Trypsin Digestion; Qin Fu1; Michael P Kowalski1; Christie L Hunter1; Mitra Mastali1; Tara R Jones-Roe1; Jennifer E Van Eyk1; 5; Cedars Sinai Medical Center, Los Angeles, CA; *Beckman Coulter Life Sciences, Indianapolis, IN, USA, Indianapolis, IN; *SCIEX, Redwood City, CA; 4Cedars Sinai Medical Center, Los Angeles, CA; *Advanced Clinical Biosystems Research Institute, Los Angeles, CA

ThP 331  
A Scalable Automated Proteomics Pipeline (ASP2) for Cerebrospinal Fluid Analysis in Large Clinical Studies; Antonio Nunez Galindo1; Martin Kussmann1; Loic Dayon1; *Nestle Institute of Health Sciences, Lausanne, Switzerland

ThP 332  
High pH Reversed-Phase Sample Fractionation for Phosphoproteomic and Glycoproteomic Workflows; Sergei I Snoevert1; Jae Choi1; Ryan Bomgardner1; Julian A Sabai1; Rosa I Viner2; John C Rogers1; *Thermo Fisher Scientific, Rockford, IL; *Thermo Fisher Scientific, San Jose, CA

ThP 333  
Design and Evaluation of Peptide Affinity Capture Formats for Selective Extraction of Antibiotics using Liquid Chromatography – Mass Spectrometry; Yu-Sheng Sung1; Veronica B. Waybright1; Dananjaya Kalu Appulage1; Abu Afzal Mohammed Shaker2; Frank W. Foss3; Kevin A Schug1; *University of Texas at Arlington, Arlington, TX

ThP 334  
A Comprehensive Evaluation of the Peptide Characteristics of Fast Digestion Methods in Discovery and Targeted Proteinomics Analysis; Zhengquang Guo1; Jie Cheng1; Wei Sun1; *School of Basic Medicine Chinese Academy of Medical Sciences, Beijing, China

ThP 335  
Determination of Oleamonic acid and Ursolic Acid in Loquat Leaf Extract by Liquid Chromatography-Tandem Mass Spectrometry; Dan Luo1; Yu-Qi Feng2; Youbaou Sun3; Jinting Yao1; Taohong Huang4; Yuki Hashi1; *Shimadzu, Shanghai, China; *Wuhan University, Wuhan, CN

ThP 336  
Rapid Online Desalting Using a Supercapromcous Reversed Phase Cartridge for Intact Monoclonal Antibody Characterization using Mass Spectrometry; Shane Bechler1; Martin Samonig1; Kelly Flook1; Remco Swart2; *Thermo Fisher Scientific, Sunnyvale, CA; *Thermo Fisher Scientific, Germering, Germany

ThP 337  
LC-MS/MS Method for the Determination of Bile Acid in Serum Sample using Cleanert MAS-MAW; Warren Chen1; Suzi Qin1; Wan Wang1; *Bonna-Agela Technologies, Tianjin, China

ThP 338  
Investigation of Protein Recovery from Restricted Access Media (RAM) for Development of a LC-MS Method to Analyze Biological Fluids; Dananjaya Kalu Appulage1; Evelyn H Wang1; Kevin A Schug1; *University of Texas at Arlington, Arlington, TX

ThP 339  
A 10-Point Time Course Pharmacokinetic Study Collected from a Single Mouse by use of the Mitra Microsampling Devices; Derek Wachtel1; Jenny Tobin1; Anna Susa1; Zijie Xia1; Evan R Williams1; *UC Berkeley, Berkeley, CA

ThP 340  
MegaFASP- Up-scaled FASP Protocol for High Yield Peptide Digest; Alon Savidor1; Alexandra Gabashvili1; Bobby Virasingh1; Adrian Sheldon1; Susan Dearborn1; Yibo Guo1; Peter Germano1; Sanjeev Fosy1; Maria Ribadeneira1; *Ironwood Pharmaceuticals, Cambridge, MA; *Necteryx, Torrance, CA; *Agilux Laboratories, Worcester, MA

ThP 341  
Efficient Extraction of Residual Pesticides in Agricultural Products and Soils for GC/MS and LC/MS Analysis using Supercritical Fluid Extraction; Takanori Hatton1; Sakai Takero1; Hayakawa Yoshishiro1; *Shimadzu Corporation, Kyoto, Japan

ThP 342  
Overcoming Challenges of Capsitol Interference in Reversed-Phase based Analytical Characterization; Hai Yue1; Barrier Teresa2; Hong Robert2; Izzyor Apostol2; Xin Zhang2; *Amgen Inc., Thousand Oaks, CA; *Amgen, Inc., Thousand Oaks, CA; *Amgen, Inc. Thousand Oaks, CA

ThP 343  
Automation Utility for Method Validation of Nicotine and Metabolites in Urine by HPLC-MS/MS; Dan Menasco1; Matthew Feldhammer1; James Ritchie2; Willa Zhang1; *Biotage, Charlotte, NC; *Emory University School of Medicine, Atlanta, GA

ThP 344  
Advantages of Rapid Automated On-Column Trypsin Digestion on Proteomics Data Quality; Raghothama Chaerkady1; Wen Yu1; Kristen Lekstrom2; Deniz BaycinHizal1; Michael Bowren1; *Medimmune, Gaithersburg, MD

ThP 345  
Optimized Protocol for In-Depth Analysis of Cell Culture Secretomes; Eike Hammer1; Daniela Suhr1; Beatrice Engelmann1; Eric Witt1; Yishan Xu2; Bonna-Agela Technologies, Tianjin, China
Mecklenburg-Vorpommern; 2University Medicine Greifswald, Greifswald, Germany

LIPIDS: QUANTITATIVE ANALYSIS

346 - 375

ThP 346 Measuring Biochemical Effects of Pulmonary Rehabilitation and OMT on COPD Patients through LC-MS-MS Analysis of Plasma Metabolites; Chen Zhang; Sherman Gorbis; John Wang; A. Daniel Jones; 1Michigan State University, East Lansing, MI

ThP 347 Identification and Comprehensive Structural Characterization of Serum Lipid Biomarkers to Type 1 Diabetes; Van Vu; Monica Narvaez-Rivas; Qibin Zhang; 1Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC; 2Center for Translational Biomedical Research, University of North Carolina at Greensboro, Kannapolis, NC

ThP 348 Comprehensive Lipidomics Approach for Platelet Analysis; Bing Peng; Patrick Münzer; Cristina Coman; Oliver Borst; Robert Ahrends; 1Leibniz-Institut für Analyt. Wissenschaft. - ISAS -, Dortmund, Germany; 2Medizinische Klinik III, Kardiologie und Kreislaufkrankungen, Universitätshilikonlinik Tübingen, Tübingen, Germany

ThP 349 Shotgun Lipidomics Analysis of Fatty Acid Esters of Hydroxy Fatty Acids Species in Biological Samples; Xiao Wang; Xianlin Han; 1Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL

ThP 350 Liquid Chromatography Tandem Mass Spectrometric Analysis of Oxidized Products of Polyunsaturated Fatty Acids and Bioactive Eicosanoids in Biological Samples; Jaeman Byun; Lixia Zeng; Subramaniam Pennathur; 1University of Michigan, Ann Arbor, MI

ThP 351 Research into Lysosomal Storage Metabolism using Plasma Lipid Characterization by LC-MS/MS; Sibylle Heidelberger; Daniel Blake; Rachel Webster; Karen Smith; Martin Roch; 1SCIEX, Phoenix House Lakeside Drive Warriington Cheshire UK; 2Queen Elizabeth Hospital Birmingham, Birmingham, UK

ThP 352 Robust Automated Lipid Extraction from Human Plasma; Dain Brademan; 1Madison, WI

ThP 353 Differential Complex Lipid Plasma Profiles Reveal Perturbations in Preeclampsia; Ben Ubbi; Katherine Williams; Susan Fischer; 1AB SCIEX, Redwood City, CA; 2UCSF, San Francisco, CA

ThP 354 Comprehensive Analysis of Polysphingosinolipid Molecular Species by Shotgun Lipidomics; Chunyan Wang; Juan Pablo Palavicini; Xianlin Han; 1Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL

ThP 355 LC-ESI-MS/MS Analysis of Oxigenated Lipid Droplets in Dendritic Cells Treated with Tumor Explant Supernatants; Vladimir Tyurin; Filippo Veglia; Andrew Amoscato; Roberto Angelini; Maureen Murphy; Alexandre Kapralov; Darush Mohammadyani; Dmitry I. Gabrilovich; Valerian Kagan; 1University of Pittsburgh, Pittsburgh, PA; 2The Wistar Institute, Philadelphia, PA

ThP 356 Identification and Quantification of Oxigenated arachidonoyl- and aradenoxy-phosphatidylethanolamines as Ferroptotic Death Signals using Oxidative Phospholipidomics; Yulia Tyurina; Andrew Amoscato; Vladimir Tyurin; Feng Gu; Gaowei Mao; Hulia Bayir; Valerian Kagan; 1University of Pittsburgh, Pittsburgh, PA

ThP 357 Analysis of Trans-Fatty Acids in Human Plasma using IsoTope Dilution-Gas Chromatography-Negative Chemical Ionization-Mass Spectrometry; Heath Clever; Na Wei; Samantha L McGunigale; Lin Zhang; Hubert W Vesper; 1CDSC, Atlanta, GA

ThP 358 Photochemical Tagging for Rapid Quantitation of Unsaturated Fatty Acids by Mass Spectrometry; Xiaoxiao Ma; Xu Zhao; Junjie Li; Ji-Xin Cheng; Zheng Ouyang; Yu Xie; 1Purdue University, West Lafayette, IN

ThP 359 Identification of Pseudomonas aeruginosa Phospholipids Involved in Surface Attachment; Sébastien Vilain; Caroline Le Senechal; Marc Crouzet; Marc Bonneau; Jean-Marie Schmitter; Corinne Bure; 1CNRS/CBMM, Bordeaux, France

ThP 360 LC-MRM for Quantitative Analysis of Endotoxins; Jianjun Li; Jacke Stupak; Kenneth Chan; 1National Research Council Canada, Ottawa, Canada

ThP 361 Development of a Wide-Targeted Quantitative Lipidomics Methodology by Supercritical Fluid Chromatography Coupled with Fast-Scanning Triple Quadrupole Mass Spectrometry; Hiroaki Takekawa; Yoshiiro Izumi; Thanai Paxton; Noriko Kato; Shinnosuke Horie; Katsutoshi Nagase; Takeshi Bamba; 1Medical Institute of Bioregulation, Kyushu Univ. Fukuoka, Japan; 2Nihon Waters K.K., Tokyo, Japan

ThP 362 An Ultrafast HPLC for Quantification of a Cationic Lipid 1,2-Dioleoyl-3-trimethylammonium Propane in Mouse Plasma by HPLC-MS/MS; Aihua Liu; Bryce Ashby; UriHong; Sherry Liu; 1Scott Reusches; 2Min Meng; 1Sanford Burnham Prebys Medicine Institute, Salt Lake City, UT; 2Covance, Salt Lake City, UT

ThP 363 Quantitative LC-MS/MS Method Development and Preliminary Analysis of Plasma Endocannabinoid Concentrations in Humans; Karolina M. Krasinska; Debra S. Karrson; Karen J. Parker; Allis S. Chien; 1Stanford University Mass Spectrometry, Stanford, CA; 2Department of Psychiatry and Behavioral Sciences, Stanford University, School of Medicine, Stanford, CA

ThP 364 Resolution of Unexpected Reference Standard Components of (5R,S)-isoprostane F2α Type VI (iPF2α-VI) using a Shallow UHPLC-MS/MS Gradient; Alan Dzerek; Miller S Patrick; Kirk E Newland; Chris J Kafonek; 1Celerion, Inc, Lincoln, NE; 2Celerion, Inc., Lincoln, NE

ThP 365 High-Throughput Approach to Separating and Quantitatively Measuring Hydroxycholesterols in Biological Matrices; Laura Dubois; Will J Thompson; Eric Benner; Kimberly Cocca; Wen Liu; Donald P McDonnell; Arthur Moseley; 1Duke University School of Medicine, Durham, NC

ThP 366 Simultaneous Measurement of 25-Hydroxyvitamin-D2, 25-Hydroxyvitamin-D3 and 27-Hydroxycholesterol Levels in Human Serum by LC-MS/MS; Ludmila Alexandria; Ken Lau; Allis C Chien; David Feldman; Sharon J Pitteri; 1Stanford University Mass Spectrometry, Stanford, CA; 2Department of Radiology, Canary Center at Stanford for Cancer Early Detection, Stanford, CA; 3Department of Medicine, Stanford University, Stanford, CA

ThP 367 Untargeted Lipidomics with Stable Isotope Labeling (H218O) used to Study Abnormal Development in Vitamin E Deficient Zebrafish Embryos; Melissa Q McDougall; 1Jawo Chiq; Jan F Stevens; 1, 2, 4, 5, 6, Lisa Truong; 1, 2, 4, 5, 6, Robert L Tanguay; 1, 2, 4, 5; Maret G. Traber; 1, 2, 4, 5, 6; 1Linus Pauling Institute, Oregon State University Corvallis, OR; 2College of Public Health and Human Sciences, Oregon State University, Corvallis, OR; 3Oregon State University, Corvallis, OR; 4College of Pharmacy, Oregon State University, Corvallis, OR; 5Environmental Health Sciences Center, Oregon State University, Corvallis, OR; 6Sinnhuber Aquatic Research Laboratory, Oregon State University, Corvallis, OR; 7Environmental and Molecular Toxicology, Oregon State.edu, Corvallis, OR

ThP 368 Methylation and Stable Isotopic Labeling-based Novel Method for Quantitative Phospholipidomics; Taniki Cal; Shu Qingbo; Liu Peibin; Niu Lili; Guo Xiaojing; Ding Xiang; Xue Peng; Xie Zhensheng; Wang Jifeng; Zhul Na; Wu Peng; Niu Lili; Yang Fuquan; 1Institute of Biophysics, CAS beijing, China

ThP 369 Differentially Expressed Nonpolar Lipids in Meibum of Dry Eye: Post-menopausal Women vs Contact Lens Wearers; Jianzhong Chen; Kari B Green; Kelly K Nichols; 1Duke University School of Medicine, Durham, NC; 2Celerion, Inc., Lincoln, NE; 3Linus Pauling Institute, Oregon State University Corvallis, OR; 4College of Public Health and Human Sciences, Oregon State University, Corvallis, OR; 5Oregon State University, Corvallis, OR; 6College of Pharmacy, Oregon State University, Corvallis, OR; 7Environmental Health Sciences Center, Oregon State University, Corvallis, OR; 8Sinnhuber Aquatic Research Laboratory, Oregon State University, Corvallis, OR; 9Environmental and Molecular Toxicology, Oregon State.edu, Corvallis, OR; 10Linus Pauling Institute, Oregon State University Corvallis, OR
MALDI: SAMPLE PREPARATION

ThP 376 Enabling HT Automated Sample Preparation Workflows with Application to MS Protein Analysis; Stoyan Stoychev1; Busisiwe Twala1; Previn Naicker1; Justin Jordaan1; CSIR Biosciences, Pretoria, Gauteng; CSIR, Pretoria, SA; CSIR, Pretoria, ZA; Rhodes University, Grahamstown, ZA

ThP 377 Analysis of Protein Profile by MALDI-TOFMS using Lyophilized Microalgae Samples Resuspended in Different TFA Content; Lidiane Andrade1; Maria Anita Mendes1; Claudio Augusto Oller do Nascimento1; University of São Paulo, São Paulo, SP

ThP 378 A New Embedding Method For Mouse Brain Tissue In Preparation For Matrix Assisted Laser Desorption Ionization Mass Spectrometry Imaging (MALDI-MSI); Emily L Gill1; Richard A Yost1; Timothy J Garrett1; Vinata Vedam-Mai1; University of Florida, Gainesville, FL

ThP 379 Improving Ion Abundances of Oligosaccharides by Decreasing Substrate Temperature During Droplet-Drying Processes in MALDI Mass Spectrometry; Yu-Meng Qu1; Yin-Hung Lai1; Hsueh Lee1; Chien-Wei Tsao1; Yi-Sheng Wang1; Academia Sinica, Genomics Research Center Taipei, Taiwan; National Taiwan University, Taipei, Taiwan

ThP 380 Structure-Property Relationship and Strategic Synthesis of MALDI Matrix for Low-Molecular-Weight Metabolites Analysis; Daisuke Miura1; Takanao Ishii2; Yoshinori Fujimura1; Daichi Yukihira1; Eisuke Hayakawa1; Hiroyuki Warishii1; Mitsuru Shinoda1; Kyushu University, Fukuoka, Kyushu; Kyushu University, Fukuoka, Japan

ThP 381 A Rapid MALDI-MS Method for the Characterization of Cardiovascular Drugs and Related Impurities; Wening Ning1; Jinlin Dong1; Jamie D Dunn1; US Food and Drug Administration, Center for Drug Evaluation and Research (CDER), Division of Pharmaceutical Analysis (DPA), St. Louis, MO

ThP 382 Gold Nanoparticles Bridging Infra-Red Spectroscopy and Laser Desorption/Ionization Mass Spectrometry for Rapid Pharmaceutical Products Screening; Siu-Leung Chau1; Ho-Wai Tang1; Kwan-Ming Ng1; University of Hong Kong, Hong Kong

ThP 383 A Trial of TLC-MALDI for Analysis of Industrial Materials; Toshiji Kudo1; Yoshikito Morishita1; Noriyuki Iwasaki1; Takashi Nirasawa2; Bruker Daltonics K.K., Yokohama, Japan

ThP 384 Fluorene Derivatives as MALDI Matrices for Electron Transfer Ionization; Juan Ramirez-Pradilla1; Laura Maria Cristancho-González2; Cristian Blanco-Tirado2; Marianne Y Combariza2; Universidad Industrial de Santander, Floridablanca, Santander; Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

ThP 385 Tryptamine as a Derivatization Matrix for Analysis of Carbonyl Compounds by MALDI Mass Spectrometry; Roman Borisov1; Mariya S. Silyundina2; Nikolai Yu. Polovkov1; Vladimir G Zaikin1; Topchiev Institute of Petrochemical synthesis, Moscow; Topchiev Institute of Petrochemical synthesis, Moscow, Russia

ThP 386 Electrowetting-controlled Sample Preparation Method for MALDI Mass Spectrometry; Olena Kudina1; Eral Burak2; Frieder Mugele1; University of Twente, Enschede, Netherlands; eMALDI BV, Enschede, The Netherlands

ThP 387 Re-evaluation and Optimisation of Common MALDI Mass Spectrometry Experimental Parameters for a Range of MALDI Matrix Compounds and Analyte Classes; Kenneth Neil Robinson1; Rory T Steven1; Josephine Bunch1,2; National Physical Laboratory, Teddington, UK; University of Nottingham, Nottingham, UK

ThP 388 Investigating the Effect of Electrospay Deposition Parameters on the Morphology of Samples and its Implications to MALDI MS Signal Intensity; Christina Emeigh1; Kevin Owens1; Drexel University, Philadelphia, PA

ThP 389 Optimized Multiply Charged Ion Production by Liquid MALDI – From High Molecular Protein Ions to Bottom-Up Proteomics using LC-MALDI MS/MS; Pavel Ryumin1; Jeffrey Brown1;2; Michael Morris1; Rainer Cramer3; University of Reading, Reading, UK; Waters Corporation, Wilmslow, UK

ThP 390 e-MALDI: An Electrowetting-Based Sample Preparation Method for MALDI Mass Spectrometry; Frieder Mugele1; Burak Eral2; Olena Kudina1; University of Twente, Enschede, Netherlands; TU Delft, Delft, NL

ThP 391 Black Phosphorus-Assisted Laser Desorption Ionization Mass Spectrometry Combined with Stable Isotope Labeling for Quantification of Small Molecules; He Xiao-Mei1; Jun Ding1; Yu Lei1; Hussain Dilshad1; Feng Yu-Qi1; Wuhan University, Wuhan, CHN

ThP 392 Investigating Complexes from Native-Like Environments: New Developments from LILBID-MS; Nina Morgner1; Tobias Lieblin2; Oliver Peetz2; Jan Hoffmann2; Nils Hellwig2; Goethe University Frankfurt, Frankfurt, Germany; Goethe University Frankfurt, Frankfurt, Germany

ThP 393 Using Simple Cell MALDI-MS to Guide Follow-Up CE-MS Assays; Troy Com1; Monika A Makurath2; Elizabeth K Neumann2; Stanislav S Rubakhin2; Jonathan V Sweedler1; University of Illinois at Urbana-Champaign, Urbana, IL; University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

ThP 394 A Comparison of Performance Characteristics of Atmospheric Pressure and Low-Pressure Matrix Assisted Laser Desorption Ionization Sources; Vladimír M Doroshenko1; Victor Laitko1; Eugene Moskovets1; MassTech, Inc Columbia, MD
ThP 395  Matrix-Coated Surface Assisting Ionization, a Sensitive and Efficient Ionization Method for Mass Spectrometry; Che-I Liao1; Kuo-Lung Ku2; 1Department of Applied Chemistry,National Chiayi University, Chiayi City, Taiwan; 2National Chiayi University, Chiayi City, Chiayi

ThP 396  Performance and Bioanalytical Applicability of MALDI-compatible Protein Chips Prepared by Ambient Ion Soft Landing. Petr Pompač1; Olďich Benada1; Jiří Hausner1; Viktor Růžička2; Michael Volný1; Petr Novák1; 1Institute of Microbiology, Prague, Czech Republic; 2Faculty of Science, Charles University in Prague, Prague, Czech Republic; 3Biovender, a.s., Brno, Czech Republic; 4AffiPro, s.r.o., Matrin, Czech Republic.

ThP 397  Nanopost and Elevated Bowtie Antenna Arrays for Laser Desorption Ionization and Fragmentation of Biomolecules; Xavier Holmes1; Sylvia Stopka1; Andrew Korte1; Scott Retterer2; Akos Vertesi1; 1George Washington University, Washington DC; 2Oak Ridge National Laboratory, CNMS Oak Ridge, TN

ThP 398  Matrix-free Laser-Induced Acoustic Desorption for Large Biomolecule Detection using Charge Monitoring Mass Spectrometer; Yung-Kun Chuang1; Jung-Lee Lin2; Szu-Hsiue Lai1; Chung-Hsun Chen1; 1Academia Sinica, Taipei, Taiwan; 2Academia Sinica, Genomics Research Center Taipei, Taiwan

ThP 399  Development of a Reduced Pressure Infrared Laser Ionization Source as a Novel Interface for Online LC/MS; Yasunari Iguchi1; Hisanao Hazama1; Kunio Akazu1; 1Graduate School of Engineering, Osaka University, Suita, Osaka, Japan

ThP 400  New User Friendly and High Sensitivity Approaches to Matrix-Assisted Ionization Directly from Vacuum; Milan Pophristic1; I-Chung Lui1; Khao Hoang1; Casey Foley1; Sarah Trimpin1; Charles N. Mcewen1; 1University of the Sciences, Philadelphia, PA; 2Wayne State University, Detroit, MI; 3Univ. of the Sciences, Philadelphia, PA

ThP 401  High Sensitivity MS Analyses by Eliminating the ‘Ion Source’: Vacuum-Assisted Ionization; Charles N. McEwen1; 1Univ. of the Sciences, Philadelphia, PA

METABOLICOMICS: IDENTIFICATION OF UNKNOWN METABOLITES 402 - 425

ThP 402  The Application of Untargeted Data Acquisition for Identifying Metabolites of ‘Designer Drug’ 25I-NBOMe in Clinical Samples; Michael Dunn1; Margaret Knight1; Clair Rooper1; Simon Thomas1; Peter Blain1; 1Medical Toxicology Centre, Newcastle University, Newcastle upon Tyne, UK

ThP 403  Metabolic Profiling of Type 1 Diabetes From Primary and Established T Cells Using Isotopic Ratio Outlier Analysis by LC-MS; Candice Ulmer1; Elizabeth Unarank Ransom1; Christopher Beecher2; Timothy Garrett2; Jing Chen1; Clayton Matthews1; Richard A Yost1; 1Bruker Daltonics, Billerica, MA; 2Bruker Daltonics Ltd, Bremen, Germany

ThP 404  A Critical Comparison of Collision Induced Dissociation and Surface Induced Dissociation for Metabolomics; Rachel Harris1; Ewa Jumeczczo1; Sophie Harvey1; Vicki H Wysocki1; John A McLean1; 1Vanderbilt University, Nashville, TN; 2The Ohio State University, Columbus, OH

ThP 405  The Use of High Resolution Mass Spec and Automated Fraction Collection for High Throughput Metabolite Identification; Jason Lamar1; PTRL West (a division of EAG, Inc.), Hercules, CA

ThP 406  Creation of Libraries of Recurring Mass Spectra: Triple Column Workflow for Improved Characterisation and Mapping of Unknowns across Multiple Samples; John M. Halket1; Anna Caldwell1; Gary Mallard2; Yuri Mirokhin2; Stephen Stein1; 1King’s College London, London, UK; 2National Institute of Standards and Technology, Gaithersburg, MD

ThP 407  Automation in the Creation of Recurrent Unidentified Spectra (RUS) Libraries; N. Rabe Andriamaharavo1; W. Gary Mallard1; Yuri A. Mirokhin1; Stephen E. Stein1; 1National Institute of Standards and Technology, Gaithersburg, MD

ThP 408  iTreeLib: Development of the MS^n Mass Spectral Tree Library of Plant Natural Products; Arpana Vaniya1; Sajjan Singh Mehta2; Oliver Fiehn1; 1UC Davis, Davis, CA; 2University of California Davis, West Coast Metabolomics Center, Genome Center, Davis, CA

ThP 409  Enabling High-Confidence Human Endogenous Metabolite Identification via High-Resolution MS/MS Retention-Time Library; Nan Wang1; Xian Luo1; Shuang Zhao1; Yiman Wu1; Zhendong Li1; Wei Han1; Jaspaul Tatlavy1; Yunong Li1; Kevin Hooton2; Dorothea Mung1; Adriana Zardini1; Xiaohang Wang1; Aiko Barsch1; Ulrike Schweiger-Hufnagel1; Liang Li1; 1Department of Chemistry, University of Alberta, Edmonton, Canada; 2Bruker Daltonik GmbH, Bremen, Germany

ThP 410  Identification of a Branched Amino Acid Metabolite Driving Fatty Acid Transport and Insulin Resistance; Sungwahn F Cho1; Choolson Jang1,2; Zofian Arany1; Dennis L Kasper1; 1Harvard Medical School, Boston, MA; 2University of Pennsylvania, Philadelphia, PA; 3Beth Israel Deaconess Medical Center, Boston, MA

ThP 411  Bioactive Compounds from Bees: Identification of Characteristic Metabolites in Propolis Extracts via UHPLC-MS and –MS/MS Based Metabolite Profiling; Sven Meyer1; Oliver Raether1; 1Bruker Daltonics Ltd, Bremen, Germany

ThP 412  Identification of Metabolites Using Isotopic Fine Structure with UPLC-FTMS; Jeremy Wolff1; Christopher J Thompson1; 1Bruker Daltonics, Billerica, MA; 2Bruker Daltonik, Billerica, MA

ThP 413  Carbonic Anhydrase Inhibitory Potential of Lagernia siceraria Stand and Identification of its Bioactive Compounds - An LC-MS/MS Approach; Joydeb Chanda1; Pulok K Mukherjee1; Rajarshi Biswas1; Dipankar Malakar1; Manoj Pillai1; 1School of Natural Product Studies, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India; 2SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India

ThP 414  Annotation of Novel Metabolites in a Pregnancy Study using Accurate Mass GC/QTOF MS and Validated Fragmentation Rules; Ziluan Lai1; Oliver Fiehn1; 1UC Davis, Davis, CA - California

ThP 415  Identifying Pregnancy Biomarkers of Dairy Cows using MALDI-MS; Tatiane Melina Guerreiro1; Mônica Ferreira1; Rodrigo Ramos Catharino1; 1Innovare Biomarkers Laboratory - UNICAMP, Campinas, SP

ThP 416  Blood Serum Metabolomics Using Comprehensive Two-Dimensional Gas Chromatography High Resolution Time-of-Flight Mass Spectrometry; David Alonso1; Joe Binkley1; Lome Fell1; Christina Kelly1; 1LECO Corporation, St. Joseph, MI; 2LECO Corporation, Saint Joseph, MI

ThP 417  Comprehensive Profiling of Bile Acids in Human and Mouse Using UPLC-MS/MS-based Metabolomics; Jun Han1; Georgia Mitsa1; David Hamelin1; Karen Lin1; Christoph H. Borchers1, 2; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

ThP 418  Elucidating Novel Cholesterol Metabolites in Mycobacterium tuberculosis using Mass Spectrometry; Israel Casabon1; Adam Crowe1; Kirsten Brown1; Jie Liu1; jason rogalinski2; Leonard Foster2; Lindsay Ellis1; 1The University of British Columbia, Vancouver, BC
ThP 419 Metabolic Profiling: Linking the IROA Metabolite Library to a Suite of Data Processing Software, Jeffrey T. Moore1; Claudia S Maier2; Michael A Stevenson3; Ian F Stevens2, 1Oregon State University, Department of Chemistry, Corvallis, OR; 2Oregon State University, Dept. of Pharmacy, Corvallis, OR

ThP 420 The Rise of Ion Mobility in Untargeted Metabolomics - Raising the Isobar in Annotation, Nicholas Ratrattay1; Cunyu Yan1; Perdita Barratt1; 1University of Manchester, Manchester, UK

ThP 421 A Software Tool to Automatically Evaluate Scan-by-Scan Spectral Accuracy of Ultra High Resolution LC/MS Data for Unique Elemental Composition Determination, Yongdong Wang1; Ming Gu1; Jeff S. Andrews1; 1Cerno Bioscience, Norwalk, CT

ThP 422 Compound Annotation Including Sulfate and Glucuronide Conjugates for Non-Targeted Analysis, Taizo Ogura1; Takeshi Bamba2; Akhiro Tai3; Eiichiro Fukusaki3, 1Shimadzu Scientific Instruments, Columbia, MD; 2Kyushu University, Fukuoka, Japan; 3Prefectural University of Hiroshima, Hiroshima, Japan; Osaka University, Osaka, Japan

ThP 423 Uncovering Cryptic Secondary Metabolites from Aspergillus nidulans with HDAC Inhibition, Matthew Henke1; Alexandra A Soukup2; Ryan A McClure3; Anthony Goering1; Regan J Thomson1; Nancy P Keller3; Neil Kelleher3, 1Northwestern University, Evanston, IL; 2University of Wisconsin Madison, Madison, WI

ThP 424 Bar Coding Tandem Mass Spectra for Metabolomic Identifications, Jonathan Spalding1; Kevin Cho1; Nathaniel G Mahieu1; Stephen L Johnson1; Gary J Patti1, 2, 1Washington University in St. Louis, St. Louis, MO; 2Washington University School of Medicine, Saint Louis, MO

ThP 425 Urinary Exposure Marker Discovery for Toxicants using UPLC-LTQ-Orbitrap and Three Untargeted Metabolomics Approaches, Jen-Yi Hsu1; Jing-Fang Hsu1; Yi-Sheng Hsu1; Tsai Shu-Han1; Pao-Chi Liao1; 1Department of Environmental and Occupational Health College of Medicine, National Cheng Kung University, Tainan, Taiwan

METABOLOMICS: QUANTITATIVE ANALYSIS 426 - 446

ThP 426 Methods for Enhancing Sensitivity and Throughput in LC-MS Analysis of BTEX Metabolites in Biological Fluid, Yehia Z. Baghdady1; C. Phillip Shelor1; Purnendu K. Dasgupta1; Kevin A. Schug1, 1Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX

ThP 427 Development and Evaluation of a Rapid LC-MS/MS Method for Accurate Quantitation of Malondialdehyde in Human and Mouse Plasma, Constance Sobsey1; Jin Han1; Karen Lin1; Walter Swartdagner2; Anthony Leviti3; Christoph H. Borchers1, 4; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2Sunnybrook Health Sciences Centre, Pharmacology and Toxicology Department, Toronto, ON, Canada; 3Sunnybrook Health Sciences Centre, Department of Psychiatry, Toronto, ON, Canada; 4Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

ThP 428 Development of a New UPLC/MRM-MS Method for Quantitation of Bile Acids in Dried Blood Spots, Jun Han1; Georgia Mitsa1; David Hamlin1; Karen Lin1; Juncong Yang1; Christoph H. Borchers2, 3; 1University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 2University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

ThP 429 Quantification of Metabolites in Plasma and Blood using a Dual Column-Switching Dual Liquid Chromatography with Tandem Mass Spectrometry Detection, Kyoko Watanabe1, 2; Yoshihiro Hayakawa2; Masami Tomita3; Gérard Hopfgartner3; 1Life Sciences Mass Spectrometry, University of Geneva, Geneva, Switzerland; 2Shimadzu Corporation, Kyoto, Japan

ThP 430 Rapid Porphyrin Quantification and Porphyria Differentiation in Urine by LC-MS/MS, Brian C Netzel1; Kimiy0 Raymond1; Silvia Tortorelli1; Mayo Clinic / DLMP, Rochester, MN

ThP 431 Detecting and Quantifying Gastrointestinal Neurotransmitters and Their Metabolites in Mice Fetes, Nitesh Sule1; Arul Jayaraman2; Lawrence J Dangott3; 1Texas A&M University, College Station, TX

ThP 432 Simultaneous Quantitation of 2-Hydroxy-4-Methoxybenzophenone, a Sunscreen Ingredient, and Its Metabolites in Harlan Sprague Dawley Rat Plasma by LC/MS/MS, Esra Mulut1; Jessica Pierfelice1; Barry S McIntyre2; Brian Burback2; Sunarama Waidyanatha2, 1University of Manchester, Manchester, UK; 2A&M University, College Station, TX

ThP 433 Analysis of Polycyclic Aromatic Hydrocarbons using LC/MS/MS: Identification of Carcinogenic Polycyclic Aromatic Hydrocarbons in Bladder Cancer, Preebi Purwaha1; Salil Kumar Bhowmik1; Rashmi Krishnapuram1; Franklin Gu1; Feng Jin1; Vadiraja B Bhat1; 1Baylor College of Medicine, Houston, TX; 2Agilent Technologies, Wilmington, DE

ThP 434 Removing Metabolomics Data Variation from LC-High Resolution Mass Spectrometry with Smart Selection of Internal Standards, Xiaojing Liu1; Jason Locasale1, 1Duke University, Durham, NC

ThP 435 Targeted Metabolomics Analysis on Aromatic Amino Acid on Yeast Strains Treated with Glyphosate, Gul M Mustafa1; Gregory Boyce1; Mark A Szewc1, 1Protea Biosciences, Inc. Morgantown, WV

ThP 436 Comparison of Metabolite Quantitation by a Triple Quadrupole vs. an Orbitrap-class Mass Spectrometer, Thomas D. Horvath1; Lin Tan1; Michael A Pontikos1; Di Du1; Yulun Chiu1; John N Weinstein1; David H Hawke1; Phil Lorenzi1, 1The University of Texas MD Anderson Cancer Center, Houston, TX

ThP 437 Metabolomics Analysis of Malonic Acid, Methylmalonic Acid and Ethylmalonic Acid in Urine of Mice with malonyl-CoA Decarboxylase Deficiency, Chandra Shekar R Ambai1; Furong Yuan1; Lutfi A Abu-Elheiga1; Vivekananda Shetty1; 1Baylor College of Medicine, Houston, TX

ThP 438 A HILIC Method for the Absolute Quantitation of Polar Metabolites in Embryo Growth Media, Sarah Marie Lyons1; Rebecca L. Krisher1; Jason Herrick1; Jay S. Kirkwood1; Corey D Broeckling1; Jessica Prenti1; 1Colorado State University, Fort Collins, CO; 2Colorado State University, Fort Collins, CO

ThP 439 LC-MRMHR QTOF MS Based Measurement of Metabolite Exchange between Pancreatic Cancer Associated Fibroblasts and Cancer Cells, Li Zhang1; Christopher Halbrook2; Daniel Kremer2; Shaokun Pang3; Kevin Cho1; Lutfi A Abu-Elheiga1; Vivekananda Shetty1; 1Baylor College of Medicine, Houston, TX

PAGE 180
64th ASMS CONFERENCE ON MASS SPECTROMETRY
ThP 440  Quantitation of Nucleotides and Nucleosides without Derivatization Using Transient Isotachophoresis-Capillary Electrophoresis Coupled to Tandem Mass Spectrometry; Jose Luis Gallegos Perez; SCIEX, Framingham, MA

ThP 441  Profiling of Polar Organic Acids in Mouse Muscle Using Ion Chromatography/Mass Spectrometry; Chris Petucel1,2; Andrew Zelenin1,2; Jeffrey A. Culver1,2; Meghan Gabriell1; Ken Kirkbride1; Terri T. Christison1; Stephen J. Gardell1,2; Sanford Burnham Prebys Medical Discovery Institute, Orlando, FL; 3Southeast Center for Integrated Metabolomics, Gainesville, FL; 4Thermo Fisher Scientific, Sunnyvale, CA

ThP 442  Data Normalization in MALDI-MSI and UHPLC-TQ-MS: A Cross-Platform Quantitative Analysis; Lin Wang1; Qian Wu1; Stanislav Rubakhin1; Jonathan Sneedler1; 'University of Illinois at Urbana-Champaign, Urbana, IL

ThP 443  LCMS Analysis of 15 Urine Steroid Hormones in Women’s Urine Samples Across a Menstrual Cycle; Cesar A Mestala1; Emily Chester1; Virginia Vitzthum1; Nicola Pohl1; Jonathan C Trinidad1; 'Indiana University Dept. Chemistry, Bloomington, IN; 2Indiana University, Bloomington, IN; 'Indiana University Department of Anthropology, Bloomington, IN

ThP 444  Predicting Concentrations of Small Molecules without Standard Substances in LC/ESI/MS via Ionization Efficiency Scales; Anneli Kruve1; Jaanus Liigand1; Piia Liigand2; Mari Sild1; Kari Kaupmees3; 'University of Tartu, Tartu, Estonia

ThP 445  Metabolomic Profiling of Beer Types by Widely-Targeted LC/MS Measurement; Mitsuhiro Kanazawa1; Daichi Yukihiro1; Tsuyoshi Nakanhishi1; Reilycs Inc., Tokyo, Japan; 2Shimadzu Corporation, Kyoto, Japan

ThP 446  Analysis of Platelet Metabolism and Function during Storage; Freyr Jonnasson1; University of Iceland, Reykjavik, Iceland

PEPTIDES: FRAGMENTATION MECHANISMS

447 - 445

ThP 447  Analysis of Coco Amphoteric Surfactants Used in Personal Care Products by Liquid Chromatography Mass Spectrometry (LCMS); Noelle Elliot1; Dale Willcox1; Jenan Elias1; Xiaoyan Mu1; Kai-cheng Huang1; 'University of California, Davis, CA

ThP 448  Chemical Characterization of Environments Containing Ultra-Small Inclusions via Nanoparticle Impacts; Aaron Clubb1; Michael J. Eller1; Rachel M Anderson2; Richard M Bloomington, IN; 3Indiana University Department of Anthropology, Bloomington, IN

ThP 449  In source-CID of CuAu144 Cluster: Evidence of Internally Bound Copper; Snigdha Boppidi1; David M. Black2; Robert L Whetten2; 'University of Texas at San Antonio, San Antonio, Texas; 2University of Texas at San Antonio, San Antonio, TX

ThP 450  Vacuum Ultraviolet Ion Mobility Mass Spectrometry of Complex Carbon Nanomaterials; Ernest K. Lewis1; Bruce Brinson1; Carter Kitrell1; Jerome Moore1; Wade Adams2; Amina S. Woods1; Robert H. Hauge1; J. Albert Schultz2; 'Ionwerks Inc., Houston, TX; 2Rice University, Houston, TX; 3Robot Nose, Lemont, IL; 4NII/NIIDA-IRP, Baltimore, MD; 5Ionwerks Inc, Houston, TX

ThP 451  Efficient Detection and Identification of Bacteria By Fluorescent Nanodiamond Labeling and Matrix-Assisted Laser Desorption Ionization Time-of-Flight Mass Spectrometry; Chih-Che Wu1; Department of Applied Chemistry, National Chi Nan University, Puli, Taiwan

ThP 452  Enhanced MALDI-MS Detection of Biomolecules Using Gold Nanoparticles and the Synergy between the Gold Core and Matrix; Alyssa L M Mansio1; Bradley Duncan1; Ryan Landis1; Vincent M Rotello1; Richard W Vachet1; 'University of Massachusetts Amherst, Amherst, MA

ThP 453  Silver Nanoparticles Assisted MALDI Mass Spectrometry for Analysis of Personal Care Products in Environmental Water; Jing-Chang Wang1; Maw-Rong Lee2; 'Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan; 2National Chung-Hsing University, Taichung, Taichung

ThP 454  Reproducibility of MILDI MS Imaging is Rationalized by Physical and Optical Characterization of AgNP Implanted Surface Layers of Brain Tissue; Samir M Shubella1; Ludovic Muller2; Viacheslav Manichev2; Damon Barbacci3; Shelley N Jackson2; Albert J Schultz4; Laura Fabbri1; Carey Balaban1; Tony Gustafsson1; Leonard Feldman1; Amina S Woods1; 'Rutgers University, Piscataway, NJ; 2NIH/NIDA-IRP, Baltimore, MD; 3Ionwerks, Gaithersburg, MD; 4Ionwerks Inc, Houston, TX; 5University of Pittsburgh, Pittsburgh, PA

ThP 455  Application of Magnetic Microbead Affinity Selection Screening (MagMASS) towards Discovery of Retinoic X Receptor-α Ligands; Ruth Muchir1; University of Illinois at Chicago, Chicago, IL

THURSDAY POSTERS

456 - 470

ThP 456  A Tandem Mass Spectrometry Study of the Transnitrosylation Products of the Dipeptide Cysteyn-tryptophan; Matias Butler1,2; Michael K W Siu1,2; Alan C Hopkinson1; 'University of Buenos Aires, Ciudad de Buenos Aires, Argentina; 2York University, Toronto, Canada; 3University of Windsor, Windsor, Canada

ThP 457  Oxidative Coupling of Cysteine Residue in Small Peptides; Ekram Hossain1; Jianhua Ren2; University of Pacific, Stockton, CA; 2University of the Pacific, Stockton, CA

ThP 458  A Comparison of Negative Electron Transfer Dissociation and Negative Ion Collision-Induced Dissociation of Acidic Peptides; Chelsea L McMullen1; Carolyn J Cassidy1; 'The University of Alabama, Tuscaloosa, AL

ThP 459  Negative Electron Transfer Dissociation Reagent Cation Discovery; Matthew J P Rush1; Nicholas M Riley1; Michael S Westphall1; Joshua J Coon1; 'University of Wisconsin-Madison, Madison, WI

ThP 460  Nucleophilic Attack by Amide Nitrogen Atoms on the Aromatic Rings of [n – H]+ ions; Xiaoyan Mu1; Kai-Chi Justin Lau2,3; Michael K W Siu2,3; Alan C Hopkinson2; Ivan K. Chu4; Hong Kong, Hong Kong; 2York University, Toronto, Canada; 3University of Windsor, Windsor, Canada; 4The University of Hong Kong, Hong Kong SAR

ThP 461  Singularly Protonated Tryptic Peptides with Penultimate Proline: Isomerization is the Gateway to Fragmentation; Shanshan Guan1; Maha T Abutokaih1; Benjamin J Bythell1; 'University of Missouri-St Louis, St. Louis, MO

ThP 462  A Systematic Investigation of Proline vs. Pipelicolic Acid-containing Peptide Fragmentation Chemistry; Maha Abutokaikh1; Shanshan Guan1; 'University of Missouri- St. Louis, St. Louis, MO

ThP 463  Development of a GC-MS Method for Identification of Dipeptides; Nino G Todaro1; Stephen E Stein1; Anzor Mikaila1; 'National Institute of Standards and Technology, Gaithersburg, MD

ThP 464  An Experimental and Computational Investigation of the Fragmentation of Dipeptide Acids, Esters and Amides; Michael J. Van Stipdonk1; Rebecca McLaughlin1; Stephen Koehler1; Anil Vishnuvajjhala1; 'Duquesne University, Pittsburgh, PA; 2Grove City College, Grove City, PA
ThP 465 Investigation of Gas Phase Fragmentation Reaction Mechanism of Doubly-Protonated bn (n=7-9) Ions by Mass Spectrometry; Ozge Gorgun1; Ahmet Emin Atik1; Tatul Yalcin2; 1IYTE, Urla-Izmir, Turkey; 2IYTE, Urla-Izmir, Turkey

ThP 466 Thermal Dissociation of the ThP 473

Mechanisms, Kinetic Parameters, and Comparison with CID; Zahra Homayoon1; Pratihar Subh1; William L Hase1; Veronica Macaluso1; Ana Martin-Somer2; Riccardo Spezia1; 1Texas Tech University, Lubbock, TX; 2CNRS, Paris, France

ThP 467 Collision Induced Dissociation Products and Mechanisms of di-protonated ThP 472Peptide by Chemical Dynamics Simulations; Veronica Macaluso1; Ana Martin-Somer1; Zahra Homayoon2; Subha Pratihar1; William L. Hase2; Riccardo Spezia1; 1CNRS, Paris, France; 2Texas Tech University, Lubbock, TX

ThP 468 Dissociation Energies of Short Doubly Protonated Tryptic Peptides with Polar Side Chains; Q. I. Obolensky1; Yi-Kuo Yu1; 1National Center for Biotechnology Information, NLM, NIH, Bethesda, MD

TXP 469 Coupled Tandem Mass Spectrometry with QM+MM Molecular Dynamic Simulations: Understanding Fragmentation Mechanisms of Protonated Uracil in the Gas Phase; Estefania Rossich Molina1; Jean-Yves Salpin2; 1CNRS UMR 8587, Evry, Ile de France; 2CNRS UMR 8587, Evry, France; 3Université d’Evr Val d’Essonne, Laboratoire Analyse et Modélisation pour la Biologie et l’Environnement., Evry, France

ThP 470 Theoretical Mass Spectrometry of Peptides: Statistical vs Non-Statistical Fragmentation; Riccardo Spezia1; Ana Martin-Somer1; Veronica Macaluso1; Zahra Homayoon2; Subha Pratihar1; William L. Hase2; 1CNRS, UMR 8587, Evry, France; 2Texas Tech University, Lubbock, TX

PEPTIDES: QUANTITATIVE ANALYSIS 471 - 504

ThP 471 Selenium Labeling Combined with LC-ICP-MS, a New Methodology in Pharmacology to Measure Protein-Ligand Interactions; Emmanuelle Cordeau1; Carine Amaudgulhern2; Brice Bouyssiere2; Agnès Hagèje1; Jean Martinez1; Gilles Subra1; Sonia Cantel2; Christine Enjalbal1; 1Institut des Biomolécules Max Mousseron (IBM, UMR 5247, Université de Montpellier, CNRS, ENSCM, Place Eugène Bataillon, 34095 Montpellier cedex 5, France, Montpellier, France; 2Laboratoire de Chimie Analytique Bioinorganique et Environnement LCABIE-IPREM, UMR 5254, Hélioparc, 64053 Pau, France, France; 3Université de Lyon, Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1, ENS Lyon, Villeurbanne, France, Lyon, France

ThP 472 Development of a Robust GLP Bioanalytical Method for a Short-lived Therapeutic Peptide; Christopher Barringer1; Daniel J Ricca1; Mary Katofiasc2; Jason Schmachtenberger3; Carole Pagen1;形2; Covance, Salt Lake City, UT; 3Covance, Salt Lake City, UT; 4Arrowhead Research Corporation, Wilmslow, UK

ThP 473 Validation and Correlation Strategies for Data Generated by Ligand Binding Assays and LC-MS to Support Product Development and Regulatory Assessment; Ryan Hill1; Trent J. Oman1; 1Dow AgroSciences, Indianapolis, IN

ThP 474 Novel Application of SCIEX 6600 TripleTOF Mass Spectrometer for Quantitative Assessment of Glucagon-Like Peptide-1 (GLP-1) Analog Pharmacokinetic Studies; Yue Huang1; Sarah Will2; Anish Konkar2; Jefferson Revel3; Marcella Petrone1; Inna Vainshtein1; Meina Liang1; Raffaella Faggioni4; Anton Rosenbaum4; 1MedImmune, Gaithersburg, MD; 2MedImmune, Mountain View, CA; 3MedImmune, Gaithersburg, MD; 4MedImmune, Cambridge, UK

ThP 475 Effect of Dimethyl Sulfoxide on Sensitivity Improvement of Therapeutic Peptides by LC/MS/MS; Eric Ma1; Moucun Yuan2; William Mylott2; Bruce Hidy1; Rand Jenkins1; 1PPD, Richmond, VA

ThP 476 Improvements in Sensitivity for Biotherapeutics using a Prototype Tandem Quadrupole Mass Spectrometer; Nikuni Tanno1; Kent Smith1; Mark Wrona1; Leonard Dillon2; Mark Roberts1; 1Waters Corporation, Milford, MA; 2Waters Corporation, Wiltshire, UK

ThP 477 Peakjuggler – A Proteome Discoverer Node for Label-free MS1 Quantification; Johannes Doblimann1; Karl Mechtler1; 1Research Institute of Molecular Pathology (IMP), Vienna, Austria; 2Institute of Molecular Biotechnology (IMBA), Vienna, Austria

ThP 478 Evaluation of the Parameters Affecting Interference Levels in Isobaric Tagging Studies; Matthew Lim1; Joao Paulo1; Steven P Gygi1; 1Harvard Medical School, Boston, MA

ThP 479 Relative Quantitative of Sites of Peptide and Protein Modification using Size Exclusion Chromatography coupled with Electron Transfer Dissociation; Boer Xie1; Joshua Sharp2; 1The University of Georgia, Athens, GA; 2The University of Mississippi, Oxford, MS

ThP 480 Quantification of Total Hepatocyte-Targeted Membrane-Lytic-Peptide (MLP-NAG) in Rat Plasma by LC/MS/MS using Solid Phase Extraction; Qingguo Tian1; Min Meng1; Roqness Juan1; Zhan Li1; 2Arrowhead Research Corporation, Madison, WI; 3Covance, Salt Lake City, UT; 3Covance, Salt Lake City, UT; 4Arrowhead Research Corporation, Madison, WI

ThP 481 MALDI Mass Spectrometry and HCCA Labeling as a Powerful Tool for Peptide Quantitation in Biology; Christine Enjalbal1; Maxime Rossich Molina2; Sonia Cantel2; Gilles Subra1; Muriel Amblard2; Jean Martinez2; Verónica Macaluso1; Zahra Homayoon2; Subha Pratihar1; William L. Hase2; 1CNRS, UMR 8587, Evry, France; 2Texas Tech University, Lubbock, TX

ThP 482 Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Human Uterine Smooth Muscle in Disparate States of Pregnancy; Christian Copley Salem1; Criag Ulrich2; David Quilici3; Rebekah Woosley1; Iain Buxton1; Heather Burkin1; 1Research Institute of Molecular Pathology (IMP), Vienna, Austria; 2CNRS UMR 8587, Evry, France; 3University Montpellier 2, Montpellier, cedex 05; 4University of Montpellier, IBMM UMR5247, Montpellier, France

ThP 483 Quantification of Synthetic Peptides by Multiple Reaction Monitoring-Liquid Chromatography-Mass Spectrometry (MRM-LC-MS); Praveena Nukareddy1; Bruce O’Rourke1; Dwight E. Matthews1; 1IYTE, Urla-Izmir, Turkey; 2IYTE, Urla-Izmir, Turkey

ThP 484 MALDI Mass Spectrometry and HCCA Labeling as a Powerful Tool for Peptide Quantitation in Biology; Christine Enjalbal1; Maxime Rossatto2; Sonia Cantel2; Gilles Subra1; Muriel Amblard2; Jean Martinez2; Verónica Macaluso1; Zahra Homayoon2; Subha Pratihar1; William L. Hase2; 1CNRS, UMR 8587, Evry, France; 2Texas Tech University, Lubbock, TX

ThP 485 Extending Targeted Proteomics to Study Molecular Signaling Events; Thierry Schmidlin1; 2; Luc Garrigue1; 2; Violette Gautier1; 2; Arjen J. Boender1; Erik L de Graaf1; 2; Roger A H Adam1; Albert J R Heck1; 2; Maarten A F Altelaar1; 2; Utrecht University, Utrecht, The Netherlands; 3Netherlands Proteomics Center, Utrecht, The Netherlands

ThP 486 Isobaric TMT 10-plex Labeled MultiNotch MS3 Analysis of Human Uterine Smooth Muscle in Disparate States of Pregnancy; Christian Copley Salem1; Criag Ulrich2; David Quilici3; Rebekah Woosley1; Iain Buxton1; Heather Burkin1; 1Research Institute of Molecular Pathology (IMP), Vienna, Austria; 2CNRS UMR 8587, Evry, France; 3University Montpellier 2, Montpellier, cedex 05; 4University of Montpellier, IBMM UMR5247, Montpellier, France

ThP 487 Quantification of Synthetic Peptides by Multiple Reaction Monitoring-Liquid Chromatography-Mass Spectrometry (MRM-LC-MS); Praveena Nukareddy1; Bruce O’Rourke1; Dwight E. Matthews1; 1IYTE, Urla-Izmir, Turkey; 2IYTE, Urla-Izmir, Turkey

ThP 488 Precise and High-Throughput Quantification of Plasma Biomarker Peptides for Alzheimer Disease at Attomole Level by SRM; Takeshi Tomonaga1; Ritsuko Maki1; Kanta Yanagida1; Shigere Yamada1; Shinji Tagami2; Masayasu
ThP 489
A High-Throughput Method for Reproducible Global Quantification of the Yeast Proteome using Data Independent Acquisition Mass Spectrometry; 
Lindsay Pino1; Gennifer E Merrinew1; William S Noble1; Michael J MacCoss1; University of Washington, Washington, WA

ThP 490
Fast and Stable LC-MS Workflow for Determination of Endogenous Secretory Peptides in Biological Fluids; 
Liangqiao Bian1; Maciej Kukula1; SCAAC, UT Arlington, Arlington, TX; SCAAC, University of Texas at Arlington, Arlington, TX

ThP 491
Quantitative Analyses of Microcystins by LC/MS/MS using an Orbitrap Fusion Tribrid Mass Spectrometer; 
Raymond West1; Dilrukshika S.W. Palagamana1; Dragan Isailovic1; University of Toledo, Toledo, OH

ThP 492
Label-free Quantitation of Opioid Induced Hyperalgesia Related-Peptides in Mice Hypothalamus using Skyline MS1 Filtering Approach; 
Nino Yang1; Krishna D Anapindi1; Stanislav S Rubakhin1; Elena V Romanova1; Aynamh Pradhan1; Jonathan v Sweeder1; University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; University of Illinois at Chicago, Chicago, IL

ThP 493
Characterization of Endoproteolytic Processing of Tachykinins and Substance P using Mouse Spinal Cord Cellular Fractions and High-Resolution Mass Spectrometry; 
Mouna Saidi1; Francis Beaudry1; Université de Montréal, St-Hyacinthe, QC

ThP 494
Selective and Sensitive Quantification of Glucagon and Glucagon-Related Peptide Hormones in Human Plasma using Conventional LC/MS/MS; 
Norhide Yokoi1; Ritsuko Hoshikawa1; Yoshiya Matsubara1;2; Ichiro Hirano1; Susumu Seino1; Kobe University Graduate School of Medicine, Kobe, Japan; Shimadzu Corporation, Kyoto, Japan

ThP 495
Quantification of Blood-Brain Barrier Permeation of Glycosylated Peptides using Microdialysis Coupled to LC-MS/MS; 
Mouna Saidi1; Francis Beaudry1; Université de Montréal, St-Hyacinthe, QC

ThP 496
Ultra Performance Liquid Chromatography–Tandem Quadrupole Mass Spectrometry for High-Sensitivity Profile Analysis of Blood Pressure Modulators Angiotensin Peptides; 
Meng Qi1; Hui Wang2; Jie Wang1; Li Yang1; Zhengtao Wang1; Shanghai University of Traditional Chinese Medicine, Shanghai, Shanghai; Waters Corporation, Shanghái, China

ThP 497
Detection of Insulin Analouges and Large Peptides in Urine for Anti-doping; 
Holly Cox1; Brittney Weber1; Daniel Eichner1; 1Sports Medicine Research and Testing Laboratory, Salt Lake City, UT

ThP 498
Validation of Vancomycin Assay in Rat Plasma by Liquid Chromatography/Tandem Mass Spectrometry; 
Xiaodong Shen1; Chantal Picard1; Rwaida Al-Eryan1; John Lord1; Gary Johnson1; 1ITR, Baie d’Urfe, Canada; 2Savara Inc., Andover, MA

ThP 499
Screening of Glyphosate-Resistant Transgenic Engineering Soy Bean and Maize by Ultra-high Performance Liquid Chromatography Coupled with Tandem Mass Spectrometry; 
Wenjuan Zang1; Meiling Yang1; John St Skilton1; Eric Carlson1; Chris Becker1; Korean German Institute of Technology, Seoul, Gangseogu, Korea; 2BioInSYSYSTEMS Inc., Seoul, Korea; 3Protein Metrics Inc., San Carlos, CA; 4Protein Metrics, San Carlos, CA

ThP 500
Systematic Comparison of TMT10-plex Quantification Accuracy and Precision in MS2 and SPS-MS3 Mode; 
Lauren Clarissa Tang1; Jana W Qiao1; Rushdy Ahmad1; Karl R Clusser1; Namrata D Udeshi1; Hasmik Keshishian1; Caitlin Feeney1; Jenn Abelin1; Jacob Jaffe1; Philipp Martens1; Steven A Carr1; 1The Broad Institute, Cambridge, MA; One and Done - HRAM MS Protein Quantitation and the Rewards of Retrospective Data Analysis in an Ever-changing Regulatory Landscape; 
Trent J Oman1; Ryan C Hill1; Jeffrey R Gilbert1; Dow AgroSciences, Indianapolis, IN

ThP 501
PTM Quantitative Analysis on Monoclonal Antibodies using LC-MS and PEAKS Software; 
Baozhen Shan1; Xin Lei1; Bioinformatics Solutions Inc., Waterloo, ON; 2Bioinformatics Solutions Inc., Waterloo, Canada

ThP 502
The Myocardial Degradome following Ischemia/Reperfusion Injury; Melanie Yvonne White1; Nina Hartcher1; Kieren A Liddy1; Joel A Cain1; Stuart J Cordwell1; 1The University of Sydney, Sydney, Australia

ThP 503
Charge Variant Identification and Quantification of Recombinant Antibody, Trastuzumab Using Automated Software; 
Jung-Keun Suh1; Kui Huy Kang2; John St Skilton1; Eric Carlson1; Chris Becker1; Korean German Institute of Technology, Seoul, Gangseogu, Korea; 2BioInSYSYSTEMS Inc., Seoul, Korea; 3Protein Metrics Inc., San Carlos, CA; 4Protein Metrics, San Carlos, CA

PEPTIDES: SEQUENCE ANALYSIS

ThP 505
LC-MS/MS – Peptide Mapping with Electron Transfer Dissociation (ETD) Reveals Enzyme-Mediated Intramolecular Bond in Transglutaminase, Thomas W Powers1; Andrew W Dawdy1; Jason C Rouse1; Olga V Friese1; Pfizer, Inc. Chesterfield, MO; 2Pfizer, Inc. Andover, MA

ThP 506
Heavyweight Champion: Iodine’s Large Mass-Defect Weighs in on the Enhancement of the Sequence Coverage of Tryptic Peptides via ETD; 
Emile Audre Vigling1; Christopher Shaffer1; František Turček1; University of Washington, Seattle, WA

ThP 507
Electron Transfer Dissociation of Trivalent Metal Cationized Acidic Phosphorylated Peptides; 
Juliette Joan Commodore1; Carolyn J. Cassady1; 1The University of Alabama, Tuscaloosa, AL

ThP 508
Comparative Study of The Skin peptidomes of Rana ridibunda from Russian and Slovenian Populations; 
Tatiana Yu Samingina1; Konstantin A Artemenko1; Jonas Bergquist1; Polonca Trebse1; Gregor Torkar1; Maria Tolpina1; Albert T. Lebedev1; 1Moscow State University, Moscow, Russia; 2Uppsala University, Uppsala, SE; 3Uppsala University, Uppsala, Sweden; 4Ljubljana University, Ljubljana, Slovenia; 5Moscow State University, Moscow, Moscow

ThP 509
Sensitive and Rapid LC/MS Method to Identify Potential T-cell Epitopes of Antibody Drugs; 
Nobuo Sekiguchi1; Chiyoumi Kudo1; Ayako Takahashi1; Kumiko Muraoka1; Akira Takei1; Mariko Yano1; Shotarote Takata1; Naoaki Murao1; Masaki Ishigai1; Chugai Pharmaceutical Co., Ltd., Gotemba, Shizuoka

ThP 510
Complete Sequence Coverage via ECD in a Q-ToF versus ETD/CID/HCD in an Orbitrap of 6+ and 7+ Protonated Ubiquitin; 
Yury Y Vasilev1; Nathan I Lopez1; Valery G Voinov1; Douglas F Barofsky1; Joseph S Beckman1; 1Linus Pauling Institute, Oregon State University Corvallis, OR; 2Oregon State University, Department of Chemistry Corvallis, OR

ThP 511
Highly Specific Peptide-Bond Dissociation of Some Peptide Model Molecules; 
Chen-Lin Liu; NSRRC, Hsinchu, Hsinchu

ThP 512
De novo Sequencing of Novel Antimicrobial Peptides from the Venom of the Scorpion Isometrus maculatus using ASDF-incorporated Curved Field Reflection; 
Yuzo Yamazaki1; Atsushi Kitakana1; Mao Yakio1; Masahiro Miyashita1; Hisashi Miyagawa1; Shimadzu Corporation, Kyoto, Japan; 2Graduate School of Agriculture, Kyoto

64TH ASMS CONFERENCE ON MASS SPECTROMETRY PAGE 183
ThP 513 Compact Mass Spectrometry (CMS) for Reaction Optimization and Quality Control of Modern Solid Phase Synthesis (SPSS) of Biologically Active Peptides; Simon J Prosser; Daniel Eikel; James P Cain; Elizabeth Restluty-Rosario; Advion, Inc. Ithaca, NY; 1Protein Technologies Inc., Tucson, AZ

ThP 514 3-Hydroxy-4-nitrobenzoic Acid (3H4NBA) as a MALDI Matrix for In-Source Decay; Yuko Fukuyama; Shunskue Izumi; Koichi Tanaka; Shimadzu Corporation, Kyoto; Hiroshima University, Hiroshima, Japan; 2Shimadzu Corporation, Kyoto, Japan

ThP 515 Application of Hydrogen Attachment/Abstraction Dissociation (HAD) for Peptide Analysis; Sadanori Sekiya; Hidenori Takahashi; Takashi Nishikaze; Shohei Yamauchi; Shinichi Iwamoto; Koichi Tanaka; Shimadzu Corporation, Kyoto, Japan

ThP 516 Selective Derivatization of Peptide Carboxyl Groups with Fluorophores for LDL-MS Analyses; Dhirukshika S. W. Palragoda; Raymond E West III; Dragan Isailovic; 1University of Illinois-Urbana Champaign, Urbana, IL; 3Beckman Institute, UIUC Urbana, IL

ThP 517 Elucidating the Mechanism of Photo-Induced Peptide Cleavage by Uranyl using Mass Spectrometry; Rasmus Elnegaard; Niels Erik Møllegaard; Thomas J D Jørgensen; Frank Kjeldsen; 1Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; 2Department of Cellular and Molecular Medicine, University of Copenhagen, Copenhagen, Denmark

ThP 518 Fragmentation of Model Deprotonated Phosphorylated Peptides by Collision-Induced Dissociation; Chelsea F. Plummer; Suma Kavati; Junjie Gao; Carolyn J Cassady; 1The University of Alabama, Tuscaloosa, AL

PEPTIDOMICS 519 - 530

ThP 519 Comparing Mass Spectrometric Platforms for Neuropeptide and Neuroproteome Discovery from Well-Defined Neuronal Tissue; Krishna D B Anapindi; Elena V Romanova; Bruce R Southey; Jonathan V Sweedler; 1University of Illinois-Urbana Champaign, Urbana, IL; 2University of Illinois at Urbana-Champaign, Urbana-Champaign, IL; 3Beckman Institute, UIUC Urbana, IL

ThP 520 Correlating Differential Peptidomics and Transcriptomics Data for Assessing Seasonal Changes in the Camel Brain; Elena Romanova; Bruce R Southey; Michael Greenwood; Charles Hindmarsh; Yea-Ling Tay; Ahmad Yamin bin Abdul Rahman; Kok-Gan Chan; Mark Rogers; Colin Campbell; F. Zahra Djazouli Ali; David Murphy; Jonathan V. Sweedler; 1University of Illinois-Urbana Champaign, Urbana, IL; 2University of Bristol, Bristol, UK; 3Queen's University, Kingston, Canada; 4BioEasy Sdn Bhd, Shah Alam, Selangor Darul Ehsan, Malaysia; 5University of Malaya, Kuala Lumpur, Malaysia; 6Université Saad Dahlab de Blida, Blida, Algeria

ThP 521 Multifaceted Mass Spectrometric Investigation of Neuropeptide Changes in Blue Crab, Callinectes sapidus, in Response to Ocean Acidification; Yang Liu; Amanda Buchberger; Lingjun Li; 1Department of Chemistry, University of Wisconsin, Madison, WI; 2School of Pharmacy, University of Wisconsin, Madison, WI

ThP 522 Mass Spectrometric Quantification and Imaging of Changes in Crustacean Neuropeptide Expression Levels Resulting from Hypoxia Stress; Kellen DeLaney; Amanda Buchberger; Yang Liu; Lingjun Li; UW Madison, Madison, WI

ThP 523 A Puzzle Approach on Single Cell Level; Susanne Neupert; Biocenter Cologne, University of Cologne 50674 Cologne, Germany

ThP 524 Large Scale Discovery and de novo-Assisted Sequencing of Native Cathion Antimicrobial Peptides (CAMPs) from the Komodo Dragon (Varanus komodoensis); Paul Russo; Melanie Juba; Megan Devine; Stephanie Barksdale; Kajal Gupta; Shalyn Scott; Kent Vliet; Joel Schnur; Monique vanHoek; Barney Bishop; 1George Mason University, Manassas, VA; 2George Mason University, Manassas, VA; 3University of Florida, Gainesville, FL

ThP 525 Immunogenic HLA-DR-presented-peptides Identified from Clinical Samples of Synovial Tissue/Fluid and Peripheral Blood from Patients with Rheumatoid Arthritis or Lyme Arthritis; Qi Wang; Elise E Drouin; Chunxiang Yao; Jiyang Zhang; Yu Huang; Deborah R Leon; Allen C Steere; Catherine E Costello; 1Boston University School of Medicine, Boston, MA; 2Massachusetts General Hospital and Harvard Medical School, Boston, MA

ThP 526 Proto-Peptidomics: A UPLC-Ion Mobility-MS/MS Proteomics Workflow for Studying Early Peptide Evolution on the Prebiotic Earth; Jay G. Forsythe; 1Anton S. Petrov; 2Sheng-Sheng Yu; 3W. Calvin Millar; 1Advion, Inc. Ithaca, NY; 2Protein Sciences, 3Protein Results, Inc.

ThP 527 LC-MS-MS identification of Small Cyclic Amphipathic Peptides (SCAmpPs) in citrus phloem; Leslie Harden; William H. Vensel; Kent F. McCue; William R. Belknap; USDA/WRRC, Albany, CA; 1U.S. Dept. of Agriculture, Albany, CA

ThP 528 Azoniaspior(4,4)azonyl Scaffold for Quantitative Peptide Analysis by LC-ESI-MS/(MS); Bartosz Selner; Monika Kijewska; Alicja Kluczyk; Piotr Stefanozczuk; Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland

ThP 529 Electroanalysis and Electrospray Ionization Mass Spectrometry of Intact and Oxidized Hormone Glucagon; Wendell P. Griffith; Sushma Karra; Robert Kennedy; Waldemar Gorski; 1University of Texas at San Antonio, San Antonio, TX; 2University of Michigan, Ann Arbor, MI

ThP 530 Peptidomic Landscapes ofPachycondila Villosa Ant Venom by Nano-Scale Chromatography and High Resolution Mass Spectrometry; Camila Takeno Cologna; Loic Quinton; Edwin De Pauw; Michel Degueldre; 1University of Liege, GIGA-Proteomics Liege, Belgium

PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION 531 - 566

ThP 531 Profiling Released High Mannose and Complex N-Glycan Structures from Monoclonal Antibodies Using Optimized Hydr: Scott McCall; Matthew Lauber; 1University of Texas at San Antonio, San Antonio, TX; 2University of Michigan, Ann Arbor, MI

ThP 532 Comprehensively Characterizing the N and O-Linked Glycosylation of a Recombinant Human EPO using HILIC-MS; Matthew Lauber; Stephan Kozza; Erin Chambers; Waters Corporation, Milford, MA

ThP 533 Mass Spectrometry Friendly Method for N-glycan Quantification; Wei Wu; Jiping Zhou; Subbarao Mantha; Zhichao Fang; Michelle Wang; Li Tao; Tapan Das; Deb Russell; Bristol-Myers Squibb Company, Bloombury, NJ; 1Bristol-Myers Squibb, Hopewell, NJ

ThP 534 Site-specific Characterization of N-O-Glycosylation on Therapeutic Human Chorionic Gonadotropins using Online LC/MS and Tandem Mass Tags; Hongbin Zhu; Ashley C Ruth; David A Keire; Hongping Ye; 1FDA, St. Louis, MO
THURSDAY POSTERS

ThP 535 Substrate- and Substrate-mimetic Chaperone Binding Sites in Human Alpha-Galactosidase Revealed by Affinity- Mass Spectrometry; Michael Przybylski; Stefan Maeser; Adrian Moise; Frederike Eggens; Mary Murphy; Jeff Bornheim; "Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; "Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim am Main, Germany; "Reichert-Ametek Technologies, Buffalo, NY

ThP 536 Hydrogen Exchange Mass Spectrometry can Reliably Detect Small Fractions of Destabilized Protein in Comparability Studies; Tyler Haugen; "Independent Research; Yu Wei; Jayant Arora; "University of Kansas, Lawrence, KS

ThP 537 Characterization of Bispecific Heteromub using LC-MS Based Methods; Yuping Zhou; Jason Tang; "Eli Lilly and Company, Indianapolis, IN

ThP 538 Disulfide Bond Mapping-A Case Study through Partial Reduction; Song Klaapeco; KBI, Durham, NC

ThP 539 Innovator and Biosimilar Infliximab: Comparability Assessment of the Host Cell Proteins and Protein Higher Order Structure; Jing Fang; Catalin E Doneanu; William R Alley; Ying-Qing Yu; Asish Chakraborty; Alain Beck; Weibin Chen; "Waters, Milford, MA; "Centre d’Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France

ThP 540 Protein Conformational Analysis of Native and Stressed Monoclonal Antibodies using Ion Mobility and LC/MS/ MS Disulfide Bond Mapping; David L Wong; Staples O Gregory; Jordy Hsiao; Te-Wei Chu; Stephen Madden; Javier Satulovisky; "Agilent Technologies, Santa Clara, CA

ThP 541 Mapping of Disulfide Bonds by Reducing Electrochemistry and Mass Spectrometry; Christian Cramer; Kim F. Haselmann; Jesper V. Olsen; Peter Kresten Nielsen; "Novo Nordisk A/S, Måløv, Denmark; "NNF Center for Protein Research, University of Copenhagen, Denmark

ThP 542 Protein Dynamics in the TGF-β Superfamily by Hydrogen Deuterium Exchange Mass Spectrometry; Roxana E. Jacob; Viet Le; Bo Zhao; Yuan Tian; Timothy A. Springer; John R. Engen; "Northeastern University, Boston and Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA; "Northeastern University, Boston, MA

ThP 543 Characterizing Deamidation and Oxidation in Adalimumab with Low pH Peptide Mapping and Middle-Up Mass Spec Analysis; Chris Hosfield; Eric Largy; Anicet Catrain; Fabrice Cantais; Gery Van Vyncht; Michael M Rosenblatt; Sergei Saveliev; Marjeta Urh; Arnaud Delobel; "Promega Corporation, Madison, WI; "Quality Assistance, Thuin, Belgium

ThP 544 Deciphering Biotherapeutic Protein Disulfide Bonds by Top and Middle-Down Mass Spectrometry; Jiao Zhang; Pilsoo Kang; Jianmei Kochling; "Sanofi Genzyme, Framingham, MA

ThP 545 Investigation of Antibody Aggregates by Hydrogen / Deuterium Exchange Mass Spectrometry and Other Biophysical Tools; Richard Yu-Cheng Huang; Deqiang Yu; Yuanli Song; Ryan K. Swanson; Zhijun Tang; Elizabeth Schultsky; Angela Lewandowski; Zhengjian Li; Guodong Chen; "Bristol-Myers Squibb, Princeton, NJ; "Bristol-Myers Squibb, Devens, MA

ThP 546 Disulfide Bond Identification of Biotherapeutic Proteins using Various Fragmentation Techniques Available on an Orbitrap Fusion Tribrid Mass Spectrometer; Stephane Houel; Jennifer Sutton; Seema Sharma; Terry Zhang; Romain Huguet; Martin Samonig; Vlad Zabrouskov; Jonathan Josephs; "Thermo Fisher Scientific, San Jose, CA; "Thermo Fisher Scientific, Germering, Germany

ThP 547 Rapid Profiling of Stressed PEGylated Protein Pharmaceuticals using Ion-Exchange Chromatography with Online Detection by Native ESI and Top-Down MS/MS; Khaja Muneruddin; Cedric E Bobst; Ruth Frenkel; Damian Houde; Iva Turyan; Zoran Sosic; Igor A Kaltashov; "University of Massachusetts, Amherst, MA; "Biogen, Cambridge, MA

ThP 548 A High-Throughput, Automated Platform Method for Multi-Attribute LC-MS Analysis of Cell Culture Harvest and Antibody Glycosylation; Jia Dong; Nicole Migliore; Steven J Mehrman; John Cunningham; Michael J Lewis; "Barnett Inst., Northeastern University Boston, MA

ThP 549 Automated Data Analysis Enabling Mass Spectrometry-based Assays for the Developability Assessment of Biotherapeutics; Maurizio Bronzetti; Cassandra Wigmore; Joe Shambaugh; David Bush; Arnd Brandenburg; Peter Haberi; "Genedata Inc, Lexington, MA; "Genedata AG, Basel, Switzerland; "Genedata GmbH, Munich, Germany

ThP 550 Characterization of Selected Therapeutic Monoclonal Antibodies under Stressed Conditions; Robert Camney; Zsuzska Lakos; Elena Demrini; John Snyder; "Eurofins Lancaster Laboratories, Inc., Lancaster, PA

ThP 551 Site-specific Glycoform Mapping of Biotherapeutics with Micro-Heterogeneity and Macro-Heterogeneity; Youngsuk Seo; "Myung Jin Oh; David Bradley; Hyun Joo An; "AGRS, Chungnam National University, Daejeon, Korea; "GRAST, Chungnam National University, Daejeon, Korea; "Agilent Technologies, Santa Clara, CA

ThP 552 Biosimilar Insulin Characterization: Top/Middle/Bottoms up Approaches; Rishikant Gupta; Mithun Bhatt; Annu Upadhyay; Manoj Pillai; Archana Krishnan; Sanjay Sonar; "Biogenomics, Thane (w), Mumbai, India; "SCIEX, 121 Udyog Vihar Phase IV Gurgaon, India

ThP 553 Mass Spectrometry Based Comparison of Rituximab Originator and Biosimilar; Ohlman Montacic; Murat Eravci; Andreas Springer; Stephan Hinderlich; Maria Kristina Parr; "Institute of Pharmaceutical and Medicinal Chemistry, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; "Institut für Chemie und Biochemie, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; "GroßgerätetechnikBioSuperMoi, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Germany, Berlin, Germany; "Beuth Hochschule für Technik Berlin - University of Applied Sciences, Department of Life Sciences and Technology, Berlin, Germany., Berlin, Germany

ThP 554 Towards the Fast and Increasingly Simplified Analysis of Trisulfide Formation in Biopharmaceutical Antibodies; Anja Resemann; Rainer Paape; Christoph Nordmann; Waltraud Evers; Lars Vonwerf; Eckhard Belau; "Barnett Inst., Northeastern University Boston, MA; "Lancaster Laboratories, Inc., Lancaster, PA; "Micro-Heterogeneity and Macro-Heterogeneity

ThP 555 Site-Specific Characterization and Quantitation of Protein Pegylation by LC-UV-MS and Standard Addition Approach; Yanjun Liu; Shiyang-Lin Wu; "William Hancock; "Barnett Inst., Northeastern University Boston, MA; "BioAnalytix Inc. Cambridge, MA

ThP 556 High Resolution Separations for Protein LC/MS; Barry Boys; Benjamin Liberti; Stephanie E Schuster; Brian E Wagner; William E Miles; Joseph Kirkland; "Barnett Inst., Northeastern University Boston, MA; "BioAnalytix Inc. Cambridge, MA

ThP 557 Complete Characterization of a Cysteine-linked Antibody-Drug Conjugate Performed on a Hybrid Quadrupole-Orbitrap Mass Spectrometer with High Mass Range; Aaron Oakley Bailey; Eugen Damoc; Kai
ThP 558 Characterization of Therapeutic Protein Charge Heterogeneity by Ion Mobility Mass Spectrometry and Native Tandem Mass Spectrometry: A Comprehensive Approach

ThP 559 Separation and Characterization of IgG2 Disulfide Isoforms by pH Gradient Cation Exchange Chromatography and Non-Reduced LC/MS - Peptide Mapping: Kristin J Bogge1; Anastasiya P Maruliov1; Thomas J Potter1; Jason C Rouse1; Tanya Q. Shang1; Matthew C Thompson1; 2Pfizer Inc, Andover, MA

ThP 560 High Throughput Screening and Characterization of Bispecifics Using Native Ion Mobility Mass Spectrometry: Caroline S. Chu1; Te-Wei Chu2; Gregory O Staples1; Patrick D Perkins1; Andy Gieschen1; Christian Klein1; Carol H. Ball1; Ning Tang1; 3Agilent Technologies, Santa Clara, CA; 4Agilent Technologies, La Jolla, CA; 5Agilent Technologies, Wilmington, DE

ThP 561 MS-Based Epitope Mapping of Malaria Antigens: DBP and MS-Tagged Malaria Peptide Analysis: J.C. Yves Leblanc1; Tanya Gamble2; 3DecipherBio, Wyndmoor, PA

ThP 562 A Workflow to Identify Mutations of Bulk Recombinant Proteins by using N-terminal Labeling Combined with the MELD method: Gabriel Mazucchelli1; Denis Morsa1; Dominique Bawir1; Nicolas Smargiasso1; Edwin De Pauw2; 1Thermo Fisher Scientific, San Jose, CA; 2Thermo Fisher Scientific, Bremen, DE

ThP 563 Higher Order Structure of Monoclonal Antibodies using Covalent Labeling Techniques and Integrative Biophysics: Mark Chance1; Pamminer Kaur1; Janna G Kiselar1; 2Case Western Reserve University, Cleveland, OH; 3NeoProteomics, Inc, Cleveland, OH

ThP 564 On-line Disulfide Cleavage for Structural Characterization: J.C. Yves Leblanc1; Tanya Gambler2; 3SCIEX, Concord, ON; 4SCIEX, Concord ON, Canada

ThP 565 Biochemical and Enzymological Characterization: Critical Quality Attribute (CQA) Mapping using LC-ESI-QToF and Automated Database Searching of Glycopeptide Analyses: Daniel Ian Richard Spencer1; Julia Smith2; Richard Andrew Gardner1; Ana Resemann1; Peter Hufnagel1; Daryl Ludger Fernandez1; 2Ludger Ltd., Oxford, UK; 3Bruker Ltd. Coventry, Coventry, UK; 4Bruker Daltonic GmbH, Bremen, Germany

ThP 566 An Investigation into Aβ/Metal Binding via MALDI TOF MS: Andrea Renee Kelley1; George Perry1; 2Ph.D. Student, University of Texas at San Antonio, San Antonio, TX

PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY

567 - 585

ThP 567 Mapping Interfaces of Protein Complexes by Deep Chemical Crosslinking Mass Spectrometry (XL-MSn): Angela Wiggins1; Eric Tse1; Daniel Southworth1; 2Philip Andrews1, 4; 1Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; 2Life Science Institute, University of Michigan, Ann Arbor, MI; 3Dept. of Chemistry, University of Michigan, Ann Arbor, MI; 4Dept. of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI

ThP 568 Crosslinking-MS Mapping of the DLL1 Histone H3K4 Methyltransferase Complex using the Fixed-Charge, CID-cleavable Crosslinker, DC4: 1Lolita Piersimoni1; 2Young-Tae Lee2; Chih-Chiang Tsou2; Alexey Nesvizhskii2; Yali Dou2; Philip C Andrews1, 4; 1Department of Biological Chemistry, University of Michigan, Ann Arbor, MI; 4Department of Pathology, University of Michigan, Ann Arbor, MI; 5Department of Chemistry, University of Michigan, Ann Arbor, MI; 6Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, MI

ThP 569 Probing GPCR Conformation by In-Cell Crosslinking and Mass Spectrometry: Bill Huang1; Ji-Won Lee1; Hee-Yong Kim1; 2NIAAA/NIH, Rockville, MD

ThP 570 Optimizing Carbene Footprinting: Br Encoding Identifies Modified Peptides and Fragments: Bojie Zhang1; Michael L Gross1; 2Washington University in St. Louis, St. Louis, MO; 3University of Massachusetts Medical School, Worcester, MA

ThP 571 Tertiary Structure Influences the Covalent Labeling Based Structural Analysis of Proteins: Patanachai Limpikiratith1; Richard V Vachtet1; 2University of Massachusetts Amherst, Amherst, MA

ThP 572 Native MS and Reporter-incorporated FPOP Platform in Studying Human SOD1 and its Mutant Variants: Ben Niu1; Brian Mackness2; Hao Zhang3; Don Rempel2; Weidong Cui4; Jill Zitzewitz5; Robert C Matthews6; Michael L Gross1; 3Washington University in St. Louis, St. Louis, MO; 4University of Massachusetts Medical School, Worcester, MA

ThP 573 Amyloid-β(1-42) Oligomer Models Developed using Combined Solid State NMR and High Resolution Hydroxyl Radical Footprinting: Janna Kiselar1; Cong Guo2; Huan-Xiang Zhou2; Anant Paravastu2; Andrew J. Nix2; Terrone L. Rosenberry3; Alexandra Klinger3; 4Case Western Reserve Univ, Cleveland, OH; 5Florida State University, Tallahassee, FL; 6FAMU & FSU College of Engineering, Florida State University, FL; 7Mayo Clinic, Jacksonville, FL; 8DecipherBio, Wyndmoor, PA

ThP 574 Characterization of a Membrane Protein in Living Cells using in-Cell Carboxyl Group Footprinting and Mass Spectrometry: Ke Sherry Li1; Weikai Li2; Yihu Yang1; Weidong Cui4; Michael L Gross1; 2Washington University, St Louis, MO; 3Washington University School of Medicine, St. Louis, MO

ThP 575 Structural Characterization of a G Protein-GEF Complex Using Top-Down Ultraviolet Photodissociation Mass Spectrometry: W. Ryan Parker1; Matthew Montana2; Quick2; Elisa Novelli1; Lauren Webb1; Jennifer S Brodbelt3; 1University of Texas at Austin, Austin, TX; 2University of Texas, Austin, TX

ThP 576 Structural Characterization of Myokinin-Ligand Complexes Using Top-Down Ultraviolet Photodissociation Mass Spectrometry: Rachel Mehaffey1; Michael Cammarata1; Jennifer S Brodbelt3; 1The University of Texas, Austin, Texas

ThP 577 Let’s Twist Again: Modulating p53 N-terminal Helicity - An Ion Mobility-Mass Spectrometry Study: Eleanor Dickinson1; Perdita Barran1; 3The University of Manchester, Manchester, Manchester, UK

ThP 578 Unfolding Pathways of Anthrax Toxin Proteins Investigated with Native Mass Spectrometry and Ion Mobility: Micah T Donor1; Simon A Ewing2; Bryan A Krantz1; 2James S Prell1; 3University of Oregon, Eugene, OR; 4University of Maryland School of Dentistry, Baltimore, MD

ThP 579 Mechanism of Prion Oligomerization as Determined by Structural Proteomics: Jason J Seppa1; Evgeniy V Petrotschenko1; Christopher H. Borchers1; 2University of Victoria - Genome BC Proteomics Centre, Victoria, BC, Canada; 3Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC, Canada

ThP 580 Unraveling Compositional Heterogeneity of Protein Complexes with a Modified Q Exactive Plus Orbitrap Instrument: Gili Ben-Nissim1; Mikhail E. Belov2; Maria G. Fuzesi-Levi1; Alexander A Makarov2; Michael Sharorn1; 1Department of Biological Chemistry, Weizmann Institute of Science, Rehovot, Israel; 2Thermo Fisher Scientific, Bremen, Germany
ThP 584
Unravelling the Mechanism of a Novel Bacterial Ferritin-Like Iron Storage System using Native Mass Spectrometry and Structural Biology; Didier He1; Alison Mackenzie1; Sally Vanden-Heuvel1; Sophia Harvey1; C. Logan Mackay2; Jon Marles-Wright2; David James Clarke1; 1University of Edinburgh, Edinburgh, UK; 2The Ohio State University, Columbus, OH

ThP 585
Higher-Throughput Native Mass Spectrometry for Protein-Ligand Screening with Application for Trimethoprim-Resistant Dihydrofolate Reductase; Michael Cammarata1; Ross Thyer1; Andrew Ellington1; Jennifer S Brodbelt1; 1University of Texas at Austin, Austin, TX

PROTEINS: PTMS (PART 2)

ThP 586
Mapping and Quantifying Protein O-GlcNAcylation in Human Brain for Studies of Alzheimer’s Disease; Sheng Wang1; Feng Yang1; Vladislav Petyuk2; Shukla Anil1; Matthew E Monroe1; Marina A Gritsenko1; Karin D Rodland1; 1Washington University in St. Louis, Chesterfield, Missouri; 2Washington University in St. Louis, St. Louis, MO; 3Washington University in St. Louis, Saint Louis, MO

ThP 587
Comparison and Optimization of First and Second Generation Quadrupole Dual Cell Linear Ion Trap Orbitrap Hybrid MS for Glycopeptide Analysis; Julian Saba; Sergei I Svidova; Christa Feasley1; Nina Soltoro1; Gauri Muradia1; Jeremy P Kunkel6; Jessica R Lavoie6; 1University of Chicago, Chicago, IL; 2Medical University of South Carolina, Charleston, SC; 3Wayne State University, Detroit, MI; 4University of Illinois at Urbana-Champaign, Urbana, IL; 5University of Texas at Arlington, Arlington, TX; 6Health Canada, Ottawa, Canada

ThP 588
Sample Displacement Chromatography (SDC) for Differentiating Glycoforms on Human Glycoproteins for Cancer Biomarker Discovery; Wonryeon Cho1; Jihoon Shin; 1Wonkwang University, IKSAN, Jeonbuk

ThP 589
Lysine β-hydroxybutyrylation is a New Type of Protein Post-Translational Modification Associated with Diverse Pathophysiology; Di Zhang1; He Huang1; Zhongyu Xie1; Dongjun Chung1; Xiaoyong Yang1; Yingming Zhao1; 1The University of Chicago, Chicago, IL; 2Medical University of South Carolina, Charleston, SC; 3Yale University, New Haven, CT

ThP 590
Comparative Analysis of Histone PTMs using DDA, DIA and PRM Methods on a QExactive HF Orbitrap; Joby Cole1; Eleanor Hanson1; David Dockrell2; 1University of Sheffield, Sheffield, UK; 2Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, UK; 3Department of Infection, Immunity and Cardiovascular Sciences, University of Sheffield Medical School, Sheffield, UK; 4Sheffield Teaching Hospitals NHS FT, Sheffield, UK; 5The Florey Institute, University of Sheffield, Sheffield, UK

ThP 591
Altered Lysine Acylation of Mitochondrial Proteins in Response to Macronutrient Stresses in the Mouse Liver; Jesse G. Meyer1; Nathan Basisty2; Samir Softic2; Birgit Schilling3; Kahn C. Ronald4; Bradford W Gibson1; 1Buck Institute for Research on Aging, Novato, CA; 2Joslin Diabetes Center and Harvard Medical School, Boston, MA; 3Proteomics of Protein Lysine Propionylation in Escherichia coli; Mingwei Sun1; Linhui Zhai1; Yingming Zhao1; 2; Minja Tan1; 3Shanghai Institute of Materia Medica, Shanghai, P. R. China; 4The University of Chicago, Chicago, IL

ThP 592
A Ubiquitin-Conjugating Enzyme Mediates Global Remodeling of the Proteome during Terminal Differentiation; Miguel Prado1; Anthony Tuan Nguyen1; Pingwei Min1; Joao A Paulo1; Yuan Shi1; Monu Kawana1; Verena Dederer1; Paul Schmidt1; Dean Campagna1; Mark D Fleming1; Steven P Gygi1; Daniel Finley1; 1Harvard Medical School, Boston, MA; 2Boston Children’s Hospital, Harvard Medical School Boston, MA

ThP 593
Acetylation Stoichiometry Analysis of Sirt3 Deficient Liver; Josue Baeza1; Michael Smallegan1; James Dowell1; Jing Fan1; John Denu1; 1University of Wisconsin Madison, Madison, WI

ThP 594
Towards Global, Quantitative and Site-Specific Characterization of the ADP-riboseylated Proteome; Yajie Wang1; Yuanli Zhen1; YONGHAO YU1; 1UT Southwestern Medical Center, Dallas, TX

ThP 595
Differential Protein Ubiquitination Profiles in Primary Human Skeletal Muscle Cells under Hyperinsulinenic Hyperglycemic Conditions Revealed by HPLC-ESI-MS/MS; Yue Qi1; Majed Alharbi1; Abdullah Mallisho2; Michael Alexander Caruso3; Nishit Shah4; Dnyasri Damchardula5; Alice Hu1; Danjun ma1; Xiaomian Zhang1; 2; Berhane Seyoum1; Zhengping Yi1; 3Wayne State University, Detroit, MI; 4Detroit Medical Center: Detroit Hospital (DMC), Detroit, MI

ThP 596
Identification and Characterization of Unexpected Degradation Pathway for Monoclonal Antibody during Process Characterization; Ratnesh Pandey1; Min (Mandy) Xie1; Lin Huang1; Yanhong Yang1; Paula Lei1; Allen Bosley1; Min Zhu1; 2MedImmune, Gaithersburg, MD

ThP 597
Identification and Characterization of Hydroxyllysines in an Immunoglobulin; Verena Niggeloh1; Georg Drabner1; 1Roche Innovation Center Penzberg, Penzberg, Germany

ThP 598
Dynamic Remodeling of Protein Acetylation in E. coli in Response to Different Carbon Sources; Birgit Schilling1; David Christensen1; Jesse G. Meyer1; Alexandria K D’Souza1; Dylan J Sorensen1; Nicholas Shulman1; Brendan McLean1; Christopher V Rao1; Alan J Wolfe1; Bradford W Gibson1; 1Buck Institute for Research on Aging, Novato, CA; 2Loyola University Chicago, Maywood, IL; 3University of Washington, Seattle, WA; 4University of Illinois at Urbana-Champaign, Urbana, IL

ThP 599
Identification of Prenylome by Chemical Oxidation and CID and ETD Tandem Mass Spectrometry; Ada Shahrizzaman1; Ruchika Bhawal1; Saiful Chowdhury1; 1University of Texas at Arlington, Arlington, TX; 2University of Texas at Arlington, Arlington, TX

ThP 600
Proteomics Analysis of Toxoplasma gondii Palmitylated Proteins and its Impact on Rhoptry Localization; Bin Deng1; Marina C Caballero1; Andres M 1

46TH ASMS CONFERENCE ON MASS SPECTROMETRY PAGE 187
ThP 604 Phosphorylation Ratio in Proteins including Protein Kinases can be Measured by Mass Spectrometry; Lonita Zenevedpot; Lennard Dekker; Noor Abdulhussein; sandor snoeijs; Jos Joore; Sieger Leenstra; Theo Luidar; Erasmus Medical Center, Rotterdam, The Netherlands; University of Amsterdam, Amsterdam, The Netherlands; Pepscpe B.V., Utrecht, Netherlands.

ThP 605 Suspension-Trapping for Rapid (< 1 hr) and Unbiased Milligram-Scale Digestions; John Wilson; Nikita Saha Turna; Rosamonde Banks; Darryl Pajpapin; Zouman Alexandre; Protifi, Huntington, NY; Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; University of Leeds, Leeds, UK.

PROTEOMICS: NEW APPROACHES (OTHER) 606 - 625

ThP 606 Dodecylen Succinyl Anhydrid (DSA)-based Depilation for Comprehensive Analysis of Protein N-terminal and C-terminal Peptides; Brian Dill; Henrik Molina; The Rockefeller University, New York, NY.

ThP 607 Supporting Alternative Bottom-Up and Middle-Down Proteomics using Neproin-1 and Tailored Informatics; Vladimir Sarpa; Christoph Schraeder; David Schriemer; University of Calgary, Calgary, Canada; Martin-Luther-Universität, Halle-Wittenberg, Germany.

ThP 608 Analysis of Specific Synaptic Proteomes in Rodent Models of Autism Spectrum Disorder; Yi-Zhi Wang; Qian Wang; William Brewer; Andrew Lee; University of South Carolina, Columbia, SC; IMCS, LLC, Columbia, SC; IMCS, Columbia, South Carolina.

ThP 609 Chemical Proteomics Approach for the Characterization of Molecular Targets of Fumaric Acid Esters; Fiona Pachl; Melanie Shackett Brennan; Robert H. Scannevin; Peter Juhasz; Biogen Inc., Cambridge, MA.

ThP 610 Evaluation of Aptamer-based Affinity Enrichment of Proteins for Mass Spectrometry; Eric Kuhn; Debby Ngo; Robert E Gerszten; Steven A Carr; Broad Institute of MIT and Harvard, Cambridge, MA; Massachusetts General Hospital, Boston, MA; Harvard Medical School, Boston, MA.

ThP 611 Utilizing Mass Spectrometry-Based Profiling System to Identify SH-SY5Y Cell Response Proteins Induced by Hyaluronic Acid Modified Biomaterials; Ming-Hui Yang; Yu-Chang Tyan; Graduate Institute of Medicine, KMU, Kaohsiung, Taiwan; Kaohsiung Medical University, Kaohsiung, Taiwan.

ThP 612 Characterization of Cardiac Myosin Heavy Chain by Middle-Down Mass Spectrometry; Yutong Jin; Loning Wei; Ying Peng; Wenxuan Cai; Ying Ge; Department of Chemistry, University of Wisconsin-Madison, Madison, WI; Institutes of Biomedical Sciences, Fudan University Shanghai, China; Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; Human Proteomics Program, University of Wisconsin-Madison, Madison, WI; Molecular and Cellular Pharmacology Training Program, University of Wisconsin-Madison, Madison, WI.

ThP 613 Integrating Carbamylation and UVPD to Facilitate Middle-Down Proteomics; James Sanders; Sylvester M Greer; Jennifer S Brodbelt; University of Texas Austin, Austin, Texas; University of Texas at Austin, Austin, TX.

ThP 614 Comparative Proteomics Reveal the Mercury Methylthion Process in Geobacter sulfurreducens PCA; Chen Qian; Alexander Joss; Chen Hongmei; Benjamin Mann; Xu Li; Paul Abraham; Baohua Gu; Robert Hetlich; Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN; Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN.

ThP 615 Reverse Phased Dispersive Micropipette Tip Extraction with Multiple Fractionation Strategy for Proteomic Profiling of Human Biofluids for Potential Clinical Applications; Yuzhe Nie; Qian Wang; Mullis Todd; William Brewer; Andrew Lee; University of South Carolina, Columbia, SC; IMCS, LLC, Columbia, SC; IMCS, Columbia, South Carolina.

ThP 616 Profiling Protein Expression in Limited Amount of Mouse Cortex using CE-ESI-HRMS; Eric Corcoran; Peter Nemes; Marta Zamard; Chiara M. Manzini; George Washington University, Washington, DC.

ThP 617 Sub-critical Processing of Proteins: Sequence Coverage, Specificity and Post-Translational Modifications; Thomas Powell; Steve Bowra; Helen J Cooper; University of Birmingham, Birmingham, UK; Pliyatec, Aberystwyth, UK.

ThP 618 Investigating the Effectiveness of Precursor Mass Exclusion List use for Proteomics on the Orbitrap Fusion; Tingting Wang; Rose E Stewart; Tony M Harvey; Tanya T Paull; Maria D Person; University of Texas at Austin, Austin, TX.

ThP 619 Combination of Cellular Thermal Shift Assay and Quantitative Proteomic Analysis to Identify Palbociclib Targets in MCF-7 Breast Cancer Cells; Julien Pelletier; Teemu Miettinen; Marek Gierliński; Matthias Trost; MRC PPU, University of Dundee, Dundee, UK; Division of Cell and Developmental Biology, University of Dundee, Dundee, UK; Division of Computational Biology, University of Dundee, Dundee, UK.

ThP 620 Surface Sampling and Mass Spectrometry Analysis of the Acquired Enamel Pellicle Formation on Hydroxyapatite Discs; Sabah Pasha; Melissa Grant; University of Birmingham, Birmingham, UK.

ThP 621 An Affinity Capture MALDI TOF MS Method for High Density Multiplexed Profiling of Total and PTM Protein Biomarker Panels; John Cammarata; Ghaith Hamza; Sergey Mamedov; Jeffrey C Silva; Vadislav Bergo; Adeptrix Corporation, Beverly, MA; Lighthouse Proteomics, Beverly, MA.

ThP 622 Protease-resistant Streptavidin for Sensitive Interaction-Proteomics; Jeroen Krijgsveeld; Mahmoud-Reza Rafiee; German Cancer Research Center, Heidelberg, Germany; University of Heidelberg, Heidelberg, Germany.

ThP 623 Mass Spectrometry-based Analysis of Potential Targets of Phenyl Vinyl Sulfone and Covalent Kinase Inhibitors by Specific Tagging Immunochemical Detection; Chi-Chi Chou; Yu Cheng-Han; Chang Geen-Dong; Khoi Kay-Hoii; Academia Sinica, Taipei; Academia Sinica, Taipei, Taiwan; National Taiwan University, Taipei, Taiwan.

ThP 624 Investigation of the Crosstalk between Phosphorylation and Cysteine Modifications using a Novel Cysteine Tag in Combination with TIO2 Chromatography; Honggang Huang; Giuseppe Palmisano; Martin R Larsen; University of Southern Denmark, Odense M, Denmark; Department of Parasitology, ICB, University of São Paulo.
PROTEOMICS: QUANTITATIVE (PRE-MS AND PLATFORMS/MULTIMICS/DYNAMICS)

626 - 649

ThP 626 Improving Speed and Robustness of DIA Quantitation Using Longer microLC Columns; Remco van Soest1; Christie Hunter1; Fischer Gavin2; SCIEX, Redwood City, CA; *SCIEX, Concord ON, Canada

ThP 627 Increasing Protein/Peptide Identification and Quantitation Using Extensive Offline Fractionation for TMT Workflows; Anthony A High1; Vishwajeet R Pagala1; Mingming Niu1; Xusheng Wang1; Hong Wang1; Haiyan Tan1; Kiran Kodali1; Kanisha Kavdia1; Yuxin Li1; Zhiping Wu1; Ashutosh Mishra1; Timothy I Shaw1; Ji-Hoon Cho1; Junmin Panse1; *STJ Children’s Research Hospital, Memphis, TN

ThP 628 Use of iOncAT Quantitation Data to Resolve ‘Hubs’ in the Protein Crosslinkome of a Relatively Rigid-Body Protein Complex; Ji-Suk Kim1; Robert Beynon2; Paul in the Protein Crosslinkome of a Relatively Rigid-Body Protein Complex; Ji-Suk Kim1; Robert Beynon2; Paul D Adams1; Christopher J Petzold1; *University of Liverpool, Liverpool, UK

ThP 629 Quantification of Low-abundant GDF-11 and GDF-8 in Human Serum/Plasma Using LC/MS/MS Analysis after Depleting Bio-Complexity by Cation Ion Exchange SPE; Limiting Peng1; Srinivasan Krishnan2; Shalender Bhaisan1; 1Brigham and Women’s Hospital, Boston, MA; *AB Sciex, Framingham, MA; *Brigham & Women’s Hospital, Harvard Boston, MA

ThP 630 Pros and Cons of Gradient Optimization in PRM Protein Assays; Sebastian Malchow1; René P Zahedi1; Albert Sickmann1; Julia M Burkhart1; Leibniz-Institut für Analytische Wissenschaften – ISAS – e. V., Dortmund, Deutschland

ThP 631 Digestion Rates and Stability of Tryptic Peptides Formed from Plasma Proteins; Adam M Hawkridge1; John Brad Mangrum2; Erika J Martin1; Donald F Brophy2; Virginia Commonwealth University, Richmond, VA; *U.S. Food and Drug Administration, College Park, MD

ThP 632 A High-Throughput Sample Preparation Workflow for Quantitative Proteomic Studies; Leanne Jade G Chen1; Yan Chen1; Huu M Tran1; Paul D Adams1; Christopher J Petzold1; Lawrence Berkeley National Laboratory, Berkeley, CA

ThP 633 Profiling the Cancer Kinome using Quantitative Chemical Proteomics; Katherine Johnson1; Jennifer Brown1; Alison Kurimchak1; James Duncan1; *Fox Chase Cancer Center, Philadelphia, PA

ThP 634 Impact of Cystinosis Mutations on Protein Degradations by Differential Dynamic SILAC and on Protein Network by Interactomics; Chiara Guerrera1; Nathalie Nevo1; Thomas Lucie1; Cerina Chhuon1; Anne Baillieux1; Joanna Lipecka1; Zuzanna Andrzzejewska1; Corinne Antignac2; 1Place de la Poterie Uni Tours Descartes, Centre Université Tours, France; 2University of Liege, Liege, Belgium; *Commissariat à l’Energie Atomique - DSV/SIMOPRO- Toxins, Receptors and Channels team, Saclay, France

ThP 635 Quantitative Analysis of AKT/mTOR Pathway using Multiplex-Immunoprecipitation and Targeted Mass Spectrometry; Bhavin Patel1; Alex Behling1; Leigh Foster1; Shouling Xu1; Ryan Bomgardan1; Carrie Clothier1; Kay Opperman1; Rosa I Viner2; Andreas Huhmer2; John C Rogers1; *Thermo Fisher Scientific, Rockford, IL; *Thermo Fisher Scientific, San Jose, CA

ThP 636 Application of Stochastic Protein Turnover Model to in vivo and in vitro Studies; Mahshubh Rahaman1; Rosshan Sadagov1; University of Texas Medical Branch at Galveston, Galveston, TX

ThP 637 Direct Measurement and Modeling of Protein Synthesis and Degradation Dynamics during Chemotherapeutic Response in Multiple Myeloma; Tzu-Yu Liu1; Hector Han-Li Huang1; DIamond D Wheeler1; Yun S Song1; Arun Paul Wiita1; UC Berkeley, Berkeley, California; *University of Pennsylvania, Philadelphia, PA; UCSI, San Francisco, CA

ThP 638 Effects of Cigarette Smoke, Cessation and Switching to Two Heat-Not-Burn Tobacco Products on Lung Lipid Metabolism Intwo Mouse Strains; Thomas Schneider1; Bjornen Titz1; Stephanie Boue1; Blaine Phillips2; Terhi Vihervaara1; Marja Talikka1; Catherine Nury1; Ashraf Elamin1; Florian Martin1; Walter Schlage1; Nikolai V. Ivanov1; Patrick Vanscheeuwijk1; Manuel C. Peitsch2; Julia Hoeng3; Philip Morris International, Neuchatel, Switzerland; *Philip Morris International Research Laboratories, Singapore, Singapore; *Zora Biosciences Oy, Biologinkuja, Finland

ThP 639 Differential Protein Expression Analysis by Mass Spectrometry as a Service; Claudia Fortes1; Jonas Grossmann1; Paolo Nanni1; Witold Wolski1; Christian Panse1; Laura Kunz2; Christian Trachsel1; Nathalie Selevsek1; Can Türker1; Ugur Gürel1; Bernd Roschitzki1; Ralph Schlapbach1; Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland

ThP 640 Targeted Proteomics Coming of Age: SRM, PRM and DIA Performance Evaluated from a Core Facility Perspective; Paolo Nanni1; Tobias Kockmann1; Christian Panse1; Christian Trachsel1; Jonas Grossmann1; Witold Wolski1; Nathalie Selevsek1; Asa Wahlander2; Ralph Schlapbach1; FGCZ, Univ Zurich Zurich, Switzerland

ThP 641 Quantitative Spatial Proteomics Analysis of the Cellular DNA Damage Response using 10-plex TMT, 4-plex iTRAQ and 8-plex iTRAQ Isobaric Tags; Sylvie Bourassa1; Benjamin Nehmé1; Jean-Philippe Gagné3; Daniel Defoy2; Frédéric Fournier1; Guy G. Poirier2; Arnaud Droit1; *Proteomics, CHU de Quebec Research Center, Quebec, QC; *Laval University, Faculty of medicine, Quebec, Quebec; *CHU de Quebec Research Center, Quebec, QC

ThP 642 Neutron-encoded Protein Quantification Integrated in the MaxQuant Platform Allows Highly Accurate and Multiplexed Quantification; Anna E Moriöl1; Katherine Overmeyer1; Derek J Bailey1; Nicholas W Kwiecien1; Alex S Hebert1; Michael S Westphall3; Stefka Tyanova1; Joshua C Coen1; Jürgen Cox2; University of Wisconsin Madison, Madison, WI; *Max-Planck-Institute of Biochemistry, Martinsried, Germany

ThP 643 Development of Universal MS Signal Processor for Improved Data Independent Acquisition Performance; Yet-Ran Chen; Academia Sinica, Taipei, Nankang

ThP 644 Extreme Discordance in Kidney Quantification Using Isobaric Labeling and Parallel Reaction Monitoring with Stable Isotope Dilution Mass Spectrometry; Robert William Sprung, Jr.1; Qiang Zhang1; Petra Erdmann-Gilmore1; Sherri R Davies1; Rose Connors1; Yiling Mi1; Gary Johnson2; Matthew R Meyer1; Shunqiang Li1; R. Reid Townsend1; Department of Medicine, Washington University School of Medicine, Saint Louis, MO; *Department of Pharmacology, University of North Carolina School of Medicine, Chapel Hill, NC
ThP 645 Integrating Protease-Specific Micorarrays (CLIP-CHIP) with Proteomics (SILAC) and Terminomics (TAILS) to Profile Macrophage Differentiation

ThP 646 2H-metabolic Labeling Approach Reveals Reduced Synthesis of Hepatic Mitochondrial Proteins in a Mouse Model of NASH

ThP 647 The Usual Subsets: Interrogating the Immune System for Proteomic Profiles of Cellular Phenotypes

ThP 648 Constructing an Immunogenome

ThP 649 Physicochemical, Proteome and Metabolome Studies to Determine Water Use Efficiency in Florida Hybrid Bunch Grape

ThP 650 Laser Capture Microdissection - Selected Reaction Monitoring for Cortical Layer Specific Protein Quantification in Postmortem Human Brain Tissue

ThP 651 Diagnosis of Thymoma Subtypes Using Proteomic Subtypes Detected by Mass Spectrometry

ThP 652 Assessment of Formalin-Fixation on Frozen Tissue Samples for Histopathologic and Proteogenomic Analyses

ThP 653 Deep Proteome Analysis of Murine Islets

ThP 654 Rapid Proteomic Profiling of Human Plasma

ThP 655 Protein Turnover Rate in Mice Gastrointestinal Tract is Affected by the Spatial Location and The Microbiota

ThP 656 A Brain Regional Proteomic Atlas in Mouse

ThP 657 Investigating Mechanisms of Preeclampsia by Probing Low Molecular Weight (LMW) Biomolecules in Human Placenta using Liquid Chromatography/Quadrupole-Orthogonal Time-of-Flight MS (LC/Q-TOF)

ThP 658 Proteomics and Imaging Mass Spectrometry of High-Grade Serous Ovarian Cancer Reveals Marked Intratumoral Alterations in Neoadjuvant Chemotherapy-Treated Patients

ThP 659 Clinical Tissue Proteomics Identifies U1 snRNP Pathology and RNA Splicing Dysfunction in Alzheimer Disease

ThP 660 Quantitative Proteomic Analysis of Human Testis Reveals System-Wide Molecular Pathways Associated with Non-Obstructive Azoospermia

ThP 661 A Proteomic Analysis of Fragile Human Bone

ThP 662 Characterizing ApoE Expression in AD Brain Tissue

ThP 663 The Protein Composition of the Human Colonic Mucus: Reduced Levels of Core Structural Components in Ulcerative Colitis patients

PAGE 190
**THURSDAY POSTERS**

**Small Molecules: Quantitative Analysis (Part 2)**

**ThP 676**
Quantitative Analysis of Thyroid Hormones by Pulsed Glow Discharge Mass Spectrometry  
Xiaqing Xu; Morgantown, WV

**ThP 677**
Development of a Surrogate Matrix for Cerebral Spinal Fluid for LC/MS Based Analytical Methods  
Shrin, Hooshfar; Babak Basiri; Michael G Bartlett;  
University of Georgia, Athens, GA

**ThP 678**
Impact of Anticoagulant on the Recovery Efficiency of Minocycline and Doxycycline in Different Matrices by LC-MS/MS; Richard Lavallée;  
Vinicio Vasquez; Nikolay I Younowskii; Milton Furtado; Anahita keyhani;  
Algorithmhe Pharma Inc., Laval, Canada

**ThP 679**
Quantitative Analysis and Protein Binding Determination of FXa Inhibitors in Human Plasma Containing Andexanet Alfa by HPLC-MS/MS; Chad Christianson; Janet M. Leeds; Sharon DeChenne;  
Tara Summer; Ryan Collins;  
Alturas Analytics, Moscow, ID; Portola Pharmaceuticals, Inc., South San Francisco, CA

**ThP 680**
LC/MS/MS Quantitation of Hydrochlorothiazide from Human EDTA Dried Whole Blood Spots; Rachel Sun; Robert Clegg; Tim Shoaf;  
Hasantha Jayaratna;  
BASI, West Lafayette, IN

**ThP 681**
High-throughput UPLC-ESI-MS/MS Method for the Simultaneous Measurement of Urinary Aliphatic Diamines, Trimethylamine N-oxide, and Beta-methylaminopropionitrile; Deepak Bhandari; Jonathan P. Rasio;  
John R. E. Ruhl; David M. Chambers;  
Centers for Disease Control and Prevention, Atlanta, GA

**ThP 682**
High Throughput Quantitation for Therapeutic Drug Monitoring with Open Access LC/MS/MS System; Miho Kawashima; Yoshishiro Hayakawa;  
Taku Tsukamoto; Masafumi Kikuchi; Masaki Tanaka; Shinya Takasaki; Hiroaki Ymaguchi; Nariyasu Mano;  
Shimadzu Corporation, Tokyo, Japan; Shimadzu Corporation, Kyoto, Japan; Tohoku University Hospital, Sendai, Japan

**ThP 683**
A Simple and Effective Strategy to Improve Bioanalysis with Capillary Microsampling (CMS): The Use of Internal Standard in Capillary (ISIC); Yonghua Ling;  
Fumin Li; PPD, Middleton, WI; Illumina, Inc, Madison, WI; PPD, Richmond, VA

**ThP 684**
Highly Sensitive LC-MS/MS Method for the Quantification of Fluticasone Propionate in Human Plasma, Feasible for Reinjection and Repeat Analysis; Jeyan Albert; Praveen V Kumar; Manoj Bob;  
Ravishekar K.; Anoop Kumar; Manoj Pillai;  
BASi, Gurgaon, Haryana; Lupin Bioresearch Center, Pune, Maharashtra; SCIEX, Gurgaon, Haryana

**ThP 685**
A Highly Sensitive Method for the Quantification of Dexamethasone in Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry; Min Chana Kim;  
Joo-Yoon Cho; Seo Hyun Yoon;  
Seoul National University College of Medicine, Seoul, South Korea

**ThP 686**
A Novel Approach to Minimize Matrix Effect in LC-MS/MS Method for Quantitation of Buprenorphine and Norbuprenorphine in Human Urine; Dawei Zhuo; Pei Li;  
Shu Zhang; Xuejun Sun; Xinping Fang;  
WUXI AppTec Co., Plainsboro, NJ

**ThP 687**
Seo Hyun Yoon; Joo-Yoon Cho;  
Seoul National University College of Medicine, Seoul, South Korea

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**Small Molecules: Quantitative Analysis (Part 2)**

**ThP 664**
Label-Free Quantitative Differential Expression Proteomics of Formalin-Fixed Paraffin-Embedded Liver Biopsy Samples from a Longitudinal Study of Hepatitis C Patients; Sarah Mabbett;  
Will J Thompson; Joseph Lucas; Keyur Patel; Arthur Moseley;  
‘Duke University Medical Center, Durham, NC; ‘University of Toronto, Toronto ON, Canada

**ThP 665**
Proteomic Mapping of Enamel Matrix in Mice with Different Susceptibilities to Dental Fluorosis by Gel-Based and Gel-Free Approaches; Aline Leite; Mileni Silva Fernandes; Senda Charone; Gary W Whittford; Eric T Everett; Marilía Afonso Rabelo Buzalaf;  
University of São Paulo, São Paulo, SP; ‘University of São Paulo, Bauru, SP-Brazil; ‘University of Georgia, Atlanta, GA; ‘University of North Carolina, Chapel Hill, NC

**ThP 666**
Quantitative Cardiovascular Proteomics of Injured Arterial Tissue by Dilu Sebacicar Labelling: Toward Novel Therapeutic Targets for Restenosis; Matthew S. Glover; Qing Yu; Bowen Wang; Xudong Shi; Lian-Wang Guo;  
C. Kent Craig; Lijun Li;  ‘University of Wisconsin-Madison, Madison, WI

**ThP 667**
Changes in Protein Expression Levels of Drug-Metabolizing Enzymes and Transporters in Liver and Kidney between Germ-Free and Specific Pathogen-Free Mice; Takuya Kuno; Mio Hirayama; Shingo Ito;  
Sumio Gu; ‘Kumamoto University, Kumamoto, Japan

**ThP 668**
Quantitative Proteomics of Mouse Skeletal Muscles after 30 Days Of Microgravity on the BION-M1 Biosatellite; Georg Tischer;  
Pauline Maes; Alain Van Dorselaere; Stephane Blanc; Guillemette Gauquel-Koch; Fabrice Berthe;  
LSMO, DSA IPHC Strasbourg, France; ‘DEPE, IPHC Strasbourg, France; ‘CINES, Paris, France

**ThP 669**
Enhanced Multiplexing to Study the Alzheimer’s Disease Proteome across Tissues; Christina King; Liqing Gu; Renä Robinson;  
‘University of Pittsburgh, Pittsburgh, PA

**ThP 670**
Unravelthe Mechanism of PP2AcPositively Regulating Liver Replication Termination in Mice through a TMT Labeling-Based Phosphoproteomic Approach; Bin Xue;  
‘University of North Carolina, Chapel Hill, NC

**ThP 671**
Label Free Proteomic Analyses of CEACAM1 Knockout Mouse Liver and Adipose Tissue; Gabriel Gugui; Ge Helen; Moore Roger; Deirdre La Placa; Zhifang Zhang; John E. Shively;  
‘City of Hope, Duarte, CA

**ThP 672**
Quantitative, Global Proteomic Analysis of the Damaged Sensory Periphery in Noise-Induced Hearing Loss; Ann E. Hickox;  
Ann C. Y. Wong; Kwang Pak; Chelsea Strojny; Allen F. Ryan; Jeffrey N. Savas;  
Northwestern Feinberg School of Medicine, Chicago, IL; ‘University of California San Diego, San Diego, CA; ‘Veterans Administration Medical Center, La Jolla, CA; ‘University of New South Wales, Sydney, Australia

**ThP 673**
Nitrite-Induced Preconditioning Elicits Significant Long-Term Alterations to Key Heart Proteins Involved in Redox Stress Protection and Mitochondrial Function; David H. Perlman; Giuseppe Infusini; Selena Bauer;  
Bernadette O Fernandez; Mark E McComb; Martin Feilisch; Catherine E Costello;  ‘Boston University School of Medicine, Boston, MA

**ThP 674**
Novel Functional Roles of Acid Sensing Ion Channel Implicated by Proteomics; Zhuhua Yang; Mingli Liu; Zhigang Xiong; An Zhou;  ‘Morehouse School of Medicine, Atlanta, GA

**ThP 675**
Proteomics and Transcriptomics of Therapeutic Ultrasound Treatment on Pancreatic Cells; S. L. Ng; S. T. Tsai; T. K. Ju; N. G. Chen; Y. P. Kuo;  
I. L. Tsai; C. H. Chen; ‘Genomic Research Center, Academia Sinica, Taipei, Taiwan (R.O.C.); ‘Institute of Biomedical Engineering/Department of Electrical and Computer Engineering, National Chiao Tung University, Hsinchu, Taiwan (R.O.C.); ‘Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taipei, Taiwan (R.O.C.)
ThP 688 Quantification of Lamotrigine and Caffeine in Human Blood using Dried Blood Spot MALDI-MS; *Anne Arnold*1; Michael Karas1; *Goethe University, Frankfurt Am Main, Germany*

ThP 689 High-Throughput Validated Method for the Quantification of Nicotine and Cotinine in Serum using Ultra Fast SPE-MS/MS; *Matthew Biergum*1; Paul J Jannetto2; Loralie J Langman2; *Mayo Clinic, Rochester, Mn; Mayo Clinic, Rochester, MN*

ThP 690 High Variation of Internal Standard Response Between Known and Incurred Samples Using LC-MS/MS Method; *Weiwei Sun*1; John Chapdelaine1; Zhao Heng Ge; Adrien Musuku1; *Pharmascience Inc., Montreal, QC; Pharmascience, Montreal, Canada*

ThP 691 Plasma 9- and 13-hydroxy-octadecadienoic Acids are Inversely Related to Granulocyte Colony Stimulating Factor and IL-6 in Runners after Heavy Exertion; David C. Nieman1; Mary Pat Meaney1; Casey John1; Kevin Knagge1; Huiyuan Chen1; *Appalachian State University, North Carolina Research Campus, Kannapolis, NC; Teknion Kannapolis, NC*

ThP 692 Evaluation of Two Sample Preparation Methods, Precipitation-Derivatization and SPE, for Quantitative LC-MS Analysis of Methylmalonic Acid in Plasma; *Mindy gao*; ThermoFisher Scientific, San Jose, CA

ThP 693 Development and Validation of a High Throughput LC-MS/MS Method for Determination of 17-desacetyl Norgestimate in Human Plasma; *Jasper X. Chu*1; Mary Hillegas1; Yuzhu Xue1; Yuan-Shek Chen2; Ben Hsu3; *QPS LLC, Newark, DE*

ThP 694 A Strategy for Maintaining Chromatographic Peak Shape Due to Incompatible Extract and Mobile Phase by LC-MS/MS; Mathieu Laheide1; Milton Furtado1; Anahita Keyhani1; *Algorithmhe Pharma Inc., Laval, Canada*

ThP 695 How Low Can We Go? Analysis of Aldosterone using a High Sensitivity Tandem Quadrupole Mass Spectrometer for Clinical Research; *Dominic Foley*1; Lisa Calton1; *Waters, Wilmslow, UK*

ThP 696 Quantitation of Pegylated Drug Conjugate Interferon Alpha-2b in Human Serum using QTRAP® 6500; Faraz Rashid1; Dipankar Malakar1; *Anoop Kumar*2; Manoj Pillai1; Praveen Kumar Vittal1; Manoj Bob1; Ravisekhar K1; SSCIEX, 121 Udyog Vihar Phase IV Gurgaon, India; SSCIEX, Gurgaon, Haryana1; SSCIEX, 121 DHR holding Udyog Vihar Phase-4, HR; *Lupin bioresearch Center, Pune Maharashtra, MH*

ThP 697 A Sub-Picomol Method for Mass Spectrometry of 65 ColoNeSt Proteomes Free DDA Quantification to Spectral Libraries for Sub-Proteomes; *Susan Klaeger*1, 2, 3; Stephanie Heinzmeir1, 2, 3; Mathias Wilhelm1; Benjamin Ruprecht1; Heiner Koch2, 4, 5; Runsheng Zheng1; Susan Klaeger1, 2, 3; Meng Chen1; Anna Jarzab1; *Technical University Munich, Munich, Germany; German Cancer Consortium (DKTK), Munich, Germany; German Cancer Research Center, Heidelberg, Germany; Freising, Germany; Center for Integrated Protein Science, Munich, Germany*

ThP 700 Intensity-Based Liquid-Phase Quantification of the Kinome and Total Proteome across 65 Colorctal Cancer Cell Lines: The CRC65 Cell Line Panel; Martin Heinrich Freiing1; Riccardo Zenezini Chiozzi1, 2; Mathias Wilhelm2; Benjamin Ruprecht1; Heiner Koch2, 4, 5; *University of Oxford, Oxford, UK; Chair of Proteomics and Bioanalytics, Technical University of Munich, Munich, Germany; University of Rome, La Sapienza, Rome, Italy; German Cancer Consortium (DKTK), Muenchen, Germany; German Cancer Research Center (DKFZ), Heidelberg, Germany; Martin-Luther-Universität, Halle-Wittenberg, Germany; Goethe University, Frankfurt Am Main, Germany; Bavarian Biomolecular Mass Spectrometry Center, Freising, Germany; Center for Integrated Protein Science, Muenchen, Germany*

ThP 701 Selectivity Profiling of Kinase Inhibitors - From Label Free DDA Quantification to Spectral Libraries for Sub-Proteomes; *Susan Klaeger*1, 2, 3; Stephanie Heinzmeir1, 2, 3; Mathias Wilhelm1; Maria Reinecke1; Dominic Helm1; Huichao Qiao1; Guillaume Médard1; Bernhard Kuster1, 2; Technical University Munich, Munich, Germany; German Cancer Research Center, Heidelberg, Germany; Freising, Germany; Center for Integrated Protein Science, Munich, Germany

ThP 702 Proteome Wide Selectivity Profiling of Cyclin-dependent Kinase Inhibitors; *Huichao Qiao*1; Susan Klaeger1, 2, 3; Mathias Wilhelm1; Stephanie Heinzmeir1, 2, 3; Dominic Helm1; Guillaume Médard1; Bernhard Kuster1, 2; University of Oxford, Oxford, UK; Chair of Proteomics and Bioanalytics, Technical University of Munich, Munich, Germany; University of Rome, La Sapienza, Rome, Italy; German Cancer Consortium (DKTK), Muenchen, Germany; German Cancer Research Center (DKFZ), Heidelberg, Germany; Martin-Luther-Universität, Halle-Wittenberg, Germany; Goethe University, Frankfurt Am Main, Germany; Bavarian Biomolecular Mass Spectrometry Center, Freising, Germany; Center for Integrated Protein Science, Muenchen, Germany

ThP 703 A Comprehensive Study of the Ponatinib-Induced Kinome Changes in Drug-Resistant Leukemia; *Laura Herrera*1; Denis Okumu1; Karim Gilbert1; Michael East1; Lee Graves1; *University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 704 MAPKi Inhibitor Induced Signaling Modulation in BRAF-mutated, BRAFi Resistant Colorectal Cancer Cells: A Step Toward Informing Clinical Combination Dose Strategy; *AN CHI*; *Merck, Boston, MA*

ThP 705 Defining Mutant and Wild-Type Colorectal Cancer Signalling Networks with an Integrated Multi-Omics Approach; *Rob Ewing*1; Zhenghe Wang2; Jing Song2; *University of Southampton, Southampton, HANTS; Case Western Reserve University, Cleveland, OH*

ThP 706 Combination of Phosphoproteomics and Machine Learning Approaches Allow Large Scale Identification of Direct Kinase Substrates in vivo; *Evgeny Kanshin*1; Sebastien Giguerue2; Jing Cheng2; Mike Tyers2; *Pierre Thibault2, 4; IRIC, Montreal, QC; IRIC-Université de Montréal, Montréal, QC; Department of Medicine, University of Montréal, Montréal Quebec, Canada; Department of Chemistry, University of Montréal, Montreal Quebec, Canada

ThP 707 PKCs and CDKs Regulate Insulin Signaling in Response to a 3-Day High Fat Diet; *Brandon Gassaway*1; Max Petersen1; Hans Rudolf Aerni1, 2; Yulio Surovtsev1; Karl W Barber1, 2; Joshua B Sheetz2; Svetlana Rogulina1; *Annie Merkle1; Varman Samuel1, 3; Gerald Shulman1, 3; Jesse Rinheat1, 8; Yale School of Medicine, New Haven, CT; Systems Biology Institute, West Haven, CT; Howard Hughes Medical Institute, Chevy Chase, MD; Yale Center for Molecular Discovery, West Haven, CT; Veterans Affairs
ThP 710  Profiling Changes in the Phosphoproteome of Hematopoietic Cells in Response to a Novel Class of Anti-Oncogenic Sphingolipid Derived Small Molecules; Peter Kubiniok1; Alison McCracken2; Michael Perryman3; Stephen Hanessian4; Aimee Edinger5; Pierre Thibault6; 1University of Montreal, Montreal QC, Canada; 2University of California - Irvine, Irvine, CA

ThP 711  Mapping the Ubiquitin Regulatory Networks by Global Proteomic Measurements; Jeremy O’Connell1; Ekaterina Stepanova2; Joao Paulo3; Steven P Gygi4; 1Harvard Medical School, Boston, MA

ThP 712  Monitoring of the AKT/mTOR Pathway using Internal Standard Triggered-Parallel Reaction Monitoring (IS-PRM); Shou Ling Xu1; Michael Blank1; Sebastien Gallien2; Bhavin Patel3; Alex Behling4; Leigh Foster5; John D Rogers6; Bruno Domon7; Andreas Humer8; “Thermo Fisher Scientific, San Jose, CA; 2Luxembourg Clinical Proteomics Center, Strassen, Luxembourg; 3Thermo Fisher Scientific, Rockford, IL

ThP 713  Targeted Proteomics-Driven Computational Modeling of Microbial Sensing and Chemotactic Signaling Pathways in Macrophages; Nathan P Manes1; Jessica M Mann1; Bastian R Angermann2; Marijke Koppenal-Raab3; Eunkyung An1,2; Virginie H Sjoelund3; Jing Sun1; Masaru Ishii3; Ronald N Germain3; Martin Meier-Schellersheim4; Aleksandra Nita-Lazar5; 1NIH/NIAID, Bethesda, MD; 2OncoPlex Diagnostics, New York, NY; 3Thermo Fisher Scientific, San Francisco, CA; 4ICN Biomedicals GmbH, Zuers, Switzerland; 5Ontario Institute for Cancer Research, Toronto, ON

ThP 714  To Interact or Not to Interact? The CLASP2 Interactome, a Case Study; Paul Langtangen1; Rikke Kruse-Sorensen1; James Krantz1; Natalie Barker1; Richard Coletta3; Kristin Ricklefs-Johnson1; Mouluin Luo1; Kurt Hojlund2; Lawrence Mandarino1; 1Mayo Clinic, Rochester, MN; 2University of Southern Denmark, Odense, Denmark; 3Arizona State University, Tempe, AZ

ThP 715  Deciphering Peptidome Network by Quantitative Proteomics and Azido-homoalanine Labeling; Haiping Tang1; Qintao Wang1; Zhenyu Zhang1; Haileng Deng1; 1Tsinghua University, Beijing, China; 2Chaoyang Hospital Affiliated to Capital Medical University, Beijing, China

ThP 716  MSCypher: A High-Throughput Peptide Identification Strategy for Complex Mixtures; Eugene Kapp1; Giuseppe Infusini1; Yunshan Zhong1; Laura Dagley1; Terry Speed1; Liam O’Connor1; Andrew Webby1; 1The Walter & Eliza Hall Institute, Parkville, Australia

ThP 717  Yeast Proteome Dynamics are Revealed by hyperLOPIT: A High Resolution Spatial Proteomics Approach; Daniel J.H. Nightingale1; Lisa M Breckels1,2; Laurent Gatto1,3; Stephen G Oliver1; Kathryn S Lilley1; 1Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge, UK; 2Computational Proteomics Unit, Department of Biochemistry, University of Cambridge, Cambridge, UK; 3Cambridge Systems Biology Centre, Department of Biochemistry, University of Cambridge, Cambridge, UK

ThP 718  Revealing the Biology between Mass Spectral Molecular Networks with a Novel Dissimilarity Measure; Ricardo Silva1; James T. Morton1; Robert Andrew Quinn1; Rob Knight1; Pieter C. Dorrestein1; 1Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA; 2Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; 3Department of Pediatrics, University of California San Diego, La Jolla, CA; 4Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA
Ultrasensitive Measurements of Endogenous and Exogenous Formaldehyde-Induced DNA-Protein Crosslinks using Nano-LC-ESI-MS/MS. Yongquan Lai; James A Swenberg; University of North Carolina at Chapel Hill, Chapel Hill, NC

Targeting the Endocannabinoid System to Enhance Innate Immunity Using Chemoproteomics. Jung Hwa Lee; Mississippi State University, Mississippi State, MS

Effect of Iron Supplementation on Lead Exposure in Liver of Rats: A Proteomic Analysis. Mileni Silva Fernandez; Aline Lima Leite; Lucas Ferreira Almeida; Fernanda Zucki; Camila Peres-Buzalaf; Marília Afonso Rabelo Buzalaf; Federal University of São Carlos, São Carlos, SP, Brazil, São Carlos, SP-Brazil; Bauru Dental School, Bauru, SP-Brazil; Faculty of Medicine of Ribeirão Preto, Ribeirão Preto, SP-Brazil; Center on Health Sciences, USC, Bauru, SP-Brazil

Non-targeted Identification of the Protein Targets of Reactive Drug Metabolites using Stable Isotopic Labeling and High-Resolution Mass Spectrometry. Michael G. Leeming; William A. Donald; Richard A.J. O’Hair; The University of Melbourne, Melbourne, Australia; The University of New South Wales, Sydney, Australia

Targeted Proteomic Analysis of Abrin. Alena Myslivcova Fucikova; Jana Klimentova; Miloslava Duracova; Jiri Dresler; Zuzana Krocova; University of Defence, Hradec Kralove, CZ; Central Military Health Institute, Prague, CZ

Arsenite Binds to the PHD-type Zinc Finger Domain of FANCL E3 Ubiquitin Ligase and Inhibits DNA Intervermillion Crosslink Repair. Ji Jia; Yinsheng Wang; University of California - Riverside, Riverside, CA

High Throughput Pharmacovigilance Screening of Nutraceuticals and Alternative Medicines. Elly Crighton; Joel Gummer; Garth Maker; Ian Mullaney; Megan Coghlan; Michael Bunce; Claire Hoban; Ian Musgrave; Roger Byard; Robert Trengove; School of Veterinary and Life Sciences, Murdoch University, WA, Australia; Perth, Australia; Separation Science and Metabolomics Laboratory, Murdoch University, Perth, Australia; Metabolomics Australia, WA Node, Perth, Australia; RMIT University, School of Science, Melbourne, Australia; Curtin University, Perth, Australia; The University of Adelaide, Adelaide, Australia; Murdoch University, Murdoch, WA

MALDI Imaging MS in Neurotoxicology: Proteomic Biomarker Discovery in the Rat Brain with Jet Fuel Inhalation Exposures. Ling Qi; Pavel Shiyano; Karen Mummy; Camilla Mausz; T11HP/RHJD, US Air Force Research Lab, WPAFB, OH; Naval Medical Research Unit-Dayton, WPAFB, OH

Integrated Proteomic Analysis of Human Airway Epithelial Cells after Exposure to Diacetyl Vapor. Matthew Foster; William Gwinn; Francine Kelly; David Brass; Ashlee Valente; Will J Thompson; Daniel Morgan; Arthur Moseley; Scott Palmer; Duke University, Durham, NC; NIEHS, RTP, NC; Duke University Medical Center, Durham, NC; NIEHS / NIH, RTP, NC
INDEX OF AUTHORS
INDEX OF AUTHORS

Benesch, Justin .................................................. ThP 186
Benesch, Justin .................................................. TOH pm 04:10
Benesch, Justin .................................................. WOB pm 04:10
Benigni, Paolo .................................................. MP 104
Benigni, Paolo .................................................. MP 105
Benigni, Paolo .................................................. TP 409
Benigni, Paolo .................................................. TP 463
Benjamin, Elifrida ........................................... WP 632
Benke, Roland .................................................. WP 414
Bener, Bruce .................................................... TP 094
Bener, Bruce .................................................... TP 015
Bener, Eric ...................................................... ThP 365
Bennett, Bryson ................................................ MP 490
Bennett, Dylan .................................................. ThP 074
Bennett, Dylan .................................................. ThP 076
Bennett, Keiryn ................................................ WOE am 10:10
Bennett, Richard ................................................ TP 030
Bennington, Leeman ........................................... ThP 170
Ben-Nissen, Gilli ................................................ WP 580
Ben-Nisse, Gilli ................................................ WP 09:00
Bensaddek, Dalila ............................................. TOE am 09:10
Bensaddek, Dalila ............................................. WP 400
Benson, Linda .................................................... MP 603
Benter, Thorsten .............................................. ThP 282
Benter, Thorsten .............................................. ThP 309
Benter, Thorsten .............................................. ThP 317
Benter, Thorsten .............................................. ThP 318
Benter, Thorsten .............................................. ThP 319
Benter, Thorsten .............................................. TP 197
Bentzen, Robert ................................................ TP 417
Bentzen, Robert .............................................. TP 428
Bentley, Mark .................................................... ThP 732
Bentley, Mark .................................................... WP 549
Bentley, Mark .................................................... WP 560
Benton, Bert ..................................................... TOG pm 03:50
Benz, Ryan ....................................................... TP 681
Berchtold, Christian ........................................ TP 098
Berchuck, Andrew .............................................. ThP 658
Berdes, Emmet .................................................. TP 573
Berden, Giel ...................................................... ThP 401
Berden, Giel ...................................................... ThP 402
Berden, Giel ...................................................... ThP 403
Berden, Giel ...................................................... ThP 404
Berejnia, Olga ................................................... ThP 063
Bereaman, Michael ............................................ WP 006
Bereaman, Michael ............................................ WP 146
Berennezen, Jacob ............................................. MP 216
Bers, Michael .................................................... TP 359
Berg, Amanda ..................................................... MP 418
Berg, Amanda ..................................................... WP 582
Berg, Christian .................................................. ThP 202
Bergen, Arthur Robert ......................................... WP 603
Bergen, Robert .................................................. ThP 548
Bergen, Scott .................................................... WOG am 08:50
Berg, Sebastian .................................................. WP 498
Bergin, Ingrid ..................................................... WP 557
Bergman, Hilde-Marlene ...................................... WP 347
Bergo, Vladislav ................................................ ThP 621
Bergquist, Jonas ................................................ ThP 508
Bergsdoerfer, Christian ...................................... TP 143
Bergstroem, Sven ............................................... MP 268
Berhow, Mark .................................................... MP 661
Berli, Joshua ...................................................... WP 146
Berim, Anna ...................................................... ThP 226
Benn, Marshall .................................................. ThP 181
Benn, Marshall .................................................. TP 033
Benn, Marshall .................................................. TP 034
Benn, Marshall .................................................. WP 626
Benn, Marshall .................................................. WP 630
Benn, Marshall .................................................. WVQ pm 04:10
Benn, Marshall .................................................. ThOB pm 04:10
Benn, Marshall .................................................. TP 375
Bernaldo, Ricardo .............................................. WP 257
Bernards, Nicholas ........................................... WOD pm 02:30
Bernet, Pascal .................................................... TP 143
Bernard, Werner ................................................ TP 270
Bernhardt, Oliver .............................................. ThOF am 09:10
Bernhardt, Oliver .............................................. ThOF am 09:30
Bernhardt, Oliver .............................................. TP 088
Bernhardt, Oliver .............................................. TP 094
Bernhardt, Ryan ................................................ WP 437
Berner, Matthew ................................................ ThP 025
Berner, Matthew ................................................ WP 406
Bersuker, Laurence E ......................................... MOF am 05:30
Bertele, Fabrice ................................................. ThP 668
Bertozi, Carolyn ................................................ ToOE am 10:10
Bertozi, Carolyn ................................................ TP 077
Bessi, Romano ...................................................... TP 069
Bessire, Andrew ................................................... MP 015
Bessonneau, Vincent ........................................... WP 446
Bessonneau, Vincent ........................................... WP 260
Bestard-Escalas, Joan ......................................... TP 335
Betancourt, Stella .............................................. MP 533
Betchy, Emily ..................................................... WP 306
Bentenbaugh, Michael ......................................... WOG am 08:30
Bentenbaugh, Michael ......................................... TP 279
Bentenbaugh, Michael ......................................... WP 309
Betgovezage, Edna ............................................... ThP 473
Betgovezage, Edna ............................................... WP 654
Bethard, Jennifer ................................................ WP 640
Betz, Daniel ....................................................... TP 515
Beu, Dominik ...................................................... TP 308
Beuerman, Roger W ........................................ ToOF am 08:50
Beveridge, Rebecca ............................................... TP 059
Beyer, Andreas ................................................... ThP 02:30
Beyer, Andreas ................................................... ThP 03:50
Beyna, Mercedes ................................................ WP 176
Beynon, Robert .................................................. ThP 088
Beynon, Robert .................................................. WP 080
Beynon, Robert .................................................. WP 169
Beynon, Robert .................................................. WP 654
Bhandari, Deepak ................................................ ThP 681
Bhandarkar, Deepthi ........................................... WP 646
Bhandarkar, Deepthi ........................................... WP 669
Bhandarkar, Deepthi ........................................... WP 854
Bhandarkar, Deepthi ........................................... WP 874
Bhandarkar, Deepthi ........................................... WP 915
Bhandarkar, Deepthi ........................................... WP 917
Bhanu, Natarajan ................................................ WP 106
Bhanu, Natarajan ................................................ WP 108
Bhanu, Natarajan ................................................ TP 366
Bhargava, Maneesh ............................................ MOF am 08:50
Bhasin, Shalender ............................................... ThP 629
Bhat, Vadiraja ..................................................... MP 527
Bhat, Vadiraja ..................................................... MP 537
Bhat, Vadiraja ..................................................... ThP 433
Bhat, Vadiraja ..................................................... WP 539
Bhat, Vadiraja ..................................................... WP 598
Bhat, Apeksha ..................................................... TP 651
Bhat, Pranay ....................................................... TP 832
Bhattacharjee, Payel ........................................... TP 036
Bhavsar, Satyendra ............................................. TP 171
Bhawal, Ruchika ................................................. WP 602
Bhune, Ankush ..................................................... MP 171
Bhune, Ankush ..................................................... MP 544
Bhune, Ankush ..................................................... ThP 147
Bhune, Ankush ..................................................... ThP 158
Bhowsik, Satil ..................................................... ThP 071
Bhowsik, Satil Kumar ........................................... ThP 077
Bhowsik, Satil Kumar ........................................... ThP 433
Bhuvanendran, Shivaprasad ................................ WP 106
Bii, Xuezi .......................................................... TP 723
Biacchi, Michael .................................................. TP 019
Bian, Liangqiao ................................................... TP 945
Bian, Yangyang ................................................... TP 584
Bianchini, Federica ............................................. WP 433
Bianucci, Raffaelea ............................................. ThOA am 09:50
Biel, Heidi ........................................................ WP 388
Bielik, Alicia ....................................................... MP 012
Bienner, Ludovic ................................................ TP 407
Bier, Mark ......................................................... ThOB pm 03:50
Bier, Mark ......................................................... TOB pm 02:30
Bierer, Veronica .................................................. MP 087
Bierbaum, Veronica ............................................. MP 389
Bierkandt, Thomas ............................................... MP 406
Bierkandt, Thomas ............................................... TOA am 03:10

Program code: M,T,W,Th = Day  O = Oral, P = Poster  Time or poster number
INDEX OF AUTHORS

Brown, Christopher ...........................................MP 086
Brown, Hilary ..................................................TP 504
Brown, Jeff .....................................................MP 319
Brown, Jeff ......................................................TP 413
Brown, Jeff .....................................................WP 436
Brown, Jeff ......................................................TP 704
Brown, Jeffrey ...................................................ThP 389
Brown, Jennifer ..................................................ThP 633
Brown, Joseph ...................................................ThP 391
Brown, Justin ....................................................ThP 072
Brown, Karen ....................................................ThP 418
Brown, Kristy ....................................................WP 106
Brown, Lauren ...................................................TP 189
Brown, Lewis M ..................................................TP 704
Brown, Murray ..................................................WP 583
Brown, Robert ...................................................WP 535
Brown, Steven ...................................................WP 187
Brown-Augsburger, Patricia ..................................WP 621
Browning, Marc ..................................................MP 435
Bruce, James ....................................................MOH pm 04:10
Bruce, James ......................................................TP 074
Bruce, James ......................................................TP 436
Bruce, James ......................................................TP 655
Bruchmann, Andreas ...........................................WP 467
Bruckner, Raphael .............................................ThOF pm 03:50
Bruderer, Roland ...............................................TP 088
Bruderer, Roland ................................................TP 094
Brüning, Merlin ..................................................WP 030
Bruinen, Anne .................................................TOD am 08:50
Bruno, Andrea ....................................................TP 708
Bruno, Alessandro ..............................................TP 276
Bruschweiler, Rafael ............................................MOG am 09:10
Brusniak, Mi-Youn .............................................WP 391
Brüttig, Christoph .............................................WP 609
Bryan, Clay .......................................................ThP 247
Bryant, Matthew .................................................TP 052
Brzezinski, Jennifer ...........................................MOA pm 04:10
Bu, Juan ............................................................MP 508
Bu, Jiexun ...........................................................ThP 298
Bu, Jiexun ...........................................................WOB am 04:10
Bu, Shuo-Lei .......................................................TP 707
Buch, Arnaud ......................................................WP 411
Buch, Greg ........................................................TP 102
Buchan, Gregory ...............................................TOC am 09:30
Buchberger, Amanda ...........................................ThP 521
Buchberger, Amanda ...........................................ThP 522
Buchberger, Amanda ...........................................TP 722
Buchberger, Amanda ...........................................ThP 174
Buchholz, Lisa ....................................................MP 364
Buck, Ash ..........................................................WP 441
Buck, Alan ........................................................TP 648
Buckley, Frank ...................................................TOB pm 03:50
Budelher, Melissa ...............................................TP 600
Buen, Zachary ....................................................WP 469
Buentello, Jerry ..................................................TP 351
Bugg, May ..........................................................WP 141
Bugianesi, Randal ...............................................TOC pm 04:10
Bugrova, Anna ...................................................TP 101
Bugrova, Anna ....................................................WP 063
Buhimschi, Catalin ..............................................WP 537
Bukichelski, Irina ...............................................WP 373
But, Anni ..........................................................WP 061
Buisson, Corinne .................................................WOF pm 03:30
Buisson, Corinne ................................................TP 071
Buist, Marjorie ...................................................TP 282
Bukasy, Nick .....................................................MP 631
Bukowski, Nick ..................................................WP 292
Bulal, Patrick ....................................................WOG am 10:10
Buljan, Marija ...................................................ThOE pm 02:30
Bulloch, Daly .....................................................TP 767
Buller, Pater ......................................................WP 697
Bunce, Michael .................................................ThP 746
Bunch, Josephine ................................................MP 509
Bunch, Josephine .................................................ThOD pm 03:50
Bunch, Josephine .................................................ThP 244
Bunch, Josephine .................................................ThP 387
Bunch, Josephine ...............................................TOF pm 03:50
Bunch, Josephine ...............................................TP 198
Bunch, Josephine ...............................................TP 355
Bunch, Josephine ...............................................TP 537
Bunch, Josephine ...............................................WP 022
Bunch, Josephine ...............................................WP 349
Bunch, Josephine ...............................................WP 360
Bunch, Josephine ...............................................WP 374
Burak, Theresa ..................................................ThP 438
Burrant, Charles ...............................................ThP 439
Burrant, Charles ...............................................WP 557
Burbank, Brian ..................................................ThP 432
Bure, Corinne ....................................................ThP 359
Burgess, Jennifer .................................................MP 145
Burgess, Jennifer ...............................................ThP 114
Burgett, Anthony ...............................................ThOE pm 04:10
Burgett, Anthony ...............................................ThP 089
Burgett, Anthony ...............................................TP 682
Burke, Adam .......................................................MOC pm 03:30
Burke, Adam .......................................................TP 024
Burke, Meghan ..................................................TP 374
Burke, Nicole ....................................................MP 408
Burke, Nicole ....................................................ThOB am 08:50
Burkert, Kathrin ...............................................TOC pm 03:50
Burkhardt, Julia ..................................................ThP 602
Burnin-Johnson, Kristin .......................................MOG am 08:30
Burns, William ..................................................MP 432
Burns, William ..................................................MP 695
Burroughs-Johnson, Kristin ..................................MOG am 08:30
Burns, William ..................................................MP 523
Burseg, Kerstin ..................................................WP 438
Burt, Michael .....................................................MP 213
Burt, Michael .....................................................MP 217
Burt, Sarah .........................................................WP 100
Burton, Keith .....................................................MP 437
Burton, Lyle .........................................................MP 304
Burton, Richard ..................................................TP 136
Byrn, Stephen ...................................................ThP 436
Byrne, Keran .....................................................MOA pm 02:30
Byrne II, Jerry ....................................................MP 169
Byrum, Stephanie ................................................WP 763
Byrum, Stephanie ................................................WP 357
Bythell, Benjamin ...............................................ThP 337
Bythell, Benjamin ...............................................ThP 462
Bythell, Benjamin ...............................................TP 474
Bythell, Benjamin ...............................................TP 506
C. Ronald, Kahn ..................................................ThP 592
Caballero, Marina ..............................................ThP 603
Cabovska, Baiba ................................................MP 535
Cabrera, Robert ..................................................MOG am 09:04
Cacchiallo, Russell .............................................MP 447
Cadene, Martine ................................................MP 562
Cadene, Martine ................................................WP 635
Caffarelli, Nicolas ...............................................TP 010
Cahill, John .......................................................MP 218
Cahours, Xavier ..................................................WP 438
Cai, Chengyuan ..................................................TP 117
Cai, Chengyuan ..................................................ThP 119
Cai, Chengyuan ..................................................TP 255
Cai, Yang ..........................................................TP 506
Cai, Qian ..........................................................WP 046
Cai, Tanxi ..........................................................ThP 029
Cai, Tie ..............................................................WP 120
Cai, Tie ..............................................................ThP 040
Cai, Wei ............................................................TP 133
Cai, Wenxuan .....................................................MP 315
Cai, Wenxuan .....................................................MP 709
Cai, Wenxuan .....................................................MP 612
Cai, Wenxuan .....................................................MP 711
Cai, Wenxuan .....................................................TP 768
Cai, Wenxuan .....................................................WOE am 09:30
Cai, Wenxuan .....................................................WOH pm 03:50
Cai, Yi ...............................................................ThOD pm 02:30
Cai, Zi ...............................................................ThP 640
Callahan, Heather ...............................................MP 512
Callahan, Heather ...............................................MP 513
Callies, Ivama .....................................................TP 163
Calligaris, David ...............................................TP 348
Calligaris, David ...............................................TP 414
Calligaris, David ...............................................WOC am 09:50
Calligaris, David ...............................................WOD pm 04:10
Calston, Lisa ......................................................ThP 695
Calvaresi, Valeria ...............................................MP 722
Camenzuli, Michelle ..........................................MP 433
Cameron, Simon ...............................................MP 03:30
Cameron, Simon ...............................................MP 506
Cameron, Simon ...............................................ThP 024
Camicioli, Richard .............................................WP 507
Cammarata, John ...............................................ThP 621
Cammarata, Michael ..........................................ThP 567
Cammarata, Michael ..........................................ThP 585
Camp, David ......................................................WP 089
Campbell, Colin ..................................................ThP 520
Campbell, Gary ...................................................MP 673
Campbell, J. Larry ...............................................TP 199
Campbell, Larry ..................................................WP 352
Campbell, Larry ..................................................WP 331
Campbell, Larry ..................................................ThOG pm 04:10
Campbell, Larry ..................................................ThP 028
Campbell, Larry ..................................................TP 513
<table>
<thead>
<tr>
<th>Index of Authors</th>
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<tbody>
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<td>Garcia-Ordonez, Ruben</td>
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INDEX OF AUTHORS

Liu, Ming ............................................... ThP 008
Livet, Sandrine ................................ MOG pm 03:10
Lyaniage, Rohana ....................................... TP 621
Lyaniage, Rohana ....................................... TP 691
Lyaniage, Rohana ....................................... WP 107
Lyu, Jinditori ........................................... MP 121
Lizhnyak, Pavel ........................................ MP 694
Lizhnyak, Pavel ........................................ MP 700
Llamas, Claire .......................................... WP 064
Lloyd, Tom .............................................. WP 706
Lloyd, Jones, Guy ........................................ WP 705
Lo, Andy .................................................. MP 196
Lobas, Anna .............................................. WP 655
Lobdeit, Nicole .......................................... MP 695
Lobinski, Ryszard ....................................... TOA am 09:50
Loboda, Andri ........................................... WP 405
Locasale, Jason ......................................... TP 591
Locasale, Jason ......................................... ThP 434
Lock, Stephen J. ......................................... ThP 473
Lock, Stephen J. ......................................... WP 654
Locke, Stephen .......................................... TP 395
Lockhausberaumper, Julia ................................ TP 699
Lockyer, Nicholas ........................................ TP 316
Loda, Massimo ........................................... ThO am 08:30
Lodes, Hong ................................................ WP 550
Lodder, Helen ............................................ WP 485
Lodder, Helen ............................................ WP 489
Lodge, Jean ............................................... TOH pm 03:50
Loecken, Beth .............................................. ThP 13
Lofuts, Neil ............................................... TP 673
Lofuts, Neil ............................................... ThP 731
Lofuts, Neil ............................................... TP 222
Lofuts, Neil ............................................... TP 233
Lofuts, Neil ............................................... TP 231
Lofuts, Neil ............................................... WP 721
Loganathan, Devan ..................................... TP 178
Loganzo, Frank .......................................... MP 015
Loh, Christina ............................................ ThO pm 03:50
Lohar, Anant .............................................. WP 234
Lohar, Anant .............................................. WP 634
Lohar, Anant .............................................. WP 715
Lohar, Anant .............................................. WP 716
Leland, Claus ............................................. ThP 175
Lombard-Bank, Camille ................................. WP 703
Lommenick, Brett ........................................ TP 664
Lommel, L ....................................................... WP 61
Loombard, Bruno ....................................... TOG pm 10:12
Loom Bairds, Stavros ................................... TP 704
Londry, Frank ............................................. TP 208
Long, Debby ............................................... TP 353
Long, Graham ............................................. WP 177
Long, Frank ................................................ TP 686
Longuespee, Remi ........................................ ThP 207
Longuespee, Remi ........................................ TP 314
Longuespee, Remi ........................................ TP 319
Longuespee, Remi ........................................ TP 674
Longuespee, Remi ........................................ TP 690
Longworth, Joseph ..................................... MP 686
Loo, Joseph ................................................ MP 078
Loo, Joseph ................................................ MP 314
Loo, Joseph ................................................ TOE am 08:30
Loo, Joseph ................................................ TP 039
Loo, Joseph ................................................ TP 494
Loo, Joseph ................................................ WP 694
Loo, Joseph ................................................ WP 712
Loo, Joseph ................................................ WOH am 10:12
Loo, Joseph ................................................ WP 133
Loo, Joseph ................................................ WP 343
Loo, Joseph ................................................ TP 214
Loo, Joseph ................................................ ThP 156
Loo, Rachel ................................................ TP 494
Loo, Rachel ................................................ WOH am 10:10
Loo, Rachel ................................................ WP 343
Loo, Rachel ................................................ ThP 107
Loostma, Wayne ......................................... TP 142
Loostma, Wayne ......................................... WP 156
Lopez, Carlos ............................................. MP 695

Program code: M,T,W,Th = Day          O = Oral, P = Poster          Time or poster number
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Race into Indy for ASMS 2017

65th Conference on Mass Spectrometry and Allied Topics

June 4 - 8, 2017

Indianapolis, Indiana

June 3 - 4
Short Courses