

**THIS YEAR WE CELEBRATE 100 YEARS OF MASS SPECTROMETRY.** Each conference registrant will receive a free reproduction of J.J. Thomson's 1913 edition of *Rays of Positive Electricity*. Pick up your copy in the "Museum" located adjacent to Exhibit Hall C. In the museum you will also find:

- Display of historical instruments and accessories
- History posters
- For sale: "Evolution of Mass Spectrometry: 1910-1940," set of two wall posters (36" X 17.5"), \$20 per set

**Don't miss these other commemorative features of the meeting.**

- Sunday, 6:45 - 7:45 pm: Michael L. Gross, The First Fifty Years of MS: Building a Foundation
- Wednesday Poster Session: Historical Posters, WP 001 and 002
- Thursday, 2:30 - 4:30 pm: Celebration of 100th Anniversary of Mass Spectrometry, Room 103

## SPONSORS

ASMS gratefully acknowledges the support of these companies.



## CONFERENCE SPONSORS



## CONTRIBUTORS

IDEX Health & Science  
New Objective  
SGE Analytical Science  
Tandem Labs  
Thermo Scientific  
Zef Scientific

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*Titles in the following sections are provided by authors. The complete abstracts are available online: [www.asms.org](http://www.asms.org)*

*The PDF document of proceedings submissions for orals and posters are online one day after presentation at the conference.*

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## GENERAL INFORMATION

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

### SUNDAY TUTORIAL SESSION, 5:00 - 6:30 pm

*Exhibit Hall A, Lower Level*



**5:00 - 5:45 pm**  
**A Wide Spectrum: Clinical  
Diagnostics for the Masses**

**Andrew Hoofnagle**  
University of Washington



**5:45 - 6:30 pm**  
**The Nuts and Bolts of Protein  
Hydrogen Exchange MS**

**John Engen**  
Northeastern University

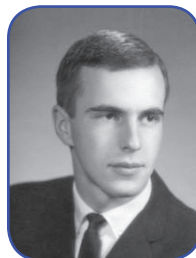
### SUNDAY CONFERENCE OPENING, 6:45 - 7:45 pm

*Exhibit Hall A, Lower Level*



**Welcome, Jenny Brodbelt**  
University of Texas, Austin  
ASMS Vice President for Programs

**Then...**



**Now...**



**The First Fifty Years of MS: Building a Foundation**  
**Michael L. Gross**

Washington University of St. Louis

### SUNDAY WELCOME RECEPTION, 7:45 - 9:00 pm

*Exhibit Hall BC.* Conference name badge is required.

## PLENARY SESSIONS

### Monday, 4:45 - 5:30 pm

*Exhibit Hall A, Lower Level*

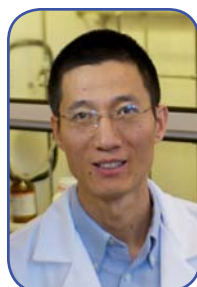


**AWARD LECTURE**  
**Award for a Distinguished  
Contribution in Mass Spectrometry**

**Richard D. Smith**  
Pacific Northwest National Laboratory

### Tuesday, 4:45 - 5:30 PM

*Exhibit Hall A, Lower Level*



**AWARD LECTURE**  
**Biemann Medal**

**Yinsheng Wang**  
University of California, Riverside

### Thursday, 4:45 - 5:30 PM

*Exhibit Hall A, Lower Level*



**PLENARY LECTURE**  
**Discovery of the Elusive Higgs Boson**

**Peter Onyisi**  
University of Texas at Austin

## DON'T MISS

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

*Ballroom A*

Enjoy a beverage while you applaud awards, hear the new initiatives under construction, and more!

### • CLOSING GALA, THURSDAY, 5:45 - 9:00 PM

*Exhibit Hall D*

*Let's celebrate!* The event features a buffet, cash bar, fun and games. Ticket is required, \$30 for conference registrant, \$20 for student.

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

Session A (MOA, TOA, WOA, ThOA).....	Exhibit Hall A (lower level)
Session B (MOB, TOB, WOB, ThOB) ....	L100 (lower level)
Session C (MOC, TOC, WOC, ThOC) .....	Ballroom B
Session D (MOD, TOD, WOD, ThOD) .....	Ballroom A
Session E (MOE, TOE, WOE, ThOE) .....	Auditorium
Session F (MOF, TOF, WOF, ThOF) .....	Room 101
Session G (MOG, TOG, WOG, ThOG) .....	Room 102
Session H (MOH, TOH, WOH, ThOH) .....	Room 103

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

**SPEAKERS** must load presentations at least one day prior to their talks. The speaker room is M101C (down to mezzanine level) and is open with a technician according to this schedule:

Sunday:	10:00 am - 8:00 pm
Monday through Wednesday:	7:30 am - 5:00 pm

**POSTERS AND EXHIBIT BOOTHS** are in Exhibit Hall BC. The Hall is open:

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

**POSTER SET-UP** is 7:30 am on the day scheduled and removal is 7:30 - 8:00 pm on the same day. Posters should not be removed early. Thursday posters must be removed by 3:30 pm. **Refer to the poster numbers in this final program for board assignments.** Presenters should supply pushpins or Velcro to mount their posters.

**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..

**LUNCH CONCESSIONS** in and near the exhibit hall are open 11:00 am - 2:00 pm.

**EXHIBITORS** must staff booths as follows:

Sunday Reception.....	7:45 pm - 9:30 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 area on level two.

**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. Visit the "Meet Minneapolis" booth for restaurant suggestions and reservations. The booth also features useful information about Minneapolis museums, shopping, attractions, nightlife and much more!

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

**CONFERENCE PROCEEDINGS** will be published online. Visit [www.asms.org](http://www.asms.org) after July 15 to view or download the Proceedings. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. Speaker web casting slides will be printed to PDF and used for speakers who fail to submit.

**WEB CASTING** includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to [www.asms.org](http://www.asms.org), select "web casting" on the annual conference page, and enter your last name and the User ID printed on your conference name badge.

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

**CORPORATE BREAKFAST SEMINARS** are hosted by some Corporate Members. Please reserve a seat at company exhibit booths. For list of companies hosting a breakfast, refer to Corporate Member listing in this program or [www.asms.org](http://www.asms.org).

**EMPLOYMENT CENTER** is located in the Poster/Exhibit Hall. The room is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. No hard copies of resumes or employment opportunities will be posted in the center. There are computers in the center for searching the database of candidates and positions. Interview booths must be reserved one day in advance.

Sunday .....	1:00 - 8:00 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.



## GENERAL INFORMATION

### MEDIA EVENTS

Corporate media sessions are scheduled on Monday and Tuesday for members of the press and financial institutions.

Company	Monday	Hilton Hotel Location
Shimadzu	8:00-9:00 am	Marquette I-III, VII-IX
Bruker Daltonics	9:30-10:30 am	Conrad
AB SCIEX	11:00-12:00 pm	Symphony Ballroom
Agilent Technologies	1:30-2:30 pm	Grand Ballroom ABC
Thermo Scientific	3:00-4:00 pm	Grand Ballroom EFG
Waters Corporation	4:30-5:30 pm	Grand Ballroom D
Company	Tuesday	Location
PerkinElmer	9:30-10:30 am	Marquette IV-VII



### CONFERENCE REGULATIONS

- Name badges are required for all conference sessions, including the exhibit hall and the employment center.
- No smoking is permitted in the convention center.
- Cell phones must be turned off in oral sessions.
- No photography or recording is allowed in oral sessions or in the Poster-Exhibit Hall.
- Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without the express written authority of ASMS and the author of the material presented. Such materials, only upon approval by ASMS and the author, may be published in print or online, and must contain appropriate credits for all quotations or photographs.
- The placement of advertising in the meeting area is strictly limited. There are poster boards and tables in the Exhibit Hall for corporate member notices and literature. No signs on easels are permitted. Other approved notices and announcements may be posted on designated Boards in the Exhibit Hall.
- Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos in slides or posters may appear only one time in the presentation.



## CONFERENCE HOTELS

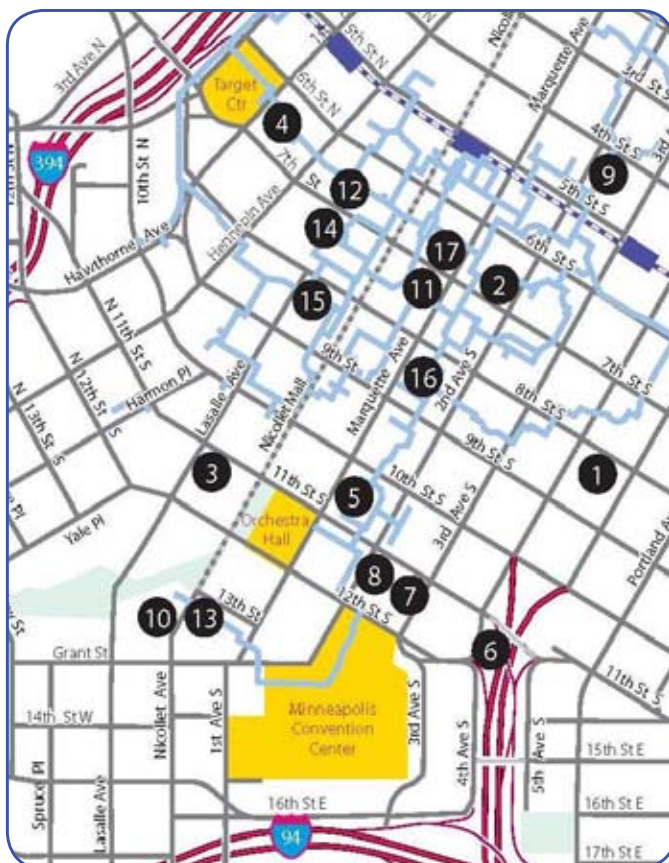
Map No.	Hotel	Telephone
1	Best Western	612-370-1400
2	Crowne Plaza	612-338-2288
3	Doubletree Suites	612-332-6800
4	Graves 601 Wyndham Grand	612-677-1100
5	Hilton Minneapolis	612-376-1000
6	Hilton Garden Inn	612-339-6633
7	Holiday Inn Express	612-341-3300
8	Hotel Ivy	612-746-4600
9	Hotel Minneapolis	612-340-2000
10	Hyatt Regency	612-370-1234
11	Marquette	612-333-4545
12	Marriott City Center	612-349-4000
13	Millenium	612-332-6000
14	Radisson Plaza	612-339-4900
15	Residence Inn	612-677-1000
16	W Minneapolis	612-215-3700
17	Westin Minneapolis	612-333-4006

## TRANSPORTATION

Travel free through the heart of downtown Minneapolis. Look for "Free Ride" buses on Nicollet Mall between the Convention Center and Washington Avenue, including a connection with the Hiawatha light-rail line, with service to the airport and Mall of America. Free bus service is available approximately every 10 minutes from 7 am to 7 pm on weekdays and roughly every 15-30 minutes on evenings and weekends.

There is also an extensive skywalk system in Minneapolis.

Image below shows bus stops.





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**Susan T. Weintraub**  
University of Texas Health Science Center  
San Antonio, TX



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**Scott A. McLuckey**  
Purdue University  
West Lafayette, IN



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**Jenny Brodbelt**  
University of Texas  
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*Vice President for Arrangements*  
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**Gavin E. Reid**  
Michigan State University  
East Lansing, MI



*Member at Large for Publications*  
**Evan Williams**  
University of California-Berkeley  
Berkeley, CA



*Member at Large for Digital Communications*  
**Michael J. MacCoss**  
University of Washington  
Seattle, WA

### Congratulations

to these members who were elected to the ASMS Board

### *Vice President for Arrangements*



**Gary Valaskovic**  
New Objective, Inc.

### *Secretary*



**Rebecca A. Jockusch**  
University of Toronto

### *Member at Large for Publications*



**David C. Muddiman**  
North Carolina State University

### Staff

Judith A. Sjoberg, *Executive Director*  
Jennifer Watson  
Cindi Lilly, Miquela Sena  
Marin Walker, Brent Watson



## INTEREST GROUP COORDINATORS

<i>Analytical Lab Managers</i>	Nathan Dalleska David Friedman
<i>Bioinformatics for MS</i>	Lucas Kall Brian Searle
<i>Clinical Chemistry</i>	Cory Bystrom Brett Holmquist
<i>DNA/RNA</i>	Fenyu Meng Norman Chiu
<i>Drug Metabolism &amp; Pharmacokinetics</i>	Don McKenzie Chandra Prakash
<i>Energy, Petroleum &amp; Biofuels</i>	Michael McGinley Wolfgang Schrader
<i>Environmental Applications</i>	Kerry Peru
<i>Flavor, Fragrance and Foodstuff</i>	Marc Engel
<i>FTMS</i>	Franklin Leach Amy McKenna
<i>Fundamentals</i>	George Khairallah Glen Jackson
<i>Hydrogen Exchange &amp; Covalent Labeling</i>	Lars Konermann David Schriemer
<i>Imaging MS</i>	Timothy Garrett Miam McDonnell
<i>Ion Mobility MS</i>	Matthew Bush
<i>LC/MS Related Topics</i>	Susan E. Abbatiello Helene Cardasis
<i>Metabolomics</i>	Gary Patti Paul West
<i>Metal Ion Coordination Chemistry</i>	Jinhua Ren Mike Van Stipdonk
<i>Peptide Fragmentation</i>	Nick Polfer Sharon Pitteri
<i>Pharmaceuticals</i>	Matthew Blatnik Brian Furmanski
<i>Polymeric Materials</i>	William Erb Gyorgy Vas
<i>Protein Therapeutics</i>	Sheng Gu Justin Sperry
<i>Quantitative Intact Proteomics</i>	Edward Dratz Julian Whitelegge
<i>Regulated Bioanalysis</i>	Fabio Garofolo
<i>Undergraduate Research in MS</i>	J.C. Poutsma
<i>Young Mass Spectrometrists</i>	Dian Su Bick Vu

## COMMITTEES

<i>Asilomar Conference</i>	Glen Jackson, Chair Carolyn Cassady Scott McLuckey Ryan Julian
<i>Corporate Liaison</i>	Lance Nicolaysen, Chair Scott McLuckey Carol Harp, Agilent Technologies Andrew Herman, Imtakt Carla Marshall-Waggett, New Objective Bez Moghadam, Thermo Scientific Qihui Ni, EMD Millipore Jon Speak, AB Sciex
<i>Digital Communications</i>	Michael MacCoss, Chair Nuno Bandeira Mike Lee Bin Ma Nathan Yates
<i>Education</i>	Gavin Reid, Chair Dieter Dorrestein Michael Fitzgerald Jennifer Grant Elaine Marzluff
<i>Nominating</i>	Alan Marshall, Chair Julia Laskin Joseph Loo Christine Miller Nathan Yates
<i>Publications</i>	Evan Williams, Chair Carthene Bazemore-Walker Lars Konermann Brandon Ruotolo Yu Xia Michael Gross ( <i>ex officio</i> )
<i>Sanibel Conference</i>	Lisa Deterding, Chair Neil Kelleher J.C. Poutsma Jon Williams

## ARCHIVIST

Michael Grayson

## AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2013 RECIPIENT: RICHARD D. SMITH

Award Lecture: 4:45 pm, Monday, Exhibit Hall A (lower level)



The increasing role of mass spectrometry (MS) in the physical and biological sciences can be attributed in a large part to the versatility afforded by the growing number of ionization methods and to mass spectrometry's increasing sensitivity. The development of the electrodynamic ion funnel in the laboratory of Dr. Richard Smith has been an important factor in the latter increase.

The ion funnel was originally created in the Smith lab in 1997 to replace ion transmission-limited skimmers and to efficiently capture ions in the expanding gas jet while radially focusing them. It has been adapted for a variety of uses and has proven to be a broadly applicable tool for ion focusing and manipulation at elevated pressures that challenged conventional approaches. Although it has undergone several iterations in the last 15 years, the defining features of the ion funnel have not changed: closely spaced ring electrodes of gradually decreasing inner diameter, out-of-phase RF potentials applied to adjacent electrodes, and a longitudinally-applied DC gradient. The ion funnel concept continues to be adapted in a growing number of applications such as ion trapping, ion cooling, low pressure electrospray, and ion mobility spectrometry; however, its original use, decreasing ion losses in the interface of high pressure sources, has remained its most prevalent. Currently, the funnel is employed by Bruker Daltonics' and Agilent Technologies and similarities can be seen in Thermo-Fisher's recent S-lens design found on the

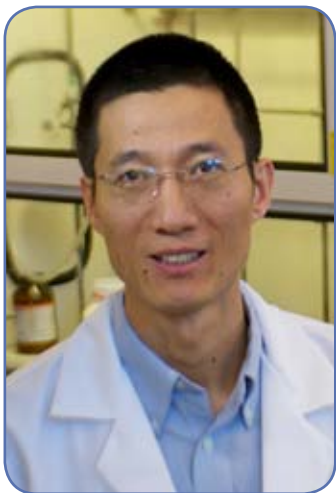
newer generations of Orbitrap instruments. In the ion funnel, Dr. Smith's obsession with sensitivity has provided a basis to greatly improve mass spectrometers, today allowing routine detection of low concentration species that would have been undetectable 15 years ago.

Dr. Richard Smith is Battelle Fellow and Chief Scientist in the Biological Sciences Division and Director of Proteomics Research at Pacific Northwest National Laboratory (PNNL).

## BIEMANN MEDAL

2013 RECIPIENT: YINSHENG WANG

Award Lecture: 4:45 pm, Tuesday, Exhibit Hall A (lower level)



Dr. Yinsheng Wang has focused his research on discovering the biological consequences of DNA damage and on unraveling mechanisms of action for anti-tumor drugs and environmental toxicants. His laboratory's use and development of mass spectrometry, synthetic organic chemistry, biochemistry and molecular biology enables us to understand and quantify, at the molecular level, how various DNA damage products are repaired, and how they perturb the efficient flow and fidelity of genetic information during DNA replication and transcription.

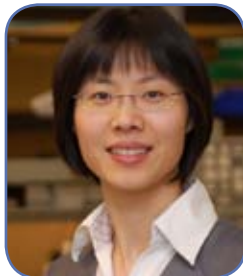
Professor Wang has identified and characterized new DNA lesions, including bulky lesions induced by reactive oxygen species. His laboratory developed LC-MS/MS combined with a plasmid-based shuttle vector to quantitatively assess how structurally defined DNA lesions alter the frequency and efficiency of DNA replication and transcription in cells, and to measure the types and frequencies of mutations induced by lesions. They also discovered that N-2-(1-carboxyethyl)-2'-deoxyguanosine (N-2-CEdG) is the major stable DNA adduct derived from methylglyoxal, and demonstrated that it is the previously unknown endogenous substrate for DinB (polymerase IV). Dr. Wang's new methods have provided some long-sought biomarkers for oxidative stress: cyclopurine lesions including 8,5'-cyclo-2'-deoxyadenosine and 8,5'-cyclo-2'-deoxyguanosine.

Dr. Yinsheng Wang is Professor of Chemistry at the University of California-Riverside.



The Research Awards are fully funded by Thermo Scientific and Waters Corporation in the amount of \$35,000 each. Awards will be presented at the Biemann Medal Award Lecture, 4:45 pm, Tuesday, Exhibit Hall A

Sponsored by  
**THERMO SCIENTIFIC**



**Yu Xia**  
Purdue University

Sponsored by  
**WATERS CORPORATION**



**Matthew F. Bush**  
University of Washington

## CALL FOR 2013 RESEARCH AWARD PROPOSALS

- OBJECTIVE** To promote academic research by young scientists in mass spectrometry.
- ELIGIBILITY** Open to academic scientists within four years of joining the tenure-track or research faculty in a North American university. Applicants may not have previously received an award under this program.
- APPLICATION** Applicants should submit the following no later than November 30.  
 1. Three-page proposal, including references and figures  
 2. One-page fiscal proposal and justification  
 3. List of current research support  
 4. *Curriculum vitae*  
 5. Two letters of recommendation may be e-mailed directly to ASMS: [office@asms.org](mailto:office@asms.org)
- DEADLINE** Application materials 1-4 should be arranged in order and assembled as one PDF and emailed to [office@asms.org](mailto:office@asms.org). File may not exceed 5 MB.
- FISCAL** The awards of \$35,000 each will be made to a university in the name of the selected individual for the researcher's exclusive use. In accepting this award, the institution will agree to not charge overhead on the funds.
- INFORMATION** Contact ASMS. Telephone: (505) 989-4517 • [office@asms.org](mailto:office@asms.org)

## RON HITES AWARD FOR OUTSTANDING RESEARCH PUBLICATION IN JASMS



The Ron Hites Award recognizes an outstanding presentation of original research. Selection is based on a paper's innovative aspects, technical quality, likely stimulation of future research, likely impact on future applications, and quality of presentation. The award is named in honor of Professor Ron Hites of Indiana University, who led the creation of JASMS in 1988 while president of ASMS. The corresponding author receives a cash award of \$2,000 and all authors are acknowledged with certificates of commendation.

The Ron Hites Award recognizes an outstanding presentation of original research. Selection is based on a paper's innovative aspects, technical quality, likely stimulation of future research, likely impact on future applications, and quality of presentation. The award is named in honor of Professor Ron Hites of Indiana University, who led the creation of JASMS in 1988 while president of ASMS. The corresponding author receives a cash award of \$2,000 and all authors are acknowledged with certificates of commendation.

The 2013 award recognizes Alexander W. G. Graham; Steven J. Ray; Christie G. Enke; Charles J. Barinaga; David W. Koppenaal; Gary M. Hieftje for "First Distance-of-Flight Instrument: Opening a New Paradigm in Mass Spectrometry," J Am Soc Mass Spectrom 2011, 22, 110-117.



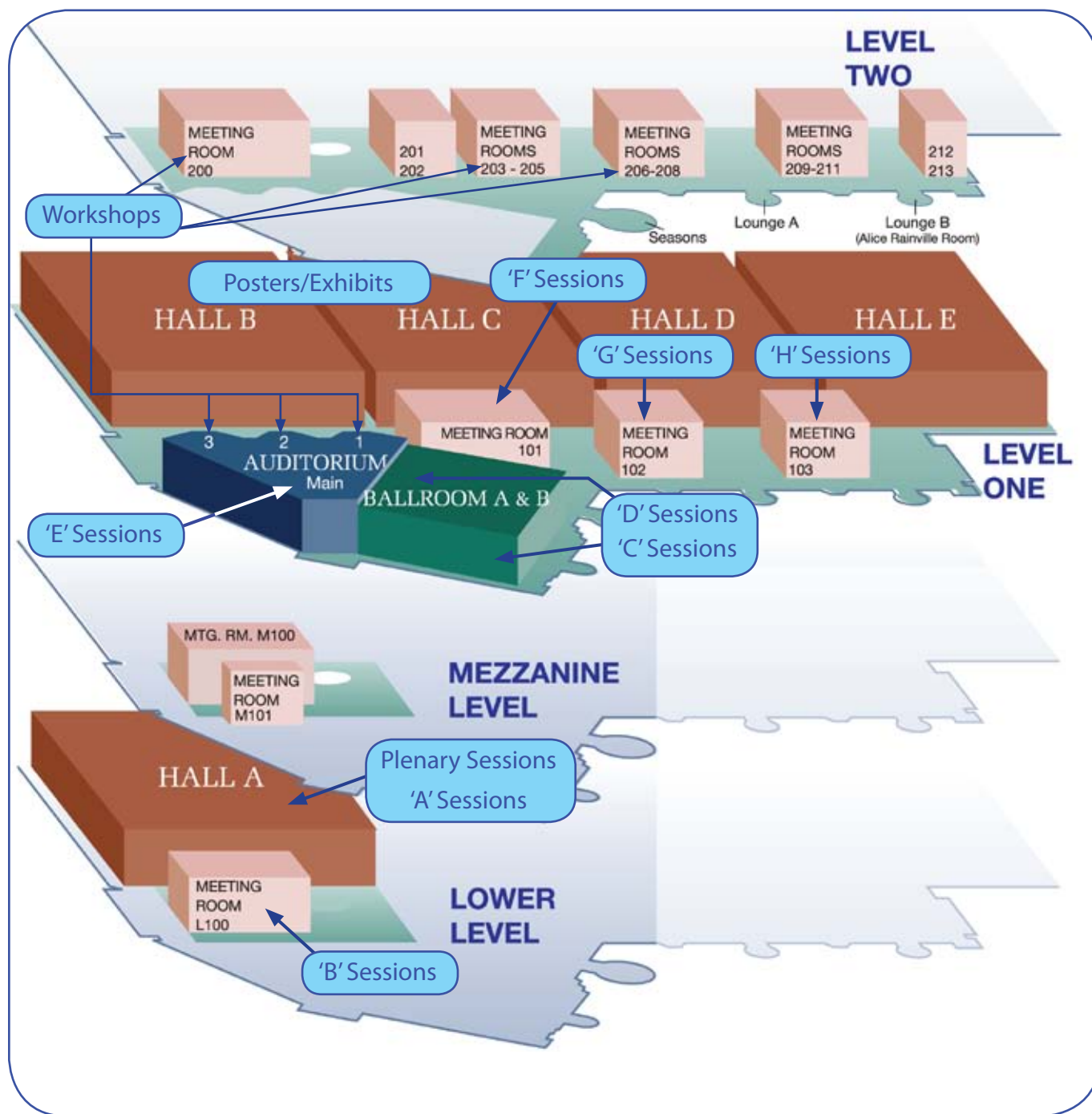
Left to right: Steven J. Ray, Gary M. Hieftje, and Alexander W. G. Graham

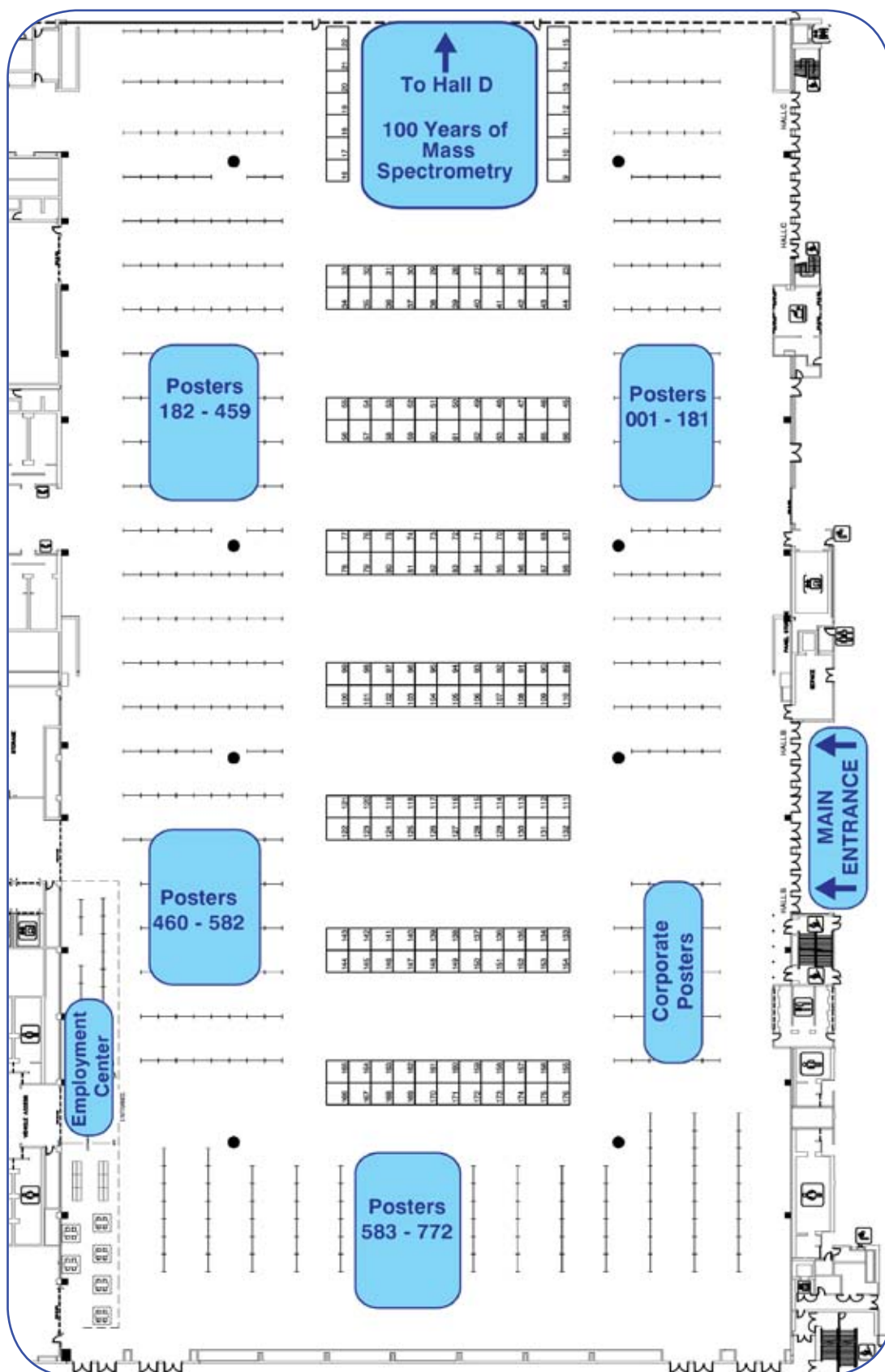


Charles J. Barinaga, David W. Koppenaal, and Christie G. Enke



## MINNEAPOLIS CONVENTION CENTER

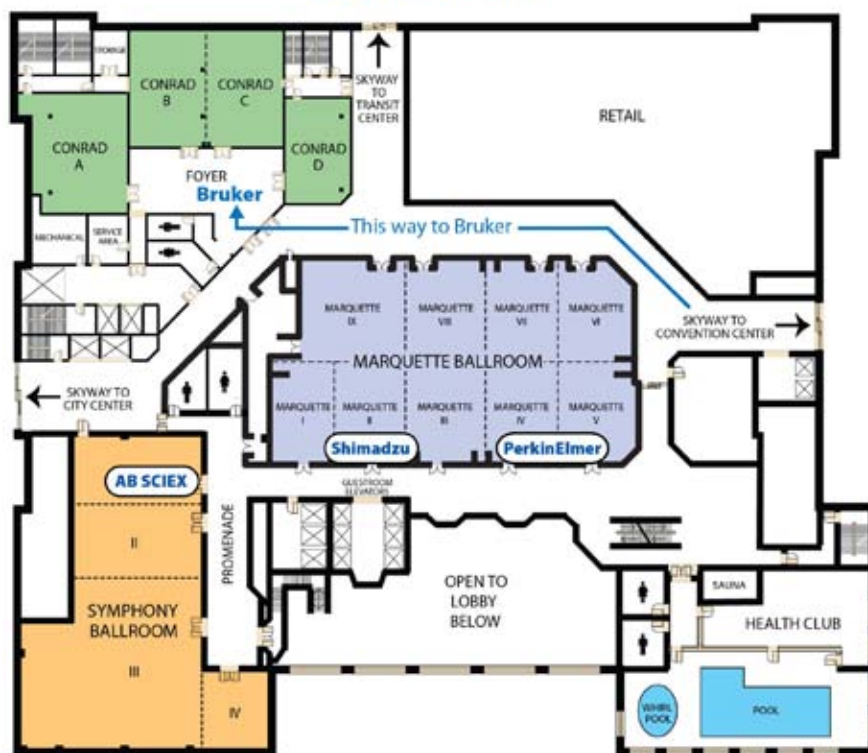




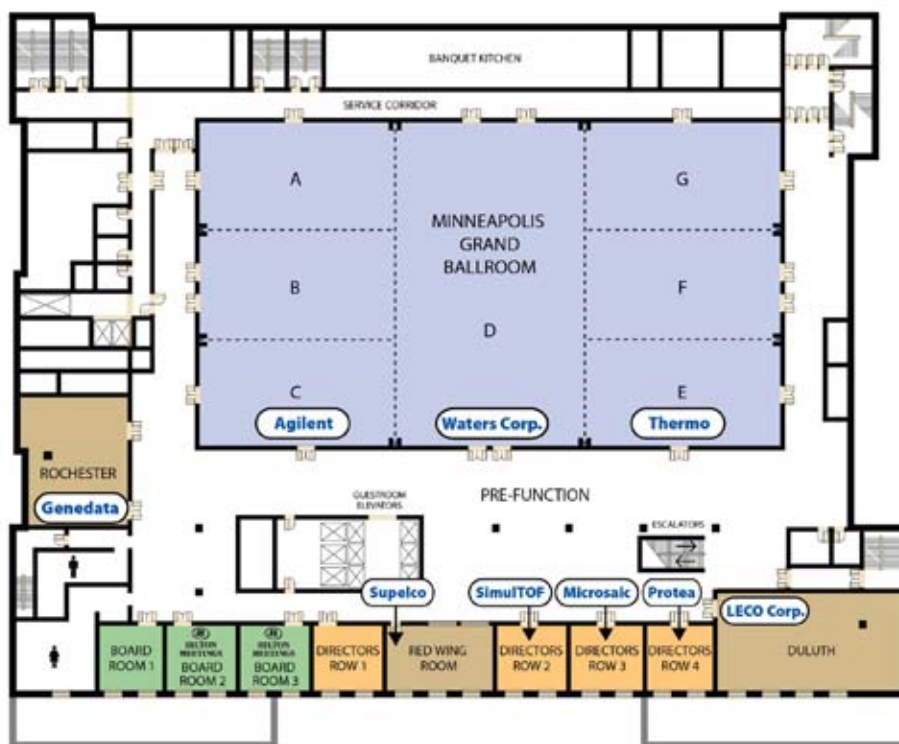




## SECOND FLOOR



## THIRD FLOOR



## ASMS CORPORATE MEMBERS

Company	Booth	Poster or Tabletop	Hilton Minneapolis Hospitality Suite	Breakfast Seminar
1st Detect .....	33 .....	Poster		
AB SCIEX .....	139 .....		Symphony Ballroom.....	Mon/Tues/Wed, 7:15 am Conv Center Room 200DE Room 200GF (Mon only) Room 208AB (Mon/Tues) Hilton Minneapolis Symphony Ballroom
Advanced Chemistry Development (ACD/Labs) .....	66 .....	Poster .....		Monday, 7:00 am Conv Center, Room 200C
Advion.....	123			
Agilent Technologies.....	109 .....	Poster .....	Grand Ballroom ABC .....	Mon/Tues/Wed, 7:00 am Conv Center, Room 205AB
Alliance Pharma, Inc.....	34 .....	Poster		
Analytical Sales & Services .....	125 .....	Poster		
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Avanti Polar Lipids, Inc. ....	21			
Bertin Technologies .....	11			
Biocompare, American Laboratory .....		Tabletop		
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Bioreclamation.....	128 .....	Poster		
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CDS Analytical.....		Poster		
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## ASMS CORPORATE MEMBERS

Company	Booth	Poster or Tabletop	Hilton Minneapolis Hospitality Suite	Breakfast Seminar
Drummond Scientific .....	168			
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EMD Millipore .....	85	Poster		Tuesday, 7:00 am Conv Center, Room 200H
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ExSAR Corporation				
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Fluid Management Systems.....	165	Poster		
Fortis Technologies.....	87	Poster		
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GMI, Inc. ....	47			
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Integrated Proteomics Applications Inc. ....	52			
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IonSense, Inc.....	142	Poster		
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## PROGRAM ACKNOWLEDGEMENTS



**Jenny Brodbelt**  
*Vice President for Programs*



**100 YEARS OF MASS SPECTROMETRY**

**Michael A. Grayson**

### 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.

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## PROGRAM OVERVIEW

### SATURDAY

9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
2:00 - 5:00 PM	<b>REGISTRATION</b>

### SUNDAY

9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
10:00 AM - 8:00 PM	<b>REGISTRATION</b>
5:00 - 6:30 PM	<b>TUTORIAL LECTURES</b> , Exhibit Hall A (lower level)  <div><p>5:00 - 5:45 pm <b>A Wide Spectrum: Clinical Diagnostics for the Masses</b>  <b>Andrew Hoofnagle</b> University of Washington</p></div> <div><p>5:45 - 6:30 pm <b>The Nuts and Bolts of Protein Hydrogen Exchange MS</b>  <b>John Engen</b> Northeastern University</p></div>
6:45 - 7:45 PM	<b>CONFERENCE OPENING</b> , Exhibit Hall A (lower level) <b>Jenny Brodbelt</b> , <i>ASMS Vice President for Programs</i>  <b>Welcome, Jenny Brodbelt</b> , University of Texas, Austin ASMS Vice President for Programs  <div><div>Then...</div><div>Now...</div></div> <b>The First Fifty Years of MS: Building a Foundation</b> <b>Michael L. Gross</b> Washington University of St. Louis
7:45 - 9:00 PM	<b>RECEPTION IN THE POSTER-EXHIBIT HALL</b> , Exhibit Hall BC

## PROGRAM OVERVIEW

### MONDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>MOA am Quantification of Targeted Proteins and Post-Translational Modifications, Exhibit Hall A (lower level)</li> <li>MOB am Instrumentation: Time-of-Flight Mass Spectrometry: In Memory of Robert J. Cotter, Room L100 (lower level)</li> <li>MOC am FAIMS and DMS: New Developments and Applications, Ballroom B</li> <li>MOD am Biotherapeutics and Biomarkers: Advances in Quantitative Analysis, Ballroom A</li> <li>MOE am Integrated Qualitative and Quantitative LC-MS for Small Molecule Analysis, Auditorium</li> <li>MOF am Covalent Labeling, Chemical Probes, and Crosslinking for Biomolecule Structural Characterization, Room 101</li> <li>MOG am Fundamentals of Peptide Fragmentation, Room 102</li> <li>MOH am Nucleic Acids, Room 103</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Exhibit Hall BC
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>MOA pm PTMs: Comprehensive Analysis, Exhibit Hall A (lower level)</li> <li>MOB pm Top-Down and Middle-Down Protein Analysis (Honoring Fred McLafferty's 90th birthday), Room L100 (lower level)</li> <li>MOC pm Clinical Chemistry: Dried Blood Spot Analysis, Ballroom B</li> <li>MOD pm Biotherapeutics, Impurities and Degradants: Structural Characterization, Ballroom A</li> <li>MOE pm High Mass Accuracy in Drug Discovery and Development, Auditorium</li> <li>MOF pm Protein-Protein and Protein-Ligand Interactions, Room 101</li> <li>MOG pm Fundamentals of Ion Activation and Dissociation, Room 102</li> <li>MOH pm Photoionization, Room 103</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>AWARD LECTURE</b> , Exhibit Hall A   <b>Award for a Distinguished Contribution in Mass Spectrometry</b>  <b>Richard D. Smith</b> Pacific Northwest National Laboratory
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments on level two. <b>Level One Rooms</b> <ul style="list-style-type: none"> <li>The Informatical Difference between Targeted and Discovery-based Proteomics (organized by the Bioinformatics for MS Interest Group), Room 1</li> <li>Have Recent LC-MS Techniques Advanced to Substitute AMS in Analyzing Microdose and other Low Level Clinical Studies for Metabolites and Drug Related Material? (organized by the DMPK Interest Group), Room 2</li> <li>Trans-Proteomic Pipeline (TPP) and Related Open-Source Proteomics Resources, Room 3</li> </ul> <b>Level Two Rooms</b> <ul style="list-style-type: none"> <li>FRAGILE Modifications, Handle with Care during Peptide Fragmentation (organized by the Peptide Fragmentation Interest Group), Room 200 DE</li> <li>Mass Spectrometry-based Characterization of Biotherapeutics (organized by the Protein Therapeutics Interest Group), Room 200 FG</li> <li>How Can MS Analysis Be Used to Improve Analytical Results and Laboratory Efficiency (organized by the Flavor, Fragrance and Foodstuff Interest Group), Room 200 H</li> <li>Nucleic Acids as Diagnostic and Therapeutic Biomarkers (organized by the DNA/RNA Interest Group), Room 200 I</li> <li>Surviving and Thriving: A Panel Discussion for Both Students and PUI Faculty on How to Get the Most out of Undergraduate Research (organized by the Undergraduate Research in MS interest Group), Room 205 AB</li> <li>Photoionization Mass Spectrometry, Room 205 CD</li> <li>Consortium for Top Down Proteomics, Room 208 AB</li> <li>Data Independent Acquisition, Room 208 CD</li> </ul>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel

## PROGRAM OVERVIEW

### TUESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA am Quantitative Proteomics, Exhibit Hall A (lower level)</li> <li>• TOB am Imaging MS: Increasing Speed and Information Content, Room L100 (lower level)</li> <li>• TOC am Functional Foods, Phytochemicals, and Supplements, Ballroom B</li> <li>• TOD am PTMs: Glycosylation, Ballroom A</li> <li>• TOE am Systems Biology/Cellular Pathways, Auditorium</li> <li>• TOF am Metabolomics/Lipidomics: New MS Technologies and Applications, Room 101</li> <li>• TOG am Ion Mobility: Separations, Room 102</li> <li>• TOH am Antibodies and Antibody-Drug Conjugates, Room 103</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Exhibit Hall BC
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA pm Instrumentation and Methods: FT, Ion Traps and Hybrid Instruments, Exhibit Hall A (lower level)</li> <li>• TOB pm Imaging MS: Biological Applications, Room L100 (lower level)</li> <li>• TOC pm Characterization of Product Variants in Biosimilars, Ballroom B</li> <li>• TOD pm Phosphoproteomics, Ballroom A</li> <li>• TOE pm Food Safety: Advances in MS for Characterization of Additives and Contaminants, Auditorium</li> <li>• TOF pm Ion Mobility: Structures, Room 101</li> <li>• TOG pm Metabolites: Unusual and Uncommon, Room 102</li> <li>• TOH pm Microorganisms: Identification and Characterization, Room 103</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>AWARD LECTURE</b> , Exhibit Hall A, Lower Level  <p><b>Biemann Medal</b></p> <p><b>Yinsheng Wang</b> University of California, Riverside</p>
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments on level two. <b>Level One Rooms</b> <ul style="list-style-type: none"> <li>• Environmental Applications of FTMS: Earth, Air &amp; Water (organized by the FTMS Interest Group), Room 1</li> <li>• Jumpstarting Your Career: a Career Development Workshop (organized by the Young Mass Spectrometrists Interest Group), Room 2</li> <li>• The Galaxy Framework as a Solution for MS-based Informatics, Room 3</li> </ul> <b>Level Two Rooms</b> <ul style="list-style-type: none"> <li>• LC-MS in the Clinical Lab: How Close is 24/7? (organized by the Clinical Chemistry Interest Group), Room 200 DE</li> <li>• Normalization Approaches to Imaging Mass Spectral Data (organized by the Imaging MS Interest Group), Room 200 FG</li> <li>• How to Work with your P.I.s More Effectively (and Without Them Knowing It) (organized by the Analytical Lab Managers Interest Group), Room 200 H</li> <li>• Current Topics in Metal Ion Chemistry (organized by the Metal Ion Coordination Chemistry Interest Group), Room 200 I</li> <li>• Ion Mobility MS: New Instrumentation &amp; Enabling Technologies (organized by the Ion Mobility MS Interest Group), Room 205 AB</li> <li>• Quantitative Intact Proteomics (organized by the Quantitative Intact Proteomics Interest Group), Room 205 CD</li> <li>• Large Molecule by LC-MS Bioanalytical Method Validation (BMV): Status, Challenges, Solutions, Recommendations (organized by the Regulated Bioanalysis Interest Group), Room 208 AB</li> <li>• Practical ETD, Room 208 CD</li> </ul>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel



## PROGRAM OVERVIEW

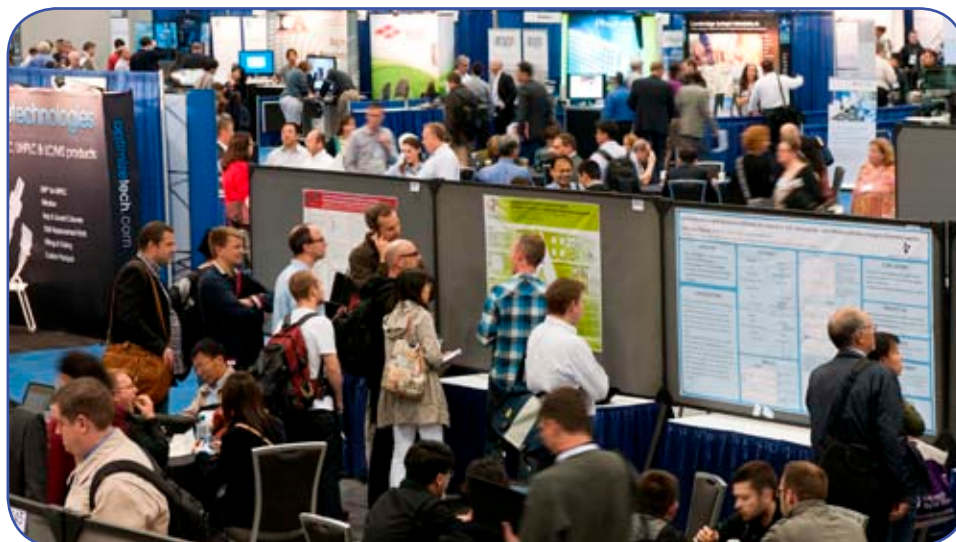
### WEDNESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>WOA am PTMS: Advances in Isolation, Derivatization and Separation, Exhibit Hall A (lower level)</li> <li>WOB am Informatics: Protein Quantification, Room L100 (lower level)</li> <li>WOC am Carbohydrates: New MS Approaches, Ballroom B</li> <li>WOD am Quantitative Analysis by MS in Drug Discovery and Development: Novel Approaches, Ballroom A</li> <li>WOE am Instrumentation: New Developments in High Resolution and Mass Accuracy, Auditorium</li> <li>WOF am Emerging Environmental Contaminants, Room 101</li> <li>WOG am Fundamentals: Ion Spectroscopy (Honoring Rob Dunbar's 70th Birthday), Room 102</li> <li>WOH am H/D Exchange: Biological Applications, Room 103</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Exhibit Hall BC
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>WOA pm Forensic Applications, Exhibit Hall A</li> <li>WOB pm Principles of Protein Identification and Characterization, Room L100</li> <li>WOC pm Gas-Phase Ions: Reactions, Dynamics and Theory, Ballroom B</li> <li>WOD pm Biomarkers of Drug Response, Efficacy and Toxicity: Novel MS Approaches, Ballroom A</li> <li>WOE pm Instrumentation: New Developments in Ionization and Sampling, Auditorium</li> <li>WOF pm Ecological and Human Health Environmental Chemistry and Toxicology, Room 101</li> <li>WOG pm Glycoproteins and Glycans: New MS Approaches, Room 102</li> <li>WOH pm H/D Exchange: New Development in Technology, Room 103</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>ASMS MEETING</b> , Ballroom A Awards, board reports, wine, beer, soft drinks - and more!
<b>5:45 - 7:00 PM</b>	<b>WORKSHOPS</b> There are light refreshments on level two <p style="text-align: center;"><b>Level One Rooms</b></p> <ul style="list-style-type: none"> <li>Fundamentals in LC-MS Troubleshooting (organized by LC/MS &amp; Related Topics Interest Group), Room 1</li> <li>H/D Exchange and Covalent Labeling (organized by H/D Exchange &amp; Covalent Labeling Interest Group), Room 2</li> <li>LC-MS of Glycans and Glycopeptides: Advantages and Challenges, Room 3</li> </ul> <p style="text-align: center;"><b>Level Two Rooms</b></p> <ul style="list-style-type: none"> <li>Fuel Analysis: Surveying Research Methods and their Application in Industrial Settings (organized by Energy, Petroleum &amp; Biofuels Interest Group), Room 200 DE</li> <li>Emerging Contaminants in Environmental Research: Hydraulic Fracturing Fluids and Shale Gas Produced Waters - Advances, Challenges and Opportunities using mass spectrometry (organized by Environmental Applications Interest Group), Room 200 FG</li> <li>The Advancement of Polymer Mass Spectrometry (organized by Polymeric Materials Interest Group), Room 200 H</li> <li>Challenges and New Directions in Plant Proteomics, Room 200 I</li> <li>CHORUS – A Community Solution for the Storage, Visualization, and Sharing of Mass Spectrometry Data on the Cloud, Room 200 J</li> <li>Ion Structures and Energetics, and Ion-Molecule Reaction Kinetics in the Gas Phase, in honor of Peter B. Armentrout's 60th birthday (organized by Fundamentals Interest Group), Room 205 AB</li> <li>Proteins and Peptides as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group), Room 205 CD</li> <li>Lipid Mass Spectrometry &amp; Lipidomics, Room 208 AB</li> <li>Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 208 CD</li> </ul>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel

## PROGRAM OVERVIEW

### THURSDAY

<b>7:00 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA am Ambient Ionization: Instrumentation and Applications, Exhibit Hall A (lower level)</li> <li>• ThOB am Informatics: Metabolomics, Room L100 (lower level)</li> <li>• ThOC am Regulated Bioanalysis and Diagnostics using High Resolution LC/MS, Ballroom B</li> <li>• ThOD am Disease Biomarkers and Pathways, Ballroom A</li> <li>• ThOE am Space Science, Astrobiology, and Atmospheric Chemistry, Auditorium</li> <li>• ThOF am Imaging MS: Pharmaceutical Applications, Room 101</li> <li>• ThOG am Energy, Petroleum, and Biofuels: Advances in MS Design and Informatics, Room 102</li> <li>• ThOH am Epigenetic Modifications and Mechanisms, Room 103</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Exhibit Hall BC Thursday posters
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA pm Ambient and Atmospheric Pressure Ionization: Fundamentals, Exhibit Hall A (lower level)</li> <li>• ThOB pm Proteomics: Infection Diseases, Room L100 (lower level)</li> <li>• ThOC pm Lipids and Profiling, Ballroom B</li> <li>• ThOD pm Biomarkers in Drug Discovery and Development, Ballroom A</li> <li>• ThOE pm Plant"omics", Auditorium</li> <li>• ThOF pm Polymer- and Packaging-Related Contaminants and Degradants in Food, Drugs, and Consumer Products, Room 101</li> <li>• ThOG pm Energy, Petroleum, and Biofuels: Advances in Sample Preparation and MS Interface Design, Room 102</li> <li>• ThOH pm History: Celebration of 100th Anniversary of Mass Spectrometry, Room 103</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>PLENARY LECTURE</b> , Exhibit Hall A (lower level)  <div data-bbox="373 1060 564 1320" data-label="Image"> </div> <div data-bbox="587 1092 1032 1123" data-label="Section-Header"> <h4>Discovery of the Elusive Higgs Boson</h4> </div> <div data-bbox="587 1148 898 1207" data-label="Text"> <p><b>Peter Onyisi</b> University of Texas at Austin</p> </div>
<b>5:45 - 9:00 PM</b>	<b>CLOSING GALA</b> , Ballroom D



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

**The Informational Difference between Targeted and Discovery-based Proteomics (organized by Bioinformatics for MS Interest Group); Brian Searle and Lukas Käll, presiding  
Room 1**

Recent developments in data acquisition strategies and instrumentation have granted proteomicists to the ability to acquire not just the mass and intensity of the peptides in large-scale proteomics samples, but also sequence specific fragment ions as well. Informatically speaking, data independent acquisition facilitates researchers to first form hypotheses about which proteins are likely to be present in samples and ask targeted questions to identify them. However, unlike traditional targeted acquisition, such as with selected reaction monitoring, data is acquired discovery-based where peptides from all proteins present in each sample are fragmented indiscriminately. These fragments can be exploited by informatics informed by database searching strategies. This workshop will be discussion-driven after both points of view are briefly introduced.

**Have Recent LC-MS Techniques Advanced to Substitute AMS in Analyzing Microdose and other Low Level Clinical Studies for Metabolites and Drug Related Material? (organized by DMPK Interest Group); Chandra Prakash and Don McKenzie, presiding  
Room 2**

Human micro dose studies require a highly sensitive analytical method such as Accelerator Mass Spectrometer (AMS). Unfortunately, the wide implementation of AMS in these analyses has been limited due to low-throughput sample preparation and high analysis cost. Over the last two decades, LC coupled with high resolution mass spectrometers (LC-HRMS) has become a reference analytical method for qualitative and quantitative analysis of pharmaceuticals. This workshop will discuss the advantages and disadvantages of LC-HRMS and AMS for the qualitative and quantitative analysis of drug and metabolites from low dose studies. The workshop will include 2 speakers (10-15 min per presentation) followed by Q&A and discussion with the audience.

**Trans-Proteomic Pipeline (TPP) and Related Open-Source Proteomics Resources;  
Eric W. Deutsch and Luis Mendoza, presiding  
Room 3**

This workshop will begin with a tutorial-style presentation on how to use the freely available and open-source suite of software tools for the analysis of proteomics shotgun datasets called the Trans-Proteomic Pipeline (TPP). The presentation will include demonstrations on use of format conversions, PeptideProphet, iProphet, PTMProphet, ProteinProphet, and related tools through the TPP graphical user interface, both in a local installation and on the Amazon EC2 cloud computing platform. Next we will present examples of how to use other resources from the Seattle Proteome Center including PeptideAtlas and SRMATlas for the planning of targeted proteomics experiments. The workshop will conclude with an open discussion on use of the tools, possible improvements, as well as future directions. There will be an opportunity to talk with the developers of the TPP.

**FRAGILE Modifications, Handle with Care during Peptide Fragmentation (organized by Peptide Fragmentation Interest Group) Nicolas Polfer and Sharon Pitteri, presiding  
Room 200 DE (level 2)**

Many post-translational modifications (PTMs) on peptides, such as phosphorylation or glycation are easily detached during collision-induced dissociation (CID). This lability seriously complicates the localization of PTMs in sequencing experiments. This workshop aims to critically assess this problem for the proteomics community and to offer solutions to eliminate or at least minimize these redundant processes.

**Mass Spectrometry-based Characterization of Biotherapeutics (organized by Protein Therapeutics Interest Group); Justin Sperry and Li Tao, presiding  
Room 200 FG (level 2)**

To provide a forum to discuss and share new techniques used to characterize and quantify biotherapeutics in various matrices by mass spectrometry. We will focus on the daily challenges faced by difficult samples such as antibodies, antibody-drug conjugates, vaccines, biosimilars, and/or heavily glycosylated proteins. The workshop will be a place for scientists to share their experiences in analyzing these samples by mass spectrometry-based methodologies. The workshop will also try to stimulate discussion on perspectives of new technologies that could improve the efficiency/throughputs in analyzing biotherapeutics.

**How Can MS Analysis Be Used to Improve Analytical Results and Laboratory Efficiency (organized by Flavor, Flavor, Fragrance and Foodstuff Interest Group); Marc Engel, presiding  
Room 200 H (level 2)**

The following questions will be addressed:

- How can I use MS to get more accurate results?
- How can MS improve the efficiency of my lab?
- Are there MS techniques that I am not using in my lab that would improve the analyses that I am performing?

**Nucleic Acids as Diagnostic and Therapeutic Biomarkers (organized by DNA/RNA Interest Group); Norman Chiu and Fanyu Meng, presiding  
Room 200 I (level 2)**

The discussion will focus on the mass spectrometry of nucleic acids biomarkers such as single nucleotide polymorphism (SNP), methylated DNA, non-coding RNA, and modified nucleosides. The use of these biomarkers for the diagnosis of diseases and therapeutic applications will be discussed. Comparison of using mass spectrometry to other analytical techniques for measuring nucleic acids biomarkers will be made during the discussion. The panelists of this workshop will include leaders from both industry and academy.

**Surviving and Thriving: A Panel Discussion for Both Students and PUI faculty on How to Get the Most out of Undergraduate Research (organized by Undergraduate Research in MS Interest Group); JC Poutsma and Chrisi Hughey presiding  
Room 205 AB (level 2)**

A two-part panel discussion will address the rewards and challenges of undergraduate (UG) research in mass spectrometry. Each panel will be comprised of 3-4 panelists. The first part of the panel discussion will focus on how undergraduates can leverage their UG research experience to set themselves apart during a job search, when applying for graduate or professional schools and graduate fellowships. Members of this panel will include ASMS members that participated in UG research and are currently in graduate school, recently employed and/or individuals who hire recent grads. The second part of the panel discussion will focus on faculty concerns. Possible topics include time management, grant writing and the formation of scholarly writing support teams. Members of this panel will include beginning, mid- and late-career faculty.

**Photoionization Mass Spectrometry;  
Jack Syage and Ralf Zimmerman presiding  
Room 205 CD (level 2)**

Photoionization based methods are playing an increasingly important role in mass spectrometry. Among the various benefits of photoionization processes, their softness and selectivity are the most important ones. With the on-going improvement of laser based and incoherent light



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

sources a further increase in techniques and applications is to be expected. The development of photoionization mass spectrometry (PIMS) based methods is also reflected in the scientific literature: In 2010 in total more than 1200 non-MALDI PIMS papers were published. The last decade has also seen the commercialization of APPI primarily for LC/MS and its emergence in important niche areas such as non-polar compounds, steroids, PAHs, petroleums, food safety, etc. PIMS is clearly making a practical and major impact in analytical MS. More recently photoionization mass spectrometers for on-line monitoring purposes were successfully commercialized.

**Consortium for Top Down Proteomics;  
Nicolas Young and Ying Ge presiding  
Room 208 AB (level 2)**

The Consortium for Top Down Proteomics was established in March 2012 with the following mission, "To promote innovative research, collaboration and education accelerating the comprehensive analysis of intact proteins". The consortium exists to bring together disparate researchers in top down proteomics and to educate the world on the

study of proteins in the intact state. At the ASMS 2013 meeting, we will review the results of current pilot projects, discuss nomenclature, data storage and data interchange. We will also review common roadblocks to successful top down proteomics experiments. A limited number of 5 minute 'lightning talks' will be available for researchers to provide updates on recent achievements and accomplishments of note. Contact workshop chairs if you are interested in presenting.

**Data Independent Acquisition; Yishai Levin presiding  
Room 208 CD (level 2)**

In recent years several alternative data acquisition modes have emerged in 'bottom-up' proteomics. Among these, Data Independent Acquisition (DIA) approaches have raised significant interest due to their improved identification reproducibility and quantitative performance. We will discuss the current status of various DIA approaches and the latest developments in instrumentation and software. We will host a panel of experts in the field and encourage discussion throughout the workshop.

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

**Environmental Applications of FTMS: Earth, Air & Water  
(organized by the FTMS Interest Group);  
Amy McKenna and Franklin Leach, presiding  
Room 1**

This workshop will focus on the application of FTMS to characterize environmental samples. The discussion will include the requirement for high resolution FTMS for complex organic mixtures, such as dissolved organic matter, petroleum and atmospheric samples. We will highlight the threshold for current capabilities with 3-4 speakers, and will outline limitations for current techniques. This workshop will combine presentations with open discussion.

**Jumpstarting Your Career: A Career Development (organized by  
the Young Mass Spectrometrists Interest Group);  
Dian Su and Bich Vu, presiding  
Room 2**

The workshop will hold panel discussions on personal career management and planning. The topics will be related to effective career planning, high impact resumes, **job search strategies, power interviewing**, industrial and corporate internships, career pathways in academia, industry, and government organizations. Recruiters and representatives from industry, academia, and government organizations inside and outside the US will be invited to share best practices on career prospects.

**The Galaxy Framework as a Solution for MS-based Informatics;  
Tim Griffin, presiding  
Room 3**

The open source, community-developed, web-based Galaxy framework enables sharing of software and analysis workflows, promoting increased transparency in data analysis and adherence to standards. Originally designed for the genomics research community, Galaxy is gaining use by those in the MS-based proteomics and metabolomics community where new informatics solutions are urgently needed. Galaxy usage is driven by its unique and powerful features, not offered by other current solutions. This workshop seeks to inform current users of Galaxy on the newest developments, and introduce the framework to interested new users. Top developers of Galaxy for MS-based informatics will give short informal presentations on their work, followed by a panel discussion and an open question and answer period from the audience.

**LC-MS in the Clinical Lab: How Close is 24/7? (organized by the  
Clinical Chemistry Interest Group);  
Brett Holmquist and Cory Bystrom, presiding  
Room 200 DE (level 2)**

Keeping a clinical LC-MS lab running smoothly is a challenge, and labs employ many strategies to keep hardware running optimally. This

workshop will discuss how clinical laboratorians view lab infrastructure, service agreements, and staff training with an eye toward maximum productivity.

**Normalization Approaches to Imaging Mass Spectral Data  
(organized by Imaging MS Interest Group);  
Timothy J. Garrett and Liam McDonnell, presiding  
Room 200 FG (level 2)**

Normalization is commonly used in imaging mass spectrometry to reduce the impact of fluctuations that can influence peak intensities. This includes fluctuation in laser intensity (MALDI), primary ion gun (SIMS), electrospray emitter (DESI), mass spectrometer performance, and matrix coating inhomogeneities. Normalization approaches can include the use of the total ion current and/or a single mass-to-charge value as well as other methods. This interactive workshop will explore the use of normalization approaches and how the approach modifies the images produced, positively or negatively.

**How to Work with your P.I.s More Effectively (and without Them  
Knowing It) (organized by the Analytical Lab Managers Interest  
Group); Nathan Dalleska and David Friedman, presiding  
Room 200 H (level 2)**

Along with a panel of three invited laboratory managers, we propose to address three topics all related to good outcomes for scientist-users and service providers in the mass spectrometry core facility environment. 1) Strategies and Models for Cost Recovery for non-tangible effort (e.g., data interpretation and translation). 2) Convincing The Scientist to do the Right Experiment. Oftentimes researchers arriving in the Mass Spectrometry lab ready to do some science have neither the inclination nor funds to do a statistically-powered experiment. How do you enter the process from a position of information provider rather than a salesperson? 3) Recognition for your contribution. This will be an expansion of last year's "Who Ran That." We will begin the session with a short introduction and perspective (ca. 3 minutes each) from the panelists, followed by an open discussion of the above topics.

**Current Topics in Metal Ion Chemistry (organized by the Metal  
Ion Coordination Chemistry Interest Group);  
Jianhua Ren and Michael van Stipdonk, presiding  
Room 200 I (level 2)**

The workshop will serve as an informal venue for active metal ion researchers to discuss the current challenges and future directions of the field. Key topics of discussion will include ion formation, reactivity, structure and energetics studied by mass spectrometry, and complementary techniques such as ion spectroscopy and ion mobility as well as calculations. Some of the potential topics include, but are not limited to, separation and quantification of metalloproteins, structural elucidation of bio-mimicking systems, structures and reactions of metal



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

clusters, micro-solvation of metals, and solving problems in metal ion chemistry using mass spectrometry experiments and theory. Those who wish to learn more about metal ion chemistry (especially young scientists) are strongly encouraged to attend.

**Ion Mobility MS: New Instrumentation & Enabling Technologies**  
(organized by the Ion Mobility MS Interest Group);

**Matthew Bush, presiding**  
Room 205 AB (level 2)

The performance of conventional and differential ion mobility mass spectrometers has escalated dramatically in recent years, which can be attributed to improved separations, more efficient ion transfer, and tighter integration of ion mobility devices into hybrid instruments. These improvements enable intricate and sensitive experiments probing mobility selected or separated ions, which has led to the adoption of ion mobility technologies in a wide range of applications, including challenges in gas-phase ion structure determination, native mass spectrometry, proteomics, and systems biology. We will showcase the latest developments in ion mobility mass spectrometry instrumentation and discuss remaining challenges.

**Quantitative Intact Proteomics** (organized by the Quantitative Intact Proteomics Interest Group);

**Edward Dratz and Julian Whitelegge, presiding**  
Room 205 CD (level 2)

A continuation of the open forum format started three years ago will include discussion directed by topics submitted to the QIP Interest Group ahead of time. The major focus of this workshop will be on quantitative methods used for intact proteins: 2D gel-based (DIGE) using fluorescent tags, multiplexing and internal standards; Top-down using GelFree-type separations etc. The goal is to achieve cross-fertilization between different areas of the community with respect to experimental design, power analysis, multivariate statistical analysis, and fitness for purpose.

**Large Molecule by LC-MS Bioanalytical Method Validation (BMV): Status, Challenges, Solutions, Recommendations** (organized by the Regulated Bioanalysis Interest Group);  
**Steve Lowes and Fabio Garofolo, presiding**  
Room 208 AB (level 2)

LBA are currently the most popular approach to Large Molecule Bioanalysis. However, recent developments in LC-MS instrumentation is evolving as a viable technique for the accurate quantitation of therapeutic proteins and large peptides in biological fluids by offering a valid alternate to LBA. LC-MS in quantification of biologics has many advantage such as no needs for high affinity reagent; uniform approach; large linear range; higher selectivity and expected to be well accepted by regulatory agencies. It is commonly performed by using tryptic digestion, then purifying and detecting one or smaller signature peptides by LCMS. The analysis of these signature peptides can be very challenging since they can interact/adsorb strongly with both plastic and glass surfaces. Preparation techniques for both intact proteins and signature peptides purification are quickly evolving based on conventional techniques and immunoaffinity-based. Sensitivity and selectivity could also be difficult to achieve even when using the most advanced LC-MS. This workshop will focus on discussing the most recent developments in large molecule quantification in Regulated Bioanalysis by LC-MS highlighting the challenges faced during the method development, validation, samples analysis.

**Practical ETD;**

**Katalin F. Medzihradszky and Robert Chalkley, presiding**  
Room 208 CD (level 2)

ETD is a relatively young technique. Discussion will focus on  
i) the available search engines – advantages and drawbacks;  
ii) unusual/unexpected fragmentations;  
iii) combination of ETD with other dissociation methods;  
iv) derivatizations  
v) intact protein analysis

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

**Fundamentals in LC-MS Troubleshooting** (organized by LC/MS & Related Topics Interest Group); **Helene Cardasis, presiding**  
Room 1

This workshop will cover fundamental principles of troubleshooting logic with the goal of helping attendees reduce LC-MS instrument down time. We'll define the terms "primary symptom" and "secondary symptom" in the context of LC-MS instrumentation problems, and as a group will work through the identification and resolution of multiple real world examples. Time will be allowed for ample discussion and questions for the expert panel, as well as an "open mic" - "has anyone seen this?" therapeutic session of communal troubleshooting of current, ongoing audience instrument problems.

**H/D Exchange and Covalent Labeling** (organized by H/D Exchange & Covalent Labeling Interest Group);

**Lars Konermann and David Schriemer, presiding**  
Room 2

The workshop will provide a forum for discussing HDX and covalent labeling approaches for protein analysis (structure, function, folding, dynamics). There will be a number of brief presentations introducing new advances in MS-based methods, experiments, data analysis and applications to the attendees. The goal of these presentations (5 min maximum) will be to stimulate discussion. The workshop will also contain a question and answer session, with questions being submitted in advance.

**LC-MS of Glycans and Glycopeptides: Advantages and Challenges;** **Yehia Mechref and Barry Boyes, presiding**

Room 3

The biosynthetic processes controlling the glycosylation of proteins and lipids invariably result in the formation of multiple glycan structures (positional and linkage isomers). A variety of glycan structures can

occupy a particular glycosylation site of a protein. Mass spectrometry alone might not be suited to attain a comprehensive characterization of all glycans associated with proteins and lipids. Accordingly, separation techniques in conjunction with mass spectrometry are currently being employed to define and quantify glycosylation of these many glycoconjugates. This workshop aims at addressing the advantages and challenges associated with LC-MS of glycans and glycopeptides. The discussion will include both condensed and gas phase separations. The use of different chromatographic modes, such as HILIC and RP, will be presented and discussed. Ion mobility mass spectrometry provides additional selectivity opportunities for the characterization of different glycans, when used both on-line and off-line with LC. Recent advances in the analysis of glycopeptides, including new formats for enrichment and separation will be also discussed.

**Fuel Analysis: Surveying Research Methods and their Application in Industrial Settings** (organized by Energy, Petroleum & Biofuels Interest Group); **Michael McGinley and Patrick Hatcher, presiding**  
Room 200 DE

Rapid advances in sample workflows, instrument technologies, and informatics have revolutionized the elemental information that one can obtain from petroleum and biofuel samples. Analytical technologies continue to impact both the industrial process control of fuel manufacturing as well as the assessing the environmental impact of fuel accidents. In this interest group workshop discussions will revolve around the most recently developed analysis methods in both biofuel and petroleum in the academic setting as well as discusses the challenges in implementing such advances in an industrial setting. Finally, industrial stakeholders will discuss unmet analytical needs in moving energy technologies forward.

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

#### **Emerging Contaminants in Environmental Research: Hydraulic Fracturing Fluids and Shale Gas Produced Waters - Advances, Challenges and Opportunities using Mass Spectrometry (organized by Environmental Applications Interest Group); Kerry Peru and Xing-Fang Li, presiding**

**Room 200 FG**

The workshop will focus on the challenges facing the environmental laboratory with emphasis on mass spectrometry analysis of emerging contaminants. The objective of the workshop is to discuss new contaminants, analytical strategies and research opportunities. This year's workshop will focus on emerging contaminants relating to hydrofracking and shale gas produced waters, discussions will be centered on how mass spectrometry can be used to fill the need of identifying and monitoring these contaminants. We welcome your questions and input to the discussion.

#### **Advancement of Polymer Mass Spectrometry (organized by Polymeric Materials Interest Group); William Erb, presiding**

**Room 200 H**

The workshop will include group discussions centered on the following topics related to synthetic polymers:

- Advancement of Polymer Separations and Chromatography
- New MS capabilities
- Academic and Industrial Applications of Polymer Analysis

Select scientists will give brief presentation (2-3 slides) on applications related to these topics to seed discussions.

#### **Challenges and New Directions in Plant Proteomics; Michelle Cilia and Brett Phinney, presiding**

**Room 200 I**

The purpose of the workshop will be to identify and discuss the unique analytical challenges that are specific to the proteomic analysis of plant and/or agricultural samples (including insects, plant pathogenic fungi, bacteria & viruses). Examples include, but may not be limited to sample prep, PTM identification, bioinformatics, functional validation and new technologies. We will select four abstracts from those submitted for consideration to the Plant Omics Oral Session that were not selected to be presented during the scientific session. Informal presentations will be limited to 15 minutes with 5 minutes for discussion. This format may be adjusted according to the number and quality of the abstracts we receive for consideration. We will preferentially select student and postdoctoral presenters to encourage participation and engagement of junior members of the society.

#### **CHORUS – A Community Solution for the Storage, Visualization, and Sharing of Mass Spectrometry Data on the Cloud; Michael MacCoss, Nathan Yates, and Andrey Bondarenko, presiding**

**Room 200 J**

The sharing and public dissemination of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a free, professionally developed solution to the mass spectrometry field's needs. The application provides a "Google Docs" type interface optimized for mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. We would like to discuss the motivations for initiating this effort, demonstrate what has been developed, describe our current short and long-term plans, obtain feedback, and encourage the involvement from the ASMS community.

#### **Ion Structures and Energetics, and Ion-Molecule Reaction Kinetics in the Gas Phase, in honor of Peter B. Armentrout's 60th birthday (organized by Fundamentals Interest Group) Glen Jackson and George Khairallah, presiding**

**Room 205 AB**

In December 2012, IJMS published a special issue edited by Mary Rodgers and David Clemmer in honor of Peter Armentrout's 60th

birthday. We plan to honor this special occasion by providing a series of invited short presentations and discussion on the major research areas in which Peter has been so influential. In the tradition of the fundamentals group, senior graduate students and postdoctoral scholars in research groups associated with ion structure, energetics and kinetics will give the presentations.

#### **Proteins and Peptides as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Matthew Blatnik and Carmen Santasania presiding**

**Room 205 CD**

The pharmaceutical industry has made a significant shift towards macromolecule based therapies. According to a Reuter's consensus sales forecast, biologics are predicted to make up the majority of sales of the top ten best-selling drugs for 2014. The inherent complexity of macromolecules requires more sophisticated analytical tools, methods, and knowledge than traditional small molecule based therapeutic programs. Historically, antigen-antibody capture techniques have been used to quantify biological targets. While ELISA assays are still the predominant method for quantitation of biologics, recent emphasis has been placed on incorporating complimentary LC-MS strategies to enhance our understanding of biological therapies. This workshop will introduce this topic with a short presentation meant to capture the field in its current state; it will open immediately afterwards for panel led discussion and audience participation. Specific topics may include but are not limited to sample preparation/handling, LC-MS in general, data management and regulatory requirements.

#### **Lipid Mass Spectrometry & Lipidomics; Gavin Reid and Stephen Blanksby, presiding**

**Room 208 AB**

*Lipidomics* involves the comprehensive analysis of lipids in biological systems, and determination of their roles in cellular structure and function in different physiological or pathological states. Recent advances in the field have been enabled by the development and application of mass spectrometry strategies for the rapid and sensitive identification, characterization and quantitative analysis of the thousands of chemically distinct lipid species that may be present within a given system of interest.

The primary goal of the inaugural ASMS Lipids and Lipidomics workshop will be to bring together like-minded people in the field to gauge the potential interest in establishing an ASMS Interest Group in this area, as well as to discuss the current status and future needs of the various mass spectrometry technologies and data analysis strategies that are associated with worldwide lipidome analysis efforts. This discussion will be facilitated by several informal presentations, followed by an extensive discussion period, from several leading researchers in the field.

#### **Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History; Mehdi Moini, presiding**

**Room 208 CD**

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

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

Jenny Brodbelt (University of Texas), presiding  
Exhibit Hall A (lower level)



5:00 - 5:45 pm  
**A Wide Spectrum: Clinical Diagnostics  
for the Masses**

**Andrew Hoofnagle**  
University of Washington



5:45 - 6:30 pm  
**The Nuts and Bolts of Protein Hydrogen  
Exchange MS**

**John Engen**  
Northeastern University

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

Jenny Brodbelt (University of Texas), presiding  
Exhibit Hall A (lower level)

**Welcome, Jenny Brodbelt**, University of Texas, Austin  
ASMS Vice President for Programs

Then...



Now...



**The First Fifty Years of MS: Building a Foundation**  
**Michael L. Gross**  
Washington University of St. Louis

7:45 - 9:00 PM, SUNDAY  
WELCOME RECEPTION  
Exhibit Hall BC

Conference name badge is required.

8:30 - 10:30 AM, MONDAY MORNING  
QUANTIFICATION OF TARGETED PROTEINS AND POST-  
TRANSLATIONAL MODIFICATIONS

Hamid Mirzaei (University of Texas Southwestern), presiding  
Exhibit Hall A (lower level)

MOA am 08:30 **Data Independent Acquisition with Improved  
Precursor Specificity on a Novel Hybrid Orbitrap  
(Q-OT-qIT) and a Q-Exactive;** Jarrett Egerton<sup>1</sup>;  
Jesse Canterbury<sup>2</sup>; Dario Amodei<sup>3</sup>; Richard  
Johnson<sup>1</sup>; Ying Ting<sup>1</sup>; Gennifer Merrihew<sup>1</sup>; Michael  
Senko<sup>2</sup>; Reiko Kiyonami<sup>2</sup>; Andreas Kuehn<sup>4</sup>; Yue  
Xuan<sup>4</sup>; Brendan MacLean<sup>1</sup>; Markus Kellman<sup>4</sup>; Parag  
Mallick<sup>3</sup>; Olga Vitek<sup>5</sup>; Vlad Zabrouskov<sup>2</sup>; Michael  
MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA;  
<sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Stanford  
University, Stanford, CA; <sup>4</sup>ThermoFisher Scientific,  
Bremen, Germany; <sup>5</sup>Purdue University, West  
Lafayette, IN

MOA am 08:50 **Using Variable Widths in Q1 Selection Windows  
to Improve Data Quality in Data Independent  
Acquisition;** Christie Hunter; Sean Seymour; AB  
SCIEX, Foster City, CA

MOA am 09:10 **Simultaneous Protein Targeting and Discovery  
Offers Reproducible, Scheduled-Free,  
Quantification of Hundreds of Proteins across  
Multiple Experiments;** Derek J. Bailey; Molly T.  
McDevitt; David J. Pagliarini; Michael S. Westphall;  
Joshua J. Coon; University of Wisconsin, Madison,  
WI

MOA am 09:30 **Improving the Quality and Production Timeline  
of Influenza Vaccines using Mass Spectrometry;**  
Tracie Williams; Wanda Santana; Emily Winne;  
James Pirkle; John Barr; Centers for Disease  
Control and Prevention, Atlanta, GA

MOA am 09:50 **Comparative Phosphoproteomic Analysis of  
Checkpoint Recovery Identifies Regulators  
of the DNA Damage Response;** Vincentius A.  
Halim<sup>1,2</sup>; Monica Alvarez-Fernández<sup>2,4</sup>; Yan Juan  
Xu<sup>3</sup>; Melinda Aprelia<sup>3</sup>; Henk W.P. van den Toorn<sup>1</sup>;  
Albert J.R. Heck<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; René  
H. Medema<sup>2,3</sup>; <sup>1</sup>Utrecht University, Utrecht, The  
Netherlands; <sup>2</sup>University Medical Center Utrecht,  
Utrecht, The Netherlands; <sup>3</sup>Netherlands Cancer  
Institute, Amsterdam, The Netherlands; <sup>4</sup>Spanish  
National Cancer Research Center (CNIO), Madrid,  
Spain

MOA am 10:10 **Quantitative Site-Specific Profiling of the  
Redox Dynamics on Protein Thiols Relevant  
to Photosynthesis in Cyanobacteria;** Jia Guo<sup>1</sup>;  
Amelia Nguyen<sup>2</sup>; Yi Qu<sup>1</sup>; Matthew J. Gaffrey<sup>1</sup>;  
Ronald J. Moore<sup>1</sup>; David G. Camp II<sup>1</sup>; Richard  
D. Smith<sup>1</sup>; Himadri B. Pakrasi<sup>2</sup>; Wei-jun Qian<sup>1</sup>;  
<sup>1</sup>Biological Sciences Division, PNNL, Richland, WA;  
<sup>2</sup>Washington University, St. Louis, MO





8:30 – 10:30 AM  
MONDAY MORNING

**INSTRUMENTATION: TIME-OF-FLIGHT MASS SPECTROMETRY**

**IN MEMORY OF ROBERT J. COTTER**  
Guido Verbeck (University of North Texas),  
presiding  
Room L100 (lower level)

- MOB am 08:30 **Opening:** Alfred L. Yergey, *National Institutes of Health*
- MOB am 08:50 **Recapturing Ions after Analysis by FT-TOF: Toward MS<sup>n</sup> using TOF;** Ryan T. Hilger; Robert E. Santini; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- MOB am 09:10 **High Resolution Ion Mobility Conformational Space Mapping Combined with Time-of-Flight Mass Spectrometry for Complex Sample Characterization;** Jody May<sup>1</sup>; Cody Goodwin<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; George Stafford<sup>2</sup>; Alexander Mordehai<sup>2</sup>; John McLean<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- MOB am 09:30 **Sub-Second CE-ESI-MS using Microfluidic Devices and a Novel Method for Acquiring High Speed TOF-MS Data;** J. Scott Mellors<sup>1</sup>; Nicholas Batz<sup>1</sup>; Martin Green<sup>2</sup>; J. Michael Ramsey<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- MOB am 09:50 **High Mass Intact Protein Detection with a Time and Position Sensitive Pixel Detector in Linear Time-of-Flight Mass Spectrometry (ToF-MS);** Shane Ellis<sup>1</sup>; Julia Jungmann<sup>1</sup>; Donald Smith<sup>1</sup>; Andras Kiss<sup>1</sup>; Chris Retif<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, Netherlands*; <sup>2</sup>*Omics2Image, Amsterdam, Netherlands*
- MOB am 10:10 **Demonstration of Constant-Momentum Acceleration in Zoom-TOF Mass Spectrometry for Improved Sensitivity in Time-of-Flight Systems;** Elise A. Dennis<sup>1</sup>; Alexander Gundlach-Graham<sup>1</sup>; Steven J. Ray<sup>1</sup>; Christie G. Enke<sup>2</sup>; Charles J. Barinaga<sup>3</sup>; David W. Koppenaal<sup>3</sup>; Gary M. Hieftje<sup>1</sup>; <sup>1</sup>*Indiana University Department of Chemistry, Bloomington, IN*; <sup>2</sup>*University of New Mexico, Albuquerque, NM*; <sup>3</sup>*Pacific Northwest National Laboratory, Richland, WA*

8:30 – 10:30 AM, MONDAY MORNING

**FAIMS AND DMS:**

**NEW DEVELOPMENTS AND APPLICATIONS**

Yves LeBlanc (AB SCIEX), presiding  
Ballroom B

- MOC am 08:30 **Performance of an Ultra-Sensitive u-FAIMS -IMS-QTOF Platform for Proteomics Measurements;** Yehia Ibrahim<sup>1</sup>; William Danielson<sup>1</sup>; Mikhail Ugarov<sup>2</sup>; Keqi Tang<sup>1</sup>; William Frazer<sup>2</sup>; Erin Baker<sup>1</sup>; Danielle Toutoungi<sup>3</sup>; Gordon Anderson<sup>1</sup>; George Stafford<sup>2</sup>; Richard Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Agilent Technologies Inc., Santa Clara, CA*; <sup>3</sup>*Owlstone Inc., Cambridge, UK*
- MOC am 08:50 **Decreased Gap Width in a Cylindrical FAIMS Device Improves Performance for Proteomics Applications;** Kristian E. Swearingen; Michael R. Hoopmann; Robert L. Moritz; *Institute for Systems Biology, Seattle, WA*

MOC am 09:10 **Differential Ion Mobility Spectrometry for the Investigation of Ion Reactions in Transfer Optics;** Samantha Isenberg; Kyle Stevens; Gary Glish; *University of North Carolina, Chapel Hill, NC*

MOC am 09:30 **FAIMS/MS/MS as an Emerging Technique for the Clinical Laboratory;** Richard A. Yost<sup>1</sup>; Christopher R. Beekman<sup>1</sup>; Jared J. Boock<sup>1</sup>; Timothy J. Garrett<sup>1</sup>; Julie A. Ray<sup>2</sup>; Mark M. Kushnir<sup>2</sup>; Alan L. Rockwood<sup>2</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*; <sup>2</sup>*ARUP Laboratories, Salt Lake City, UT*

MOC am 09:50 **FAIMS Mass Spectrometry for the Identification of Sites of Glycosylation in Flagellin A from *Campylobacter jejuni*;** Helen Cooper; Sam Xin Hui; Gloria N. Ulasi; Alistair McIntosh; Andrew J. Creese; Charles W. Penn; *University of Birmingham, Birmingham, UK*

MOC am 10:10 **Gas-phase Separation of Drugs and Metabolites using Modifier-Assisted Differential Ion Mobility Spectrometry after Liquid Extraction Surface Analysis;** Tiffany Porta; Emmanuel Varesio; Gérard Hopfgartner; *University of Geneva, Geneva, Switzerland*

8:30 – 10:30 AM, MONDAY MORNING

**BIOTHERAPEUTICS AND BIOMARKERS: ADVANCES IN QUANTITATIVE ANALYSIS**

Sheng Gu (Biogen Idec), presiding  
Ballroom A

MOD am 08:30 **Evolution of Candidate Biomarkers for Breast Cancer from Discovery to Large-Scale Assay Design and Assessment in patient plasma;** Thomas Lau<sup>1</sup>; Michael Gillette<sup>1</sup>; Regine Schoenherr<sup>2</sup>; Eric Kuhn<sup>1</sup>; Jeffrey Whiteaker<sup>2</sup>; Jennifer Ross<sup>1</sup>; Lola Fagbami<sup>1</sup>; Tao Liu<sup>3</sup>; Pei Wang<sup>2</sup>; ChenWei Lin<sup>2</sup>; Dave Camp<sup>3</sup>; Francisco Esteva<sup>4</sup>; Amanda Paulovich<sup>2</sup>; Steven Carr<sup>1</sup>; Richard Smith<sup>3</sup>; <sup>1</sup>*Broad Institute, Cambridge, MA*; <sup>2</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>3</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>4</sup>*MD Anderson Cancer Center, Houston, TX*

MOD am 08:50 **Toward the Absolute Quantification of CSF Tau Isoforms in the Picogram/Milliliter Range by a Simple and Cost-Effective Purification and  $\mu$ LC-SIM-HRMS;** Nicolas Barthélemy<sup>1</sup>; Christophe Hirtz<sup>2</sup>; Jerome Vialaret<sup>2</sup>; Susanna Schraen-Maschke<sup>3</sup>; Nicolas Sergeant<sup>3</sup>; Guy Lippens<sup>4</sup>; Isabelle Huvent<sup>4</sup>; François Fenaile<sup>1</sup>; Christophe Junot<sup>1</sup>; Sylvain Lehmann<sup>2</sup>; François Becher<sup>1</sup>; <sup>1</sup>*CEA, iBiTec-S/SPI/LEMM, Gif-sur-Yvette, France*; <sup>2</sup>*LBPC-IRB, CHU de Montpellier, Montpellier, France*; <sup>3</sup>*Inserm, UMR 837, Lille, France*; <sup>4</sup>*CNRS, UMR 8576, LGSF, Villeneuve d'Ascq, France*

MOD am 09:10 **Mass Analyzer Comparison for Quantitative and Confirmatory Determination of OPNA Biomarker Butyrylcholinesterase Peptides from Human Serum by Liquid Chromatography-Mass Spectrometry;** Caroline Watson<sup>1</sup>; Melissa Carter<sup>2</sup>; Thomas Blake<sup>2</sup>; Brian Crow<sup>2</sup>; Brooke Pantazides<sup>1</sup>; Rudolph Johnson<sup>2</sup>; <sup>1</sup>*ORISE Centers for Disease Control and Prevention, Atlanta, GA*; <sup>2</sup>*Centers for Disease Control and Prevention, Atlanta, GA*

MOD am 09:30 **Determining and Monitoring with Quantitation the Site-Specific Glycosylation of Proteins in Serum;** Qiuting Hong<sup>1</sup>; L. Renee Ruhaak<sup>1</sup>; Suzanne Miyamoto<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*Chemistry, UC, Davis, CA*; <sup>2</sup>*Comprehensive Cancer Center, UC, Davis, CA*



MOD am 09:50 **2D-LC/MS Technique for the Identification of Proteins in Biological Matrices: Is It Possible to Do It Quantitatively?** Luca Genovesi; Barbara Marsiglia; Luca Barbero; *Merck-Serono, Colletterto Giacosa, Italy*

MOD am 10:10 **Development and Application of LC-MS Methods for the Evaluation of Therapeutic Oligonucleotides**; Michael G. Bartlett; Buyun Chen; A. Cary McGinnis; *University of Georgia, Athens, GA*

**8:30 – 10:30 AM, MONDAY MORNING  
INTEGRATED QUALITATIVE AND QUANTITATIVE LC-MS FOR  
SMALL MOLECULE ANALYSIS**

**Kevin Schug (Univ of Texas at Arlington), presiding  
Auditorium**

MOE am 08:30 **Integrated Quantitative and Qualitative Work-Flow for *in-vivo* Discovery Bioanalysis using Hybrid Quadrupole-Time-of-Flight Mass Spectrometry**; Asoka Ranasinghe; Celia D'Arienzo; Timothy Olah; *Bristol-Myers Squibb Company, Princeton, NJ*

MOE am 08:50 **Quantitative Monitoring of Tamoxifen Extended to Forty Metabolites in Human Plasma using LC-HR-MS: New Investigation Capabilities for Clinical Pharmacology**; Elyes Dahmane<sup>1</sup>; Chantal Csajka<sup>1</sup>; Serge Rudaz<sup>2</sup>; Julien Boccard<sup>2</sup>; Khalil Zaman<sup>1</sup>; Laurent Decosterd<sup>1</sup>; Eric Genin<sup>3</sup>; Bénédicte Duret<sup>3</sup>; Maciej Bromirski<sup>3</sup>; Serge Leyvraz<sup>1</sup>; Bernard Testa<sup>1</sup>; Bertrand Rochat<sup>1</sup>; <sup>1</sup>*University Hospital of Lausanne, CHUV, Lausanne, Switzerland*; <sup>2</sup>*University of Geneva, Geneva, Switzerland*; <sup>3</sup>*Thermo Fisher, Paris - Bremen, European Union*

MOE am 09:10 **A Quantitative LC-MS Method Allows Rapid Identification of Fungal Natural Products, their Biosynthetic Pathways, and Complex Mechanisms Regulating their Production**; Jessica Albright<sup>1</sup>; Matthew Henke<sup>1</sup>; Alexandra Soukup<sup>2</sup>; Nancy Keller<sup>2</sup>; Neil Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*University of Wisconsin, Madison, WI*

MOE am 09:30 **Workflow to Validate Compounds Identified in Enriched Autophagosome Fractions and Activated Mast Cell by UPLC-MSE**; Chad Satori<sup>1</sup>; Joseph Koopmeiners<sup>1</sup>; Jose Antonio Rodriguez-Navarro<sup>2</sup>; Audrey Meyer<sup>1</sup>; Christy Haynes<sup>1</sup>; Edgar A. Arriaga<sup>1</sup>; Joseph J. Dalluge<sup>1</sup>; <sup>1</sup>*University of Minnesota-Twin Cities, Minneapolis, MN*; <sup>2</sup>*Albert Einstein College of Medicine, Bronx, NY*

MOE am 09:50 **Integrated High Throughput Quantitative and Qualitative Approaches for Pharmaceutical Research with HRMS (QqTOF)**; Ian Moore<sup>1,1</sup>; Brendon Kapinos<sup>2</sup>; Hui Zhang<sup>2</sup>; Veronica Zelesky<sup>2</sup>; Rick Schneider<sup>2</sup>; Gary Impey<sup>1</sup>; John Janiszewski<sup>2</sup>; Loren Olson<sup>1</sup>; <sup>1</sup>*AB SCIEX, Foster City, CA*; <sup>2</sup>*Pfizer, Groton, CT*

MOE am 10:10 **Evaluation and Integration of Picoliter Dispensing Technology for LC-MS/MS Analysis of Small Molecules in High Throughput ADME and PK Workflows**; Brian Furmanski<sup>1</sup>; Daniela Zima Kropf<sup>1</sup>; Jeff Nielsen<sup>2</sup>; X. Steven Yan<sup>1</sup>; Ken Ward<sup>2</sup>; Dennis Hruby<sup>1</sup>; Robert Allen<sup>1</sup>; <sup>1</sup>*Siga Technologies, Corvallis, OR*; <sup>2</sup>*Hewlett-Packard Company, Corvallis, OR*

**8:30 – 10:30 AM, MONDAY MORNING  
COVALENT LABELING, CHEMICAL PROBES, AND  
CROSSLINKING FOR BIOMOLECULE STRUCTURAL  
CHARACTERIZATION**

**David Hamby (Amgen, Inc.), presiding  
Room 101**

MOF am 08:30 **Protein-RNA interactions: Large-Scale Identification of Peptides Crosslinked to RNA through Database Searches against Entire Proteomes**; Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Saadia Qamar<sup>1</sup>; Oliver Kohlbacher<sup>2</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>*Max Planck Institute for Biophysical Chemistry, Göttingen, Germany*; <sup>2</sup>*Eberhard Karls University, Tübingen, Germany*

MOF am 08:50 **Structure, Function and Regulation of an Intact F-type ATPase Revealed by Chemical Crosslinking and Native Mass Spectrometry**; Carla Schmidt; Carol V. Robinson; *University of Oxford, Oxford, UK*

MOF am 09:10 **Inter-Subunit Contacts in Prion Oligomers Studied by Crosslinking of <sup>15</sup>N-metabolically Labeled Prion Proteins**; Jason Serpa<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; David Wishart<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*University of Alberta, Edmonton, Canada*; <sup>3</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*

MOF am 09:30 **Covalent Labeling of Oncogenic HER2-HER3 Tyrosine Kinase Dimers on Lipid Surfaces Reveals Key Intermolecular Interactions that Mediate Phosphorylation- Independent Activation**; Timothy Collier<sup>1</sup>; John Monsey<sup>1</sup>; Wei Shen<sup>1</sup>; Karthikeyan Diraviyam<sup>2</sup>; David Sept<sup>2</sup>; Ron Bose<sup>1</sup>; <sup>1</sup>*Washington University, St. Louis, MO*; <sup>2</sup>*University of Michigan, Ann Arbor, MI*

MOF am 09:50 **Monitoring Large Scale Protein Conformational Changes Using Covalent Protein Footprinting and Mass Spectrometry**; Taylor A. Poor<sup>1</sup>; Lisa M. Jones<sup>2</sup>; Manolo D. Plasencia<sup>3</sup>; Don L. Rempel<sup>4</sup>; George P. Leser<sup>1,5</sup>; Michael L. Gross<sup>4</sup>; Robert A. Lamb<sup>1,5</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Indiana University-Purdue University Indianapolis, Indianapolis, IN*; <sup>3</sup>*WUSTL School of Medicine, St. Louis, MO*; <sup>4</sup>*Washington University, St. Louis, MO*; <sup>5</sup>*Howard Hughes Medical Institute, Evanston, IL*

MOF am 10:10 **pH-Dependent Changes in the Selectivity Filter of KcsA Assessed by Radiolytic Footprinting and Structural Mass Spectrometry**; Rhijuta D'mello<sup>1</sup>; Vassiliy N Bavro<sup>2</sup>; Sayan Gupta<sup>1</sup>; Mark R Chance<sup>1</sup>; Stephen J Tucker<sup>2</sup>; <sup>1</sup>*Center for Proteomics and Bioinformatics, CWRU, Cleveland, OH*; <sup>2</sup>*Clarendon Lab., Dept. of Physics, Univ. of Oxford, Oxford, UK*

**8:30 – 10:30 AM, MONDAY MORNING  
FUNDAMENTALS OF PEPTIDE FRAGMENTATION**  
**Kristina Hakansson (University of Michigan), presiding  
Room 102**

MOG am 08:30 **Evidence of Third Residue Involvement in Diketopiperazine and Oxazolone b<sub>2</sub> Ion Formation in NAXIG and QAXIG Pentapeptides**; Lindsay Morrison<sup>1</sup>; Julia Chamot-Rooke<sup>2</sup>; Vicki Wysocki<sup>1</sup>; <sup>1</sup>*Ohio State University, Columbus, OH*; <sup>2</sup>*Pasteur Institute, Paris, France*

## MONDAY MORNING ORAL SESSIONS

- MOG am 08:50 **Regioselective<sup>18</sup>O-Labeling to Quantify Competing H<sub>3</sub>PO<sub>4</sub> versus HPO<sub>3</sub>+H<sub>2</sub>O Side Chain Neutral Losses from Protonated Phosphopeptide Ions during CID-MS/MS;** Li Cui; Ipek Yapici; Babak Borhan; Gavin Reid; *Michigan State University, East Lansing, MI*
- MOG am 09:10 **In-source Decay during MALDI Combined with Collisional Process in FTICR Mass Spectrometer;** Daiki Asakawa; David Calligaris; Edwin De Pauw; *University of Liège, Liège, Belgium*
- MOG am 09:30 **Peptide Fragmentation Patterns as a Measure of Antioxidant Capacity;** Omar Hamdy; Ryan Julian; *UC-Riverside, Riverside, CA*
- MOG am 09:50 **Gas-phase Fragment Ion Isomer Analysis Reveals the Mechanism of Peptide Sequence Scrambling;** Chenxi Jia; Zhe Wu; Christopher Lietz; Zhidan Liang; Qiang Cui; Lingjun Li; *University of Wisconsin, Madison, WI*
- MOG am 10:10 **Electron Transfer Dissociation of Conformationally Restricted Heptapeptides;** Robert Pepin; Alex Marek; Bo Peng; Frantisek Turecek; *U of Washington, Chemistry, Seattle, WA*

**8:30 – 10:30 AM, MONDAY MORNING  
NUCLEIC ACIDS**

**Natalia Tretyakova (University of Minnesota), presiding  
Room 103**

- MOH am 08:30 **Structure/Dynamics Investigation of a Tertiary Interaction in the HIV-1 Genome Packaging Signal by Concerted MS and IMS-MS Approaches;** Jennifer Lippens; Maria Basanta-Sanchez; D. Fabris; *The RNA Institute, University at Albany, Albany, NY*

- MOH am 08:50 **Targeted tRNA identification by Tandem Mass Spectrometry;** Collin Wetzel; Patrick Limbach; *University of Cincinnati, Cincinnati, OH*
- MOH am 09:10 **Protein-RNA Interactions Identified in Megadalton Ribonucleoprotein Complexes: the Human Spliceosomal U1, U2, and U6/U4.U5 snRNPs;** Romina Hofele<sup>1</sup>; Katharina Kramer<sup>1</sup>; Florian Richter<sup>2</sup>; Chung-Tien Lee<sup>1</sup>; Dmitry Agafonov<sup>1</sup>; Reinhard Lührmann<sup>1</sup>; Henning Urlaub<sup>1,3</sup>; <sup>1</sup>*MPI for Biophysical Chemistry, Goettingen, Germany*; <sup>2</sup>*MPI of Immunobiology and Epigenetics, Freiburg, Germany*; <sup>3</sup>*University Medical Center, Goettingen, Germany*
- MOH am 09:30 **Characterization of Modified RNA by Top-Down Mass Spectrometry;** Monika Taucher; Kathrin Breuker; *University of Innsbruck, Innsbruck, Austria*
- MOH am 09:50 **ESI-MS Study of a Cyclic Polyamide Selectively Targeting the G-Quadruplex in c-myc Oncogene Promoter;** Xiaoqie Cui; Han Chen; Qiang Zhang; Jiang Zhou; Gu Yuan; *College of Chemistry and Molecular Engineering, Pe, Beijing, China*
- MOH am 10:10 **Oxidation of the Methyl Group of Thymine and 5-Methylcytosine in DNA: Product Analyses by LC-MS/MS and Mechanistic Studies;** Guru S Madugundu; J. Richard Wagner; *Université de Sherbrooke, Sherbrooke, Canada*

**10:30 AM - 2:30 PM  
MONDAY POSTER SESSION  
Exhibit Hall BC**

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

## MONDAY AFTERNOON ORAL SESSIONS

**2:30 – 4:30 PM, MONDAY AFTERNOON  
PTMs: COMPREHENSIVE ANALYSIS  
Katalin Medzihradsky (UCSF), presiding  
Exhibit Hall A (lower level)**

- MOA pm 2:30 **Quantitative Proteomic and Phosphoproteomic Analysis of iPS-Derived Cardiomyocytes following Transfection with a miRNA Upregulated in Heart Failure;** Justin Blethrow<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Derek Lemons<sup>2</sup>; Mark Mercola<sup>2</sup>; Laurence Brill<sup>2</sup>; <sup>1</sup>*Thermo Scientific, San Jose, CA*; <sup>2</sup>*Sanford Burnham Medical Research Institute, San Diego, CA*
- MOA pm 2:50 **Expanding the Depth of Coverage in Quantitative Phosphoproteomics through the Combination of Metal Oxide and Motif-Specific Antibody Enrichment Strategies;** Erik J. Soderblom<sup>1</sup>; J. Will Thompson<sup>1</sup>; Charles L. Farnsworth<sup>2</sup>; Brenna M. Richardson<sup>1</sup>; Jeffrey C. Silva<sup>2</sup>; M. Arthur Moseley<sup>1</sup>; <sup>1</sup>*Duke University School of Medicine, Durham, NC*; <sup>2</sup>*Cell Signaling Technologies, Danvers, MA*
- MOA pm 3:10 **Dynamic Phosphorylation Regulates Histone Deacetylase Localization, Interactions, and Cell Cycle-Dependent Functions;** Amanda Guise; Rommel Mathias; Todd Greco; Irene Zhang; Ileana M. Cristea; *Princeton University, Princeton, NJ*

- MOA pm 3:30 **Quantitative Proteomics Reveals Important Roles for Mitochondrial Acetylation in Metabolic Transitions;** Amelia J. Still; Brendan J. Floyd; Molly Mcdevitt; Alex S. Hebert; Joshua J. Carson; Drew R. Gunderson; Brendan K. Dolan; Paul A. Grimsrud; Michael S. Westphall; David J. Pagliarini; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- MOA pm 3:50 **Quantification of Lysine Acetylation in *Escherichia coli* Using Label-Free Proteomics: Assessing the Role of Acetyl-CoA and Acetyl-Phosphate;** Birgit Schilling<sup>1</sup>; Linda Hu<sup>2</sup>; Alexandria K. D'Souza<sup>1</sup>; Misty L. Kuhn<sup>3</sup>; Dylan J. Sorensen<sup>1</sup>; Bozena Zemaitaitis<sup>2</sup>; Bruno Lima<sup>2</sup>; Michael Scholle<sup>3</sup>; Milan Mrksich<sup>3</sup>; Wayne F. Anderson<sup>3</sup>; Alan J. Wolfe<sup>2</sup>; Bradford W. Gibson<sup>1</sup>; <sup>1</sup>*Buck Institute for Research on Aging, Novato, CA*; <sup>2</sup>*Loyola University Chicago, Maywood, IL*; <sup>3</sup>*Northwestern University, Chicago, IL*
- MOA pm 4:10 **High-throughput Identification of Protein Disulfide Bonds from Complex Samples;** Shan Lu<sup>1,2</sup>; Bing Yang<sup>2</sup>; Sheng-Bo Fan<sup>3</sup>; Jia-Ming Meng<sup>3</sup>; Long Wu<sup>3</sup>; Kun Zhang<sup>3</sup>; Mei-Jun Zhang<sup>2</sup>; En-Zhi Shen<sup>2</sup>; Chun-Qing Song<sup>2</sup>; Yu-Xin Li<sup>2</sup>; Rui-Xiang Sun<sup>3</sup>; Si-Min He<sup>3</sup>; Meng-Qiu Dong<sup>1,2</sup>; <sup>1</sup>*College of Life Science, Beijing Normal University, Beijing, China*; <sup>2</sup>*National Institute of Biological Sciences, Beijing, China*; <sup>3</sup>*ICT, Chinese Academy of Sciences, Beijing, China*



2:30 – 4:30 PM,  
MONDAY AFTERNOON

**TOP-DOWN AND MIDDLE-DOWN PROTEIN ANALYSIS  
HONORING FRED MCLAFFERTY'S 90<sup>TH</sup> BIRTHDAY**

Joseph Loo (UCLA), presiding  
Room L100 (lower level)

- MOB pm 2:30 **Fragmenting Intact Macromolecules and Protein Assemblies: Native ESI and Top-down MS for Protein Biophysics and Analysis;** Michael L. Gross<sup>1</sup>; Hao Zhang<sup>1</sup>; Weidong Cui<sup>1</sup>; Lisa M. Jones<sup>2</sup>; Justin Sperry<sup>3</sup>; James A Carroll<sup>3</sup>; Robert E. Blankenship<sup>1</sup>; Weikai Li<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO; <sup>2</sup>IUPUI, Indianapolis, IN; <sup>3</sup>Pfizer, Chesterfield, MO
- MOB pm 2:50 **Top-down Mass Spectrometry Enabled Cardiac Proteomics for Understanding Heart Failure;** Ying Ge; *University of Wisconsin, Madison, WI*
- MOB pm 3:10 **Unequivocal Determination of Site-Specific Protein Disulfide Bond Reduction Potentials by Top-Down FT-ICR MS/MS;** Alan G. Marshall; Jenna Scotcher; Nicolas Young; *Ion Cyclotron Resonance Prog, Tallahassee, FL*
- MOB pm 3:30 **Detailed Characterization of Complex Protein and RNA Modification Patterns by Top-Down Mass Spectrometry;** Barbara Ganis; Kathrin Breuker; *University of Innsbruck, Innsbruck, Austria*
- MOB pm 3:50 **Antibody Characterization by Top-Down and Middle-Down Electron Transfer Dissociation using a High-Field Orbitrap FTMS;** Luca Fornelli<sup>1</sup>; Anton N. Kozhinov<sup>1</sup>; Ünige A. Laskay<sup>1</sup>; Daniel Ayoub<sup>2</sup>; Alain Beck<sup>2</sup>; Yuri O. Tsybin<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Centre d'Immunologie Pierre Fabre, St Julien-en-Genevois, France
- MOB pm 4:10 **Comprehensive Top Down Proteomics of Human Cells: The Role of Mitochondria and Membrane Proteins in Cellular Senescence;** Adam Catherman; Kenneth Durbin; Owen Skinner; Dorothy Ahlf; Bryan Early; Philip Compton; Paul Thomas; Neil Kelleher; *Northwestern University, Evanston, IL*

**2:30 – 4:30 PM, MONDAY AFTERNOON  
CLINICAL CHEMISTRY, DRIED BLOOD SPOT ANALYSIS  
Karen Phinney (NIST), presiding  
Ballroom B**

- MOC pm 2:30 **Multiplex Newborn Screening of Lysosomal Storage Diseases using Flow Injection Tandem Mass Spectrometry;** Mariana Barcenas<sup>1</sup>; Martin Sadilek<sup>1</sup>; Frantisek Turecek<sup>1</sup>; Michael Gelb<sup>1,2</sup>; Ronald Scott<sup>3</sup>; <sup>1</sup>Department of Chemistry, University of Washington, Seattle, WA; <sup>2</sup>Department of Biochemistry, University of Washington, Seattle, WA; <sup>3</sup>Department of Pediatrics, University of Washington, Seattle, WA
- MOC pm 2:50 **HPLC-ESI-MS/MS Analysis of Hemoglobin Peptides in Tryptic Digests of Dried-Blood Spot Extracts Detects HbS, HbC, HbE, HbO-Arab and HbG-Philadelphia Mutations;** Christopher A. Haynes<sup>1</sup>; Stephanie Guerra<sup>2</sup>; Victor De Jesus<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>Harvard University, Cambridge, MA

- MOC pm 3:10 **In-Paper Dried Blood Spot Enzyme Assays for the Reliable Determination of Plasma Enzyme Activities;** Eszter Szabo<sup>1</sup>; Ildiko Szatmari<sup>2</sup>; Julia Denes<sup>3</sup>; Laszlo Szonyi<sup>2</sup>; Zoltan Takats<sup>3</sup>; <sup>1</sup>Eötvös Lóránd University, Budapest, HUNGARY; <sup>2</sup>1st Dept. of Pediatrics, Semmelweis University, Budapest, Hungary; <sup>3</sup>Imperial College London, London, UK
- MOC pm 3:30 **Application of LC-MS/MS to Determine the Exposure to Methyl and Propyl Parabens in Preterm Neonates using Dried Blood Spot (DBS);** Shirish Yakkundi<sup>1</sup>; James McElroy<sup>1</sup>; Mark Turner<sup>2</sup>; <sup>1</sup>Queen's University Belfast, Belfast, UK; <sup>2</sup>Liverpool Women's NHS Foundation Trust, Liverpool, UK
- MOC pm 3:50 **Detergent-Assisted Elution: Method Optimization to Improve Analyte Elution and Assay Performance for Dried Matrix Spots (DMS) by uHPLC-MS/MS;** Naiyu Zheng<sup>1</sup>; Jianing Zeng<sup>1</sup>; Qin C. Ji<sup>1</sup>; Aida Angeles<sup>1</sup>; Shenita Basdeo<sup>1</sup>; Anne-Francoise Aubry<sup>1</sup>; Ishani Savant<sup>2</sup>; Navin Jariwala<sup>2</sup>; Mark E. Arnold<sup>1</sup>; <sup>1</sup>Bioanalytical Sciences, Bristol-Myers Squibb Co., Princeton, NJ; <sup>2</sup>DMCP, Bristol-Myers Squibb Co., Pennington, NJ
- MOC pm 4:10 **Sensitive Quantification of Insulin-like Growth Factor-1 and Its Synthetic Analogues in Dried Blood Spots;** Holly Cox; Daniel Eichner; *Sports Medicine Research and Testing Laboratory, Salt Lake City, UT*

**2:30 – 4:30 PM, MONDAY AFTERNOON  
BIOTHERAPEUTICS, IMPURITIES AND DEGRADANTS:  
STRUCTURAL CHARACTERIZATION  
Justin Sperry (Pfizer), presiding  
Ballroom A**

- MOD pm 2:30 **The Main Cause of Amino Acid Misincorporations in Recombinant Proteins;** Zhongqi Zhang; Bhavana Shah; Pavel Bondarenko; *Amgen, Inc., Thousand Oaks, CA*
- MOD pm 2:50 **Rapid Characterization and Comparison of Stressed anti-CD20 Drugs using Middle Down Mass Spectrometry;** Ashley Gucinski; Timothy Toby; Michaela Levy; Bo Wang; Michael Boyne; *U.S. FDA, Division of Pharmaceutical Analysis, Saint Louis, MO*
- MOD pm 3:10 **Assessing the Impact of Chemical Modifications on mAb Conformational Dynamics using Hydrogen/Deuterium Exchange Mass Spectrometry (HDX-MS);** Aming Zhang; Paul MacGregor; Yu Xue; Aston Liu; Leonard Olszewski; Ping Hu; *GlaxoSmithKline, King of Prussia, PA*
- MOD pm 3:30 **Characterization of Non-Native, Intermolecular Disulfide Linkages in a Recombinant Protein by LC-MS/MS;** Chris Morgan; Xiaoying Jin; X. Kate Zhang; *Genzyme, A Sanofi Company, Framingham, MA*
- MOD pm 3:50 **Comprehensive Comparison of Biosimilar Protein Drugs by High-Separation and High-Resolution LC-MS;** David Horn<sup>1</sup>; Shiaw-Lin Wu<sup>2</sup>; Zhiqi Hao<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Barnett Institute, Northeastern University, Boston, MA
- MOD pm 4:10 **One-Dimensional Liquid Chromatography Analysis of Host Cell Proteins in Therapeutic Antibodies using an Orbitrap Velos;** Ashley Bell; Richard Rogers; Tom Kowski; Bailey Robert; *Amgen, Seattle, WA*



**2:30 – 4:30 PM, MONDAY AFTERNOON  
HIGH MASS ACCURACY IN DRUG DISCOVERY AND  
DEVELOPMENT**

**Karin Keller (Cleveland HeartLab), presiding  
Auditorium**

- MOE pm 2:30 **Rapid Antibody de novo Sequencing by Reference Sequence Matching;** Bianca Gruenwalder; Stefan Klostermann; Maximiliane Hilger; Roche Diagnostics GmbH, pRED, Penzberg, Germany
- MOE pm 2:50 **Evaluation of LC-HRMS Full Scan with Positive-Negative Switching for Increasing Throughput of Human In Vitro Cocktail Drug-Drug Interaction Assay;** Ragu Ramanathan<sup>1</sup>; Brad Yuska<sup>1</sup>; Kate Comstock<sup>2</sup>; Lakshmi Ramanathan<sup>1</sup>; Tim Stratton<sup>2</sup>; Patrick Bennett<sup>2</sup>; Helen Shen<sup>1</sup>; Zamas Lam<sup>1</sup>; <sup>1</sup>QPS, LLC, Newark, DE; <sup>2</sup>ThermoFisher, San Jose, CA
- MOE pm 3:10 **From MS Data to Information and from Information to Knowledge;** Ismael Zamora<sup>1</sup>; Andreas Brink<sup>2</sup>; Eickhoff Kirsten<sup>2</sup>; Cece Esra Nurten<sup>3</sup>; Axel Paehler<sup>2</sup>; <sup>1</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, SPAIN; <sup>2</sup>F. Hoffmann-La Roche Ltd, Basel, Switzerland; <sup>3</sup>Pompeu Fabra University, Barcelona, Spain
- MOE pm 3:30 **Combining Sub-PPM Mass Accuracy and Isotopic Fine Structures for Structural Elucidation in Pharmaceutical Drug Development;** Guilong (Charles) Cheng; Ron Morris; Victor Soliman; Pfizer, Inc., Groton, CT
- MOE pm 3:50 **Comparative Analysis of Pharmaceutical Excipients using High Performance Time to Flight Mass Spectrometry – Purity Evaluation and Impurity Identification;** Jeffrey Patrick; Joe Binkley; Stephanie Amaya; Kevin Siek; LECO Corporation, St. Joseph, MI
- MOE pm 4:10 **Quality Control for Shuxuetong Injection by High Resolution Mass Spectrometry Based Statistical Analysis;** Zheng-Xiang Zhang; Tao Bo; Wei Chen; Zhi-Xu Zhang; Agilent Technologies, Beijing, China

**2:30 – 4:30 PM, MONDAY AFTERNOON  
PROTEIN- PROTEIN AND PROTEIN-LIGAND INTERACTIONS**  
**David Russell (Texas A&M University), presiding  
Room 101**

- MOF pm 2:30 **Dissecting Large Non-covalent Ring Protein Complexes by Surface Induced Dissociation Combined with Ion Mobility;** Mowei Zhou; Yun Zhang; Vicki Wysocki; Ohio State University, Columbus, OH
- MOF pm 2:50 **Probing the Limits of Mass Spectrometry in Analyzing Mega Dalton Assemblies;** Joost Snijder<sup>1</sup>; Rebecca J. Rose<sup>1</sup>; David Veessler<sup>2</sup>; John E. Johnson<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>The Scripps Research Institute, La Jolla, CA
- MOF pm 3:10 **Time Window Expansion for HDX Analysis of an Intrinsically Disordered Protein;** Patrick Griffin<sup>1</sup>; Devrishi Goswami<sup>1</sup>; Srikrupa Devarakonda<sup>2</sup>; Michael Chalmers<sup>1</sup>; Bruce Pascal<sup>1</sup>; Bruce Spiegelman<sup>2</sup>; <sup>1</sup>The Scripps Research Institute, Jupiter, FL; <sup>2</sup>Harvard Medical School, Dana-Farber Cancer INST, Boston, MA
- MOF pm 3:30 **Proteomic Mapping of Mitochondria in Living Cells via Spatially-Restricted Enzymatic Tagging;** Hyun-Woo Rhee<sup>1</sup>; Peng Zou<sup>1</sup>; Namrata Udeshi<sup>2</sup>; Jeffrey Martell<sup>1</sup>; Tanya Svinkina<sup>2</sup>; Vamsi Mootha<sup>2,3</sup>; Steven Carr<sup>2</sup>; Alice Ting<sup>1,2</sup>; <sup>1</sup>Massachusetts Institute of Technology, Cambridge, MA; <sup>2</sup>The Broad Institute of MIT and Harvard, Cambridge, MA; <sup>3</sup>Harvard Medical School, Boston, MA

- MOF pm 3:50 **Utilization of Epitope-Tagged Knock-in Mice for IP-MS/MS Analysis of the Effects of Drug Treatments on the Dopamine Transporter Interactome;** Sarah Rogstad<sup>1,2</sup>; John Caltagarone<sup>1</sup>; Shiqi Ma<sup>1</sup>; Alexander Sorkin<sup>1</sup>; Christine Wu<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>University of Colorado, Anschutz Medical Campus, Aurora, CO

- MOF pm 4:10 **Monitoring the Pathways of Fibril Formation and Inhibition from the Amyloidogenic Protein IAPP using ESI-IMS-MS;** Lydia Young; Sheena E Radford; Alison E. Ashcroft; Faculty of Biological Sciences, University of Leeds, Leeds, UK

**2:30 – 4:30 PM, MONDAY AFTERNOON  
FUNDAMENTALS OF ION ACTIVATION AND DISSOCIATION**  
**Eric Dodds (University of Nebraska-Lincoln), presiding  
Room 102**

- MOG pm 2:30 **Charge Reversal Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Vladislav Lobodin<sup>1,2</sup>; Joshua Savory<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Ryan Rodgers<sup>1,2</sup>; Alan Marshall<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Tallahassee, FL; <sup>3</sup>Florida State University, Tallahassee, FL
- MOG pm 2:50 **Factors that Influence Competitive Intermolecular Solvation of Protonated Groups in Peptides and Proteins in the Gas Phase;** Yuanqi Tao; Ryan Julian; UC Riverside, Riverside, CA
- MOG pm 3:10 **Systematic nECD Mechanistic Exploration with Synthetic Peptides and Fixed-Charge Tags;** Ning Wang; Kristina Hakansson; University of Michigan, Ann Arbor, Michigan
- MOG pm 3:30 **Using Dissociation Energies to Predict Observability of b- and y- Peaks in Mass Spectra of Tryptic Hexapeptides;** Oleg Obolensky<sup>1</sup>; Wells Wu<sup>2</sup>; Rong-Fong Shen<sup>2</sup>; Yi-Kuo Yu<sup>1</sup>; <sup>1</sup>National Center for Biotechnology Information, NLM, Bethesda, MD; <sup>2</sup>Center for Biologics Evaluation and Research, FDA, Bethesda, MD
- MOG pm 3:50 **Elucidation of Heterolytic N-C<sub>α</sub> Bond Cleavage in ECD/ETD Mass Spectrometry;** Matthew D. Wodrich; Konstantin O. Zhurov; Clémence Corminboeuf; Yury O. Tsybin; Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
- MOG pm 4:10 **Development of a Detailed Molecular Model for the Collision Induced Unfolding of Multiprotein-Ligand Complexes;** Shuai Niu; Brandon Ruotolo; University of Michigan, Ann Arbor, MI

**2:30 – 4:30 PM, MONDAY AFTERNOON  
PHOTOIONIZATION**  
**Jack Syage (Syagen/Morpho Detection), presiding  
Room 103**

- MOH pm 2:30 **Gas Chromatography – Atmospheric Pressure Photoionization – Tandem Mass Spectrometry (GC-APPI-MS/MS) in Neurosteroid Analysis;** Tina Suominen<sup>1</sup>; Markus Haapala<sup>1</sup>; Anna Takala<sup>1</sup>; Raimo A Ketola<sup>2</sup>; Risto Kostianen<sup>1</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland; <sup>2</sup>Hjelt Institute, Helsinki, Finland
- MOH pm 2:50 **Studying the Effects of Simulated Solar Radiation upon Crude Oil using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Matthew Griffiths; Raffaello da Campo; Peter O'Connor; Mark Barrow; University of Warwick, Coventry, UK



## MONDAY AFTERNOON ORAL SESSIONS

- MOH pm 3:10 **A New APPI Ion Source for Low Flow LC-MS and CE-MS Analysis of Small Molecules;** Sheng-Suan (Victor) Cai<sup>1</sup>; Andy Gieschen<sup>2</sup>; Martin Greiner<sup>3</sup>; Brian Nies<sup>1</sup>; Stefan Lukow<sup>1</sup>; Michael Patterson<sup>1</sup>; <sup>1</sup>Morpho Detection, Inc., Santa Ana, CA; <sup>2</sup>Agilent Technologies, Inc., La Jolla, CA; <sup>3</sup>Agilent Technologies, Waldbronn, Germany
- MOH pm 3:30 **GC and the Exactive Orbitrap – Two Approaches for Powerful GC APPI Interfaces;** Hendrik Kersten; Kai Kroll; Thorsten Benter; University of Wuppertal, Wuppertal, Germany
- MOH pm 3:50 **Fast Switchable Photon/Electron Ionization for Time-of-Flight Mass Spectrometry and Its Application for Gas Chromatography – Mass Spectrometry;** Thomas Groeger<sup>1,2</sup>; Mohammad Reza Saraji-Bozorgzad<sup>2</sup>; Ralf Zimmermann<sup>3</sup>; <sup>1</sup>Joint Mass Spectrometry Centre, Oberschleissheim, Germany; <sup>2</sup>Photonion GmbH, Schwerin, Germany; <sup>3</sup>University of Rostock, Rostock, Germany
- MOH pm 4:10 **Thermal Analysis--Single Photon Ionization Mass Spectrometry for Highly Resolved Thermo-Chemical Evolved Gas Speciation: Coffee Roasting and Crude Oil Characterization;** Mohammad Reza Saraji-Bozorgzad; Andreas Walte; Thomas Groeger; Matthias Bente-von Frowein; Photonion GmbH, Neuherberg, Germany

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

Susan T. Weintraub (Univ of Texas HSC-San Antonio), presiding  
Exhibit Hall A, Lower Level



Award for a Distinguished Contribution in  
Mass Spectrometry

Richard D. Smith  
Pacific Northwest National Laboratory

### 5:45 - 7:00 PM, MONDAY AFTERNOON WORKSHOPS

Light snacks are provided on level two.

#### LEVEL ONE ROOMS

- **The Informatical Difference between Targeted and Discovery-based Proteomics** (organized by the Bioinformatics for MS Interest Group), Room 1
- **Have Recent LC-MS Techniques Advanced to Substitute AMS in Analyzing Microdose and other Low Level Clinical Studies for Metabolites and Drug Related Material?** (organized by the DMPK Interest Group), Room 2
- **Trans-Proteomic Pipeline (TPP) and Related Open-Source Proteomics Resources**, Room 3

#### LEVEL TWO ROOMS

- **FRAGILE Modifications**, Handle with Care during Peptide Fragmentation (organized by the Peptide Fragmentation Interest Group), Room 200 DE
- **Mass Spectrometry-based Characterization of Biotherapeutics** (organized by the Protein Therapeutics Interest Group), Room 200 FG
- **How Can MS Analysis Be Used to Improve Analytical Results and Laboratory Efficiency** (organized by the Flavor, Fragrance and Foodstuff Interest Group), Room 200 H
- **Nucleic Acids as Diagnostic and Therapeutic Biomarkers** (organized by the DNA/RNA Interest Group), Room 200 I
- **Surviving and Thriving: A Panel Discussion for Both Students and PUI Faculty on How to Get the Most out of Undergraduate Research** (organized by the Undergraduate Research in MS interest Group), Room 205 AB
- **Photonization Mass Spectrometry**, Room 205 CD
- **Consortium for Top Down Proteomics**, Room 208 AB
- **Data Independent Acquisition**, Room 208 CD

### AFTER 8:00 PM CORPORATE HOSPITALITY SUITES HILTON MINNEAPOLIS HOTEL

## TUESDAY MORNING ORAL SESSIONS

### 8:30 – 10:30 AM, TUESDAY MORNING QUANTITATIVE PROTEOMICS

David Muddiman (North Carolina State Univ), presiding  
Exhibit Hall A (lower level)

- TOA am 08:30 **18-plex SILAC, and there's room to grow;** Christopher M. Rose<sup>1</sup>; Alexander S. Hebert<sup>1</sup>; Anna E. Merrill<sup>1</sup>; Derek J. Bailey<sup>1</sup>; Joel C. Bradley<sup>2</sup>; William W. Wood<sup>2</sup>; Marwan Elmasri<sup>2</sup>; Michael S. Westphall<sup>1</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Cambridge Isotope Laboratories, Andover, MA
- TOA am 08:50 **Highly Sensitive Proteomic Analysis of Age-Related Protein Aggregation;** Dirk M. Walther; Franz-Ulrich Hartl; Matthias Mann; MPI of Biochemistry, Martinsried, Germany
- TOA am 09:10 **Quantitative Proteomic Analysis of Reversible Cysteine Oxidation in Hearts from Mice Fed a Western Diet;** Jessica B Behring; Vikas Kumar; Pratibha Chauhan; Stephen A Whelan; Deborah A Siwik; Catherine E Costello; Wilson S Colucci; Richard A Cohen; Mark E McComb; Markus M Bachschmid; Boston University School of Medicine, Boston, Ma
- TOA am 09:30 **Increasing the Breadth and Depth of Multi-Notch MS3-based TMT Quantitation using a Hybrid Q-OT-qIT Mass Spectrometer;** Graeme McAlister<sup>1</sup>; Edward Huttlin<sup>1</sup>; Mark P. Jedrychowski<sup>1</sup>; Martin Wuehr<sup>1</sup>; Ramin Rad<sup>1</sup>; David Nusinow<sup>1</sup>; Philip Remes<sup>2</sup>; Jesse Canterbury<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Justin Blethrow<sup>2</sup>; Shannon Eliuk<sup>2</sup>; Mike Senko<sup>2</sup>; Wilhelm Haas<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TOA am 09:50 **Peptide Barcodes: A Genetic Approach for N-Plexing Protein Quantification for Synthetic Biology Applications;** Pragya Singh<sup>1,2</sup>; Becky J. Rutherford<sup>1,2</sup>; Vikram R. Ramakrishnan<sup>3</sup>; Paul D. Adams<sup>1,2</sup>; Jay D. Keasling<sup>1,2</sup>; Christopher J. Petzold<sup>1,2</sup>; <sup>1</sup>Lawrence Berkeley National Lab, Berkeley, CA; <sup>2</sup>Joint BioEnergy Institute, Emeryville, CA; <sup>3</sup>University of California, Berkeley, CA
- TOA am 10:10 **Highly Multiplexed and Sensitive Quantitation of Candidate Disease-related Biomarker Proteins in Human Plasma by 1-D and 2-D LC/MRM-MS;** Andrew Percy<sup>1</sup>; Andrew Chambers<sup>1</sup>; Juncong Yang<sup>1</sup>; Martin Eisinger<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada

**8:30 – 10:30 AM, TUESDAY MORNING  
IMAGING MS: INCREASING SPEED AND  
INFORMATION CONTENT**  
**Kevin Schey (Vanderbilt University), presiding**  
**Room L100 (lower level)**

- TOB am 08:30 **High Speed AP-MALDI Imaging at High Spatial Resolution;** Bernhard Spengler<sup>1</sup>; Andreas Römpf<sup>1</sup>; Karl-Christian Schäfer<sup>1</sup>; Sabine Guenther<sup>1</sup>; Oliver Schulz<sup>1</sup>; Alfons Hester<sup>1</sup>; Christian Schinz<sup>1</sup>; Christian Lotze<sup>1</sup>; Jörg-Ulrich Pötzl<sup>1</sup>; Oliver Lange<sup>2</sup>; Kerstin Strupat<sup>2</sup>; <sup>1</sup>*Justus Liebig University, Giessen, Germany*; <sup>2</sup>*Thermo Fisher Scientific GmbH, Bermer, Germany*
- TOB am 08:50 **High-Speed Imaging using Nanospray Desorption Electrospray Ionization Mass Spectrometry: Toward 3D and MS/MS Imaging;** Julia Laskin<sup>1</sup>; Ingela Lanekoff<sup>1</sup>; Mathew Thomas<sup>1</sup>; James Carson<sup>1</sup>; Kristin Burnum<sup>1</sup>; Jeeyeon Cha<sup>2</sup>; Sudhansu K Dey<sup>2</sup>; Mari Prieto<sup>3</sup>; Pengxiang Yang<sup>3</sup>; <sup>1</sup>*Pacific NW National Laboratory, Richland, WA*; <sup>2</sup>*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- TOB am 09:10 **Mass Spectrometry Imaging with a LAESI Hybrid Iontrap FT-ICR Mass Spectrometer;** Andras Kiss<sup>1</sup>; Donald F. Smith<sup>1</sup>; Brent R. Reschke<sup>2</sup>; Matthew J. Powell<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, Netherlands*; <sup>2</sup>*Protea Biosciences, Inc., Morgantown, WV*
- TOB am 09:30 **Ambient Molecular Imaging and Quantitative Analysis by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation;** Hang Li<sup>1</sup>; Brian K. Smith<sup>1</sup>; Peter Nemes<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*The George Washington University, Washington, DC*; <sup>2</sup>*Food and Drug Administration, Silver Spring, MD*
- TOB am 09:50 **Polarity Switching Multiplex MALDI Imaging on an LTQ-Orbitrap Hybrid Mass Spectrometer;** Andrew Korte<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames Laboratory/USDOE, Ames, IA*
- TOB am 10:10 **Visualizing Biomolecular Modifications in Tissue: Integrating Mass Difference ( $\Delta m/z$ ) Scanning Algorithms and MALDI FT-ICR Imaging Mass Spectrometry;** Jeffrey Spraggins; Raf Van de Plas; Kerri Grove; David Rizzo; Richard Caprioli; *Vanderbilt University, Nashville, TN*

**8:30 – 10:30 AM, TUESDAY MORNING  
FUNCTIONAL FOODS, PHYTOCHEMICALS, AND SUPPLEMENTS**  
**Nadja Cech (Univ of North Carolina-Greensboro), presiding**  
**Ballroom B**

- TOC am 08:30 **Analysis of an Adulterated Herbal Medicinal Product using UPLC-Qtof-MS;** Mark Powell<sup>1</sup>; Margaret Maziarz<sup>2</sup>; Michael D. Jones<sup>2</sup>; Warren Potts<sup>2</sup>; Kate Yu<sup>2</sup>; <sup>1</sup>*Quay Pharmaceuticals, Flintshire, UK*; <sup>2</sup>*Waters Corporation, Milford, MA*
- TOC am 08:50 **Screening Herbal Supplements using Statistical Modeling to Find and Identify Adulterants and Contaminants using Direct Analysis in Real Time (DART)-MS;** Nick Levitt<sup>1</sup>; Joseph LaPointe<sup>2</sup>; Michael Festa<sup>2</sup>; Elizabeth Crawford<sup>2</sup>; <sup>1</sup>*TwoCenter Technologies, Cambridge, MA*; <sup>2</sup>*IonSense Inc., Saugus, MA*

- TOC am 09:10 **Solvent- and Gas-Phase Deuteration of Polyphenolics Informs their Identification by Mass Spectrometry;** Mikel R. Roe; Jerry Cohen; Adrian Hegeman; *University of MN, St. Paul, MN*
- TOC am 09:30 **Human Pharmacokinetics of Xanthohumol, a Flavonoid with Anti-Diabetic Activity Derived from Hops;** LeeCole Legette<sup>1</sup>; Chanida Karnpracha<sup>1</sup>; Ralph Reed<sup>1</sup>; Jaewoo Choi<sup>1</sup>; J. Mark Christensen<sup>1</sup>; Jonathan Purnell<sup>2</sup>; J. Fred Stevens<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*Oregon Health Sciences University, Portland, OR*
- TOC am 09:50 **How Can Mass Spectrometry Help to Decipher Bioactive Peptides in Functional Food?** Michael Affolter; Alexandre Panchaud; *Nestle Research Centre, Lausanne, Switzerland*
- TOC am 10:10 **EnzymePredictor: A Tool for Predicting and Visualizing Enzymatic Cleavages of Digested Proteins;** Nora Khaldi<sup>1,2</sup>; Vaishnavi Vijayakumar<sup>1</sup>; Andrés Guerrero<sup>2</sup>; Norman Davey<sup>3</sup>; Carlito Lebrilla<sup>2</sup>; Denis Shields<sup>1</sup>; <sup>1</sup>*University College Dublin, Dublin, Ireland*; <sup>2</sup>*University College Davis, CA*; <sup>3</sup>*European Molecular Biology Laboratory, Heidelberg, Germany*

**8:30 – 10:30 AM, TUESDAY MORNING  
PTMs: GLYCOSYLATION**  
**Heather Desaire (University of Kansas), presiding**  
**Ballroom A**

- TOD am 08:30 **Development of a Fully Characterized N-Glycan Library from Human Serum with Structures and Relative Abundances;** Ting Song; Danielle Aldredge; Javier González; Carlito Lebrilla; *University of California, Davis, CA*
- TOD am 08:50 **Applications of Aldehyde-Reactive Thermo Scientific Tandem Mass Tag (TMT) Reagents for Mass Spectrometry-based Quantitative Glycomics;** Sergei Snovidia<sup>1</sup>; Karsten Kuhn<sup>2</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>*ThermoFisher Scientific, Rockford, IL*; <sup>2</sup>*Proteome Sciences, Frankfurt, Germany*
- TOD am 09:10 **Increasing the Accessibility of N-Glycopeptide Determination via an Integrated Informatics and Instrumental Strategy;** John Froehlich<sup>1,2</sup>; Oliver Serang<sup>1,2</sup>; Peter Warren<sup>1</sup>; Hui Zhou<sup>1,2</sup>; Judith Steen<sup>1,2</sup>; Richard Lee<sup>1,2</sup>; <sup>1</sup>*Boston Children's Hospital, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- TOD am 09:30 **The Occurrence of Extracellular O-glycosylation in Murine Synaptosomes;** Katalin F. Medzihradszky<sup>1</sup>; Jonathan C. Trinidad<sup>1,2</sup>; Ralf Schoepfer<sup>3</sup>; Al Burlingame<sup>1</sup>; <sup>1</sup>*UCSF, San Francisco, CA*; <sup>2</sup>*Department of Chemistry, Indiana University, Bloomington, IN*; <sup>3</sup>*Department of Pharmacology, UCL, London, UK*
- TOD am 09:50 **Glycoproteomic Analysis of Mycobacterium Tuberculosis Culture Filtrate Proteins using Multiple Fragmentation Techniques;** Geoffrey T. Smith; Michael J Sweredoski; Sonja Hess; *Caltech, Pasadena, CA*
- TOD am 10:10 **Comparative Glycoproteomics Analysis of Influenza Hemagglutinin (H5N1) Expressed in Vaccine and Vaccine Research Relevant Cell Substrates;** Yanning An; John Cipollo; *FDA, Bethesda, MD*

**8:30 – 10:30 AM, TUESDAY MORNING  
SYSTEMS BIOLOGY/CELLULAR PATHWAYS**  
**Ileana Cristea (Princeton University), presiding**  
**Auditorium**

TOE am 08:30 **Exploring Communication in the Tumor Microenvironment;** Catherine Fenselau<sup>1</sup>; Meghan Burke<sup>1</sup>; Waeowalee Choksawangkam<sup>1</sup>; Rebecca Rose<sup>1</sup>; Avantika Dhabaria<sup>1</sup>; Nathan Edwards<sup>2</sup>; Suzanne Ostrand-Rosenberg<sup>3</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>Georgetown University Medical Center, Washington, DC; <sup>3</sup>UMBC, Baltimore, MD

TOE am 08:50 **Global Quantitative Phosphoproteomic Analysis of RSK-Dependent Signal Transduction;** Jacob A. Galan<sup>1</sup>; Kathryn M. Geraghty<sup>2</sup>; Evgeny Kanshin<sup>1</sup>; Joseph Tcherkezian<sup>1</sup>; Geneviève Lavoie<sup>1</sup>; Benjamin E. Turk<sup>3</sup>; Bryan A. Ballif<sup>4</sup>; John Blenis<sup>2</sup>; Pierre Thibault<sup>1,5</sup>; Philippe P. Roux<sup>1,5</sup>; <sup>1</sup>Institute for Research in Immunology and Cancer, Montreal, Canada; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Yale University School of Medicine, New Haven, CT; <sup>4</sup>University of Vermont, Burlington, VT; <sup>5</sup>Université de Montréal, Montréal, Canada

TOE am 09:10 **Key Contribution of Post-Transcriptional Mechanisms to Circadian Metabolism Regulation Revealed by Perseus Analysis of Quantitative Proteomics and Cross-Omics Data;** Juergen Cox; Maria S Robles; Matthias Mann; Max-Planck-Institute of Biochemistry, Martinsried, Germany

TOE am 09:30 **Acetylome Machinery Interactome Revealed by Data Dependent and Independent Mass Spectrometry Acquisition;** Jean-Philippe Lambert<sup>1</sup>; Sarah Picaud<sup>2</sup>; Brett Larsen<sup>1</sup>; Beatriz Gonzalez Badillo<sup>1</sup>; Tony Pawson<sup>1,3</sup>; Stefan Knapp<sup>2</sup>; Panagis Filippakopoulos<sup>2</sup>; Anne-Claude Gingras<sup>1</sup>; <sup>1</sup>Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, Canada; <sup>2</sup>Nuffield Department of Clinical Medicine, SGC, Oxford, UK; <sup>3</sup>Department of Molecular Genetics, U Toronto, Toronto, Canada

TOE am 09:50 **Quantitative Dynamics of the Link between Cellular Metabolism and Histone Acetylation;** Adam Everts<sup>1</sup>; Barry Zee<sup>2</sup>; Peter DiMaggio<sup>3</sup>; Michelle Cope<sup>2</sup>; Hilary Collier<sup>1</sup>; Benjamin Garcia<sup>2</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>University of Pennsylvania School of Medicine, Philadelphia, PA; <sup>3</sup>Imperial College London, London, UK

TOE am 10:10 **Multi-notch MS3-based 8-Plex TMT Quantification of 8 Colorectal Cancer Cell Line Proteomes Reveals Functional Reflections of Tumor Mutation Profiles;** David P. Nusinow; Graeme McAlister; Edward L. Huttlin; Mark Jedrychowski; Wilhelm Haas; Steven P. Gygi; Harvard Medical School, Boston, MA

**8:30 – 10:30 AM, TUESDAY MORNING  
METABOLOMICS/LIPIDOMICS:  
NEW MS TECHNOLOGIES AND APPLICATIONS**  
**Mark Emmett (UTMB), presiding**  
**Room 101**

TOF am 08:30 **Metabolomics: A Review of Issues Affecting Translational Research;** Paul Wood; Lincoln Memorial University, Harrogate, TN

TOF am 08:50 **Identification of Unknown Metabolites Involved in Type 2 Diabetes with Accurate Mass GC-QTOF Mass Spectrometry;** John Meissen<sup>1</sup>; Kohei Takeuchi<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Kao Corporation, Tokyo, Japan

TOF am 09:10 **Comprehensive Pathway-Specific Metabolite Analysis of Central Carbon Metabolism using Three Complementary LC/ESI-MS Methods;** Jun Han<sup>1</sup>; Adrien Nyakas<sup>1</sup>; Tobias Eckle<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Department of Anesthesiology, U Colorado, Denver, CO; <sup>3</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada

TOF am 09:30 **Multi-Omics Profiling of Methionine-Restricted MCF7 Cells in 24 Hours using a Prototype UPLC-Compatible Microfluidic Device;** J. Will Thompson<sup>1</sup>; Jay Johnson<sup>2</sup>; Giuseppe Astarita<sup>2</sup>; Xiaohu Tang<sup>1</sup>; Giuseppe Paglia<sup>3</sup>; Jim Murphy<sup>2</sup>; Steven Cohen<sup>2</sup>; Mark Bennett<sup>4</sup>; Jen-Tsan Chi<sup>1</sup>; James Langdridge<sup>2</sup>; Geoff Gerhardt<sup>2</sup>; M. Arthur Moseley<sup>1</sup>; <sup>1</sup>Duke University School of Medicine, Durham, NC; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Center for Systems Biology, Univ of Iceland, Reykjavik, Iceland; <sup>4</sup>Nonlinear Dynamics, Durham, NC

TOF am 09:50 **Identification of Nuclear Lipids;** Huan He<sup>1</sup>; Nicolas L. Young<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; <sup>2</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL

TOF am 10:10 **The Use of Ion-Mobility Mass Spectrometry for Separation and Structural Elucidation of Lipids in Human Plasma. Application in Lipidomics Studies;** Carola W.N. Damen<sup>1,2</sup>; Giorgis Isaac<sup>3</sup>; Jonathan P. Williams<sup>4</sup>; Johannes P.C. Vissers<sup>4</sup>; James I. Langridge<sup>4</sup>; Thomas Hankemeier<sup>1,2</sup>; Rob J. Vreeken<sup>1,2</sup>; <sup>1</sup>Netherlands Metabolomics Centre, Leiden University, Leiden, The Netherlands; <sup>2</sup>Analytical Biosciences, LACDR, Leiden University, Leiden, The Netherlands; <sup>3</sup>Waters Corporation, Milford, MA, Waters Corporation., Manchester, UK

**8:30 – 10:30 AM, TUESDAY MORNING  
ION MOBILITY: SEPARATIONS**  
**John McLean (Vanderbilt University), presiding**  
**Room 102**

TOG am 08:30 **An Efficient Approach for Flexible Ion Transport, Mobility Separation, and Reaction;** Richard D. Smith; Xinyu Zhang; Erin Baker; Yehia Ibrahim; Gordon Anderson; Keqi Tang; PNNL, Richland, WA

TOG am 08:50 **Characterization of a New Uniform-Field Ion Mobility-Quadrupole Time-of-Flight Mass Spectrometer and its Application in Biomolecular Analyses;** Ruwan Kurulugama; Alexander Mordehai; Nathan Sanders; Ed Darland; Christian Klein; Crystal Cody; Bill Barry; George Stafford; John Fjeldsted; Agilent Technologies, Santa Clara, CA

TOG am 09:10 **Toward Calibration Standards for Ion Mobility Spectrometry (IMS);** William F. Siems<sup>1</sup>; Larry A. Viehland<sup>2</sup>; Herbert H. Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Chatham University, Pittsburgh, PA

TOG am 09:30 **Stereoisomers Separation by Ion Mobility-Mass Spectrometry;** Virginie Domalain<sup>1</sup>; Marie Hubert-Roux<sup>1</sup>; Catherine Lange<sup>1</sup>; Vincent Tognetti<sup>1</sup>; Jacques Rouden<sup>2</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>Normandie Univ UMR 6014, FR 3038; Univ Rouen; CNRS, Mont St Aignan, France; <sup>2</sup>Normandie Univ UMR 6507, FR 3038; ENSICAEN; CNRS, Caen, France



## TUESDAY MORNING ORAL SESSIONS

- TOG am 09:50 **Petroleomics by TWIM-MS: Development, Optimization and Applications of a Powerful Analytical Tool for Crude Oil and Petrofuel Characterization;** Maíra Fasciotti<sup>1,2</sup>; Clécio F. Klitzke<sup>2</sup>; Priscila M. Lalli<sup>2,3</sup>; Yuri E. Corilo<sup>3</sup>; Renan S. Galaverna<sup>2</sup>; Marcos A. Pudenzí<sup>2</sup>; Heliara L. Nascimento<sup>2</sup>; Ramsés Capilla<sup>4</sup>; Wagner Bastos<sup>4</sup>; Erica Morais<sup>4</sup>; Romeu J. Daroda<sup>1</sup>; Rosana Pereira<sup>4</sup>; Marcos N. Eberlin<sup>2</sup>; <sup>1</sup>*inmetro, Duque De Caxias, Brazil*; <sup>2</sup>*University of Campinas, Campinas, Brazil*; <sup>3</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>4</sup>*petrobras, Rio de Janeiro, Brazil*
- TOG am 10:10 **Exploiting IM-MS Separation to Overcome Heterogeneity in Protein Self Assembly;** Justin Benesch; *University of Oxford, Oxford, UK*

### 8:30 – 10:30 AM, TUESDAY MORNING ANTIBODIES AND ANTIBODY-DRUG CONJUGATES Yury Tsybin (Ecole Polytechnique Federale), presiding Room 103

- TOH am 08:30 **An Integrated Top-Down and Bottom-Up Proteomic Approach to Characterize Antibodies;** Lennard Dekker<sup>1</sup>; Si Wu<sup>2</sup>; Martijn Vanduijn<sup>1</sup>; Nikola Tolić<sup>2</sup>; Christoph Stingl<sup>1</sup>; Rui Zhao<sup>2</sup>; Theo Luider<sup>1</sup>; Ljiljana Paša-Tolić<sup>2</sup>; <sup>1</sup>*Erasmus Medical Center, Rotterdam, Netherlands*; <sup>2</sup>*Pacific Northwest National Laboratories, Richland, WA*
- TOH am 08:50 **In-Depth Mass Spectrometry Characterization of Therapeutic Antibodies for Efficient Biosimilar Development;** Wolfgang Jabs<sup>1</sup>; Anja Resemann<sup>1</sup>; Waltraud Evers<sup>1</sup>; Catherine Evans<sup>2</sup>; Laura Main<sup>3</sup>; Carsten Baessmann<sup>1</sup>; Detlev Suckau<sup>1</sup>; Daniel Ayoub<sup>4</sup>; Elsa Wagner-Rousset<sup>4</sup>; Alain Beck<sup>4</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics GmbH, Fällanden, Switzerland*; <sup>3</sup>*Bruker Daltonics Ltd, Coventry, UK*; <sup>4</sup>*Centre d'Immunologie Pierre Fabre, St Julien-en-Genevois, France*

- TOH am 09:10 **Rapid Qualitative and Quantitative Characterization of Antibody Glycosylation Profiles by Native Mass Spectrometry using an Orbitrap Mass Analyzer;** Sara Rosati<sup>1</sup>; Ewald T.J. van den Bremer<sup>2</sup>; Paul Parren<sup>2</sup>; Janine Schuurman<sup>2</sup>; Albert J. R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*Genmab, Utrecht, Netherlands*
- TOH am 09:30 **An Online Top-Down Mass Spectrometry Based Strategy Aimed at Complete *de novo* Sequencing of Monoclonal Antibodies;** Weihan Wang<sup>1</sup>; A. Michelle English<sup>1</sup>; Lissa Anderson<sup>1</sup>; John Syka<sup>2</sup>; Sushma Shivaswamy<sup>3</sup>; Kevin Sunley<sup>3</sup>; John Simard<sup>3</sup>; Jeffrey Shabanowitz<sup>1</sup>; Dina Bai<sup>1</sup>; Donald Hunt<sup>1,4</sup>; <sup>1</sup>*Department of Chemistry, University of Virginia, Charlottesville, VA*; <sup>2</sup>*Thermo Fisher Sci, San Jose, CA*; <sup>3</sup>*XBiotech USA Inc., Austin, TX*; <sup>4</sup>*Department of Pathology, University of Virginia, Charlottesville, VA*
- TOH am 09:50 **Micro-Scale Native Top-Down LCMS of Cysteine-Linked Antibody-Drug Conjugates;** Shawna M. Hengel; Russell Sanderson; William McFee; Jay Jones; John Valliere-Douglass; Stephen C. Alley; *Seattle Genetics, Bothell, WA*
- TOH am 10:10 **New Technology for Producing Large Repertoires of Bacterially Expressed High-Affinity Antibodies;** Yinyin Li<sup>1</sup>; Peter C. Fridy<sup>1</sup>; Mary K. Thompson<sup>1</sup>; Sarah Keegan<sup>2</sup>; David Fenyo<sup>2</sup>; Michael P. Rout<sup>1</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*New York University, New York, NY*

10:30 AM - 2:30 PM  
TUESDAY POSTER SESSION  
Exhibit Hall BC  
Lunch concessions are open 11:00 am - 2:00 pm

## TUESDAY AFTERNOON ORAL SESSIONS

### 2:30 – 4:30 PM, TUESDAY AFTERNOON INSTRUMENTATION AND METHODS: FT, ION TRAPS AND HYBRID INSTRUMENTS

Jim Bruce (University of Washington), presiding  
Exhibit Hall A (lower level)

- TOA pm 2:30 **Improving Data Dependent MS<sup>n</sup> Performance with a Multitasking Mass Spectrometer;** Michael W. Senko<sup>1</sup>; Philip Remes<sup>1</sup>; Qingyu Song<sup>1</sup>; Jesse Canterbury<sup>1</sup>; Justin Blethrow<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Oliver Lange<sup>2</sup>; Alexander Makarov<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific GmbH, Bremen, Germany*
- TOA pm 2:50 **Development of a Mass Spectrometer for Gas Phase Ion-Radical Reactions;** Ziqing Lin<sup>1</sup>; Tsungchi Chen<sup>1</sup>; Linfan Li<sup>1</sup>; Yu Xia<sup>2</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>*BME, Purdue University, West Lafayette, IN*; <sup>2</sup>*Chemistry, Purdue University, West Lafayette, IN*
- TOA pm 3:10 **2D FT-ICR Optimized Pulse Sequence: Application to Human Plasma Triglycylglycerols (TAG) Analyzed by nanoESI/IRMPD;** Fabrice Bray<sup>1</sup>; Maria Van Agthoven<sup>1</sup>; Lionel Chiron<sup>2,3</sup>; Marie-Aude Coutouly<sup>3</sup>; Marc-André Delsuc<sup>2</sup>; Caroline Tokarski<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>*Université Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France*; <sup>2</sup>*Université de Strasbourg, Strasbourg, France*; <sup>3</sup>*NMRTEC, Illkirch-Graffenstaden, France*

- TOA pm 3:30 **Particle-in-Cell Simulation of Image Charge in Cylindrical and Harmonized ICR Cells;** Joshua Driver<sup>1</sup>; Andriy Kharchenko<sup>1,2</sup>; Ron Heeren<sup>2</sup>; Eugene Nikolaev<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands*; <sup>3</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russia*
- TOA pm 3:50 **The Structure and the Performance of Mesh-Electrode Linear Ion Trap (MeLIT) Mass Analyzer;** Chuan-Fan Ding; Liang Wang; Fuxing Xu; *Fudan University, Shanghai, CHINA*
- TOA pm 4:10 **Intact Protein Characterization by 193 nm Ultraviolet Photodissociation in an Orbitrap Elite;** Jared B. Shaw; Jennifer S. Brodbelt; *The University of Texas, Austin, TX*

### 2:30 – 4:30 PM, TUESDAY AFTERNOON IMAGING MS: BIOLOGICAL APPLICATIONS Pierre Chaurand (University of Montreal), presiding Room L100 (lower level)

- TOB pm 2:30 **On-Tissue Micro-Extraction: The Key to Success for Identification of Less Abundant Proteins in MALDI MSI;** Jusal Quanicó<sup>1,2</sup>; Julien Franck<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Claire Dauly<sup>3</sup>; Robert Day<sup>2</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>*FABMS, Villeneuve D'Ascq, France*; <sup>2</sup>*Institute de Pharmacologie de Sherbrooke, Sherbrooke, Canada*; <sup>3</sup>*Thermo Fisher Scientific France, Paris, France*



- TOB pm 2:50 **Molecular Diagnosis of Atypical Spitzoid Neoplasms using Direct Tissue Profiling Mass Spectrometry**; Erin H. Seeley<sup>1</sup>; Rossitza Lazova<sup>2</sup>; Alireza Sepehr<sup>3</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Yale University, New Haven, CT; <sup>3</sup>Harvard Beth Israel Deaconess Medical Center, Boston, MA
- TOB pm 3:10 **Differential Molecular Profiling of Lipids and Glycans at the Tumor Margin of Clear Cell Renal Carcinoma Tissues by MALDI-MS Imaging**; Richard R Drake<sup>1</sup>; Thomas Powers<sup>1</sup>; E. Ellen Jones<sup>1</sup>; Anand Mehta<sup>2</sup>; Raymond Lance<sup>3</sup>; Dean Troyer<sup>4</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Drexel Institute for Biotechnology and Virology, Doylestown, PA; <sup>3</sup>Urology of Virginia, Norfolk, VA; <sup>4</sup>Eastern Virginia Medical School, Norfolk, VA
- TOB pm 3:30 **Development of Mass Spectrometry Imaging and LESA Techniques to Assess Region-Specific Corticosteroid Regeneration in Brain Assessed by Mass Spectrometry Imaging**; C. Logan Mackay<sup>1</sup>; Diego Cobice<sup>2</sup>; Andrew McBride<sup>2</sup>; Pat Langridge Smith<sup>1</sup>; Scott Webster<sup>2</sup>; Brian Walker<sup>2</sup>; Ruth Andrew<sup>2</sup>; <sup>1</sup>School of Chemistry, University of Edinburgh, Edinburgh, UK; <sup>2</sup>QMRI, University of Edinburgh, Edinburgh, UK
- TOB pm 3:50 **Molecular Signatures of Mouse Embryo Implantation Sites using Nanospray Desorption Electrospray Ionization Imaging Mass Spectrometry**; Ingela Lanekoff<sup>1</sup>; Kristin Burnum<sup>1</sup>; Jeeyeon Cha<sup>2</sup>; Mathew Thomas<sup>1</sup>; James Carson<sup>1</sup>; Sudhansu K Dey<sup>2</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>PNNL, Richland, WA; <sup>2</sup>Cincinnati Children's Hospital Medical Center, Cincinnati, OH
- TOB pm 4:10 **Macroscopic Imaging Mass Spectrometry: 3D Surface Mass Spectrometry of a Man and a Woman**; Christopher M Rath<sup>1,2</sup>; Mingxun Wang<sup>3</sup>; Guo Yurong<sup>1</sup>; Antonio Gonzalez Pena<sup>4</sup>; Donna Berg-Lyons<sup>4</sup>; Gail Ackermann<sup>4</sup>; Kathleen Dorrestein<sup>1</sup>; Robert Knight<sup>4</sup>; Nuno Bandeira<sup>3</sup>; Theodore Alexandrov<sup>1,5</sup>; Pieter Dorrestein<sup>1,6</sup>; <sup>1</sup>School of Pharmacy, U. California, San Diego, CA; <sup>2</sup>Current: Novartis Institute for Biomedical Res., Emeryville, CA; <sup>3</sup>Center for Computational Mass Spectrometry, UCSD, San Diego, CA; <sup>4</sup>Chemistry and Biochemistry, U. Colorado Boulder, Boulder, CO; <sup>5</sup>Center for Industrial Mathematics, U. Bremen, Bremen, Germany; <sup>6</sup>Chemistry and Biochemistry, UCSD, San Diego, CA

**2:30 – 4:30 PM, TUESDAY AFTERNOON  
CHARACTERIZATION OF  
PRODUCT VARIANTS IN BIOSIMILARS**

**Tracie Williams (Ctr for Disease Control & Prevention), presiding  
Ballroom B**

- TOC pm 2:30 **Use of Stable Isotope-Labeled Reference Standards and Antioxidants for Reliable Evaluation of Methionine Oxidation by LC-MS/MS in Therapeutic Proteins**; Pilsoo Kang<sup>1</sup>; Tanya Mezhebovsky<sup>1</sup>; Wei Chen<sup>2</sup>; James A. McCordle<sup>2</sup>; Sheng Zhang<sup>2</sup>; Eric Routhier<sup>1</sup>; Philip Sass<sup>1</sup>; <sup>1</sup>Morphotek, Exton, PA; <sup>2</sup>Cornell University, Ithaca, NY
- TOC pm 2:50 **Comparability Analysis of Anti-CD20 mAb from Commercial (MabThera) and RNAi-Mediated Fucosylation Molecules by Two Orthogonal LC-MS Approaches**; Chen Li<sup>1</sup>; Greg Thill<sup>2</sup>; Anthony Rossomando<sup>2</sup>; Shiaw-Lin Wu<sup>1</sup>; Barry Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Alnylam Pharmaceuticals, Cambridge, MA
- TOC pm 3:10 **Characterization of an IgG1 Biosimilar Candidate by High-Resolution Mass Spectrometry Methods**; Susanne Hensel; Stefanie Janzen; Gerhard Koerting; Stephanie Felske-Mueller; Andreas Wattenberg; Martin Blueggel; *Protogen Protein Services GmbH, Dortmund, Germany*
- TOC pm 3:30 **Assessing 'Scrambled' Disulfide Linkages: A Comprehensive Workflow for Routine Characterization of Biotherapeutics using High-Resolution LCMS and Electron Transfer Dissociation**; Asish Chakraborty; Stephane Houel; Henry Shion; Scott Berger; Weibin Chen; *Waters Corporation, Milford, MA*
- TOC pm 3:50 **Detailed Glycomic Characterization of Commercial Erythropoietin (EPO) Variants**; Myung Jin Oh<sup>1</sup>; Serenus Hua<sup>1</sup>; Chanyoung Han<sup>1</sup>; Ha Neul Jeong<sup>1</sup>; Gregory Staples<sup>2</sup>; Jong Shin Yoo<sup>1,3</sup>; Rudolf Grimm<sup>1,2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>Chungnam National University, Daejeon, Korea; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Korea Basic Science Institute, Ochang, Korea
- TOC pm 4:10 **LC-Fluorescence-MS/MS Assessment of Bioreactor Parameters on IgG Glycosylation**; John Schiel<sup>1</sup>; Karen Phinney<sup>1</sup>; Cyrus Agarabi<sup>2</sup>; Erik Read<sup>2</sup>; Kurt Brorson<sup>2</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>CDER, FDA, Silver Spring, MD

**2:30 – 4:30 PM, TUESDAY AFTERNOON  
PHOSPHOPROTEOMICS**

**Susan Abbatiello (Broad Inst of Harvard & MIT), presiding  
Ballroom A**

- TOD pm 2:30 **A Lower Limit on the Size of the Human Cancer Cell Line Phospho-Proteome**; Kirti Sharma; Rochelle C J D'souza; Juerger Cox; Igor Paron; Stefka Tyanova; Matthias Mann; *Max Planck Institute for Biochemistry, Martinsried (Near Munich), Germany*
- TOD pm 2:50 **LuciPHOR: A Powerful Algorithm for Phosphorylation Site Localization with False Localization Rate Estimation using Target-Decoy Approach**; Damian Fermin<sup>1</sup>; Scott Walmsley<sup>1</sup>; Anne-Claude Gingras<sup>2,3</sup>; Hyungwon Choi<sup>4</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>University of Toronto, Toronto, ON; <sup>3</sup>Samuel Lunenfeld Research Institute, Toronto, ON; <sup>4</sup>National University of Singapore, Singapore
- TOD pm 3:10 **A Novel Phosphopeptide Standard to Evaluate Data Interpretation in a Realistic Phosphoproteomic Environment**; Sonja Radau<sup>1</sup>; Marc Vaudel<sup>1</sup>; Florian Beck<sup>1</sup>; Ingo Feldmann<sup>1</sup>; Lennart Martens<sup>2</sup>; Albert Sickmann<sup>1</sup>; René Zahedi<sup>1</sup>; <sup>1</sup>Leibniz – Institut für Analytische Wissenschaften, Dortmund, Germany; <sup>2</sup>Department of Medical Protein Research, VIB, Ghent, BE
- TOD pm 3:30 **Effect of Post-Excision-Delay-to-Freezing Time on Protein Phosphorylation of Tumors: A Study by the NCI Clinical Proteomics Tumor Analysis Consortium (CPTAC)**; Philipp Mertins<sup>1</sup>; DR Mani<sup>1</sup>; Vladislav Petyuk<sup>2</sup>; Tao Liu<sup>2</sup>; Feng Yang<sup>2</sup>; Aaron Gajadhar<sup>3</sup>; Hannah Johnson<sup>3</sup>; Hui Zhang<sup>4</sup>; Douglas Levine<sup>5</sup>; Reid Townsend<sup>6</sup>; Sherri Davies<sup>8</sup>; Michael Gillette<sup>1</sup>; Kelly Ruggles<sup>7</sup>; David Fenyo<sup>7</sup>; Karl Clauser<sup>1</sup>; Jana Qiao<sup>1</sup>; Marina Gritsenko<sup>2</sup>; Shunqiang Li<sup>6</sup>; Bai Zhang<sup>4</sup>; Yuan Tian<sup>4</sup>; Ronald Moore<sup>2</sup>; Narcisco Olvera<sup>5</sup>; Fanny Dao<sup>5</sup>; Daniel Chan<sup>4</sup>; Daniel Liebler<sup>9</sup>; Karin Rodland<sup>2</sup>; Gordon Mills<sup>8</sup>; Richard Smith<sup>2</sup>; Amanda Paulovich<sup>10</sup>; Matthew Ellis<sup>6</sup>; Forest White<sup>3</sup>; Steven Carr<sup>1</sup>; NCI CPTAC Consortium<sup>11</sup>; <sup>1</sup>The Broad



## TUESDAY AFTERNOON ORAL SESSIONS

*Institute, Cambridge, MA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Massachusetts Institute of Technology, Cambridge, MA; <sup>4</sup>Johns Hopkins, Baltimore, MD; <sup>5</sup>Memorial Sloan Kettering Cancer Center, New York, NY; <sup>6</sup>Washington University, Saint Louis, MO; <sup>7</sup>New York University, New York, NY; <sup>8</sup>MD Anderson, Houston, TX; <sup>9</sup>Vanderbilt University, Nashville, TN; <sup>10</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>11</sup>National Cancer Institute, Bethesda, MD*

TOD pm 3:50 **SWATH MS Targeted Data Extraction: A Powerful Method to Resolve False Phospho-Site Assignments in Phosphopeptides;** Ludovic C. Gillet<sup>1</sup>; Alessio Maiolica<sup>1</sup>; Pedro Navarro<sup>1</sup>; Umut Toprak<sup>1</sup>; Christina Ludwig<sup>1</sup>; Ruedi Aebersold<sup>1,2</sup>; <sup>1</sup>Dept Biology, IMSB, ETH Zurich, Zurich, Switzerland; <sup>2</sup>Faculty of Science, University of Zurich, Zurich, Switzerland

TOD pm 4:10 **Investigating Kinase Targets in Neurodegeneration using Mass Spectrometry;** Donald S Kirkpatrick; Daisy Bustos; Zejuan Sheng; Shuo Zhang; Sarah Huntwork-Rodriguez; Christine Pozniak; Tracy Kleinheinz; Claire Le Pichon; Anthony Estrada; Kimberley Searce-Levie; John Moffat; Joseph Lewcock; Haitao Zhu; *Genentech, Inc., South San Francisco, CA*

### 2:30 – 4:30 PM, TUESDAY AFTERNOON FOOD SAFETY: ADVANCES IN MS FOR CHARACTERIZATION OF ADDITIVES AND CONTAMINANTS

**Adrian Hegeman (University of Minnesota), presiding  
Auditorium**

TOE pm 2:30 **Screening Large Sample Sets for Contaminants by DART-MS: Limitations & Advantages;** Luke Ackerman<sup>1</sup>; Karim Bentayeb<sup>2</sup>; Timothy Begley<sup>1</sup>; <sup>1</sup>FDA Center for Food Safety, College Park, MD; <sup>2</sup>Univ. Zaragoza, Analytical Chem, Zaragoza, Spain

TOE pm 2:50 **Mass Accuracy and Isotopic Abundance Measurements in Complex Sample Matrices: Capabilities of HR-MS Instrumentation for Non-Targeted Analyses;** Ann M. Knolhoff; Timothy R. Croley; John H. Callahan; *FDA/CFSAN, College Park, MD*

TOE pm 3:10 **Sample Class Prediction for the Determination of Off-Flavors in Cranberries by GC/MS;** Jean Francois Sylvain<sup>2</sup>; Cindy Ricard<sup>2</sup>; Stephan Baumann<sup>1</sup>; Dave Peterson<sup>1</sup>; Marcus Kim<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Atoka Cranberries Inc, Manseau (Québec), Canada

TOE pm 3:30 **On-Site Screening for Plasticizers, Melamine, and Residual Pesticides in Tainted Foods via Mobile Ambient Mass Spectrometry (MAMS);** Christopher Shiea<sup>1</sup>; Chih-Chiang Chou<sup>2</sup>; Min-Zong Huang<sup>2</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan

TOE pm 3:50 **Preventing Wine Spoilage: Rapid Screening and Quantitative Analysis of Off-flavor Phenolic Compounds by DART Mass Spectrometry;** Elizabeth Crawford<sup>1</sup>; Paola Domizio<sup>2</sup>; Brian Musselman<sup>3</sup>; Lucy Joseph<sup>4</sup>; Linda Bisson<sup>4</sup>; Bart Weimer<sup>5</sup>; Richard Jeannotte<sup>5</sup>; <sup>1</sup>Institute of Chemical Technology Prague, Prague, Czech Republic; <sup>2</sup>Università degli Studi di Firenze, Florence, Italy; <sup>3</sup>IonSense, Inc., Saugus, MA; <sup>4</sup>UC-Davis Dept. of Viticulture & Enology, Davis, CA; <sup>5</sup>UC-Davis Dept. of Health and Reproduction, Davis, CA

TOE pm 4:10 **Non-Volatile Profiling of Whiskies using UHPLC/QTOF-MS;** Thomas S. Collins<sup>1,3</sup>; Jerry Zweigenbaum<sup>2</sup>; Susan E. Ebeler<sup>1</sup>; <sup>1</sup>U.C. Davis, Davis, CA; <sup>2</sup>Agilent Technologies, Wilmington, DE; <sup>3</sup>Treasury Wine Estates, Napa, CA

### 2:30 – 4:30 PM, TUESDAY AFTERNOON ION MOBILITY: STRUCTURES

**Erin Baker (Pacific Northwest National Lab) presiding  
Room 101**

TOF pm 2:30 **Structure and Interactions of Membrane-Bound Peptides and Proteins Studied in Detergent Micelles by nano-ESI IMS-MS/MS;** Albert Konijnenberg<sup>1</sup>; Jeroen van Dyck<sup>1,3</sup>; Jens Obbels<sup>1</sup>; Frederik Lermyte<sup>1</sup>; Frank Sobott<sup>1,2</sup>; <sup>1</sup>Biomolecular Mass Spec., University of Antwerp, Antwerpen, Belgium; <sup>2</sup>Center for Proteomics, University of Antwerp, Antwerpen, Belgium; <sup>3</sup>Radboud University, Nijmegen, The Netherlands

TOF pm 2:50 **MS-based Investigation of Tertiary and Quaternary Interactions in the 5'-Untranslated Region of HIV-1 Genomic RNA;** Daniele Fabris; Papa-Nii Asare Okai; Jennifer Lippens; Maria Basanta Sanchez; Matteo Scalabrin; *The RNA Institute, University at Albany, Albany, NY*

TOF pm 3:10 **Structural Mass Spectrometry to Interrogate Microbial Metabolomes for Natural Product Prioritization;** Cody Goodwin<sup>1</sup>; Dagmara Derewacz<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Brian Bachmann<sup>1</sup>; John McLean<sup>1</sup>; <sup>1</sup>Vanderbilt Univ Dept of Chem, Nashville, TN; <sup>2</sup>Agilent Technologies, Santa Clara, CA

TOF pm 3:30 **Application of Ion Mobility Mass Spectrometry to Analysis of Biological Samples;** Qi Wang<sup>1</sup>; Kshitij Khatari<sup>1</sup>; Ying Zhou<sup>1</sup>; Crystal Cody<sup>2</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Erin Baker<sup>3</sup>; Joseph Zaia<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA

TOF pm 3:50 **Do Electrosprayed Protein Ions Retain Memory of their Solution Phase Structure? Insights from Ion Mobility Mass Spectrometry;** Siavash Vahidi; Bradley B. Stocks; Lars Konermann; *Univ. of Western Ontario, London, Canada*

TOF pm 4:10 **Collision Cross Sections: The Effects of Size, Shape and Bath Gas;** Michael T. Bowers; Christian Bleiholder; Thomas Wytenbach; *University of California, Santa Barbara, CA*

### 2:30 – 4:30 PM, TUESDAY AFTERNOON METABOLITES: UNUSUAL AND UNCOMMON Paul Thomas (Northwestern University), presiding Room 102

TOG pm 2:30 **Network Based Discovery of Known Unknowns;** Laura Sanchez<sup>1</sup>; Jane Yang<sup>1</sup>; Chris Rath<sup>1</sup>; Paul Boudreau<sup>2</sup>; Xueting Liu<sup>1</sup>; Nicole Bruns<sup>2</sup>; Anne Wodtke<sup>2</sup>; Rafael de Felicio<sup>2</sup>; Amanda Fenner<sup>2</sup>; Evgenia Glukhov<sup>2</sup>; William Gerwick<sup>2</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Scripps Institution of Oceanography, La Jolla, CA

TOG pm 2:50 **The World of Acylpolyamines, Beta Carbolines, and Biogenic Amines: Understanding the Diversity of Spider Venoms through LC-IT-TOF Mass Spectrometry;** Daniel Menezes Saidenberg<sup>1</sup>; Nicolí Barão Baptista Saidenberg<sup>2</sup>; Mario Sergio Palma<sup>3</sup>; <sup>1</sup>Shimadzu do Brasil, São Paulo/SP, BRAZIL;

<sup>2</sup>Endocrine Pancreas Laboratory/IB/UNICAMP, Campinas/SP, Brazil; <sup>3</sup>LBEZ/CEIS/IB/UNESP, Rio Claro/SP, Brazil

TOG pm 3:10 **Integrated Metabolomics Approach Enables Discovery of Novel Natural Products from *Streptomyces coelicolor* A3(2)**; Erin Carlson; Indiana University, Bloomington, IN

TOG pm 3:30 **Identification of Imidacloprid Metabolites in Onion using High Resolution Mass Spectrometry and Accurate Mass Tools**; Jerry Zweigenbaum<sup>1</sup>; Michael Thurman<sup>2</sup>; Imma Ferrer<sup>2</sup>; Paul Zavitsanos<sup>1</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>University of Colorado, Boulder, Co

TOG pm 3:50 **Effective Detection and Structural Characterization of Uncommon Drug Metabolites using High Resolution Mass Spectrometry and Real-Time Polarity-Switching**; Qian Ruan; Mingshe Zhu; Bristol-Myers Squibb, Princeton, NJ

TOG pm 4:10 **Automated Structure Elucidation of Unknown Metabolites In Metabolomics and Pharmaceutical Studies using the Masspec Algorithm and Tandem Mass Spectral Data**; Marshall M. Siegel; Gary Walker; MS Mass Spec Consultants, Fair Lawn, NJ

#### 2:30 – 4:30 PM, TUESDAY AFTERNOON

#### MICROORGANISMS: IDENTIFICATION AND CHARACTERIZATION Franco Basile (University of Wyoming), presiding Room 103

TOH pm 2:30 **Specialized Metabolite Discovery in Microorganisms through Visualization of Living Metabolomes using Live-Colony Mass Spectrometry and Molecular Networking**; Jeramie Watrous<sup>1</sup>; Paul Boudreau<sup>2</sup>; Mingxun Wang<sup>1</sup>; Menno vander Voort<sup>3</sup>; George Dimopoulos<sup>4</sup>; Nuno Bandeira<sup>1</sup>; William Gerwick<sup>2</sup>; Pieter Dorrestein<sup>1,2</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Scripps Institute of Oceanography, La Jolla, CA; <sup>3</sup>Wageningen University, Wageningen, Netherlands; <sup>4</sup>Johns Hopkins University, Baltimore, MD

TOH pm 2:50 **Applications of an *in situ* Microextraction Based Surface Sampling System to Microorganism Analysis**; Mariam S Elnaggar<sup>1</sup>; Cheng-Chih Hsu<sup>2</sup>; Xueting Liu<sup>3</sup>; Pieter Dorrestein<sup>2</sup>; Bartek Rajwa<sup>4</sup>; Justin Wiseman<sup>1</sup>; <sup>1</sup>Prosoia, Inc., Indianapolis, IN; <sup>2</sup>University of California, San Diego, CA; <sup>3</sup>Inst. of Microbiology, Chinese Academy of Sciences, Peking, China; <sup>4</sup>Purdue University, Lafayette, IN

TOH pm 3:10 **Identification of Bacteria Using Rapid Evaporative Ionization Mass Spectrometry**; Nicole Strittmatter; Emrys A. Jones; Monica Rebec; Zoltan Takats; Imperial College London, London, UK

TOH pm 3:30 **Rapid Identification of Intact Biothreat Viruses using MALDI Mass Spectrometry**; Lisa H. Cazares<sup>1</sup>; Julie Constantino<sup>2</sup>; Rekha Panchal<sup>2</sup>; Sina Bavari<sup>2</sup>; <sup>1</sup>Geneva Foundation/USAMRIID, Frederick, MD; <sup>2</sup>USAMRIID, Ft. Detrick, MD

TOH pm 3:50 **Combination of Intact Cell Immunocapture and Multiplexed SRM Mass Spectrometry for the Sensitive and Specific Detection of *Yersinia Pestis***; Jérôme Chénau<sup>1,2</sup>; Stéphanie Simon<sup>1</sup>; Sofia Filali<sup>2</sup>; François Fenaille<sup>1</sup>; Hervé Volland<sup>1</sup>; Christophe Junot<sup>1</sup>; Elisabeth Carniel<sup>2</sup>; François Becher<sup>1</sup>; <sup>1</sup>CEA, DSV/iBiTec-S/SPI, Gif Sur Yvette Cedex, France; <sup>2</sup>Institut Pasteur, Unité de recherche *Yersinia*, Paris, France

TOH pm 4:10 **Development and Application of Assays for Targeted MS Analysis of the Complete Proteome of *Mycobacterium tuberculosis* by SRM and SWATH-MS**; Olga Schubert<sup>1</sup>; Christina Ludwig<sup>1</sup>; Jeppe Mouritsen<sup>1</sup>; Hannes Roest<sup>1</sup>; George Rosenberger<sup>1</sup>; Patrick Arthur<sup>2</sup>; Manfred Claassen<sup>1</sup>; Dave Campbell<sup>3</sup>; Zhi Sun<sup>3</sup>; Terry Farrah<sup>3</sup>; Martin Gengenbacher<sup>4</sup>; Stefan H. E. Kaufmann<sup>4</sup>; Robert Moritz<sup>3</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>University of Ghana, Accra, Ghana; <sup>3</sup>Institute for Systems Biology, Seattle, WA; <sup>4</sup>Max Planck Institute for Infection Biology, Berlin, Germany

#### 4:45 - 5:30 PM, TUESDAY

#### AWARD LECTURE

Susan T. Weintraub (Univ of Texas HSC-San Antonio), presiding  
Exhibit Hall A, Lower Level



Biemann Medal

Yinsheng Wang  
University of California, Riverside

#### 5:45 - 7:00 PM, TUESDAY AFTERNOON WORKSHOPS

Light snacks are provided on level two.

#### LEVEL ONE ROOMS

- Environmental Applications of FTMS: Earth, Air & Water (organized by the FTMS Interest Group), Room 1
- Jumpstarting Your Career: a Career Development Workshop (organized by the Young Mass Spectrometrists Interest Group), Room 2
- The Galaxy Framework as a Solution for MS-based Informatics, Room 3

#### LEVEL TWO ROOMS

- LC-MS in the Clinical Lab: How Close is 24/7? (organized by the Clinical Chemistry Interest Group), Room 200 DE
- Normalization Approaches to Imaging Mass Spectral Data (organized by the Imaging MS Interest Group), Room 200 FG
- How to Work with your P.I.s More Effectively (and Without Them Knowing It) (organized by the Analytical Lab Managers Interest Group), Room 200 H
- Current Topics in Metal Ion Chemistry (organized by the Metal Ion Coordination Chemistry Interest Group), Room 200 I
- Ion Mobility MS: New Instrumentation & Enabling Technologies (organized by the Ion Mobility MS Interest Group), Room 205 AB
- Quantitative Intact Proteomics (organized by the Quantitative Intact Proteomics Interest Group), Room 205 CD
- Large Molecule by LC-MS Bioanalytical Method Validation (BMV): Status, Challenges, Solutions, Recommendations (organized by the Regulated Bioanalysis Interest Group), Room 208 AB
- Practical ETD, Room 208 CD

AFTER 8:00 PM  
CORPORATE HOSPITALITY SUITES  
HILTON MINNEAPOLIS HOTEL



**8:30 – 10:30 AM, WEDNESDAY MORNING  
PTMs: ADVANCES IN ISOLATION,  
DERIVATIZATION AND SEPARATION  
Laszlo Prokai (University of North Texas), presiding  
Exhibit Hall A (lower level)**

- WOA am 08:30 **Tyrosine-Selective Phosphopeptide Enrichment by Chemical and Immuno-Affinity Approaches;** Shigeharu Yoshida; Mayu Ogura; Masaki Wakabayashi; Naoyuki Sugiyama; Yasushi Ishihama; *Kyoto University, Kyoto, Japan*
- WOA am 08:50 **A General Strategy for Enrichment, Site-Specific Identification, and Quantification of Multiple Types of Redox Modifications on Protein Thiols;** Jia Guo; Dian Su; Matthew Gaffrey; Yi Qu; Anil Shukla; Ronald Moore; Brian Thrall; Richard Smith; Weijun Qian; *Pacific Northwest National Lab, Richland, WA*
- WOA am 09:10 **Reductive Methylation of Ubl Isopeptides (RUBl): An Elegant Method for the Enhanced Detection of SUMO and Ubiquitin Modified Peptides;** Navin Chicooree<sup>1,2</sup>; Yvonne Connolly<sup>1</sup>; Duncan Smith<sup>1</sup>; John Griffiths<sup>1</sup>; <sup>1</sup>*Paterson Institute for Cancer Research, Manchester, UK*; <sup>2</sup>*School of Chemistry, University of Manchester, Manchester, UK*
- WOA am 09:30 **Improved Enrichment of S-Nitrosylated Peptides using Iodoacetyl Tandem Mass Tag Reagents, Immobilized Anti-TMT Antibody Resin and TMT Elution Buffer;** Ryan Bomgarden<sup>1</sup>; Zhe Qu<sup>3</sup>; Eric Hommema<sup>1</sup>; Rosa Viner<sup>2</sup>; Zezong Gu<sup>3</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>*ThermoFisher Scientific, Rockford, IL*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*University of Missouri, Columbia, MO*
- WOA am 09:50 **Evaluation of a Novel Tandem Mass Tag for Profiling of Protein Carbonylation;** Somi Afuni<sup>1</sup>; Sergei I. Snovida<sup>2</sup>; Ryan D. Bomgarden<sup>2</sup>; John C. Rogers<sup>2</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*Thermo Fisher Scientific, Rockford, IL*
- WOA am 10:10 **Serial Enrichment of Post-Translationally Modified Peptides Enables Deep and Quantitative Analysis of the Proteome, Phosphoproteome, Ubiquitinome, and Acetylome;** Jana Qiao; Philipp Mertins; Jinal Patel; Karl Clauser; DR Mani; Michael Burgess; Michael Gillette; Jacob Jaffe; Steven Carr; *Broad Institute, Cambridge, MA*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
INFORMATICS: PROTEIN QUANTIFICATION  
Brian Searle (Proteome Software, Inc.), presiding  
Room L100 (lower level)**

- WOB am 08:30 **Slice: Scalable Data Sharing for Remote Mass Informatics;** Manor Askenazi<sup>1</sup>; David Fenyo<sup>2</sup>; <sup>1</sup>*The Ionomix Initiative, Arlington, MA*; <sup>2</sup>*NYU Langone Medical Center, New York City, NY*
- WOB am 08:50 **IldpQuantify : Combining Precursor Intensity with Spectral Counts for Protein and Peptide Quantification;** Yao-Yi Chen<sup>1</sup>; Matthew Chambers<sup>1</sup>; Amy-Joan Ham<sup>2</sup>; Ming Li<sup>1</sup>; David Tabb<sup>1</sup>; <sup>1</sup>*Vanderbilt University Medical School, Nashville, TN*; <sup>2</sup>*Belmont University College of Pharmacy, Nashville, TN*
- WOB am 09:10 **Avoiding Arbitrary Parameters in Quantitative Proteomics: Is “Differential” a 1.1-Fold or 1.2-Fold Change?** Oliver Serang; Ertugrul Cansizoglu; Hanno Steen; Judith Steen; *Harvard Medical School/ Boston Children's Hospital, Boston, MA*

- WOB am 09:30 **Electrospray Current Fluctuations and other Instrumental Response Instabilities –*In silico* Correction Method Improves Precision of Label-free Proteomics Quantification;** Yaroslav Lyutvinskiy<sup>1</sup>; Hongqian Yang<sup>1</sup>; Dorothea Rutishauser<sup>1</sup>; Roman Zubarev<sup>1,2</sup>; <sup>1</sup>*Karolinska Institutet, MBB, Stockholm, Sweden*; <sup>2</sup>*Science for Life Laboratory, Stockholm, Sweden*
- WOB am 09:50 **Pre- and Postprocessing Steps in Affinity Purification Mass Spectrometry Data – More Reliable Detection of Interaction Candidates;** Martina Fischer<sup>1</sup>; Susann Zilkenat<sup>2</sup>; Samuel Wagner<sup>2,3</sup>; Bernhard Y Renard<sup>1</sup>; <sup>1</sup>*Robert-Koch-Institute, Berlin, Germany*; <sup>2</sup>*IMIT, Eberhard Karls University Tübingen, Tübingen, Germany*; <sup>3</sup>*German Center for Infection Research (DZIF), Tübingen, Germany*
- WOB am 10:10 **Statistical Selection of Informative Features for Protein Quantification in Data-Independent Spectral Acquisition;** Ching-Yun Chang<sup>1</sup>; Nathalie Selevsek<sup>2</sup>; Ludovic Gillet<sup>2</sup>; Hannes Roest<sup>2</sup>; Ruedi Aebersold<sup>2,3</sup>; Olga Vitek<sup>1,4</sup>; <sup>1</sup>*Department of Statistics, Purdue University, West Lafayette, IN*; <sup>2</sup>*IMSB, ETH, Zürich, Switzerland*; <sup>3</sup>*Faculty of Science, University of Zürich, Zürich, Switzerland*; <sup>4</sup>*Department of Computer Science, Purdue University, West Lafayette, IN*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
CARBOHYDRATES: NEW MS APPROACHES  
Yehia Mechref (Texas Tech University), presiding  
Ballroom B**

- WOC am 08:30 **Obtaining Linkage Information from Linear Oligosaccharides via MS<sup>n</sup> (>2) and Z<sub>1</sub> Ions;** Chiharu Konda<sup>1</sup>; Brad Bendiak<sup>2</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of Colorado Denver, Aurora, CO*
- WOC am 08:50 **Trivalent Metal-Assisted Electron Capture Dissociation and Electron Transfer Dissociation of Underivatized Glycans;** Di Gao; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WOC am 09:10 **Glycan Structural Analysis on the LC Time Scale Employing Electron Activated Dissociation (ExD) Methods;** Cheng Lin; Xiang Yu; Yan Jiang; Yu Huang; Joseph Zaia; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- WOC am 09:30 **Semi-Automated Sequencing Of Affinity-Purified Heparan Sulfate Oligosaccharides;** Rongrong Huang; Eduard Condac; Yulun Chiu; Christian Heiss; Mayumi Ishihara; Muchena J. Kailemia; Jon Amster; Parastoo Azadi; Lianchun Wang; Joshua S. Sharp; *University of Georgia, Athens, GA*
- WOC am 09:50 **Use of Field Asymmetrical Ion Mobility Spectrometry (FAIMS) and Tandem Mass Spectrometry for Structural Characterization of Isobaric Mixtures of Glycosaminoglycans;** Muchena Kailemia<sup>1</sup>; Yuejie Zhao<sup>1</sup>; Isaac Agyekum<sup>1</sup>; Andre Venot<sup>1</sup>; Melvin Park<sup>2</sup>; Desmond Kaplan<sup>2</sup>; Geert-Jan Boons<sup>1</sup>; Robert Linhardt<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*; <sup>3</sup>*Rensselaer Polytechnic Institute, Troy, NY*
- WOC am 10:10 **Production of a <sup>13</sup>C-Labeled Internal Standard for Quantitative Glycomics;** Evelyn Rampler<sup>1</sup>; Shujuan Tao<sup>2</sup>; Stephan Hann<sup>1</sup>; Friedrich Altmann<sup>1</sup>; Ron Orlando<sup>2</sup>; Gunda Koellensperger<sup>1</sup>; <sup>1</sup>*University Boku Vienna, Vienna, Austria*; <sup>2</sup>*University of Georgia, Athens, GA*



**8:30 – 10:30 AM, WEDNESDAY MORNING  
QUANTITATIVE ANALYSIS BY MS IN DRUG DISCOVERY AND  
DEVELOPMENT: NOVEL APPROACHES**  
**Jim Shen (Bristol-Myers Squibb), presiding**  
**Ballroom A**

- WOD am 08:30 **A New Twist on an Old Experiment: Leveraging Automation and LC-MS/MS to Understand and Reduce Variability in Plasma Protein Binding;** Lucinda Cohen<sup>1</sup>; Haiping Wang<sup>1</sup>; Matt Zrada<sup>2</sup>; Ken Anderson<sup>2</sup>; Ravi Katwaru<sup>1</sup>; Xinchun Tong<sup>1</sup>; Bernard Choi<sup>1</sup>; Paul Harradine<sup>1</sup>; Vince Tong<sup>1</sup>; Natasa Pajkovic<sup>2</sup>; Kathy Cox<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Rahway, NJ; <sup>2</sup>Merck & Co., Inc, West Point, PA
- WOD am 08:50 **Using 13C and 15N Isotopomer Metabolic Flux via Glucose and Glutamine to Understand Cancer's Metabolic Dependencies by SRM-LC-MS/MS;** Susanne Breitkopf<sup>1,2</sup>; Min Yuan<sup>1</sup>; Costas Lyssiotis<sup>1,2</sup>; John M Asara<sup>1,2</sup>; <sup>1</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- WOD am 09:10 **PaperSpray Technology for Quantitative Analysis: Applications in Research and Regulated Bioanalysis;** Jennifer Cunliffe<sup>1</sup>; Luis Ramos<sup>1</sup>; Ann Brown<sup>2</sup>; Shawn Harriman<sup>2</sup>; Michael Hayes<sup>1</sup>; Jakal Amin<sup>2</sup>; Jimmy Flarakos<sup>1</sup>; <sup>1</sup>Novartis DMPK, East Hanover, NJ; <sup>2</sup>Novartis MAP, Cambridge, MA
- WOD am 09:30 **Strategies for the Quantitation of Nucleotides in Human Plasma using Novel Ion-Pair Hydrophilic Interaction Chromatography Coupled with Tandem Mass Spectrometry;** Guodong Zhang; Annie Walker; Zhaosheng Lin; Xiaogang Han; Matthew Blatnik; Rick Steenwyk; Elizabeth Groeber; Pfizer Inc., Groton, CT
- WOD am 09:50 **Optimization of a High-Throughput Metabolic Soft Spot Assay with Pooled Sample Analysis and Software-Assisted Structure Elucidation;** Anthony Paiva; Cheryl Klakouski; Tatyana Zvyaga; Benjamin Johnson; Jonathan Josephs; W. Griffith Humphreys; Harold Weller; Wilson Shou; Bristol-Myers Squibb Company, Wallingford, CT
- WOD am 10:10 **New Quadratic Calibration Approaches for LC-MS Bioanalysis: Impact of Calibrator Concentrations and Their Distribution on Accuracy of Quadratic Regression;** Aimin Tan; Kayode Awaieye; Fethi Trabelsi; BioPharma Services Inc., Toronto, Canada

**8:30 – 10:30 AM, WEDNESDAY MORNING  
INSTRUMENTATION: NEW DEVELOPMENTS IN HIGH  
RESOLUTION AND MASS ACCURACY**  
**Steve Patrie (UT Southwestern Medical Center), presiding**  
**Auditorium**

- WOF am 08:30 **The Way to Isotopic Resolution of Mega Dalton Protein Mass Spectra for Top-Down Proteomics;** Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia
- WOF am 08:50 **Accelerating High Resolution Mass Spectrometry by Advanced Signal Processing and Allied Technique Development;** Yury O. Tsybin<sup>1</sup>; Tagir Aushev<sup>2</sup>; Luca Fornelli<sup>1</sup>; Kristina Srzentić<sup>1</sup>; Konstantin O. Zhurov<sup>1</sup>; Ünige A. Laskay<sup>1</sup>; Philippe Dugourd<sup>3</sup>; Jérôme Lemoine<sup>3</sup>; Anton N. Kozhinov<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Federale, Lausanne, Switzerland; <sup>2</sup>Institute for Theoretical and Experimental Physics, Moscow, Russia; <sup>3</sup>Université Lyon 1, Villeurbanne, France

- WOF am 09:10 **Autophaser GA – Absorption Mode Spectra for All;** David Kilgour; Rebecca Wills; Yulin Qi; Peter O'Connor; Warwick University, Coventry, UK
- WOF am 09:30 **Measurement of Intact Proteins under Non-Denaturing Conditions with nLC-MS Technique on an Orbitrap Instrument;** Olaf Scheibner<sup>1</sup>; Michael Trnka<sup>2</sup>; Shenheng Guan<sup>2</sup>; Alma Burlingame<sup>2</sup>; Phillip Robinson<sup>3</sup>; Roger Kornberg<sup>3</sup>; Eugen Damoc<sup>1</sup>; Eduard Denisov<sup>1</sup>; Maciej Bromirski<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>2</sup>University of California, San Francisco, CA; <sup>3</sup>Stanford University School of Medicine, Stanford, CA
- WOF am 09:50 **27-Plex Protein Quantification using Neutron-Encoded Chemical Tags, Resolution in Excess of One Million, and a New Hybrid Orbitrap Mass Spectrometer;** Alexander S. Hebert<sup>1</sup>; Anna E. Merrill<sup>1</sup>; Christopher M. Rose<sup>1</sup>; Derek J. Bailey<sup>1</sup>; Jonathan A. Stefely<sup>1</sup>; David J. Pagliarini<sup>1</sup>; Jesse Canterbury<sup>2,3</sup>; Vlad Zabrouskov<sup>2,3</sup>; Michael Senko<sup>2,3</sup>; Eduard Denisov<sup>2,3</sup>; Alexander Makarov<sup>2,3</sup>; Michael S. Westphall<sup>1</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany
- WOF am 10:10 **High Density, High Resolution MS Scans Dramatically Boost the Number of Precursors Identifiable and Quantifiable at the MS Level;** Annette Michalski; Nagarjuna Nagaraj; Juergen Cox; Matthias Mann; MPI of Biochemistry, Martinsried, Germany

**8:30 – 10:30 AM, WEDNESDAY MORNING  
EMERGING ENVIRONMENTAL CONTAMINANTS**  
**Kerry Peru (Environment Canada), presiding**  
**Room 101**

- WOF am 08:30 **Organic Components in a Wildfire-Applied Fire Retardant by Positive And Negative Electrospray Ionization High Resolution Mass Spectrometry;** Colleen Rostad<sup>1</sup>; Edward Furlong<sup>2</sup>; <sup>1</sup>USGS, WRD, National Research Program, Denver, CO; <sup>2</sup>USGS, NWQL, Methods Research & Development Program, Denver, CO
- WOF am 08:50 **Mass Spectrometry Characterization and Determination of Emerging Disinfection Byproducts in Swimming Pools;** Xing-Fang Li; Wei Wang; Yichao Qian; Jessica Boyd; Rongfu Huang; University of Alberta, Edmonton, Canada
- WOF am 09:10 **Integrating Comprehensive Two-Dimensional Gas Chromatography, (Ultra)High Resolution Mass Spectrometry and Mass Defect Analysis for the Identification of Halogenated Environmental Contaminants;** Karl J Jobst<sup>1</sup>; Eric J Reiner<sup>1</sup>; Vince Y Taguchi<sup>1</sup>; Trudy Watson-Leung<sup>1</sup>; Dave Poirier<sup>1</sup>; Dave Alonso<sup>2</sup>; Joe Binkley<sup>2</sup>; Lorne Fell<sup>2</sup>; <sup>1</sup>Ontario Ministry of the Environment, Toronto, Canada; <sup>2</sup>LECO Corporation, St. Joseph, MI
- WOF am 09:30 **Exact Mass Screening of 1024 Pharmaceuticals in Wastewater Samples using QExactive Mass Spectrometer;** Heinz Singer; Annika Woessner; Christa McArdell; Kathrin Fenner; Eawag - Swiss Federal Institute of Aquatic Science, Duebendorf, Switzerland
- WOF am 09:50 **Large Volume Injection of 900 µL Landfill Leachate Extracts for Fluorochemicals Analysis by Orthogonal Diol/C18 HPLC-MS/MS;** Mckay Alled<sup>1</sup>; Johnsie Lang<sup>2</sup>; Morton Barlaz<sup>2</sup>; Jennifer Field<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>North Carolina State University, Raleigh, NC

## WEDNESDAY MORNING ORAL SESSIONS

WOF am 10:10 **Are the Results of Non-Target Screening for Water Contaminants Very Surprising?** Christian Zwiener; Marco Zedda; Christina Schmalz; *University of Tuebingen, Tuebingen, Germany*

### 8:30 – 10:30 AM, WEDNESDAY MORNING FUNDAMENTALS: ION SPECTROSCOPY (HONORING ROB DUNBAR'S 70<sup>TH</sup> BIRTHDAY)

**Peter Armentrout (University of Utah), presiding  
Room 102**

WOG am 08:30 **HisGly as a Model for Metal-Ion Binding to Peptides**; Robert C. Dunbar<sup>1</sup>; Jos Oomens<sup>2</sup>; Giel Berden<sup>2</sup>; Justin Kai-Chi Lau<sup>3</sup>; Udo H. Verkerk<sup>3</sup>; Alan C. Hopkinson<sup>3</sup>; K. W. Michael Siu<sup>3</sup>; <sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>Radboud University, Nijmegen, Netherlands; <sup>3</sup>York University, Toronto, Canada

WOG am 08:50 **Infrared Spectroscopy of Anionic Polyaromatic Hydrocarbons**; Juehan Gao<sup>2</sup>; Giel Berden<sup>1,2</sup>; Jos Oomens<sup>1,2</sup>; <sup>1</sup>FOM Rijnhuizen, Nieuwegein, Netherlands; <sup>2</sup>Radboud University Nijmegen, Nijmegen, Netherlands

WOG am 09:10 **Polycyclic Aromatic Hydrocarbon Fragment Ions Studied with an FTICR Mass Spectrometer Coupled to FELICE**; Annemieke Pettrignani<sup>1,2</sup>; A.F.G. van der Meer<sup>1</sup>; Britta Redlich<sup>1</sup>; A.G.G.M. Tielens<sup>2</sup>; Martin Vala<sup>4</sup>; John R. Eyler<sup>4</sup>; Jos Oomens<sup>1,3</sup>; <sup>1</sup>FOM Rijnhuizen, Nieuwegein, The Netherlands; <sup>2</sup>Leiden Observatory, Leiden University, Leiden, The Netherlands; <sup>3</sup>IMM, Radboud University, Nijmegen, The Netherlands; <sup>4</sup>University of Florida, Gainesville, FL

WOG am 09:30 **Cold Ion Spectroscopy for Structural Determination of Peptides and Proteins**; Oleg V. Boyarkine; Natalia S. Nagornova; Thomas R. Rizzo; Vladimir Kopysov; *EPFL, Lausanne, Switzerland*

WOG am 09:50 **IRMPD Spectroscopy: When Does It Reveal What's Present?** Jacob Schmidt; Steven Kass; *University of Minnesota, Minneapolis, MN*

WOG am 10:10 **UV Spectroscopy on a Model Hydrogen Storage Cluster, [Ag<sub>3</sub>H<sub>2</sub>(Ph<sub>3</sub>P)<sub>2</sub>CH<sub>2</sub>]<sup>+</sup>**; Richard A. J. O'Hair<sup>1</sup>; Athanasios Zavras<sup>1</sup>; George Khairallah<sup>1</sup>; Marion Girod<sup>2,3</sup>; Rodolphe Antoine<sup>2,4</sup>; Philippe Dugourd<sup>2,4</sup>; Luke MacAleese<sup>2,4</sup>; Marjan Krstić<sup>5</sup>; Vlasta Bonačić-Koutecký<sup>5,6</sup>; <sup>1</sup>University of Melbourne, Victoria, Australia; <sup>2</sup>Université Lyon 1, Lyon, France; <sup>3</sup>Institut des Sciences Analytiques, Lyon, France; <sup>4</sup>Institut Lumière Matière, Lyon, France; <sup>5</sup>University of Split, Split, Croatia; <sup>6</sup>Humboldt-Universität Berlin, Institut für Chemie, Berlin, Germany

### 8:30 – 10:30 AM, WEDNESDAY MORNING H/D EXCHANGE: BIOLOGICAL APPLICATIONS Thomas Jorgensen (Univ of Southern Denmark), presiding Room 103

WOH am 08:30 **The Influence of Adnectin on the Extracellular Domain of Epidermal Growth Factor Receptor as Measured by Hydrogen/Deuterium Exchange Mass Spectrometry**; Roxana E. Jacob<sup>1</sup>; Guodong Chen<sup>2</sup>; Hui Wei<sup>2</sup>; Jingjie Mo<sup>2</sup>; Daniel Cohen<sup>2</sup>; Dianlin Xie<sup>2</sup>; Zheng Lin<sup>2</sup>; Paul Morin<sup>2</sup>; Michael Doyle<sup>2</sup>; Adrienne A. Tymiak<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Bristol-Myers Squibb Company, Princeton, NJ

WOH am 08:50 **Effector Binding Causes Major Changes in the Structure and Dynamics of the ClpP Protease Complex: A HDX/MS Investigation**; Modupeola Sowole<sup>1</sup>; John Alexopoulos<sup>2</sup>; Joaquin Ortega<sup>2</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Canada; <sup>2</sup>McMaster University, Hamilton, ON, Canada

WOH am 09:10 **Epitope-Distal Effects Accompany the Binding of Two Distinct Antibodies to Hepatitis B Virus Capsids**; Jessica Bereszczak<sup>1</sup>; Rebecca Rose<sup>1</sup>; Esther van Duijn<sup>1</sup>; Norman Watts<sup>2</sup>; Paul Wingfield<sup>2</sup>; Alasdair Steven<sup>2</sup>; Albert Heck<sup>1</sup>; <sup>1</sup>Biomolecular Mass Spectrometry and Proteomics, Utrecht, The Netherlands; <sup>2</sup>National Institutes of Health, Bethesda, MD

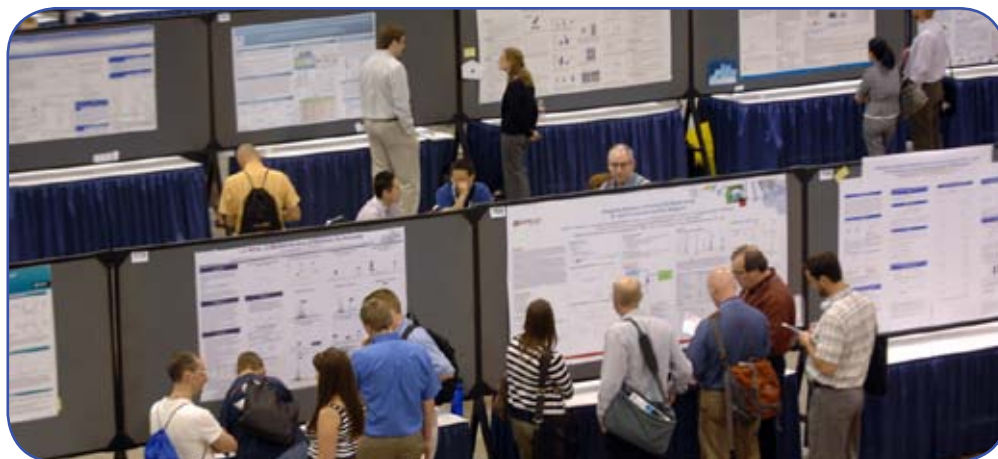
WOH am 09:30 **Characterization of Residual Structure in the Native and Amyloidogenic Tau**; Shaolong Zhu; Tamanna Rob; Derek Wilson; *York University, Toronto, Canada*

WOH am 09:50 **Rational Design of Novel Insulin Sensitizers Guided with HDX**; David Marciano; Scott Novick; Bruce Pascal; Michael Chalmers; Theodore Kamenecka; Patrick Griffin; *The Scripps Research Institute, Jupiter, FL*

WOH am 10:10 **Higher-Order Structure Characterization of a Fusion Protein Biopharmaceutical by Hydrogen/Deuterium Exchange Mass Spectrometry**; George M. Bou-Assaf; Steven A. Berkowitz; *Protein Pharmaceutical Development, Biogen Idec, Cambridge, MA*

### 10:30 AM - 2:30 PM WEDNESDAY POSTER SESSION Exhibit Hall BC

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



**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
FORENSIC APPLICATIONS**  
**Mary Satterfield (NIST), presiding**  
**Exhibit Hall A (lower level)**

- WOA pm 2:30 **Development and Validation of a Liquid-Chromatography-High Resolution Mass Spectrometry Method for the Simultaneous Analysis of 28 Synthetic Cathinones in Urine;** Sebastien Anizan; Kayla Ellefsen; Marta Concheiro-Guisan; Marilyn A. Huestis; *Chemistry and Drug Metabolism, NIDA / NIH, Baltimore, MD*
- WOA pm 2:50 **Differentiation of African and Brazilian Mahogany Wood based on the Chemical Profile of Methanolic Extractives by Electrospray Ionization Mass Spectrometry;** Maira Fasciotti<sup>1</sup>; Rodrigo Leal<sup>1</sup>; Valnei Cunha<sup>1</sup>; Romeu Daroda<sup>1</sup>; Rosana Alberici<sup>1,2</sup>; Marcos Eberlin<sup>2</sup>; *<sup>1</sup>inmetro, Duque De Caxias, Brazil; <sup>2</sup>University of Campinas, Campinas, Brazil*
- WOA pm 3:10 **Analysis of Propofol (2,6-Diisopropylphenol) and Its Metabolites in One Injection using a Dual Ionization Source;** Adrian Taylor<sup>1</sup>; Larry Campbell<sup>1</sup>; Carmai Seto<sup>1</sup>; Oscar Cabrices<sup>2</sup>; Takeo Sakuma<sup>1</sup>; *<sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>Gerstel Inc, Linthicum, MD*
- WOA pm 3:30 **Development of Species Specific Dating Technique for Human Bone with Minimal Sample Consumption;** Christopher Rollman; Mehdi Moini; *Smithsonian Institution, Suitland, MD*
- WOA pm 3:50 **Identification of Non-Synonymous Single Nucleotide Polymorphisms (nsSNPs) in Hair Shaft Protein and Utilization to Obtain Measures of Identity;** Tami Leppert<sup>1</sup>; Krishna Parsawar<sup>1</sup>; Jonathan Hilmer<sup>2</sup>; Lisa Baird<sup>1</sup>; Brandon Hanberg<sup>3</sup>; Jacquie Howard<sup>3</sup>; Chad Nelson<sup>1</sup>; Brian Bothner<sup>2</sup>; Mark Leppert<sup>1</sup>; Glendon Parker<sup>3</sup>; *<sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>Montana State University, Bozeman, MT; <sup>3</sup>Utah Valley University, Orem, UT*
- WOA pm 4:10 **LC-MS/MS Analysis of Opioids in Urine: Evaluation of LC-MS/MS Conditions for Interferences Due to Oxycodone Metabolites;** Marc Rumpfer; Lindsay Bazydlo; Bruce Goldberger; Timothy Garrett; *University of Florida, Gainesville, FL*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
PRINCIPLES OF PROTEIN IDENTIFICATION AND  
CHARACTERIZATION**  
**Neil Kelleher (Northwestern University), presiding**  
**Room L100 (lower level)**

- WOB pm 2:30 **The Utility of Prior Information such as GPMdb Frequency and RNAseq Transcript Abundance for Improved Protein Identification in Shotgun Proteomics;** Avinash Shanmugam; Anastasia K. Yocum; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- WOB pm 2:50 **CPTAC Proteogenomics : Proteogenomics Analysis of Cancer MS/MS Spectra by Peptide Level Identification of Genomic Mutations Expressed in RNA-Seq Data;** Sunghye Woo; Seong Won Cha; Vineet Bafna; *UCSD, San Diego, CA*
- WOB pm 3:10 **Discovery and Mass Spectrometric Analysis of Novel Splice-Junction Peptides using RNA-Seq;** Gloria Sheynkman; Michael Shortreed; Lloyd Smith; *Univ. of Wisconsin Madison, Madison, WI*
- WOB pm 3:30 **An Unsupervised Machine Learning Algorithm for Positioning Modifications on Phosphopeptides;** Oliver Horlacher; Frederic Nikitin; Frederique Lisacek; Markus Muller; *SIB, Geneva, Switzerland*

- WOB pm 3:50 **Using Prior Knowledge to Improve Scoring in High-Throughput Top-Down Proteomics Experiments;** Richard LeDuc; Le-Shin Wu; *Indiana University, Bloomington, IN*

- WOB pm 4:10 **Proteogenomics of Immunoglobulins: Applications to the Clinical Laboratory;** Surendra Dasari; Jason Theis; Robert Bergen, III; Diana Gil; David Barnidge; Marina Ramirez-Alvarado; Diane Jelinek; David Murray; Ahmet Dogan; *Mayo Clinic, Rochester, MN*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
GAS-PHASE IONS: REACTIONS, DYNAMICS AND THEORY**  
**Mike Van Stipdonk (Lawrence University), presiding**  
**Ballroom B**

- WOC pm 2:30 **Energetics and Dynamics of the Reactions of Thorium Cations with Dihydrogen and Methane;** Richard Cox; Peter B. Armentrout; *University of Utah, Salt Lake City, UT*
- WOC pm 2:50 **Charge Site Mass Spectra: Gaseous Protein Ions Have an Unusual Common Secondary Structure;** Fred W. McLafferty<sup>1</sup>; Owen S. Skinner<sup>2</sup>; Kathrin Breuker<sup>3</sup>; *<sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Northwestern University, Evanston, IL; <sup>3</sup>University of Innsbruck, Innsbruck, Austria*
- WOC pm 3:10 **Model Compound Fragmentation Pathways as an Entry to Structural Analysis of Crude Oil;** Benjamin J. Bythell<sup>1</sup>; Yuri Corilo<sup>1,2</sup>; Vladislav V. Lobodin<sup>1,2</sup>; Ryan Rodgers P.<sup>1,2</sup>; Alan G. Marshall<sup>1,3</sup>; *<sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University Future Fuels Institute, Tallahassee, FL; <sup>3</sup>Florida State University, Tallahassee, FL*
- WOC pm 3:30 **A Catalytic Cycle for the Formation of a C-C Bond Catalysed by Bimetallic Ag/Cu;** George N. Khairallah; Halal Al Sharif; Krista Vikse; Richard A. J. O'Hair; *Bio21 Inst, Uni of Melbourne, Melbourne, Australia*
- WOC pm 3:50 **Variable Temperature Ion Trap Mass Spectrometer for the Study of Gas-Phase Reactions;** David Derkits; Jared Lamp; Jasmine Harge; Russell Snead; Alexander Wiseman; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- WOC pm 4:10 **Investigating Electron-Induced Chemiluminescence in Ru<sup>3+</sup> (bipy)<sub>3</sub> Acetonitrile Clusters;** Maria Demireva; Evan R. Williams; *University of California, Berkeley, CA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
BIOMARKERS OF DRUG RESPONSE, EFFICACY AND TOXICITY:  
NOVEL MS APPROACHES**  
**Fanyu Meng (Merck & Co), presiding**  
**Ballroom A**

- WOD pm 2:30 **N-terminal Labeling Reveals Circulating Proteomic Signatures of Cell Death Post-Chemotherapy;** Arun Wiita; James Wells; *University of California, San Francisco, CA*
- WOD pm 2:50 **Protein C Inhibitor Proteotypic Peptide Quantitation by LC-Free SISCAPA-MALDI Mass Spectrometry Predicts Recurrence of Prostate Cancer after Radiotherapy;** N. Leigh Anderson<sup>1</sup>; Morteza Razavi<sup>2</sup>; Terry Pearson<sup>2</sup>; Lisa Johnson<sup>3</sup>; Julian Lum<sup>3</sup>; Gary Kruppa<sup>4</sup>; *<sup>1</sup>SISCAPA Assay Technologies, Washington, DC; <sup>2</sup>University of Victoria, Victoria, BC, Canada; <sup>3</sup>Deeley Research Ctr, BC Cancer Agency, Victoria, BC, Canada; <sup>4</sup>Bruker Daltonics Inc., Billerica, MA*



WOD pm 3:10 **Evaluation of a Novel Microfluidic Device for Robust and Ultrasensitive Quantitative Analysis of Biomarkers and Bio-Therapeutics by LC-MS/MS;** Jose Castro-Perez<sup>1</sup>; Haihong Zhou<sup>1</sup>; Vinit Shah<sup>1</sup>; Kevin Bateman<sup>1</sup>; David McLaren<sup>1</sup>; Anita Lee<sup>1</sup>; Stephen Previs<sup>1</sup>; Kitshiri Herath<sup>1</sup>; James Murphy<sup>2</sup>; Paul Rainville<sup>2</sup>; Alan Millar<sup>2</sup>; Angela Doneanu<sup>2</sup>; Michele Cleary<sup>1</sup>; Thomas Roddy<sup>1</sup>; <sup>1</sup>Merck, Kenilworth, NJ; <sup>2</sup>Waters Corp, Milford, MA

WOD pm 3:30 **Quantifying Proteoforms using High-Throughput Top-Down Proteomics for Cell-Based Biomarker Discovery;** John P. Savaryn<sup>1</sup>; Adam D. Catherman<sup>1</sup>; Archer D. Smith IV<sup>1</sup>; Ryan T. Fellers<sup>1</sup>; Richard D. LeDuc<sup>2</sup>; Paul M. Thomas<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Indiana University, Bloomington, IN

WOD pm 3:50 **Proteomic Analysis Reveals Differences between Xenograft Models of Triple-Negative Breast Cancer Associated with Therapy Response;** Nadine Mascini<sup>1</sup>; Gert Eijkel<sup>1</sup>; Petra ter Brugge<sup>2</sup>; Jelle Wesseling<sup>2</sup>; Jos Jonkers<sup>2</sup>; Ron Heeren<sup>1</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>2</sup>The Netherlands Cancer Institute, Amsterdam, The Netherlands

WOD pm 4:10 **Development of Urinary Biomarkers to Monitor Oligomer Treatment in Duchenne Muscular Dystrophy;** Aiping Zhang; Kitipong Uaesoontrachoon; Kathryn White; Sree Rayavarapu; Kristy J Brown; Patricia Ray; Kanneboyina Nagaraju; John N. van den Anker; Eric P Hoffman; Yetrib Hathout; children's National Medical center, Washington, DC

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION  
AND SAMPLING**

**Richard Vachet (University of Massachusetts), presiding  
Auditorium**

WOE pm 2:30 **A Novel ConDUCT Interface for Transmitting ~100% Ions from an ESI Source into a Mass Spectrometer;** Andrew N. Krutchinsky; Julio C. Padovan; Herbert Cohen; Brian T. Chait; *Rockefeller University, New York, NY*

WOE pm 2:50 **A New Ionization Method for Volatile and Nonvolatile Compounds Requiring only Vacuum and Matrix Assistance;** Sarah Trimpin; Wayne State University, Detroit, MI

WOE pm 3:10 **Nanoliter Segmented-Flow Sampling Mass Spectrometry: Introducing On-line Compartmentalization while Avoiding Sample Dilution;** Michael Volny<sup>1</sup>; Bejan Hakimi<sup>1</sup>; Joelle Rolfs<sup>1</sup>; Petr Frycak<sup>2</sup>; Thomas Schneider<sup>1</sup>; Gloria Yen<sup>1</sup>; Dingsheng Liu<sup>1</sup>; Daniel Chiu<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Palacky University, Olomouc, Czech Republic

WOE pm 3:30 **Coupling Gel Electrophoresis to Mass Spectrometry by Electrostatic Spray Ionization;** Elena Tobolkina<sup>1</sup>; Liang Qiao<sup>1</sup>; Liu Baohong<sup>2</sup>; Hubert Girault<sup>1</sup>; <sup>1</sup>École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Institute of Biomedical Sciences, Fudan University, Shanghai, China

WOE pm 3:50 **Large Surface Area Analysis by Spray Desorption Collection Coupled to Paper Spray Mass Spectrometry;** Andre Venter; Gregg Hasman; Kevin Douglass; Western Michigan University, Kalamazoo, MI

WOE pm 4:10 **Off-line Capillary Electrophoresis Mass Spectrometry Using Patterned Deposition Nanostructure Assisted Laser Desorption Ionization;** Jon Beusse; Kermit K. Murray; Louisiana State University, Baton Rouge, LA

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
ECOLOGICAL AND HUMAN HEALTH ENVIRONMENTAL  
CHEMISTRY AND TOXICOLOGY  
Paul Chiarelli (Loyola University), presiding  
Room 101**

WOF pm 2:30 **Real-Time, Geospatially-Resolved Atmospheric Contaminant Monitoring by Membrane Introduction Tandem Mass Spectrometry (MIMS-MS/MS) Near Oil and Gas Operations in Alberta, Canada;** Ryan J. Bell<sup>4</sup>; Nicholas G. Davey<sup>1,4</sup>; Morten Martinsen<sup>2,4</sup>; Alexander J. Thompson<sup>4</sup>; Isobel J. Simpson<sup>3</sup>; Donald R. Blake<sup>3</sup>; Erik T. Krogh<sup>1,4</sup>; Christopher G. Gill<sup>1,4</sup>; <sup>1</sup>University of Victoria, Victoria, BC, Canada; <sup>2</sup>NTNU, Trondheim, Norway; <sup>3</sup>University of California, Irvine, CA; <sup>4</sup>AERL, Vancouver Island University, Nanaimo, BC, Canada

WOF pm 2:50 **LC -Q-TOF-MS and LC -HR-TOF-MS Methods for the Determination of Metabolites of Polycyclic Aromatic Hydrocarbons in Urine: A Comparison;** Jutta Lintelmann<sup>1</sup>; Evelyn Huebner<sup>1</sup>; Juergen Wendt<sup>2</sup>; Ralf Zimmermann<sup>1</sup>; <sup>1</sup>Helmholtz Zentrum Muenchen, Neuherberg, Germany; <sup>2</sup>LECO European LSCA Centre, Moenchengladbach, Germany

WOF pm 3:10 **Simultaneous Determination of Polybrominated Diphenyl Ethers (BDEs) and Polychlorinated Biphenyls (PCBs) in Plasma by GC Triple Quadrupole Mass Spectrometer;** Yan-Ping Lin<sup>1</sup>; Birgit Puschner<sup>1</sup>; Isaac N. Pessah<sup>1</sup>; Keyu Zhou<sup>2</sup>; Gwen Lim<sup>2</sup>; Helen Sun<sup>2</sup>; Kefei Wang<sup>2</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>Bruker, Chemical and Applied Market (CAM) Division, Fremont, CA

WOF pm 3:30 **Investigation of Human Body Adaptation to the High Temperature and High CO<sub>2</sub> Level by MS Analysis of Exhaled Breath Condensate;** Alexey Kononikhin<sup>1,2</sup>; Anna Ryabokon<sup>2</sup>; Igor Popov<sup>2,5</sup>; Nataliia Starodubtseva<sup>1,3</sup>; Viktoria Kurova<sup>2</sup>; Evgeny Kukaev<sup>2,5</sup>; Maria Indeykina<sup>1,2</sup>; Alexander Spassky<sup>1</sup>; Stanislav Pekov<sup>1</sup>; Sergey Varfolomeev<sup>2</sup>; Irina Larina<sup>4</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>3</sup>Research Center for Obstetrics, Gynecology, Moscow, Russia; <sup>4</sup>Institute for Biomedical Problems, Moscow, Russia; <sup>5</sup>Moscow Institute of Physics and Technology, Moscow, Russia

WOF pm 3:50 **A New Method for the Analysis of Cyanotoxins using Laser Diode Thermal Desorption-Atmospheric Pressure Chemical Ionization-Tandem Mass Spectrometry (LDTD-APCI-MS/MS);** Audrey Roy-Lachapelle; Pascal Lemoine; Sébastien Sauvé; Université de Montréal, Montréal, Canada

WOF pm 4:10 **Quantitative Determination and Simultaneous Confirmation by UPLC-MS/MS of Methylhippuric Acids in the Urine of Workers Exposed to Xylenes;** Sebastien Gagne; IRSST, Montreal, Canada



**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
GLYCOPROTEINS AND GLYCANS: NEW MS APPROACHES**  
Carthene Bazemore-Walker (Brown University), presiding  
Room 102

- WOG pm 2:30 **Site-Specific Glycan-Peptide Analysis for Determination of N-Glycoproteome Heterogeneity**; Benjamin Parker<sup>1</sup>; Morten Thaysen-Andersen<sup>2</sup>; Nestor Solis<sup>1</sup>; Nichollas Scott<sup>1,3</sup>; Martin Larsen<sup>4</sup>; Mark Graham<sup>5</sup>; Nicolle Packer<sup>2</sup>; Stuart Cordwell<sup>1</sup>; <sup>1</sup>The University of Sydney, Sydney, Australia; <sup>2</sup>Macquarie University, Sydney, Australia; <sup>3</sup>University of British Columbia, Vancouver, Canada; <sup>4</sup>The University of Southern Denmark, Odense, Denmark; <sup>5</sup>Children's Medical Research Institute, Sydney, Australia
- WOG pm 2:50 **Insights on the Glycopeptides and Glycosylation Site Mapping of the Atypical Glycans of the Methanogen Archaeon *Methanosarcina mazei***; Deborah R. Leon<sup>1</sup>; Xiang Yu<sup>1</sup>; Cheng Lin<sup>1</sup>; Nancy Leymari<sup>1</sup>; Rachel R. Ogorzalek Loo<sup>2</sup>; Joseph A. Loo<sup>3</sup>; Robert P. Gunsalus<sup>4</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Dept of Biological Chemistry UCLA, Los Angeles, CA; <sup>3</sup>Dept of Chem and Biochem UCLA, Los Angeles, CA; <sup>4</sup>Microbiol, Immunol and Molec Genetics Dept UCLA, Los Angeles, CA
- WOG pm 3:10 **Low-Flow Sheathless Capillary Electrophoresis - Mass Spectrometry for Sensitive High-Resolution Glycoform Profiling of Intact Pharmaceutical Proteins**; Rob Haselberg<sup>1</sup>; Gerhardus J. de Jong<sup>2</sup>; Govert W. Somsen<sup>1</sup>; <sup>1</sup>AIMMS Division of BioMolecular Analysis, Amsterdam, the Netherlands; <sup>2</sup>Biomolecular Analysis, Utrecht, the Netherlands
- WOG pm 3:30 **In Depth Characterization of N-Linked Oligosaccharides using Fluoride-Mediated Negative Ion Microfluidic Chip LC-MS**; Jonathan Bones<sup>1,2</sup>; Wenqin Ni<sup>1</sup>; Victoria Berger<sup>1</sup>; Barry Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>National Institute for Bioprocessing Research, Dublin, Ireland
- WOG pm 3:50 **Selected Reaction Monitoring to Differentiate and Relatively Quantitate Isomers of Sulfated Core 1 O-Glycans from Salivary MUC7 in Rheumatoid Arthritis**; Sarah Flowers<sup>1</sup>; Liaqat Ali<sup>1</sup>; Catherine Lane<sup>2</sup>; Niclas Karlsson<sup>1</sup>; <sup>1</sup>Gothenburg University, Gothenburg, Sweden; <sup>2</sup>AB Sciex, Warrington, UK
- WOG pm 4:10 **Computational Approach for Identifying Sulfation Pattern of Heparan Sulfate using High Resolution Tandem Mass Spectrometry Data**; Han Hu; Yu Huang; Yu Xia; Joseph Zaia; Boston University, Boston, MA

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
H/D EXCHANGE: NEW DEVELOPMENTS IN TECHNOLOGY**  
David Weis (University of Kansas), presiding  
Room 103

- WOH pm 2:30 **Electrochemical Reduction of Disulphide Bonds for Use in Protein Hydrogen/Deuterium Exchange Monitored by Mass Spectrometry**; Simon Mysling; Thomas J. D. Jorgensen; BMB, University of Southern Denmark, Odense, Denmark
- WOH pm 2:50 **Improvement of Peptic Peptide Identification for Amide H/D Exchange using High Mass Accuracy Combined with a Statistical Approach**; Jianqing Wu<sup>1</sup>; Guillaume van der Rest<sup>2</sup>; <sup>1</sup>Ecole Polytechnique, Palaiseau, France; <sup>2</sup>Université Paris-Sud, Orsay, France
- WOH pm 3:10 **Nepenthesin-I – Recombinant Carnivorous Plant Protease as a Tool for Hydrogen / Deuterium Exchange Mass Spectrometry**; Alan Kadek<sup>1,2</sup>; Hynek Mrazek<sup>1,2</sup>; Vyacheslav Tretyachenko<sup>2</sup>; Martial Rey<sup>3</sup>; David Schriemer<sup>3</sup>; Petr Halada<sup>1</sup>; Petr Man<sup>1,2</sup>; <sup>1</sup>Institute of Microbiology ASCR, Prague, Czech Republic; <sup>2</sup>Charles University, Prague, Czech Republic; <sup>3</sup>University of Calgary, Calgary, Canada
- WOH pm 3:30 **Microfluidics-Enabled, Sub-Second Hydrogen/Deuterium Exchange Pulse Labeling Reveals Allosteric 'Hotspots' in Enzymes**; Derek Wilson; Tamanna Rob; Preet Gill; Dasantila Golemi-Kotra; York University, Toronto, Canada
- WOH pm 3:50 **Using Isotopic Fine Structure to Resolve Individual Hydrogen/Deuterium Exchanges**; Qian Liu<sup>1</sup>; Michael Easterling<sup>2</sup>; Jeffrey Agar<sup>1</sup>; <sup>1</sup>Brandeis University, Waltham, MA; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA
- WOH pm 4:10 **Information Independent Acquisition of MS/MS Data for High Efficiency HDX-MS Experiments**; Vladimir Sarpe; David Schriemer; University of Calgary, Calgary, Canada

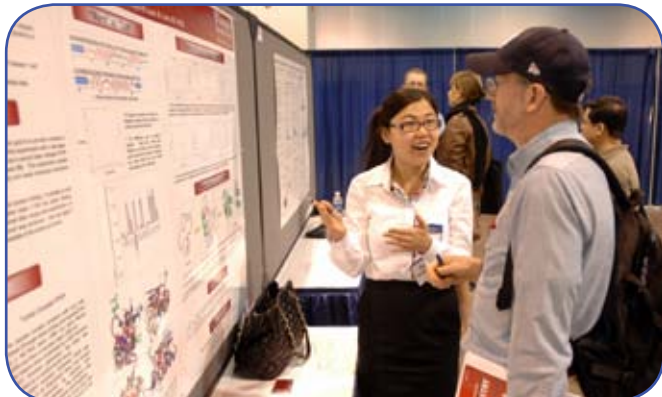
**4:45 - 5:30 PM, WEDNESDAY AFTERNOON  
ASMS MEETING**  
Susan T. Weintraub, presiding  
Ballroom A

Don't miss awards, Board reports and more.

**5:45 - 7:00 PM, WEDNESDAY AFTERNOON  
WORKSHOPS**  
Light snacks are provided on level two.

**LEVEL ONE ROOMS**

- Fundamentals in LC-MS Troubleshooting (organized by LC/MS & Related Topics Interest Group), Room 1
- H/D Exchange and Covalent Labeling (organized by H/D Exchange & Covalent Labeling Interest Group), Room 2
- LC-MS of Glycans and Glycopeptides: Advantages and Challenges, Room 3



## WEDNESDAY AFTERNOON ORAL SESSIONS

### Wednesday Workshops continued

#### LEVEL TWO ROOMS

- Fuel Analysis: Surveying Research Methods and their Application in Industrial Settings (organized by Energy, Petroleum & Biofuels Interest Group), Room 200 DE
- Emerging Contaminants in Environmental Research: Hydraulic Fracturing Fluids and Shale Gas Produced Waters - Advances, Challenges and Opportunities using mass spectrometry (organized by Environmental Applications Interest Group), Room 200 FG
- The Advancement of Polymer Mass Spectrometry (organized by Polymeric Materials Interest Group), Room 200 H
- Challenges and New Directions in Plant Proteomics, Room 200 I
- CHORUS – A Community Solution for the Storage, Visualization, and Sharing of Mass Spectrometry Data on the Cloud, Room 200 J

- Ion Structures and Energetics, and Ion-Molecule Reaction Kinetics in the Gas Phase, in honor of Peter B. Armentrout's 60th birthday (organized by Fundamentals Interest Group), Room 205 AB
- Proteins and Peptides as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group), Room 205 CD
- Lipid Mass Spectrometry & Lipidomics, Room 208 AB
- Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 208 CD

**AFTER 8:00 PM**  
**CORPORATE HOSPITALITY SUITES**  
**HILTON MINNEAPOLIS HOTEL**

## THURSDAY MORNING ORAL SESSIONS

### 8:30 – 10:30 AM, THURSDAY MORNING AMBIENT IONIZATION: INSTRUMENTATION AND APPLICATIONS Justin Wiseman (Prosolia, Inc.), presiding Exhibit Hall A (lower level)

ThOA am 08:30 **Progress toward Universal Ionization by Combining Different Ambient Ionization Methods**; Robert B. Cody; John Dane; JEOL USA, Inc., Peabody, MA

ThOA am 08:50 **Development of a Ruggedized AI-MS with Remote Sampling for Explosives Trace Detection**; Mitch Wells; Mike Stump; Bruce Solomon; Mark Gregory; Dennis Barket; FLIR Mass Spectrometry, West Lafayette, IN

ThOA am 09:10 **Microscopy Guided Atmospheric Ionization in situ Top-Down Protein Mass Spectrometry**; Cheng-Chih Hsu<sup>1</sup>; Tiffany Poon<sup>2</sup>; Eugene C. Lin<sup>1</sup>; Nick White<sup>2</sup>; Marito Hayashi<sup>2</sup>; Indroneel Banerjee<sup>3</sup>; Ju Chen<sup>3</sup>; Samuel L. Pfaff<sup>2</sup>; Eduardo R. Macagno<sup>4</sup>; Pieter C. Dorrestein<sup>1,5</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, UCSD, La Jolla, CA; <sup>2</sup>Salk Institute, La Jolla, CA; <sup>3</sup>Department of Medicine, UCSD, La Jolla, CA; <sup>4</sup>Division of Biological Sciences, UCSD, La Jolla, CA; <sup>5</sup>Skaggs School of Pharmacy, UCSD, La Jolla, CA

ThOA am 09:30 **Embryonic Metabolic Status Evaluated BY Combining DESI-HRMS Positive and Negative Ion Mode Mass Spectral Data by Data Fusion Strategy**; Valentina Pirro<sup>1</sup>; Christina R. Ferreira<sup>2</sup>; Paolo Oliveri<sup>3</sup>; Andres F. Gonzales-Serrano<sup>4</sup>; Livia S. Eberlin<sup>2</sup>; Julia Heinzmann<sup>4</sup>; Andrea Lucas-Hahn<sup>4</sup>; Heiner Niemann<sup>4</sup>; Robert G. Cooks<sup>2</sup>; <sup>1</sup>Università degli Studi di Torino, Torino, ITALY; <sup>2</sup>Department of Chemistry, Purdue University, West Lafayette, Indiana; <sup>3</sup>Department of Pharmacy, University of Genova, Genova, Italy; <sup>4</sup>Department of Biotechnology, Friedrich-Loeffler-In, Neustadt, Germany

ThOA am 09:50 **Combining Atomic Force Microscopy and Thermal Desorption-Based Surface Sampling/Ionization Mass Spectrometry for Submicrometer Scale Multimodal Chemical Imaging**; Olga S. Qvichinnikova<sup>1</sup>; Kevin Kjoller<sup>2</sup>; Gary J. Van Berkel<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>Anasys Instruments, Santa Barbara, CA

ThOA am 10:10 **Rapid Evaporative Ionization Mass Spectrometry – Mechanism and Applications**; Dániel Szalay<sup>1</sup>; Lajos Gödörházy<sup>1</sup>; Tamás Karancsi<sup>1</sup>; Andor Rozsnyai<sup>1</sup>; Ottmar Golf<sup>2</sup>; Karl-Christian Schäfer<sup>2</sup>; Steven Pringle<sup>3</sup>; Mike Morris<sup>3</sup>; Zoltán Takáts<sup>2</sup>; <sup>1</sup>Medimass Ltd., Budapest, Hungary; <sup>2</sup>Imperial College London, London, UK; <sup>3</sup>Waters Corporation, Manchester, UK

### 8:30 – 10:30 AM, THURSDAY MORNING METABOLOMICS Lloyd Sumner (Samuel Roberts Noble Fndn), presiding Room L100 (lower level)

ThOB am 08:30 **Multivariate and Network Tools for Analysis and Visualization of Metabolomic Data**; Dmitry Grapov<sup>1,2</sup>; Oliver Fiehn<sup>1,2</sup>; <sup>1</sup>West Coast Metabolomics Center, Davis, CA; <sup>2</sup>University of California, Davis, CA

ThOB am 08:50 **A Novel Approach for Processing LC-Ion Mobility-MS Metabolomics Data**; Giorgis Isaac<sup>2</sup>; Martin Palmer<sup>3</sup>; Mark Bennett<sup>1</sup>; James Langridge<sup>3</sup>; John P. Shockcor<sup>2</sup>; Andy Borthwick<sup>1</sup>; <sup>1</sup>Nonlinear Dynamics, Newcastle, upon Tyne, UK; <sup>2</sup>Waters Corporations, Milford, MA; <sup>3</sup>Waters Corporation, Manchester, UK

ThOB am 09:10 **High(er) Throughput Metabolite Annotation in LC/MS Metabolomics**; Steffen Neumann<sup>1</sup>; Michael Gerlich<sup>1</sup>; Carsten Kuhl<sup>1</sup>; Andrea Thum<sup>2</sup>; Christoph Böttcher<sup>1</sup>; <sup>1</sup>Leibniz Institute of Plant Biochemistry, Halle, Germany; <sup>2</sup>Martin Luther Universität, Halle, Germany

ThOB am 09:30 **RAMClust: An Unsupervised Feature Clustering Method for Non-Targeted Metabolomics Datasets**; Corey D. Broeckling; Fayyaz A. Afsar; Asa Ben-Hur; Jessica E. Prenni; Colorado State University, Fort Collins, CO

ThOB am 09:50 **MRMPROBS: Data Assessment and Metabolite Identification Tool for Large-scale MRM-based Widely Targeted Metabolomics**; Tsugawa Hiroshi<sup>1</sup>; Arita Masanori<sup>1</sup>; Kanazawa Mitsuhiro<sup>3</sup>; Ogiwara Atsushi<sup>3</sup>; Bamba Takeshi<sup>2</sup>; Fukusaki Eiichiro<sup>2</sup>; <sup>1</sup>RIKEN, Yokohama, Japan; <sup>2</sup>Osaka University, Suita, Japan; <sup>3</sup>Reifys, Inc., Minato-ku, Japan

ThOB am 10:10 **Untargeted Metabolomics: From Statistical Objects to the Efficient Identification of “Known Unknowns”**; Robert Mistrik; Juraj Lütisan; *HighChem, Bratislava, Slovakia*

**8:30 – 10:30 AM, THURSDAY MORNING  
REGULATED BIOANALYSIS AND DIAGNOSTICS USING HIGH  
RESOLUTION LC/MS**

**David Burinsky (Alcon Laboratories), presiding  
Ballroom B**

ThOC am 08:30 **Balancing Sensitivity Gains and Method Simplification: Investigating HR/AM and a new Nanospray Source for a Challenging Bioanalytical Method**; Min Meng<sup>3</sup>; Hongxia Wang<sup>1</sup>; Kate Comstock<sup>1</sup>; Spencer Carter<sup>2</sup>; Patrick Bennett<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*WIL Research, Ashland, OH*; <sup>3</sup>*Tandem Labs, Salt Lake City, UT*

ThOC am 08:50 **Monitoring Phosphodiesterase-4 Inhibitors using LC-MS/MS in Sports Drug Testing**; Mario Thevis<sup>1</sup>; Oliver Krug<sup>2</sup>; Wilhelm Schänzer<sup>1</sup>; <sup>1</sup>*German Sport University, Cologne, Germany*; <sup>2</sup>*Europ. Monitoring Center f. Emerging Doping Agents, Cologne/Bonn, Germany*

ThOC am 09:10 **A Single Multi-Attribute Method for Quality Control and Release Testing of Therapeutic Biomolecules**; Rich Rogers<sup>1</sup>; Brittney Livingston<sup>1</sup>; Jenn Kerr<sup>1</sup>; Nancy Nightlinger<sup>1</sup>; Becky Scott<sup>1</sup>; Sihong Deng<sup>1</sup>; Brittany Affholter<sup>1</sup>; David Bassett<sup>1</sup>; Jim Bailey<sup>1</sup>; Steve Cockrill<sup>1</sup>; Quanzhou Luo<sup>1</sup>; Oleg Borisov<sup>1</sup>; Bob Bailey<sup>1</sup>; Scott Peterman<sup>2</sup>; Amol Prakash<sup>2</sup>; Hongxia Wang<sup>2</sup>; Kevin Wheeler<sup>2</sup>; Patrick Bennett<sup>2</sup>; Alain Balland<sup>1</sup>; <sup>1</sup>*Amgen, Seattle, WA*; <sup>2</sup>*ThermoFisher, San Jose, CA*

ThOC am 09:30 **Determination of Colistin Pharmacokinetics in Human Plasma and Bronchoalveolar Lavage by a Novel UPLC-ESI QTOF MS/MS Methodology**; Demetris Anagnostopoulos<sup>1</sup>; Evangelos Gikas<sup>1,2</sup>; Konstantinos Papanikolaou<sup>4</sup>; Panagiotis Haritidis<sup>2</sup>; Athanassios Skoutelis<sup>3</sup>; George Daikos<sup>4</sup>; Anthony Tsarbopoulos<sup>1,5</sup>; <sup>1</sup>*The Goulandris Natural History Museum, Kifissia, Greece*; <sup>2</sup>*University of Athens, Pharmacy Department, Athens, Greece*; <sup>3</sup>*Evangelismos Hospital, Dpt. of Internal Medicine, Athens, Greece*; <sup>4</sup>*University of Athens Medical School, Internal Med., Athens, Greece*; <sup>5</sup>*University of Athens Medical School, Pharmacology, Athens, Greece*

ThOC am 09:50 **Validation of a Glycan Biomarker Set for the Detection of Ovarian Cancer using Mass Spectrometry**; L. Renee Ruhaak<sup>1</sup>; Sandra Taylor<sup>1</sup>; Cynthia Williams<sup>1</sup>; UyenThao Nguyen<sup>1</sup>; Lauren Dimapasoc<sup>1</sup>; Sureyya Ozcan<sup>1</sup>; Carol Stroble<sup>1</sup>; <sup>2</sup>Suzanne Miyamoto<sup>2</sup>; Kyoungmi Kim<sup>1</sup>; Gary Leiserowitz<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*UC Davis Comprehensive Cancer Center, Sacramento, CA*

ThOC am 10:10 **Quantification of Purine Biomarkers by UPLC-MS/MS for Clinical Diagnostic of Rare Kidney Stones and Kidney Failure**; Margrét Thorsteinsdóttir<sup>1,2</sup>; Finnur Freyr Eiríksson<sup>1,2</sup>; Vidar O Edvardsson<sup>1,3</sup>; Runolfur Pálsson<sup>1,3</sup>; <sup>1</sup>*University of Iceland, Reykjavik, Iceland*; <sup>2</sup>*ArcticMass, Reykjavik, Iceland*; <sup>3</sup>*Landspítali University Hospital, Reykjavik, Iceland*

**8:30 – 10:30 AM, THURSDAY MORNING  
DISEASE BIOMARKERS AND PATHWAYS**  
**Carol Nilsson (UTMB), presiding  
Ballroom A**

ThOD am 08:30 **Deciphering Breast Cancer Proteogenomics using Bioinformatics Methods**; Kelly V. Ruggles<sup>1</sup>; Zuojian Tang<sup>1</sup>; Manor Askenazi<sup>2</sup>; Olexandra Ovsy<sup>1</sup>; Christopher Maher<sup>3</sup>; Li Ding<sup>3</sup>; Stuart Brown<sup>1</sup>; Steven Shen<sup>1</sup>; Meera Prasad<sup>1</sup>; Jeremy Hoog<sup>3</sup>; Shunqiang Li<sup>3</sup>; Robert T. Kitchens<sup>3</sup>; Charles M. Perou<sup>4</sup>; Sherri R. Davies<sup>3</sup>; Matthew J. Ellis<sup>3</sup>; R. Reid Townsend<sup>3</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>*NYU Langone Medical Center, New York, NY*; <sup>2</sup>*The Ionomix Initiative, Arlington, MA*; <sup>3</sup>*Washington University, St. Louis, MO*; <sup>4</sup>*University of North Carolina, Chapel Hill, NC*

ThOD am 08:50 **Proteomic Profiling of Breast Cancer Cell Line Secretome for Basal-type Specific Tumor Biomarker Discovery using Skyline MS1 Filtering**; Anna M. Zawadzka; Birgit Schilling; Michael P. Cusack; Christopher Benz; Bradford W. Gibson; *Buck Institute for Research on Aging, Novato, CA*

ThOD am 09:10 **Comparative Proteome Analysis Reveals an 11-Protein Signature that Predicts Clinical Outcome in Triple Negative Breast Cancer**; Ning Qing Liu<sup>1</sup>; Tommaso De Marchi<sup>1</sup>; Annemieke M. Timmermans<sup>1</sup>; Christoph Stingl<sup>1</sup>; Anita M.A.C. Trapman-Jansen<sup>1</sup>; Renée Foekens<sup>1</sup>; Maxime P. Look<sup>1</sup>; Marcel Smid<sup>1</sup>; Carolien H.M. van Beurden<sup>1</sup>; René B.H. Braakman<sup>1</sup>; Paul N. Span<sup>2</sup>; Fred C.G.J. Sweep<sup>2</sup>; Barbro K. Linderholm<sup>3</sup>; Anita Mangia<sup>4</sup>; Angelo Paradiso<sup>4</sup>; Luc Y. Dirix<sup>5</sup>; Steven J. Van Laere<sup>5</sup>; Julie Benedicte Brask<sup>6</sup>; Vera Timmermans-Wielenga<sup>6</sup>; Theo M. Luiders<sup>1</sup>; John W.M. Martens<sup>1</sup>; John A. Foekens<sup>1</sup>; Arzu Umar<sup>1</sup>; <sup>1</sup>*Erasmus University Medical Center, Rotterdam, Netherlands*; <sup>2</sup>*University Nijmegen Medical Centre, Nijmegen, Netherlands*; <sup>3</sup>*Karolinska Institute, Stockholm, Sweden*; <sup>4</sup>*National Cancer Centre Giovanni Paolo II, Bari, Italy*; <sup>5</sup>*GZA hospitals St-Augustinus, Antwerp, Belgium*; <sup>6</sup>*Copenhagen University Hospital, Copenhagen, Denmark*

ThOD am 09:30 **Targeting the Multi-Hit Mechanism of IgA Nephropathy through Systematic Serum Analysis of Circulating Components and Upstream Effector's**; Jennifer Cushing<sup>1</sup>; Audra Hargett<sup>1</sup>; Stacy Hall<sup>1</sup>; Blake P. Moore<sup>1</sup>; Greg Bowersock<sup>1</sup>; Monica W. Stinnett<sup>1</sup>; Kazuo Takahashi<sup>1,2</sup>; Hitoshi Suzuki<sup>1</sup>; Tyler J. Stewart<sup>1</sup>; LeeAnn J. Boerma<sup>1</sup>; Scott Peterman<sup>3</sup>; Amol Prakesh<sup>3</sup>; Milan Raska<sup>1</sup>; Jiri Mestecky<sup>1</sup>; Bruce A. Julian<sup>1</sup>; Jan Novak<sup>1</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*Fujita Health University School of Medicine, Toyoake, Japan*; <sup>3</sup>*ThermoFisher Scientific, San Jose, CA*

ThOD am 09:50 **Cell Membrane Glycan Profiling Differentiates Cancer Cell Origin and Molecular Subtype**; Serenus Hua<sup>1</sup>; Lauren Dimapasoc<sup>2</sup>; Bum Jin Kim<sup>1</sup>; Seung Hyup Jeong<sup>1</sup>; Jae Han Kim<sup>1</sup>; Carlito Lebrilla<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*GRASST, Chungnam National University, Daejeon, South Korea*; <sup>2</sup>*University of California, Davis, CA*

ThOD am 10:10 **Elucidating Pathways Associated with Sudden Infant Death Syndrome (SIDS) using Quantitative Proteomics to Analyze Various Regions Isolated from Autopsied Brainstems**; Kevin G. Broadbelt<sup>1</sup>



<sup>2</sup>; Claire F. Magiotto<sup>2</sup>; Catherine A. Hassett<sup>2</sup>; Jan Muntel<sup>1,2</sup>; Elisabeth A. Haas<sup>3</sup>; Henry F. Krous<sup>3</sup>; Hannah C. Kinney<sup>2</sup>; Hanno Steen<sup>1,2</sup>; <sup>1</sup>*Proteomics Center, Boston Children's Hospital, Boston, MA*; <sup>2</sup>*Department of Pathology, Boston Children's Hospital, Boston, MA*; <sup>3</sup>*Rady Children's Hospital San Diego and UCSD, San Diego School of Medicine, La Jolla, CA*

**8:30 – 10:30 AM, THURSDAY MORNING  
SPACE SCIENCE, ASTROBIOLOGY, AND  
ATMOSPHERIC CHEMISTRY**

**Veronica Bierbaum (University of Colorado), presiding  
Auditorium**

ThOE am 08:30 **Micro-AirCore: Spatial Mapping of Atmospheric Species**; Kristin Favela<sup>1</sup>; Pieter Tans<sup>2</sup>; Thomas Jaeckle<sup>1</sup>; William Williamson<sup>1</sup>; <sup>1</sup>*Southwest Research Institute, San Antonio, TX*; <sup>2</sup>*National Oceanic and Atmospheric Administration, Boulder, CO*

ThOE am 08:50 **Development of a Dual Ion Source Linear Ion Trap Mass Spectrometer for *in situ* Detection of Organics on Mars**; Ryan M. Danell<sup>1</sup>; Veronica Pinnick<sup>2</sup>; Friso Van Amerom<sup>3</sup>; Ricardo Arevalo<sup>2</sup>; Xiang Li<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Paul Mahaffy<sup>2</sup>; <sup>1</sup>*Danell Consulting, Inc., Winterville, NC*; <sup>2</sup>*NASA Goddard Space Flight Center, Greenbelt, MD*; <sup>3</sup>*SRI International, St Petersburg, FL*

ThOE am 09:10 **Cluster Ion Imaging of the "Paris" Meteorite**; Manale Noun<sup>1,2</sup>; Bilal Nsouli<sup>2</sup>; Donia Baklouti<sup>3</sup>; Rosario Brunetto<sup>3</sup>; Frédéric Jamme<sup>4</sup>; Christophe Sandt<sup>4</sup>; Paul Dumas<sup>4</sup>; Louis Hendecourt<sup>3</sup>; Serge Della-Negra<sup>1</sup>; <sup>1</sup>*Institut de Physique Nucleaire d'Orsay, Orsay Cedex, FRANCE*; <sup>2</sup>*Lebanese Atomic Energy Commission, CNRSL, Beirut, Lebanon*; <sup>3</sup>*Institut d'Astrophysique Spatiale, CNRS, UMR-8617, Orsay, France*; <sup>4</sup>*Synchrotron SOLEIL, Gif-sur-Yvette-France, Orsay, France*

ThOE am 09:30 **Mass Spectrometric-based Investigations of Polymerized Biomolecules Synthesized in Miller's Unreported Cyanamide Spark Discharge Experiment**; Eric Parker<sup>1</sup>; Manshui Zhou<sup>1</sup>; Aaron Burton<sup>2</sup>; Daniel Glavin<sup>2</sup>; Jason Dworkin<sup>2</sup>; Facundo Fernández<sup>1</sup>; Jeffrey Bada<sup>3</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, U.S.A.*; <sup>2</sup>*NASA Goddard Space Flight Center, Greenbelt, MD*; <sup>3</sup>*Scripps Institution of Oceanography, La Jolla, CA*

ThOE am 09:50 **Structural Determination of Titan's Tholins Components by Tandem FTMS, by Standard Comparison and Action Spectroscopy**; Roland Thissen<sup>1</sup>; Arpad Somogyi<sup>2</sup>; Véronique Vuitton<sup>1</sup>; Laurene Flandinet<sup>1</sup>; Anne Millet<sup>3</sup>; Carlos Perez del Valle<sup>3</sup>; Istvan Komaromi<sup>4</sup>; <sup>1</sup>*IPAG, Grenoble, France*; <sup>2</sup>*University of Arizona, Tucson, AZ*; <sup>3</sup>*Département de Chimie Moléculaire, UJF, Grenoble, France*; <sup>4</sup>*University of Debrecen, Debrecen, Hungary*

ThOE am 10:10 **Polycyclic Aromatic Hydrocarbon Evolution in a Nitrogen Environment Driven by Collisional Activation, Cold Plasma Discharge, or UV Radiation: A Tholin Study**; Anyin Li<sup>1</sup>; Fred Jjunju<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*King Abdullah University of Science and Technology, CEMSE KAUST, Thuwah, KSA*

**8:30 – 10:30 AM, THURSDAY MORNING  
IMAGING MS: PHARMACEUTICAL APPLICATIONS  
Walter Korfmacher (Genzyme), presiding  
Room 101**

ThOF am 08:30 **Mass Spectrometry Imaging for Pharmaceutical R&D Employing Cassette Drugs Dosing for Higher Throughput High Resolution Pharmacokinetic and Biodistribution Analysis**; Richard Goodwin<sup>1</sup>; John Swales<sup>1</sup>; Michael Rooney<sup>2</sup>; C. Logan Mackay<sup>3</sup>; Per Andren<sup>4</sup>; Peter Webb<sup>1</sup>; <sup>1</sup>*AstraZeneca, UK, Macclesfield, UK*; <sup>2</sup>*AstraZeneca, USA, Waltham, MA*; <sup>3</sup>*University of Edinburgh, Edinburgh, UK*; <sup>4</sup>*Uppsala University, Uppsala, Sweden*

ThOF am 08:50 **Label-Free Mass Spectrometry Imaging of Drug and Metabolites in Target Tissue**; Angela Wehr; Lin Xu; Chandra Prakash; *Biogen Idec, Cambridge, MA*

ThOF am 09:10 **Drug and Metabolism Studies using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Mass Spectrometry Imaging (IR-MALDESI MSI) Coupled to FT-ICR MS**; Jeremy A. Barry<sup>1</sup>; Reid Groseclose<sup>2</sup>; Guillaume Robichaud<sup>1</sup>; David Wagner<sup>2</sup>; Stephen Castellino<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*GlaxoSmithKline, Research Triangle Park, NC*

ThOF am 09:30 **Muscarinic Receptor Antagonist Target Disposition in Lung Disease Utilizing 10-µm Spatial Resolution of AP SMALDI Tissue Imaging**; Akos Vegvari<sup>1</sup>; Kerstin Strupat<sup>3</sup>; Magnus Dahlbäck<sup>2</sup>; Thomas Fehniger<sup>1</sup>; György Marko-Varga<sup>1</sup>; <sup>1</sup>*Lund University, Lund, Sweden*; <sup>2</sup>*Astra Zeneca R&D, Mölndal, Sweden*; <sup>3</sup>*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThOF am 09:50 **MALDI-MS Imaging and Quantitation of Primary Amine Neurotransmitters Dopamine, GABA and Glutamate Directly in Brain Tissue Sections**; Mohammadreza Shariatgorji<sup>1</sup>; Anna Nilsson<sup>1</sup>; Richard Goodwin<sup>1</sup>; Xiaoqun Zhang<sup>2</sup>; Nicoletta Schintu<sup>2</sup>; Per Svenningsson<sup>2</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*; <sup>2</sup>*Karolinska Institutet, Stockholm, Sweden*

ThOF am 10:10 **Evaluation of Quantitative MSI Approaches Applied to Small and Large Molecules Analysis in tissue**; Gregory Hamm; Guillaume Hochart; Fabien Pamelard; raphael legouffe; David Bonnel; Jonathan Stauber; *ImaBiotech, MS Imaging Department, Lille, France*

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

**Steven Kass (University of Minnesota), presiding  
Room 102**

ThOG am 08:30 **Ultra-Fast, High Mass-Resolution Multi-Reflection-Time-of-Flight-Mass Spectrometer as Detector for One-Dimensional and Comprehensive Two-Dimensional Gas Chromatography: Characterization of Highly Complex Petrochemical Mixtures**; Ralf Zimmermann<sup>1,2</sup>; Thomas Gröger<sup>1</sup>; Jürgen Wendt<sup>3</sup>; <sup>1</sup>*JMSC, CMA Helmholtz Zentrum Muenchen, Neuherberg, Germany*; <sup>2</sup>*JMSC, Analytical Chemistry, University of Rostock, Rostock, Germany*; <sup>3</sup>*LECO European LSCA Centre, Moenchengladbach, Germany*



ThOG am 08:50 **Validation of High Resolution Time-of-Flight Petroleomics: Linearity, Repeatability, and Accuracy of Heteroatomic Species Measurements in Crude Petroleum;** Clécio F. Klitzke<sup>1</sup>; Kevin Siek<sup>2</sup>; Julie A.B. Hernández<sup>3</sup>; Rubens Maciel-Filho<sup>3</sup>; Marcos N. Eberlin<sup>1</sup>; Joe Binkley<sup>2</sup>; Jeffrey S. Patrick<sup>2</sup>; Wibke Peters<sup>4</sup>; <sup>1</sup>UNICAMP, Institute of Chemistry, Campinas, Brazil; <sup>2</sup>LECO Corporation, St. Joseph, MI; <sup>3</sup>UNICAMP, Chemical Engineering Faculty, Campinas, Brazil; <sup>4</sup>LECO Instrumente GmbH, Mönchengladbach, Germany

ThOG am 09:10 **A New Apparatus for Study of Pressure-Dependent Laminar Premixed Flames with VUV Photoionization Mass Spectrometry;** Zhongyue Zhou; Yu Wang; Xiaofeng Tang; Wuhua Wu; Fei Qi; University of Science and Technology of China, Hefei, China

ThOG am 09:30 **Analysis of Hydrocarbon Based Oil from Hydrothermal Treatment of Algal Biomass by Complementary 2D GC and ESI-FTICR-MS;** Wassim Obeid; Patrick Hatcher; Old Dominion University, Norfolk, VA

ThOG am 09:50 **Climate Change Effects on Biomass Emissions and Biofuels;** Simin Maleknia<sup>1</sup>; Andreas Klingberg<sup>2</sup>; Juergen Odermatt<sup>2</sup>; <sup>1</sup>University of New South Wales, Sydney, Australia; <sup>2</sup>Institute for Wood Chemistry, Hamburg, Germany

ThOG am 10:10 **Characterization of Organosolv Switchgrass by High Performance Liquid Chromatography/High Resolution Multiple Stage Tandem Mass Spectrometry Using Hydroxide-Doped Electrospray Ionization;** Tiffany Jarrell<sup>1</sup>; Christopher Marcum<sup>1</sup>; Benjamin Owen<sup>1</sup>; Joseph Bozell<sup>2</sup>; Hilka Kenttämää<sup>1</sup>; <sup>1</sup>Purdue University, Lafayette, IN; <sup>2</sup>University of Tennessee, Knoxville, TN

8:30 – 10:30 AM, THURSDAY MORNING  
**EPIGENETIC MODIFICATIONS AND MECHANISMS**  
Ben Garcia (University of Pennsylvania), presiding  
Room 103

ThOH am 08:30 **Mass Spectrometry Based Quantification of Epigenetic DNA Modifications *in vivo*;** Delshanee Kotandeniya; Brock Matter; Jungmin Song; Xuemin Qian; Fekadu Kassie; Natalia Tretyakova; University of Minnesota, Minneapolis, MN

ThOH am 08:50 **Toward Solving the Histone Code: A Novel Method to Identify Histone PTM Crosstalk using Quantitative Mass Spectrometry;** Yael David<sup>1</sup>; Anna Arnaudo<sup>2</sup>; Tom Muir<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>University of Pennsylvania, Philadelphia, PA

ThOH am 09:10 **RapidFire MS/MS Enables Both Rapid Evaluation of Multiple Histone Methyltransferases and Label-Free High Throughput Screening of Targeted Compound Libraries;** Patrick Bingham; Cody Krivacic; Dawn Nowlin; Karen Maegley; Pfizer, San Diego, CA

ThOH am 09:30 **The Functional Interactome Landscape of the Human Histone Deacetylase Family: A Proteomics-Bioinformatics Approach for Profiling Relative Interaction Stabilities;** Preeti Joshi<sup>1</sup>; Todd Greco<sup>1</sup>; Amanda Guise<sup>1</sup>; Yang Luo<sup>1</sup>; Fang Yu<sup>1</sup>; Alexey Nesvizhskii<sup>2</sup>; Ileana M. Cristea<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>University of Michigan Medical School, Ann Arbor, MI

ThOH am 09:50 **Comprehensive Maps of Ribonucleotide Modifications as Possible Indicators of Cell Identity, Epigenetic, and Metabolic State;** Rebecca E. Rose; Ryan Quinn; D. Fabris; The RNA Institute, University at Albany, Albany, NY

ThOH am 10:10 **MS-based Measurement and Modeling of Histone Methylation Kinetics (M4K) in Multiple Myeloma Cells Carrying Methyltransferase Mutations;** Yupeng Zheng<sup>1</sup>; Nir Yungster<sup>1</sup>; Relja Popovic<sup>2</sup>; Teresa Ezponda-Itoiz<sup>2</sup>; Paul Thomas<sup>1</sup>; Jonathan Licht<sup>2</sup>; William Kath<sup>1</sup>; Neil Kelleher<sup>1,2</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Feinberg School of Medicine, Northwestern Univ, Chicago, IL



10:30 AM - 2:30 PM  
**THURSDAY POSTER SESSION**  
Exhibit Hall BC  
Lunch concessions are open 11:00 am - 2:00 pm



**2:30 – 4:30 PM, THURSDAY AFTERNOON  
AMBIENT AND ATMOSPHERIC PRESSURE IONIZATION:  
FUNDAMENTALS**

**Gary Van Berkel (Oak Ridge National Laboratory), presiding  
Exhibit Hall A**

- ThOA pm 2:30 **Dissociative Electron Transfer Desorption: A Non-Thermal Desorption Mechanism in Plasma-Based Ambient Ionization;** Joshua Wiley; Jacob Shelley; Jobin Cyriac; Graham Cooks; *Purdue University, West Lafayette, IN*
- ThOA pm 2:50 **A New Ambient Ionization Method for Ionization of Volatile and Nonvolatile Compounds;** Shubhashis Chakrabarty; Vincent S. Pagnotti; Charles N. McEwen; *University of the Sciences, Philadelphia, PA*
- ThOA pm 3:10 **Visualization of Mass Transfer in the Flowing Atmospheric-Pressure Afterglow Source for Ambient Desorption/Ionization Mass Spectrometry;** Kevin Pfeuffer; Steven Ray; Gary Hieftje; *Indiana University, Bloomington, IN*
- ThOA pm 3:30 **Sorting Surface Affinity of Analytes in Droplets by Pulsed Nanospray Ionization;** Carina Minardi; Haopeng Wang; Kaveh Jorabchi; *Georgetown Univ., Washington, DC*
- ThOA pm 3:50 **Elucidation of Reagent Species and Mechanisms in the Direct Sampling Analysis (DSA) Source;** Sharanya Reddy; Thomas White; George Perkins; Craig Whitehouse; *PerkinElmer, Shelton, CT*
- ThOA pm 4:10 **Development of Atmospheric Pressure Laser Ionization Method using a Novel 6  $\mu$ m-Band Mid-Infrared Tunable Laser and Solvent as Matrix;** Ryuji Hiraguchi; Hisanao Hazama; Kunio Awazu; *Osaka University, Suita, Japan*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
PROTEOMICS: INFECTIONS DISEASES  
Mark E. Bier (Carnegie Mellon University), presiding  
Room L100**

- ThOB pm 2:30 **Neutron-Encoded (NeuCode) Mass Signatures for the Absolute Quantification of Vesicular Stomatitis Virus Proteins during Infection;** Gregory K. Potts; Emily A. Voigt; John Yin; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- ThOB pm 2:50 **Probing the Hijacking of the Dynamic Epigenome during Viral Infection;** Benjamin Garcia<sup>1</sup>; Peter DiMaggio<sup>2</sup>; Christine O'Connor<sup>4</sup>; Tom Shenk<sup>3</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Imperial College, London, UK*; <sup>3</sup>*Princeton University, Princeton, NJ*; <sup>4</sup>*Cleveland Clinic, Cleveland, OH*
- ThOB pm 3:10 **Defining the HIV-1 Interactome using Insertional Mutagenesis Tagging and I-DIRT;** Yang Luo<sup>2</sup>; Erica Jacobs<sup>1</sup>; Todd Greco<sup>3</sup>; Sarah Keegan<sup>4</sup>; David Fenyö<sup>4</sup>; Michael Rout<sup>1</sup>; Ileana Cristea<sup>3</sup>; Mark Muesing<sup>2</sup>; Brian Chait<sup>1</sup>; <sup>1</sup>*Rockefeller University, New York, NY*; <sup>2</sup>*Aaron Diamond Aids Research Center, New York, NY*; <sup>3</sup>*Princeton University, Princeton, NJ*; <sup>4</sup>*New York University, New York, NY*
- ThOB pm 3:30 **Combining Fragmentation Data with an Interactive de novo Sequencing Program to Characterize Circulating Antibodies against Malaria;** Jessica Chapman<sup>1</sup>; Wilfred Tang<sup>2</sup>; Yong Kil<sup>2</sup>; Chris Becker<sup>2</sup>; Marshall Bern<sup>2</sup>; David Fenyö<sup>1</sup>; Matthias Muellenbeck<sup>3</sup>; Hedda Wardemann<sup>3</sup>; Beatrix Ueberheide<sup>1</sup>; <sup>1</sup>*New York University Langone Medical*

*Center, New York, NY*; <sup>2</sup>*Protein Metrics, San Carlos, CA*; <sup>3</sup>*Max Planck Institute for Infection Biology, Berlin, Germany*

- ThOB pm 3:50 **Exploring *Neisseria meningitidis* Virulence with Top-Down Mass Spectrometry;** Joseph Gault<sup>1</sup>; Christian Malosse<sup>4</sup>; Marie-Cécile Ploy<sup>3</sup>; Catherine E. Costello<sup>2</sup>; Guillaume Duménil<sup>3</sup>; Julia Chamot-Rooke<sup>4</sup>; <sup>1</sup>*Institut Pasteur, Paris, France*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*; <sup>3</sup>*Hôpital Européen G. Pompidou, INSERM, Paris, France*; <sup>4</sup>*Institut Pasteur, CNRS, Paris, France*; <sup>5</sup>*CHU Limoges, INSERM, Limoges, France*
- ThOB pm 4:10 **A Systems Biology Approach for the Discovery of Drug and/or Vaccine Targets in *Plasmodium falciparum* using Irradiated Long-Lived Merozoites;** Krishan Kumar<sup>1</sup>; Prakash Srinivasan<sup>2</sup>; Michael J. Nold<sup>3</sup>; Dan Sturdevant<sup>4</sup>; J. Kathleen Moch<sup>5</sup>; Karine Reiter<sup>1</sup>; Steve F. Porcella<sup>4</sup>; Scott Geromanos<sup>3</sup>; Julian C. Rayner<sup>6</sup>; J. David Haynes<sup>5</sup>; David L. Narum<sup>1</sup>; <sup>1</sup>*LMIV, NIAID, NIH, Rockville, MD*; <sup>2</sup>*LMVR, NIAID, NIH, Rockville, MD*; <sup>3</sup>*Waters Corporation, Milford, MA*; <sup>4</sup>*RTB, NIAID, NIH, Hamilton, MT*; <sup>5</sup>*Walter Reed Army Institute of Research, Silver Spring, MD*; <sup>6</sup>*Wellcome Trust Sanger Institute, Hinxton, Cambridge, UK*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
LIPIDS AND PROFILING  
David Goodlett (University of Maryland), presiding  
Ballroom B**

- ThOC pm 2:30 **Novel Application of Reversed-Phase UHPLC–QTOFMS for Comprehensive Analysis of Plasma Lipids;** Tomas Cajka; William Wikoff; Carlos Leon; Brian DeFelice; Dmitry Grapov; Oliver Fiehn; *University of California, Davis, CA*
- ThOC pm 2:50 **Lipidomic Profiling of Commensal Microbe *Bacteroides Fragilis* and Identification of Immunomodulatory Sphingolipids;** Sungwan Oh; Dingding An; Fikri Avci; Dennis Kasper; *Harvard Medical School, Boston, MA*
- ThOC pm 3:10 **High-Throughput Lipid Profiling System for Dried Plasma Spots using Online-Supercritical Fluid Extraction-Supercritical Fluid Chromatography/ Mass Spectrometry;** Takeshi Bamba; Takato Uchikata; Atsuki Matsubara; Eiichiro Fukusaki; *Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, Japan*
- ThOC pm 3:30 **Gas-Phase Transformation of Phosphatidylcholine Cations to Structurally Informative Anions via Ion/Ion Chemistry;** John Stutzman<sup>1</sup>; Stephen Blanksby<sup>2</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of Wollongong, Wollongong, Australia*
- ThOC pm 3:50 **Long-Term Performance and Stability of Shotgun Lipidomic Analysis of Human Plasma Samples;** Laura Heiskanen; Kirill Tarasov; Hung Xuan Ta; Tuulia Sylvänne; Helena Simolin; Dimple Kauhanen; Kim Ekroos; *Zora Biosciences Oy, Espoo, Finland*
- ThOC pm 4:10 **Nanomanipulation-Coupled to Mass Spectrometry for Direct Organelle Analysis to Explore Lipid Localization Chemistry within Single Cells;** Kristina Clemons<sup>1</sup>; Sheida Torabi<sup>2</sup>; Huanbiao Mo<sup>2</sup>; Guido Verbeck<sup>1</sup>; <sup>1</sup>*Univ. of North Texas, Denton, TX*; <sup>2</sup>*Texas Women's University, Denton, TX*



**2:30 – 4:30 PM, THURSDAY AFTERNOON  
BIOMARKERS IN DRUG DISCOVERY AND DEVELOPMENT**  
Chandra Prakash (Biogen Idec), presiding  
Ballroom A

- ThOD pm 2:30 **Challenges and Considerations for Multi-component LC/MS Biomarker Assays: Lysophosphatidic Acids as Biomarkers;** Petia Shipkova; Joelle Onorato; Michael Furlong; Anne Minnich; *Bristol Myers Squibb, Princeton, NJ*
- ThOD pm 2:50 **LC-MS Strategies for Separation and Detection of Endogenous Organic Acids and Polar Metabolites in Pharmaceutical R&D;** David Pirman; Matthew Blatnik; *Pfizer, Groton, CT*
- ThOD pm 3:10 **The “Off Targets” of Angiotensin Converting Enzyme – A Peptidomic Approach;** Teresa B. Hong<sup>1</sup>; Gabriel B. Gugiu<sup>1</sup>; Tea Janjulia<sup>2</sup>; Kenneth E. Bernstein<sup>2</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>*City of Hope, Duarte, CA*; <sup>2</sup>*Cedars-Sinai Medical Center, Los Angeles, CA*
- ThOD pm 3:30 **LC/SRM Reveals Amyloid-Beta Isoforms’ Metabolic Differences and Diurnal Fluctuations in Alzheimer’s Disease;** Kwasi Mawuenyega; Vitaliy Ovod; Tom Kasten; Yafei Huang; Wendy Sigurdson; Randall Bateman; *Washington University School of Medicine, Saint Louis, MO*
- ThOD pm 3:50 **Using Mass Spectrometry to Identify a Novel Protein Responsible for Adrenal Amyloidosis;** Stephanie M. Cologna; Mitra L. Rauschecker; Peter S. Backlund; Robert D. Shamburek; James E. Balow; Alfred L. Yergey; Constantine A. Stratakis; Smita B. Abraham; *National Institutes of Health, Bethesda, MD*
- ThOD pm 4:10 **Development and Qualification of a Multiplexed Selected Reaction Monitoring-Mass Spectrometry Based Assay for Evaluation of Candidate Alzheimer’s Disease Progression Markers;** Daniel S. Spellman<sup>1</sup>; Weixun Wang<sup>1</sup>; Katie Southwick<sup>2</sup>; Rachel Korn<sup>1</sup>; Ronald A. Miller<sup>1</sup>; Mary J. Savage<sup>1</sup>; Daniel J. Holder<sup>1</sup>; Nathan A. Yates<sup>3</sup>; Ronald C. Hendrickson<sup>4</sup>; Bonnie J. Howell<sup>1</sup>; <sup>1</sup>*Merck and Co., Inc., West Point, PA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*University of Pittsburgh, Pittsburgh, PA*; <sup>4</sup>*Memorial Sloan-Kettering Cancer Center, New York, NY*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
PLANT“OMICS”**  
Michelle Cilia (US Department of Agriculture), presiding  
Auditorium

- ThOE pm 2:30 **An Overview of Label-Free Quantitative Shotgun Proteomics in Rice and Grapevines;** Paul A. Haynes<sup>1</sup>; Karlie Neilson<sup>1</sup>; Mehdi Mirzaei<sup>1</sup>; Iniga George<sup>1</sup>; Shila Shabshazian<sup>1</sup>; C. Gayani Gammulla<sup>1</sup>; Steve Van Sluyter<sup>1</sup>; Brian Atwell<sup>1</sup>; G. Hosseini Salekdeh<sup>2</sup>; Anne Fennell<sup>3</sup>; Grant Cramer<sup>4</sup>; <sup>1</sup>*Macquarie University, North Ryde, Sydney, Australia*; <sup>2</sup>*Agricultural Biotechnology Institute of Iran, Tehran, Iran*; <sup>3</sup>*South Dakota State University, Brookings, SD*; <sup>4</sup>*University of Nevada, Reno, NV*
- ThOE pm 2:50 **Integrating the Malting Barley Metabolome, Phenome and Genome using a Novel Non-Targeted UPLC-MS Metabolomics Workflow;** Adam Heuberger<sup>1</sup>; Corey Broeckling<sup>1</sup>; Kaylyn Kirkpatrick<sup>1</sup>; Gary Hanning<sup>2</sup>; Jessica Prenni<sup>1</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*Anheuser-Busch, Inc., St. Louis, MO*

- ThOE pm 3:10 **Improving the Identification Rate of Data Independent Label-Free Quantitative Analysis: A Proteomics Case Study on Apple Fruit;** Kim Buts<sup>1</sup>; Sebastien Carpentier<sup>2,3</sup>; Servaas Michielssens<sup>4</sup>; Eisuke Hayakawa<sup>5</sup>; Maarten Hertog<sup>1</sup>; Bart Nicolaï<sup>1</sup>; <sup>1</sup>*BIOST-MeBioS, KU Leuven, Heverlee, Belgium*; <sup>2</sup>*SYBIOMA, KU Leuven, Leuven, Belgium*; <sup>3</sup>*BIOST-Crop biotechnics, KU Leuven, Heverlee, Belgium*; <sup>4</sup>*Quantum and Physical Chemistry Section, KU Leuven, Heverlee, Belgium*; <sup>5</sup>*Research Group of Functional Genomics & Proteomics, Leuven, Belgium*
- ThOE pm 3:30 **A Novel GC/quadrupole-Orbitrap for Untargeted Metabolomics and Combined Multi-Omics Analysis of Symbiosis in *Medicago truncatula*;** Allison J. Balloon<sup>1</sup>; Amelia C. Peterson<sup>2</sup>; Jens Griep-Raming<sup>2</sup>; Christopher M. Rose<sup>1</sup>; Benjamin Minkoff<sup>1</sup>; Muthusubramanian Venkateshwara<sup>1</sup>; Jeremy Volkening<sup>1</sup>; Derek J. Bailey<sup>1</sup>; Paul A. Grimsrud<sup>1</sup>; Junko Maeda<sup>1</sup>; Michael S. Westphall<sup>1</sup>; Michael R. Sussman<sup>1</sup>; Jean-Michel Ané<sup>1</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*The University of Wisconsin, Madison, WI*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- ThOE pm 3:50 **Dissect Snf1-Related Protein Kinases (SnRKs) Signaling Network in the Abscissic Acid (ABA) Pathway-based on Kinase Assay Linked Phosphoproteomics;** Liang Xue<sup>1</sup>; Pengcheng Wang<sup>2</sup>; Jian-kang Zhu<sup>2</sup>; W. Andy Tao<sup>1</sup>; <sup>1</sup>*Biochemistry, Purdue University, West Lafayette, IN*; <sup>2</sup>*Horticulture & Landscape Architecture, Purdue Univ, West Lafayette, IN*
- ThOE pm 4:10 **Using Formaldehyde Crosslinking and Label-Free LC/MS/MS Quantification to Develop an LRR RLK Interactome in *Arabidopsis thaliana*;** Tara Nash; Kevin Blackburn; Steven Clouse; Michael B. Goshe; *North Carolina State University, Raleigh, NC*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
POLYMER-AND PACKAGING-RELATED CONTAMINANTS AND DEGRADANTS IN FOOD, DRUGS, AND CONSUMER PRODUCTS**  
David Stranz (Sierra Analytics, Inc.) and Luke Ackerman (FDA Center for Food Safety), presiding  
Room 101

- ThOF pm 2:30 **Migration and Identification of Leachables from Drug Product Container Closure Systems; Case Studies;** Alan Hendrick; James Mclean; Thomas Feinberg; *Catalent Pharma Solutions, Morrisville, NC*
- ThOF pm 2:50 **Analysis of Thermoplastic Copolymers by Mild Thermal Degradation Coupled to Ion Mobility Mass Spectrometry;** Nadrah Alawani; Chrys Wedemiotis; *The University of Akron, Akron, OH*
- ThOF pm 3:10 **Transformation Products of Packaging Additives as Leachables in Ophthalmic Drug Products;** Christopher Houston; *Bausch & Lomb, Rochester, NY*
- ThOF pm 3:30 **Leachable and Extractable Analysis of IV Bag by HR-LCMS, GCMS, and ICPMS ,** Kate Comstock; Ekong Bassey; John Schmelzel; *Thermo Fisher Scientific, San Jose, CA*
- ThOF pm 3:50 **Determination of Ultra Low Level Leachable Components from Permanent Implantable Medical Devices, Using Stir Bar Sorptive Extraction and GC-MS/MS Detection;** Gyorgy Vas; Barbara Armstrong; Lori Alquier; *Johnson and Johnson Company, Raritan, NJ*



## THURSDAY AFTERNOON ORAL SESSIONS

ThOF pm 4:10 **The Composition of d- $\alpha$ -Tocopheryl Polythylene Glycol Succinate: A Different View from FTICR Tandem MS;** Juan Wei<sup>1</sup>; Anthony Bristow<sup>2</sup>; Eileen McBride<sup>2</sup>; Peter O'Connor<sup>1</sup>; <sup>1</sup>*University of Warwick, Coventry, UK*; <sup>2</sup>*AstraZeneca UK Limited, London, UK*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN SAMPLE  
PREPARATION AND MS INTERFACE DESIGN**  
**Michael McGinley (Phenomenex), presiding**  
**Room 102**

ThOG pm 2:30 **Novel Analytical Methods for the On-Line Analysis of the Primary Products of Fast Pyrolysis of Cellulose and their Manipulation;** Matthew Hurt; John Degenstein; Piotr Gamecki; David Borton; Nelson Vinuesa; Rakesh Agrawal; Nicholas Delgass; Fabio Ribeiro; Hilka Kentamaa; *Purdue University, West Lafayette, IN*

ThOG pm 2:50 **Pyrolysis and Reactive Pyrolysis GCMS Investigation of Intractable Deposits and Spent Catalysts;** Michael T. Cheng; *Chevron Research, Richmond, CA*

ThOG pm 3:10 **A High Resolution Mass Spectrometry Platform for Studying Kinetics of Biomass Pyrolysis: Single Particle Pyrolysis Utilizing  $\mu$ Py-APCI-TOF;** Erica Smith; Carolyn Hutchinson; D. Paul Cole; Young-Jin Lee; *Chemistry Department, Iowa State University, Ames, IA*

ThOG pm 3:30 **Chemical Characterization and Molecular Weight Distribution from Distillation Products of Colombian Crude Oils by MALDI TOF-TOF;** Enrique Mejía Ospino<sup>1</sup>; Rafael Cabanzo<sup>1</sup>; Diana Catalina Palacio Lozano<sup>1</sup>; Jorge Armando Orrego<sup>2</sup>; Neisy Calderon<sup>1</sup>; <sup>1</sup>*Universidad Industrial de Santander, Bucaramanga, Colombia*; <sup>2</sup>*Ecopetrol, Bucaramanga, Colombia*

ThOG pm 3:50 **Structural Diversity of Petroporphyrins Isolated from Natural Petroleum Seeps and Weathered Oil by FT-ICR MS;** Amy McKenna<sup>1</sup>; Christoph Aeppli<sup>2</sup>; David Valentine<sup>3</sup>; Huan Chen<sup>1</sup>; Ryan Rodgers<sup>1</sup>; Robert Nelson<sup>2</sup>; David Podgorski<sup>1</sup>; Karin Lemkau<sup>2</sup>; Christopher Reddy<sup>2</sup>; Steven Rowland<sup>1</sup>; Winston Robbins<sup>1</sup>; Alan Marshall<sup>1</sup>; Nathan Kaiser<sup>1</sup>; <sup>1</sup>*Natl High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*Woods Hole Oceanographic Institute, Woods Hole, MA*; <sup>3</sup>*University of California, Santa Barbara, CA*

ThOG pm 4:10 **Studying Crude Oil Samples with Normal-Phase HPLC Coupled to Atmospheric Pressure Laser Ionization FT-ICR MS: Selective Analysis of Nitrogen Compounds;** Wolfgang Schrader<sup>1</sup>; Sami Lababidi<sup>1</sup>; Saroj Panda<sup>1</sup>; Jan T. Andersson<sup>2</sup>; <sup>1</sup>*Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany*; <sup>2</sup>*University Münster, Münster, Germany*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
HISTORY:  
CELEBRATION OF 100<sup>TH</sup> ANNIVERSARY OF  
MASS SPECTROMETRY**  
**Mike Grayson, presiding**  
**Room 103**

ThOH pm 2:30 **Mass Spectrometry in Russia: From Static Instruments to Electrospray;** Lidia Gall; *Institute of Analytical Instrumentation, Saint Petersburg, Russia*

ThOH pm 2:50 **More than 100 years of Mass Spectrometry – Developments in Germany;** Simone Koenig; *University of Muenster, Muenster, Germany*

ThOH pm 4:10 **The More than Sixty-Year History of Mass Spectrometry in Japan;** Yoshinao Wada; *Osaka MCHRI / Osaka University, Osaka, Japan*

ThOH pm 4:30 **J.J. Thomson, Kenneth Bainbridge, and Special Relativity;** Robert K. Boyd; *National Research Council, Vancouver, Canada*

ThOH pm 4:50 **Promoters as Catalysts of the Advance of Mass Spectrometry;** Keith Nier

ThOH pm 5:10 **The Crucial Roles of Mass Spectrometry in the Manhattan Project;** Keith Nier<sup>1</sup>; A. Karl Yergey<sup>2</sup>; Alfred L. Yergey<sup>3</sup>; <sup>1</sup>*Independent, Madison, NJ*; <sup>2</sup>*Educator, Hagerstown, MD*; <sup>3</sup>*NIH, Bethesda, MD*

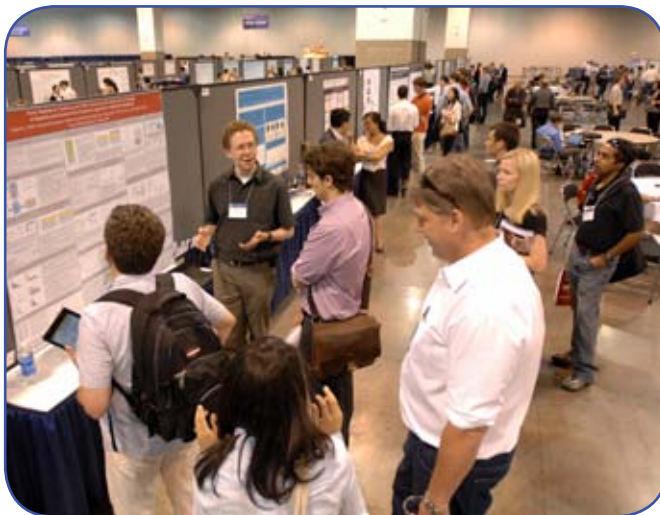
**4:45 - 5:30 PM, THURSDAY  
PLENARY LECTURE**  
**Jenny Brodbelt (University of Texas), presiding**  
**Exhibit Hall A, Lower Level**



**Discovery of the Elusive Higgs Boson**

**Peter Onyisi**  
University of Texas at Austin

**5:45 - 9:00 PM, THURSDAY AFTERNOON  
TIME TO CELEBRATE  
CLOSING GALA (ticket required)  
FOOD, CASH BAR, FUN AND GAMES**  
**Exhibit Hall D**





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

Small Molecules: Quantitative Analysis I.....	001-030
Drug Metabolism: High Throughput Analysis.....	031-040
Metabolomics: Identification of Unknown Metabolites.....	041-059
Metabolomics: Untargeted Metabolite Profiling (Methods).....	060-080
Metabolomics: Sample Preparation.....	081-084
LC-MS: Chromatography.....	085-130
LC-MS: Sample Preparation (Small Molecules).....	131-150
MALDI Sample Preparation.....	151-167
Diagnostic Clinical Chemistry: Peptides/Proteins.....	168-182
Imaging MS: Disease Markers.....	183-206
Lipids General.....	207-220
Lipids: Identification and Structural Analysis.....	221-232
Nucleic Acids: General.....	233-250
Nucleic Acids: RNA.....	251-262
Instrumentation: New Developments in Ionization and Sampling.....	263-293

Instrumentation: New Developments in Mass Analyzers.....	294-329
Ambient Ionization: Instrumentation.....	330-356
Informatics: General.....	357-373
Informatics: Workflow and Data Management.....	374-386
Informatics: Crosslinking and Structure Analysis.....	387-392
Crosslinking.....	393-412
H/D Exchange: Protein Structure/Function.....	413-440
Proteins: General.....	441-462
New Advances in Quantitative Proteomics.....	463-493
Protein Therapeutics: Quantitative Analysis.....	494-521
Biomarker Quantitation: Proteins and Peptides.....	522-549
Biomarker Discovery: Cancer.....	550-567
Immunology.....	568-575
Molecular Systems Biology and Disease.....	576-603
Forensics.....	604-628
Environmental Analysis: General I.....	629-652
Plant"omics".....	653-671
Agriculture.....	672-682
Natural Products.....	683-714
Astrobiology & Atmospheric Chemistry.....	715-720
Polymers.....	721-749

These posters will be displayed Monday through Thursday

- Museum **From Radio Tube Cathodes to Cells in Mitosis: The Evolution of Secondary Ion Mass Spectrometry (SIMS) Instrumentation and Applications;** P. Jane Gale<sup>1</sup>; Bryan L. Bentz<sup>2</sup>; <sup>1</sup>Gale-Bentz Consulting, Southborough, MA; <sup>2</sup>Waters Corporation, Milford, MA
- Special **2013 Ron Hites Award Recipient: First Combination of an Inductively Coupled Plasma Ion Source with Distance-of-Flight Mass Spectrometry (ICP-DOFMS);** Alexander Gundlach-Graham<sup>1</sup>; Elise A. Dennis<sup>1</sup>; Steven J. Ray<sup>1</sup>; Christie G. Enke<sup>2</sup>; Charles J. Barinaga<sup>3</sup>; David Koppenaal<sup>3</sup>; Gary Hieftje<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Department of Chemistry, University of New Mexico, Albuquerque, NM; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA
- Special **Ability of the Glycoproteomics Community to Profile N-glycosylation of Prostate Specific Antigen by Mass Spectrometry: An ABRF 2013 Interlaboratory Study;** Nancy Leymarie<sup>1</sup>; Paula Griffin<sup>1</sup>; Chuanhua Xing<sup>1</sup>; Karen Jonscher<sup>2</sup>; Daniel Kolarich<sup>3</sup>; Ron Orlando<sup>4</sup>; Mark McComb<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>CBMS, Boston University School of Medicine, Boston, MA; <sup>2</sup>Dept of Anesthesiology University of Colorado, Denver Aurora, CO; <sup>3</sup>Max Planck Institute of Colloids and Interfaces, Berlin, Germany; <sup>4</sup>CCRC, University of Georgia, Athens, GA

Small Molecules: Quantitative Analysis I, 001 - 030

- MP 001 **Lithium Adduct as Precursor Ion for Sensitive and Rapid Quantification of 20 (S)-protopanaxadiol in Rat Plasma by LC-MS/MS;** Yuanwu Bao<sup>1</sup>; Pingming Tang<sup>2</sup>; <sup>1</sup>Sundia MediTech Company Ltd., Shanghai, China; <sup>2</sup>Suzhou Kangrun Pharmaceutical Testing Service, Inc, Suzhou, China
- MP 002 **An Isomeric Impurity Caused Bioanalytical Data Discrepancy between +ESI and -ESI LC-MS/MS Quantification of a Drug Discovery Compound;** Guifen Xu; Tom Huang; Thuy Tran; Qiuping Ye; Lixia Jin; Timothy Carlson; Amgen, South San Francisco, CA
- MP 003 **Development of a Method for Evaluation of Mass Spectrometer Performance in Real Time;** Terry Olney; Huy Nguyen; Oleg Silivra; Thermo Fisher Scientific, San Jose, CA

- MP 004 **A Quantitative Inspection of ESI Glucuronide Degradation;** Jeffrey R. Enders; Cade Park; Ayodele Morris; Gregory McIntire; Ameritox, Ltd., Greensboro, NC
- MP 005 **Oxidation of Analytes during Positive Ion Electrospray Mass Spectrometric Analysis;** Luis Sojo; Navjot Chahal; Xenon Pharmaceutical, Burnaby, Canada
- MP 006 **Using Synthetic Sample Matrices to Optimize Ion Source Parameters and Evaluate Nozzle Geometry for Improved Quantitative Analysis of Small Molecules;** Craig Love; Alex Mordehai; Agilent Technologies, Inc, Santa Clara, CA
- MP 007 **Mass Spectrometric Analysis of Retinoid Binding Protein Receptor Substrate Specificity;** Riki Kawaguchi<sup>1</sup>; Ming Zhong<sup>2</sup>; Hui Sun<sup>2</sup>; <sup>1</sup>UCLA Physiology, Los Angeles, CA; <sup>2</sup>Howard Hughes Medical Institute, UCLA, Los Angeles, CA
- MP 008 **Impact of Immunosuppressant Interactions in LC-MS/MS Analysis;** Josh Cooper; Beth Marek; Isil Dilek; Uma Sreenivasan; Cerilliant, Round Rock, TX
- MP 009 **Secondary Crosstalk Case Report for Amprenavir and Darunavir in the LC-MS/MS Quantification Method of 15 Anti-retroviral Drugs Measured Simultaneously;** Denis Thibeault; Rose Djiana; David Blank; Royal-Victoria Hospital, Montreal, Canada
- MP 010 **Novel High-Throughput Bioanalysis for Basic Drug Candidates Formulated in PEG;** Ling Xu; Shaoxia Yu; Jing-Tao Wu; Millennium30 Pharmaceutical, Cambridge, MA
- MP 011 **Development and Validation of Methods for Chemotherapy Drugs on the New Prelude SPLC™ LC-MS/MS System;** Kerry Hassell; Dayana Argoti; Sarah Fair; Joseph Herman; ThermoFisher Scientific, Franklin, MA
- MP 012 **Validated Ultra-trace Quantification Method for Estrogens in Human Cerebrospinal Fluid using Bulk Derivatization and Restricted Access Media with LC-MS/MS;** Hui Fan<sup>1</sup>; Barbora Papoušková<sup>2</sup>; Jane Wigginton<sup>3</sup>; Karel Lemr<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>University of Texas Arlington, Arlington, TX; <sup>2</sup>Palacký University, Olomouc, Czech Republic; <sup>3</sup>University of Texas Southwestern Medical School, Dallas, TX
- MP 013 **Expanding the Linear Dynamic Range for Quantitative Liquid chromatography-High Resolution Mass Spectrometry Utilizing Natural isotopologue Signals;** Hanghui Liu<sup>1</sup>; Bert Chi<sup>1</sup>; Lily Lam<sup>1</sup>; Lin Yan<sup>1</sup>; Purnendu Dasgupta<sup>2</sup>; <sup>1</sup>Senomyx, San Diego, CA; <sup>2</sup>Dept of Chem & Biochem, UT Arlington, Arlington, TX

- MP 014 **Investigation on Internal Standard Response Variability during LCMSMS Analysis of Fesoterodine**; Nicolas Jean; Marie-Claude Théberge; Sylvain Lachance; Nadine Boudreau; Sofi Gagnon-Carignan; Ann Lévesque; *PharmaNet Canada, Québec, Canada*
- MP 015 **Deception in the Deuteriums: Errors Associated with Deuterated Internal Standards in LC-MS/MS Bioanalysis**; Brian Rappold; Audrey Harvey; Matthew Salske; Patrick Bell; Jennifer Andre; Michele Glinn; *Essential Testing, Collinsville, IL*
- MP 016 **Improved Assay Selectivity for the Determination of Hydroxymidazolam in Capillary Microsampling Extracts using LC-MS<sup>3</sup> on a Hybrid Linear Ion Trap**; Jeffrey Plomley; Mohamed Makhlofi; Alexandre Pimenov; *Charles River Laboratories, Senneville, Canada*
- MP 017 **Development and Validation of LC/MS/MS Method with Extra Small Injection Volume for Quantitative Determination of Alprazolam in Human Plasma**; Zhaoqi Zhan<sup>1</sup>; Jie Xing<sup>1</sup>; Gabriel Onn Kit Loh<sup>2</sup>; Kok Khian Peh<sup>2</sup>; <sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; <sup>2</sup>School of Pharmaceutical Sciences, Universiti Sain, Malaysia, Minden, Penang, Malaysia
- MP 018 **Determination of Diuretics in urine Using Multi-Walled Carbon Nanotubes Dispersive Solid Phase Extraction Combined with Liquid Chromatography-Tandem Mass Spectrometry**; Tse-Tsung Ho; Chung-Yu Chen; Maw-Rong Lee; *National Chung-Hsing University, Taichung, TAIWAN*
- MP 019 **TurbolonSpray vs. APCI for the Determination of Furosemide in Human Plasma by LCMSMS**; Jason Bilodeau; Marie-Claude Théberge; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 020 **Importance of Assessing Whole Blood Stability during Validation of Serum and Plasma LCMSMS Methods**; Sylvain Lachance; Nadine Boudreau; Sofi Gagnon-Carignan; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 021 **Interferences from Borosilicate Laboratory Material: Investigation and Application to LC-MS/MS Bioanalysis of Valproic Acid**; Pierre-Yves Caron; Nathalie Pelletier; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 022 **Ultra Low Limit of Detection of Mometasone Furoate in Human Plasma by UPLC-MS/MS**; Pierre-Yves Caron; Nicolas Jean; Marie-Claude Théberge; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 023 **Investigation of Long-Term Stability of Rabepazole Thioether Metabolite and Its Impact on Rabepazole Quantitation**; Sébastien Gagné; François Viel; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 024 **Hemolysis and Matrix Effect Issues during Method Development of Promethazine in Human Plasma**; Eric Morin; Nathalie Pelletier; Sylvain Lachance; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Quebec, Canada*
- MP 025 **Comparison of LDTD-MSMS and LCMSMS for the Determination of Testosterone in Human Serum**; Sylvain Lachance<sup>1</sup>; Nadine Boudreau<sup>1</sup>; Ann Lévesque<sup>1</sup>; Serge Auger<sup>2</sup>; Pierre Picard<sup>2</sup>; <sup>1</sup>PharmaNet Canada, Quebec, Canada; <sup>2</sup>Phytronix Technologies, Québec, Canada
- MP 026 **Low Detection Limit and Stability Issues during Method Development of Apomorphine in Human Plasma**; Guy Havar; Marie-Claude Théberge; Nadine Boudreau; Ann Lévesque; *PharmaNet Canada, Québec, Canada*
- MP 027 **Analysis of Ocular Tissues: Investigation of Potential Matrix Effects**; Vikki Tsefrikas; Dylan Bennett; Kyle Goodsell; Allysen Meymaris; *Agilux Laboratories, Worcester, MA*

- MP 028 **Effect of Special Population Matrices on Quantitation of Drugs with Wide Range of Plasma Protein Binding Levels Using LC-MS/MS Method**; Dongmei Zhou; David Wilson; Mai Nguyen; Erin Harmon; Kyle Nishikawa; Li-Tain Yeh; *Ardea Biosciences, San Diego, CA*
- MP 029 **Ion Suppression in Rat Brain Due to Phospholipids and Its Impact on Sensitivity and Electrospray Response Function for Small Molecules**; Navjot Chahal; Luis Sojo; *Xenon Pharmaceuticals, Burnaby, Canada*
- MP 030 **Improving the Sensitivity, Precision and Accuracy of PGIs Analysis by LC-MS**; Peng Wang; Alwyn Forbes; Naijun Wu; *Celgene Corporation, Summit, NJ*

**Drug Metabolism: High Throughput Analysis, 031 - 040**

- MP 031 **Computer Assisted Metabolite Identification, Application in Cytochrome Reaction Phenotyping**; Esra Nurten Cece<sup>1</sup>; Kristen Eickhoff<sup>2</sup>; Andreas Brink<sup>2</sup>; Ismael Zamora<sup>3</sup>; Axel Paehler<sup>2</sup>; <sup>1</sup>Pompeu Fabra University, Barcelona, Spain; <sup>2</sup>F. Hoffmann-La Roche Ltd, Basel, Switzerland; <sup>3</sup>Molecular Discovery, London, UK
- MP 032 **Combining *in vitro* Intrinsic Clearance and Metabolic Soft Spot Identification in Early Drug Discovery**; Marina Slavsky<sup>1</sup>; Keeley Murphy<sup>2</sup>; Ismael Zamora<sup>3</sup>; Thomas O'Shea<sup>1</sup>; Maria Fitzgerald<sup>1</sup>; <sup>1</sup>DMPK, Sanofi, Waltham, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Lead Molecular Design, Barcelona, Spain
- MP 033 **Integrating Qualitative and Quantitative Measures across HRMS and Qtrap MS Platforms in Early Stage Metabolic Stability Screening in Drug Discovery**; Jianhua Liu<sup>1</sup>; Veronica A. Zelesky<sup>1</sup>; Anthony J. Romanelli<sup>2</sup>; Loren Y. Olson<sup>2</sup>; John S. Janiszewski<sup>1</sup>; <sup>1</sup>Pfizer, Inc, Groton, CT; <sup>2</sup>AB Sciex, Framingham, MA
- MP 034 **Differential Mobility Spectrometry as a Measure of Physicochemical Properties Related to *in vitro* Absorption (Permeability, Solubility and Lipophilicity)**; John Janiszewski<sup>1</sup>; Yves LeBlanc<sup>2</sup>; Bradley Schneider<sup>2</sup>; Tom Covey<sup>2</sup>; George Chang<sup>1</sup>; Charles Rotter<sup>1</sup>; Manthena Varma<sup>1</sup>; Troutman Matthew<sup>1</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>AB Sciex, Concord, Ontario, Canada
- MP 035 **Microsampling Method Using 1 µL of Human Blood to Determine Pharmacokinetic Parameters of Dextrophan Using LDTD-MS/MS**; Jean Lacoursiere; Annick Dion; Serge Auger; Pierre Picard; *Phytronix Technologies, Quebec City, Canada*
- MP 036 **A High-Throughput, Accurate-Mass Approach for Plasma Protein Binding Analysis Using SPE/TOF-MS**; Kari Schlicht; Vaughn Miller; William LaMarr; Can Ozbai; *Agilent Technologies, Wakefield, MA*
- MP 037 **Determination of a DGAT1 Inhibitor in Human Plasma Using microLC-MS/MS: Comparison of microLC vs. Conventional LC Methods for Bioanalysis**; Tapán Majumdar; Shari Wu; Adam Bentley; Jimmy Flarakos; *Novartis Pharmaceuticals Corporation, East Hanover, NJ*
- MP 038 **Reducing Gradient Cycle Time for Increased Throughput Using Dual-Stream LC/MS/MS Bioanalysis**; Mary Piotrowski<sup>1</sup>; Carrie Funk<sup>1</sup>; John Janiszewski<sup>1</sup>; Hui Zhang<sup>1</sup>; Brendon Kapinos<sup>1</sup>; Anthony Romanelli<sup>2</sup>; <sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>AB Sciex, Framingham, MA
- MP 039 **Optimizing High-Throughput LC/MS/MS "trap-and-elute" Bioanalysis in Drug Discovery**; Brendon Kapinos<sup>1</sup>; John Janiszewski<sup>1</sup>; Mary Piotrowski<sup>1</sup>; Hui Zhang<sup>1</sup>; Carrie Funk<sup>1</sup>; Wayne Lootsma<sup>2</sup>; Will Schramm<sup>2</sup>; <sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>Sound Analytics, Niantic, CT
- MP 040 **Development of High Speed CYP Cocktail Inhibition Assay Using UHPLC-MS/MS**; Ichiro Hirano; Miho Kawashima; Natsuyo Asano; Kiyomi Arakawa; Yoshihiro Hayakawa; *Shimadzu Corporation, Kyoto, Japan*

**Metabolomics: Identification of Unknown Metabolites, 041-059**

- MP 041 **Improved Unknown Metabolite Identification by Combining Smart Isotope Tags and Ratio Analysis MS and NMR Heterospectroscopy**; G. A. Nagana Gowda<sup>1</sup>; Haiwei Gu<sup>1</sup>; Fariba Tayyari<sup>2</sup>; Daniel Raftery<sup>1,3</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Purdue University, West Lafayette, IN; <sup>3</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 042 **Metab-ID: An Automated Tool for Metabolite Identification from MS1 Data**; T. Mamie Lih<sup>1</sup>; Ke-Shiuan Lynn<sup>1</sup>; Hui-Yin Chang<sup>1</sup>; Mei-Ling Cheng<sup>2</sup>; Ming-Shi Shiao<sup>2</sup>; Wen-Harn Pan<sup>3,4</sup>; Ting-Yi Sung<sup>1</sup>; Wen-Lian Hsu<sup>1</sup>; <sup>1</sup>Institute of Information Science, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Chang Gung University, Taoyuan, Taiwan; <sup>3</sup>National Health Research Institutes, Mialoli, Taiwan; <sup>4</sup>Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan
- MP 043 **Annotation and Identification of Fragmentation of Known Metabolites and Elucidation of Possible Known Unknowns with Fragmentation Analysis**; Hongping Dai; Annie Evans; Corey DeHaven; *Metabolon, Durham, NC*
- MP 044 **Automated Compound Identification Using Product Ion Scanning with Accurate Mass Measurement and Compound Database Searching for Non-Targeted Metabolomics**; Tairo Ogura<sup>1,2</sup>; Faith Hays<sup>3</sup>; Takeshi Bamba<sup>1</sup>; Eiichiro Fukusaki<sup>1</sup>; <sup>1</sup>Graduate School of Engineering, Osaka University, Osaka, Japan; <sup>2</sup>Shimadzu corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD
- MP 045 **A Platform to Identify Endogenous Metabolites Using a Novel High Performance Orbitrap and the m/zCloud Library**; Junhua Wang<sup>1</sup>; David Peake<sup>1</sup>; Robert Mistrík<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific Inc, San Jose, CA; <sup>2</sup>HighChem, Ltd., Bratislava, Slovakia
- MP 046 **Utilization of Metabolic Network Information for Improved Metabolite Identification by LC-MS**; Bin Zhou; Habtom Resson; *Georgetown University, Washington, DC*
- MP 047 **Testing the Limits of a New, Extremely Accurate HPLC Retention Prediction Methodology (www.retentionprediction.org)**; Allison Haaning; Jonathan Schellenberg; Paul Boswell; *University of Minnesota, Saint Paul, MN*
- MP 048 **The Ideal Stationary Phase for an HPLC Retention Database**; Joseph Manulik; Paul Boswell; *University of Minnesota, St. Paul, MN*
- MP 049 **An Inter-Laboratory Study on a New, Extremely Accurate Retention Prediction Methodology for GC-MS (www.retentionprediction.org)**; Brian Barnes<sup>1</sup>; Michael Wilson<sup>1</sup>; Panhia Yang<sup>1</sup>; Mark Vihta<sup>2</sup>; Amanda Tawfall<sup>3</sup>; Lloyd Sumner<sup>6</sup>; Adam Heuberger<sup>3</sup>; Corey Broeckling<sup>3</sup>; Jessica Prenni<sup>3</sup>; Henry Corcoran<sup>4</sup>; Gregory Janis<sup>4</sup>; Shilpi Chopra<sup>5</sup>; Nicholas Snow<sup>5</sup>; Paul Boswell<sup>1</sup>; <sup>1</sup>University of Minnesota, St. Paul, MN; <sup>2</sup>Drake University, Des Moines, IA; <sup>3</sup>Colorado State University, Fort Collins, CO; <sup>4</sup>Medtox Scientific, Inc., St. Paul, MN; <sup>5</sup>Seton Hall University, South Orange, NJ; <sup>6</sup>Samuel Roberts Noble Foundation, Ardmore, OK
- MP 050 **'Sequencing' the First Plant Metabolome, and the Systematic Annotation of the Metabolic Composition of the Model Legume *Medicago truncatula***; Lloyd Sumner<sup>1</sup>; Zhentian Lei<sup>1</sup>; Dennis Fine<sup>1</sup>; Daniel Wherritt<sup>1</sup>; David Huhman<sup>1</sup>; Kota Kera<sup>2</sup>; Hidezaki Suzuki<sup>2</sup>; Kazuki Saito<sup>3</sup>; <sup>1</sup>The Samuel Roberts Noble Foundation, Ardmore, OK; <sup>2</sup>Kazusa DNA Research Institute, Chiba, Japan; <sup>3</sup>RIKEN Plant Science Center, Yokohama, Japan
- MP 051 **FT-ICR Based "Ultrafast Statistical Profiling": Myxobacterial Secondary Metabolite Profiling for Quickly Pinpointing and Identifying Marker Compounds**; Aiko Barsch<sup>1</sup>; Matthias Witt<sup>1</sup>; Christopher

Thompson<sup>2</sup>; Daniel Krug<sup>3</sup>; Thomas Hoffmann<sup>3</sup>; Rolf Mueller<sup>3</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonik Inc., Billerica, MA; <sup>3</sup>Helmholtz Institute for Pharmaceutical Research, Saarbruecken, Germany

- MP 052 **Defensive Chemistry: MS-based Characterization of Sesquiterpene Lactone - and Hydroxybenzeneacetic Acid-Derived Defensive Metabolites of *Taraxacum officinale* Root Latex**; Sven Heiling<sup>1</sup>; Meret Huber<sup>1</sup>; Andrea Kiehne<sup>2</sup>; Christian Paetz<sup>1</sup>; Michael Reichelt<sup>1</sup>; Sandy Yates<sup>3</sup>; Aiko Barsch<sup>2</sup>; Matthias Erb<sup>1</sup>; Jonathan Gershenzon<sup>1</sup>; Ian T. Baldwin<sup>1</sup>; <sup>1</sup>Max Planck Institute for Chemical Ecology, Jena, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Bruker Daltonics, Fremont, CA
- MP 053 **LC-MS/MS-based Structural Analysis of Novel Enniatins Produced by Canadian Strains of *Fusarium avenaceum* in Liquid Culture**; Azeret Zuniga<sup>1,2</sup>; Whyann Bosnich<sup>1</sup>; Kanak Bala<sup>1</sup>; Linda Harris<sup>1</sup>; Steve Gleddie<sup>1</sup>; Zoltan Mester<sup>2</sup>; <sup>1</sup>Agriculture and Agri-Food Canada, Ottawa, Canada; <sup>2</sup>National Research Council, Ottawa, Canada
- MP 054 **Online Study on Metabolites Profiles of Sixteen Clausenamide Enantiomers *in vitro* by Liquid Chromatography/Quadrupole Ion Trap/Time-of-Flight Mass Spectrometry**; Ma Chao<sup>1,2</sup>; Feng Ru<sup>1</sup>; Wang Yan<sup>1</sup>; Qiu xiongxiong<sup>2</sup>; <sup>1</sup>Chinese Academy of Medical Sciences, Beijing, China; <sup>2</sup>Shimadzu Global COE, Shimadzu (China) Co., Ltd., Beijing, China
- MP 055 **Profiling Biosynthetic Intermediates from *Camptotheca acuminata* Using Liquid Chromatography, Multiplexed Collision-Induced-Dissociation and Time-of-Flight Mass Spectrometry**; Sujana Pradhan; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 056 **Evidence for Glucuronide and Glutathione Conjugation of Glyceollins in Rats by On-Line Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry**; Syeda S. Quadri<sup>1</sup>; Robert E. Stratford<sup>2</sup>; Richard B. Cole<sup>1,3</sup>; <sup>1</sup>Dept. of Chemistry, Univ. Of New Orleans, New Orleans, LA; <sup>2</sup>College of Pharmacy, Xavier Univ., New Orleans, LA; <sup>3</sup>Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France
- MP 057 **The *in vitro* Study of the Metabolism of 3, 4-Methylenedioxymethamphetamine (MDMA) in Human Hepatocytes**; Chengan Du; *Hampton University, Hampton, VA*
- MP 058 **Metabolomics Approach to Determine A. *flavus* Cluster 27 Polyketide Synthase Metabolites: Evaluation of UHPLC-Orbitrap MS and micro-LC-tripleTOF**; José Diana Di Mavungu<sup>1</sup>; Svetlana V. Malysheva<sup>1</sup>; Natalia Aroyo-Manzanares<sup>2</sup>; Jeffrey W. Cary<sup>3</sup>; Kenneth C. Ehrlich<sup>3</sup>; Julie Vanden Bussche<sup>1</sup>; Lynn Vanhaecke<sup>1</sup>; Deepak Bhatnagar<sup>3</sup>; Sarah De Saeger<sup>1</sup>; <sup>1</sup>Ghent University, Ghent, Belgium; <sup>2</sup>University of Granada, Granada, Spain; <sup>3</sup>U.S. Department of Agriculture, New Orleans, LA
- MP 059 **NanoLC-MS/MS Metabolomics of Urinary Biomolecules Following Intake of Grape Seed Extract in a Rodent Model of Menopause**; John Cutts; Landon Wilson; Scott Sweeney; D. Ray Moore; Jeevan Prasain; Stephen Barnes; Helen Kim; *University of Alabama at Birmingham, Birmingham, AL*

**Metabolomics: Untargeted Metabolite Profiling (Methods), 060-080**

- MP 060 **Quality Control and Data Extraction Validation for High-Resolution Metabolomics**; Vilinh Tran<sup>1</sup>; Karan Uppal<sup>1</sup>; Milam Brantley<sup>2</sup>; Arshed Quyyumi<sup>1</sup>; Greg Gibson<sup>3</sup>; Dean Jones<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Georgia Institute of Technology, Atlanta, GA





- MP 061 **Global Characterization of SRM 1950 (Metabolites in Human Plasma) Using Liquid Chromatography-Mass Spectrometry;** Kelly H. Telu; William E. Wallace III; Stephen E. Stein; Yamil Simón-Manso; *NIST, Gaithersburg, MD*
- MP 062 **Sheathless Capillary Electrophoresis Mass Spectrometry: Investigation Using High Resolution Accurate Mass MS for Metabolome Analysis;** Junhua Wang<sup>1</sup>; John Hudson<sup>2</sup>; Maria Prieto Conaway<sup>1</sup>; David Peake<sup>1</sup>; Yingying Huang<sup>1</sup>; Andreas Huhmer<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific Inc, San Jose, CA*; <sup>2</sup>*Beckman Coulter, Inc., Brea, CA*
- MP 063 **Combination of Double Isotopic Labeling and High Resolution Mass Spectrometry: A Novel Method for Untargeted Fungal Metabolic Profiling;** Patricia M. Cano<sup>1,2</sup>; Emilien L. Jamin<sup>1,2</sup>; Souria Tadriss<sup>1,2</sup>; Pascal Bourdaudhui<sup>1,2</sup>; Michel Péan<sup>3,4</sup>; Laurent Debrauwer<sup>1,2</sup>; Isabelle P. Oswald<sup>1,2</sup>; Marcel Delaforge<sup>5</sup>; Olivier Puel<sup>1,2</sup>; <sup>1</sup>*INRA, Toxalim, Research Center in Food Toxicology, Toulouse, France*; <sup>2</sup>*Université de Toulouse, INP, Toxalim, Toulouse, France*; <sup>3</sup>*CEA, DSV, IBEB & CNRS Bio. Vég. et Microbio. Envir, Saint-Paul-les-Durance, France*; <sup>4</sup>*Aix-Marseille Université, Saint-Paul-les-Durance, France*; <sup>5</sup>*CEA Saclay, iBiTec-S, SB2SM and URA CNRS 8221, Gif sur Yvette, France*
- MP 064 **Evaluation of Different Dansylation Reaction Conditions for Isotope Labeling of Metabolites in Metabolome Profiling of Biological Samples;** Jared Curle; Liang Li; *University of Alberta - Department of Chemistry, Edmonton, Canada*
- MP 065 **Variety and Specificity of Granules in a Cell, Detected by Live Single-Cell Mass Spectrometry;** Yuki Yamamoto<sup>2</sup>; Tsuyoshi Esaki<sup>1</sup>; Hajime Mizuno<sup>1</sup>; Sachiko Date<sup>1</sup>; Naohiro Tsuyama<sup>2</sup>; Tsutomu Masujima<sup>1</sup>; <sup>1</sup>*Quantitative Biology Center (QBiC), Riken, Suita, Japan*; <sup>2</sup>*Hiroshima University, Hiroshima, Japan*
- MP 066 **Isotope Labeling Liquid Chromatography-Mass Spectrometry in Metabolite Biomarker Discovery for Mild Cognitive Impairment Disease;** Tran Tran; Roger A. Dixon; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 067 **xMSanalyzer: Automated Pipeline for Improved Feature Detection and Downstream Analysis of Large-Scale, Non-Targeted Metabolomics Data;** Karan Uppal<sup>1,2</sup>; Dean Jones<sup>1</sup>; <sup>1</sup>*Emory University, Atlanta, GA*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*
- MP 068 **An Improved Isotopic Labeling Protocol for LC-MS Metabolomic Profiling of Carboxylic Acids in Biofluids and Cell Extracts;** Jun Peng; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 069 **Understanding the Biology of Higher Organisms through GoogleMAPS-type Visualization of Specialized Metabolites Found to be Associated with Microbial Communities;** Pieter Dorrestein; Christopher Rath; Vanessa Phelan; Guo Yurong; Jeramie Watrous; Mingxun Wang; Robbie Quinn; Yan Wei Lim; Kathleen Dorrestein; Nuno Bandeira; Theodore Alexandrov; *University of California, San Diego, Skaggs school, La Jolla, CA*
- MP 070 **Novel Software Solutions for Liquid Chromatography-High Resolution MS (LC-HRMS) Metabolite Profiling of Legumes under Drought and Fungal Infection Conditions;** Michael Dickinson<sup>1</sup>; Martin Wells<sup>2</sup>; Mark Harrison<sup>1</sup>; Rosario Romero<sup>1</sup>; Adrian Charlton<sup>1</sup>; Jackson Pope<sup>2</sup>; <sup>1</sup>*The Food and Environment Research Agency, York, UK*; <sup>2</sup>*Nonlinear Dynamics, Newcastle upon Tyne, UK*
- MP 071 **Unexpected Complexity of In-Source Fragmentation: The Utility of Spectral Searching for Compound Annotation in Non-Targeted Metabolite Profiling Studies;** Corey Broeckling; Jessica Prenni; *Colorado State University, Fort Collins, CO*
- MP 072 **Metabolite Profiling and Metabolic Fingerprinting of Arabidopsis Mutants Using Atmospheric Pressure GC-MS<sup>E</sup> Approach and Multivariate Statistical Analysis;** Carolina Salazar; Nobuhiro Suzuki; Ron Mittler; Vladimir Shulaev; *University of North Texas, Denton, TX*
- MP 073 **Improved Methodology for Metabolomics Data Acquisition Workflow: Utilization of Electron Impact and Chemical Ionization High Resolution Time-Of-Flight Mass Spectrometry;** David Alonso; Joe Binkley; John Heim; *Leco Corporation, St. Joseph, MI*
- MP 074 **Rapid Clinical Biofluid Profiling with Rapid Evaporative Ionisation Mass Spectrometry;** Kate Leary; Sabine Guenther; Zoltán Takáts; *Imperial College London, London, UK*
- MP 075 **Comprehensive Liquid Chromatography Coupled to High Resolution Mass Spectrometry Methods for the Global Metabolic Profiling of Human Serum;** Samia Boudah<sup>1,2</sup>; Sandrine Aros-Calt<sup>1,3</sup>; Marie-Françoise Olivier<sup>1</sup>; François Fenaille<sup>1</sup>; Christophe Junot<sup>1</sup>; <sup>1</sup>*LEMM-CEA-Saclay, Gif-Sur-Yvette, France*; <sup>2</sup>*GlaxoSmithKline - Centre de recherche F.Hyafil, Villebon-sur-Yvette, France*; <sup>3</sup>*bioMérieux S.A, Chemin de l'Orme, Marcy l'Etoile, France*
- MP 076 **An Efficient Automated Dual pH Dual Polarity HILIC Based LC-MS Approach to the Analysis of the Metabolome;** James Cox; *University of Utah, Salt Lake City, UT*
- MP 077 **LC-HRMS Based Stable Isotopic Labeling-Assisted Metabolomics: Using MetExtract Software for the Global Characterization of the Plant Pathogenic Fungus *Fusarium graminearum*;** Christoph Büschl; Bernhard Kluger; Gerlinde Wiesenberger; Stefan Bödi; Romana Stücker; Joseph Strauss; Gerhard Adam; Rainer Schuhmacher; *University of Natural Resources and Life Sciences, Tulln, Austria*
- MP 078 **Utilization of GC-TOFMS for Metabolomics Using a Standardized Global Approach from Sample Preparation to Data Interpretation;** John R. Heim; Joe Binkley; David Alonso; *LECO Corporation, St. Joseph, MI*
- MP 079 **Isotopic Ratio Outlier Analysis (IROA) of Genetically Engineered *Myxococcus xanthus* Strains Using Ultra High Resolution Mass Spectrometry;** Daniel Krug<sup>1</sup>; Aiko Barsch<sup>2</sup>; Rolf Müller<sup>1</sup>; Chris Beecher<sup>3</sup>; Felice de Jong<sup>3</sup>; <sup>1</sup>*Helmholtz-Institute for Pharmaceutical Research, Saarbrücken, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*NextGen Metabolomics Inc, Ann Arbor, Michigan*
- MP 080 **MsCompare: An Untargeted GC/MS Metabolomics Platform for Quality Control and Accurate Deconvolution;** Claartje Van Der Kroft; *MsMetrix, Maarssen, Netherlands*
- Metabolomics: Sample Preparation, 081-084**
- MP 081 **Development of Isotope Labeling LC-MS for Metabolic Profiling of Bacterial Cells and Its Application for Bacterial Differentiation;** Yiman Wu; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 082 **Effective Extraction Method and Stable-Isotope Dansylation Labeling Combined with RPLC-FTMS for the Analysis of Arabidopsis Thaliana Metabolome;** Chiao-Li Tseng; Michael Deyholos; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 083 **Development of a Dilute-and-Shoot LC/MS/MS Method with 21 Opiates in Urine;** Simon Sheng; Kate Evans; Francois Espourteille; *Thermo, San Jose, CA*
- MP 084 **Metabolomics of *Elaeis guineensis* Leaves: From Optimization of the Sample Preparation Steps to Untargeted Metabolite Profiling Analysis;** Luiz Henrique Vargas<sup>2</sup>; José Antônio Ribeiro<sup>1</sup>; Daniel Sifuentes<sup>1</sup>;



Anselmo E. de Oliveira<sup>3</sup>; Manoel T. Souza Júnior<sup>1</sup>; Clenilson Rodrigues<sup>1</sup>; Patrícia Verardi Abdelnur<sup>1</sup>; *Embrapa Agroenergy, Brasília, Brazil; <sup>2</sup>Federal University of Lavras, Lavras, Brazil; <sup>3</sup>Federal University of Goiás, Goiânia, Brazil*

**LC-MS: Chromatography, 085-130**

- MP 085 **Development of a HILIC-MS/MS Method for Quantification of Decitabine in Human Plasma by Using Lithium Adducts**; Wenyi Hua; Michael Lesslie; Brian T. Hoffman; Daniel Mulvana; *Advion Bioanalytical Labs, a Quintiles Company, Ithaca, NY*
- MP 086 **LC-MS Separation Tuning for Polar Hydrophilic Metabolites on Complementary Zwitterionic HILIC Columns**; Tobias Jonsson<sup>1</sup>; Wen Jiang<sup>1</sup>; Anders Nordstrom<sup>2</sup>; Petrus Hemstrom<sup>1</sup>; Patrik Appelblad<sup>1</sup>; *<sup>1</sup>Merck SeQuant AB, Umeå, Sweden; <sup>2</sup>Umea University, Umea, Sweden*
- MP 087 **Separation Efficiency and Selectivity of Ultra Performance Columns for Hydrophilic Interaction Liquid Chromatography (HILIC)**; Wen Jiang; Lena Westin; Tobias Jonsson; *Merck SeQuant AB, Umeå, Sweden*
- MP 088 **Ibuprofen Chiral Resolution Improvement by Water/Acetonitrile Endotherm from LC-Pump Mixer**; Pierre-Yves Caron; Guy Havard; Nathalie Pelletier; Nadine Boudreau; Ann Lévesque; *PnarmaNet Canada, Québec, Canada*
- MP 089 **Evaluation of Polar-Embedded ODS Column in Supercritical Fluid Chromatography**; Chiaki Aoyama<sup>1</sup>; Takayuki Yamada<sup>2</sup>; Megumi Ishibashi<sup>2</sup>; Kensuke Okusa<sup>1</sup>; Masakazu Takahashi<sup>1</sup>; Masayoshi Ohira<sup>1</sup>; Eiichiro Fukusaki<sup>2</sup>; Takeshi Bamba<sup>2</sup>; *<sup>1</sup>GL Sciences Inc., Iruma, Japan; <sup>2</sup>Graduate School of Engineering, Osaka University, Suita, Japan*
- MP 090 **Mass-Directed Chiral SFC Separations Versus Asymmetric Synthesis in Drug Discovery**; Kanaka Hettiarachchi; *Theravance, South San Francisco, CA*
- MP 091 **A Multidimensional System for Phosphopeptide Analysis using TiO<sub>2</sub> Enrichment and Ion-Exchange Chromatography with Mass Spectrometry**; Kun Cho; Jisun Yoo; Eunmin Kim; Jong Shin Yoo; *KBSI, Ochang, South Korea*
- MP 092 **Quantitation of Adsorbed Plasma Proteins on Coated and Non-Coated PLGA (poly(lactic-co-glycolic acid)) Nanoparticles by LC-MALDI**; Tobias Schorge; Karim Sempf; Michael Karas; Jörg Kreuter; *Goethe-University Frankfurt, Frankfurt, Germany*
- MP 093 **Increasing Peak Capacities for Peptide Separations Using Long Microcapillary Columns and Sub 2 µm Particles at 30,000+ psi**; Kaitlin Fague; Justin Godinho; Edward Franklin; Jordan Stobaugh; James Jorgenson; *University of North Carolina, Chapel Hill, NC*
- MP 094 **High pH Reversed Phase and Isoelectric Focusing as Pre-fractionation Approaches for Complex Proteome Analysis**; Derek R Stein<sup>1</sup>; Xiaojie Hu<sup>2</sup>; Stuart J McCorrister<sup>2</sup>; Garrett R Westmacott<sup>2</sup>; Francis A Plummer<sup>1, 2</sup>; T Blake Ball<sup>1, 2</sup>; Michael S Carpenter<sup>1, 2</sup>; *<sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Public Health Agency of Canada, Winnipeg, CA*
- MP 095 **Understanding Separation Parameters For Intact Protein LC/MS Analysis Using Wide-Pore Core-Shell Media**; Michael McGinley; Jeff Layne; Jason Anspach; *Phenomenex, Torrance, CA*
- MP 096 **High Resolution LC-MS Peptide Separations with Formic Acid Mobile Phases Using Charge Surface Modified C18 Columns**; Matthew Lauber; Stephan Koza; Kenneth Fountain; *Waters Corporation, Milford, MA*
- MP 097 **In Depth Characterization of C18 and C18-like Solid Phase Extraction materials, Indented for Sub-Microgram Applications in Proteomic Workflows**; Lasse Falkenby<sup>1</sup>; Lena Haubro<sup>2</sup>; Nicolai Bache<sup>2</sup>; Martin R Larsen<sup>1</sup>; Jens S Andersen<sup>1</sup>; *<sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Thermo Scientific, Odense, Denmark*
- MP 098 **In-house Construction of a UHPLC System in Combination with Ti4+-IMAC aLLows Comprehensive (phospho)Proteomic Profiling**; Alba Cristobal; Marco L. Hennrich; Houjiang Zhou; Albert J.R. Heck; Shabaz Mohammed; *Biomolecular Mass Spectrometry and Proteomics Group, Utrecht, The Netherlands*
- MP 099 **Bio-Solid Phase Extraction and Information Dependent Tandem Mass Spectrometry for Deconvolution of Complex Mixtures**; Erica Forsberg; John Brennan; *McMaster University, Hamilton, Canada*
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- MP 118 **How to Accurately Measure Your HPLC Gradient with a Mass Spectrometer ([www.measureyourgradient.org](http://www.measureyourgradient.org));** Megan H. Magee; Brian B. Barnes; Joseph Manulik; Paul G. Boswell; University of Minnesota, St. Paul, MN
- MP 119 **Automated 2D UHPLC/MS Workflow on an EASY-nLC 1000;** Fabio Marino<sup>1</sup>; Alba Cristobal<sup>1</sup>; Peter A. Nielsen<sup>2</sup>; Nicolai Bache<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; <sup>1</sup>Biomolecular Mass Spectrometry and Proteomics Group, Utrecht, The Netherlands; <sup>2</sup>Thermo Fisher Scientific, Odense, Denmark
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- MP 128 **Intact Protein LC-MS, How to Overcome the Challenges?** Evert-Jan Sneekes<sup>1,2,3</sup>; Laurent Rieux<sup>1,2,3</sup>; Mauro De Pra<sup>1,2,3</sup>; Christian Ravensborg<sup>1,2,3</sup>; Dafydd Milton<sup>1,2,3</sup>; Remco Swart<sup>1,2,3</sup>; <sup>1</sup>Thermo Fisher Scientific, Amsterdam, Netherlands; <sup>2</sup>Thermo Fisher Scientific, Odense, Denmark; <sup>3</sup>Thermo Fisher Scientific, Runcorn, UK
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- MP 133 **Determination of Sulfonamide Residues in Whole Milk Using a Novel Lipid-Stripping Filtration Cartridge and LC/MS/MS;** Irina Dioumaeva; Agilent Technologies, Inc., Lake Forest, CA
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- Layne; Erica Pike; Stuart Kushon; Shahana Huq; Michael McGinley; *Phenomenex, Torrance, CA*
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- MP 171 **A novel Mass Spectrometry-Based Assay for the Accurate Measurement of Thyroglobulin from Patient Samples Containing Antithyroglobulin Autoantibodies;** Yanni Zhang; Nigel J. Clarke; Richard E. Reitz; *Quest Diagnostics, San Juan Capistrano, CA*
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- MP 173 **Quantitative Determination of Tamm-Horsfall Glycoprotein (THP, Uromodulin) in Urine Samples Using LC-MS/MS Analysis;** Nick Voskoboev; Olga Bondar, PhD; John Lieske, M.D.; *Mayo Clinic, Rochester, MN*
- MP 174 **A New Approach to Lipoprotein Fingerprinting Using the Mass Spectrometry of Proteins Associated with High Density Lipoprotein (HDL) Nanoparticles;** Ronald D. Macfarlane; *Texas A & M University, College Station, TX*
- MP 175 **Diagnosing Monoclonal Gammopathies Using Top-Down Analysis of Immunoglobulin Light Chains in Serum and Urine by LC-ESI-QTOF Mass Spectrometry;** David Barnidge<sup>1</sup>; Chad Botz<sup>1</sup>; Surendra Dasari<sup>2</sup>; Melissa Snyder<sup>1</sup>; Jerry Katzmann<sup>1</sup>; David Murray<sup>1</sup>; <sup>1</sup>*Mayo Clinic/DLMP, Rochester, MN*; <sup>2</sup>*Mayo Clinic/Health Sciences Research, Rochester, MN*
- MP 176 **Analysis of Disease-Related Hemoglobin Modifications by Top-Down Mass Spectrometry;** Didia Coelho Graça<sup>1</sup>; Adelina Acosta Martin<sup>1,2</sup>; Lorella Clerici<sup>2</sup>; Yury O. Tsybin<sup>3</sup>; Ralf Hartmer<sup>4</sup>; Markus Meyer<sup>4</sup>; Kaveh Samii<sup>2</sup>; Denis Hochstrasser<sup>1,2</sup>; Pierre Lescuyer<sup>1,2</sup>; Alexander Scherl<sup>1</sup>; <sup>1</sup>*University of Geneva, Geneva, Switzerland*; <sup>2</sup>*Geneva University Hospitals, Geneva, Switzerland*; <sup>3</sup>*Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*; <sup>4</sup>*Bruker Daltonics, Bremen, Germany*
- MP 177 **Quantitation of Insulin Grow Factors, IGF1 and IGF2 in Human Serum Using UHPLC-TOF;** Sharanya Reddy; Andrew Tyler; George Perkins; *PerkinElmer, Shelton, CT*
- MP 178 **Quantification of Serum C-peptide by Isotope-Dilution Mass Spectrometry Using Immobilized Antibody and N-terminal Modification by Isotope-Dilution Mass Spectrometry;** Tomoya Kinumi; Ryoko Mizuno; Akiko Takatsu; *Bio-Medical Std Section, NMIJ AIST, Tsukuba, Ibaraki, Japan*
- MP 179 **Simultaneous Transferrin and Apolipoprotein CIII Glycoforms Analysis by Online Immuno-Affinity Chromatography Electrospray Ionization Mass Spectrometry;** Coleman Turgeon<sup>1</sup>; Francesco Porta<sup>2</sup>; Mark Magera<sup>1</sup>; Kristen Liedtke<sup>1</sup>; Dimitar Gavrilov<sup>1</sup>; Devin Oglesbee<sup>1</sup>; Silvia Tortorelli<sup>1</sup>; Piero Rinaldo<sup>1</sup>; Dietrich Matern<sup>1</sup>; Kimiyo Raymond<sup>1</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*; <sup>2</sup>*Department of Pediatrics, University of Torino, Torino, Italy*
- MP 180 **Developing an iMALDI MS Assay for the Clinical Determination of Plasma Renin Activity;** Alexander Camenzind<sup>1</sup>; J Grace van der Gugten<sup>2</sup>; Daniel Holmes<sup>3</sup>; Christoph Borchers<sup>1,4</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*St. Paul's Hospital, Vancouver, Canada*; <sup>3</sup>*University of British Columbia, St Paul's Hospital, Vancouver, Canada*; <sup>4</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*

- MP 181 **Extending the Information Content of the MALDI Analysis of Biological Fluids (Deep MALDI);** Mark W. Duncan<sup>1,2</sup>; Senait Asmellash<sup>2</sup>; Jenna Allen<sup>2</sup>; Maxim Tsylin<sup>2</sup>; Joanna Roder<sup>2</sup>; Heinrich Roder<sup>2</sup>; <sup>1</sup>Univ. Colorado, School of Medicine, Aurora, CO; <sup>2</sup>Biodesix Inc., Boulder, CO
- MP 182 **Applications of Mass Tags for Diagnostic Microchips;** Martina Lorey<sup>1</sup>; Ville Jokinen<sup>2</sup>; Belinda Adler<sup>3</sup>; Hong Yan<sup>3</sup>; Rabah Soliymani<sup>1</sup>; Simon Ekström<sup>3</sup>; Thomas Laurell<sup>3</sup>; Marc Baumann<sup>1</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland; <sup>2</sup>Aalto University, Espoo, Finland; <sup>3</sup>Lund University, Lund, Sweden
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- MP 183 **Vitamin D Induced Regulation of Lipids in a Mouse Model of Breast Cancer Using Imaging MS and Gene Array Analysis;** Ami Grunbaum<sup>1</sup>; Pierre Chaurand<sup>2</sup>; Richard Kremer<sup>1</sup>; <sup>1</sup>McGill University Health Centre, Montreal, Canada; <sup>2</sup>University of Montreal, Montreal, Canada
- MP 184 **Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) Imaging Reveals Cholesterol Overload in the Cerebral Cortex of Alzheimer Disease Patients;** Alain Brunelle<sup>1</sup>; Adina N Lazar<sup>2,3</sup>; Claudia Bich<sup>1</sup>; Maï Panchal<sup>2,3</sup>; Nicolas Desbenoit<sup>1</sup>; Vanessa W. Petit<sup>4</sup>; David Touboul<sup>1</sup>; Catherine Marquer<sup>2,3</sup>; Olivier Laprévotte<sup>5</sup>; Charles Duyckaerts<sup>2,3</sup>; <sup>1</sup>CNRS, Institut de Chimie des Substances Naturelles, Gif-sur-Yvette, France; <sup>2</sup>Hôpital de la Salpêtrière, AP-HP, Paris, France; <sup>3</sup>Centre de Recherche de l'ICM, Paris, France; <sup>4</sup>LRTS, ICM, DSV, CEA, Fontenay-aux-Roses, France; <sup>5</sup>Université Paris-Descartes, Paris, France
- MP 185 **Profiling and Imaging MS of the Post-Injection b-Amyloid Mobility in Mouse Brain Tissues Sections;** Aurelien Thomas<sup>1</sup>; Nathan Heath Patterson<sup>1</sup>; Stéphane Epelbaum<sup>2</sup>; Pascale Laco<sup>3</sup>; Benoît Delatour<sup>2</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>University of Montreal, Montreal, Canada; <sup>2</sup>Inserm/CNRS/UPMC, Hôpital de la Pitié-Salpêtrière, Paris, France; <sup>3</sup>Cognitive Neurology and Alzheimer's Disease Center, Chicago, IL
- MP 186 **Imaging Mass Spectrometry Helps Predict Healing Course in Acute Wound Healing;** Domenico Taverna<sup>1,3</sup>; Jeffrey M. Spraggins<sup>2,3</sup>; Joshua J. Nicklay<sup>3</sup>; Lillian B. Nanney<sup>4</sup>; Alonda C. Pollins<sup>4</sup>; Giovanni Sindona<sup>1</sup>; Richard M. Caprioli<sup>2,3</sup>; <sup>1</sup>Università della Calabria, Dept. of Chemistry, Arcavacata Di Rende, CS, Italy; <sup>2</sup>Vanderbilt University, Dept. of Biochemistry, Nashville, TN; <sup>3</sup>Vanderbilt University, Mass Spec. Research Center, Nashville, TN; <sup>4</sup>Vanderbilt University, Dept. of Plastic Surgery, Nashville, TN
- MP 187 **Imaging Mass Spectrometry of Normal and PKD Mouse Kidney Tissues Using MALDI-MS;** Rachel Marvin; Yang Xu; Maki Takahashi; Leif Hanson; Surya Nauli; Dragan Isailovic; University of Toledo, Toledo, Ohio
- MP 188 **Matrix-assisted Laser Desorption Ionization Imaging Mass Spectrometry (MALDI-IMS) of Aging in Rat Skeletal Muscle;** Laetitia Theron<sup>1</sup>; Daniel Bechet<sup>1</sup>; Didier Viala<sup>1</sup>; Jeremy Pinguet<sup>2</sup>; Christophe Chambon<sup>1</sup>; <sup>1</sup>INRA, Theix, France; <sup>2</sup>CHU, Clermont-Ferrand, France
- MP 189 **Mass Spectrometric Imaging of Myelin Basic Protein and Its Breakdown Products in Traumatic Brain Injury;** Manasi Mangaonkar; Kevin Wang; Richard Yost; David Powell; University of Florida, Gainesville, FL
- MP 190 **Multimodality Imaging Mass Spectrometry for Co-localization of Trace Metals and Proteins in Abscesses in Murine Tissue from *Staphylococcus aureus* Infection;** Jessica L. Moore; Yaofang Zhang; Thomas E. Kehl-fie; Joshua J. Nicklay; Eric P. Skaar; Richard M. Caprioli; Vanderbilt University, Nashville, TN
- MP 191 **Analysis of Bacterial Biofilms Using MALDI Imaging Mass Spectrometry: Protein Spatial Distribution within Uropathogenic *E. coli* Biofilms;** Kyle A. Floyd; Jessica L. Moore; Carrie L. Shaffer; Maria Hadjifrangiskou; Richard M. Caprioli; Vanderbilt University, Nashville, TN
- MP 192 **Identifying Lipid, Glycan and Protein Correlates of Vitamin D3 Supplemented Prostate Tissues Using MALDI-MS Imaging;** Sebastiano Gattoni-Celli; Ellen Jones; Drew Schoenling; Stephen Savage; Richard Drake; Medical University of South Carolina, Charleston, SC
- MP 193 **Imaging Mass Spectrometry (IMS) Approach for the Assessment of Meniscus Degeneration;** Jörg Kriegsmann<sup>1,2</sup>; Rita Casadonte<sup>1</sup>; Friederike Zweynert<sup>2</sup>; Vanessa Schommer<sup>2</sup>; Jenny Petzold<sup>3</sup>; Axel W. Baltzer<sup>3</sup>; Markus Granrath<sup>3</sup>; Jens Fuchser<sup>4</sup>; Sören Deininger<sup>4</sup>; Mike Otto<sup>1,2</sup>; <sup>1</sup>Proteopath GbR, Trier, Germany; <sup>2</sup>Institute for Molecular Pathology, Trier, Germany; <sup>3</sup>Center for Molecular Orthopedics, Düsseldorf, Germany; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany
- MP 194 **Typing of Renal Amyloidosis in Formalin-Fixed Paraffin-Embedded (FFPE) Biopsy Specimens by MALDI Imaging Mass Spectrometry (IMS);** Rita Casadonte<sup>1</sup>; Jens Fuchser<sup>2</sup>; Sören Deininger<sup>2</sup>; Kerstin Amann<sup>3</sup>; Mike Otto<sup>1,4</sup>; Jörg Kriegsmann<sup>1,4</sup>; <sup>1</sup>Proteopath GbR, Trier, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>University Erlangen-Nürnberg, Erlangen, Germany; <sup>4</sup>Histology, Cytology and Molecular Diagnostics, Trier, Germany
- MP 195 **Discovery and Localization of Modified Lipids in Kidneys of Diabetic Mouse Model using Mass Difference Scanning and Imaging Mass Spectrometry;** Kerri Grove; Raf Van de Plas; Jeffery Spraggins; Paul Vozyan; Raymond Harris; Billy Hudson; Richard Caprioli; Vanderbilt University, Nashville, TN
- MP 196 **Identification of Potential Biomarkers of Atherosclerotic Plaque Vulnerability by Imaging Mass Spectrometry;** Patricia Schneider Yogi<sup>1</sup>; Gabriela Venturini<sup>1</sup>; Karina Helena Moraes Cardozo<sup>2</sup>; Pamela Araújo Malagrino<sup>1</sup>; Valdemir Melechco Carvalho<sup>2</sup>; Paulo Sampaio Gutierrez<sup>1</sup>; José Eduardo Krieger<sup>1</sup>; Alexandre da Costa Pereira<sup>1</sup>; <sup>1</sup>Heart Institute (InCor) - Medical School, USP, Sao Paulo, Brazil; <sup>2</sup>Fleury Group, Sao Paulo, Brazil
- MP 197 **Matrix Assisted Laser Desorption Ionization Imaging Mass Spectrometry Reveals a Different Molecular Composition in Human Healthy and Osteoarthritic Synovial Membrane;** Berta Cillero Pastor<sup>1</sup>; Gert B. Eijkel<sup>1</sup>; Francisco J. Blanco<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>2</sup>INIBIC-CH Universitario A Coruña, A Coruña, Spain
- MP 198 **Towards Lipidomics of Low-Abundant Species for Exploring Biological Relevance Guided by High-Resolution Mass Spectrometry Imaging;** Cimino Jonathan<sup>1,2</sup>; Calligaris David<sup>2</sup>; Far Johann<sup>2</sup>; Debois Delphine<sup>2</sup>; Blacher Silvia<sup>1</sup>; Sounni Nor Eddine<sup>1</sup>; Noel Agnès<sup>1</sup>; De Pauw Edwin<sup>2</sup>; <sup>1</sup>Laboratory of Tumor and Development Biology, GIGA, Belgium, Liege; <sup>2</sup>Mass Spectrometry Laboratory, GIGA-R, Belgium, Liege
- MP 199 **Integrating Multivariate Data Analysis and +/- Mode MALDI Imaging MS for Interrogating Animal Models of Myocardial Infarction;** Robert Menger<sup>1</sup>; Andras Kiss<sup>2</sup>; Raquel Hendershot<sup>1</sup>; Brad Wacker<sup>3</sup>; Gert Eijkel<sup>2</sup>; Ron Heeren<sup>2</sup>; David Ford<sup>3</sup>; Richard Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>3</sup>Saint Louis University, St. Louis, MO
- MP 200 **MALDI Imaging and FTICR MS Mapping of Lipids Alterations in Spinal Cord Injury;** Huiling Liu<sup>1</sup>; Karin B. Nilsson<sup>1,2</sup>; Huan He<sup>3,4</sup>; Alexander Shavkunov<sup>1</sup>; Young S. Gwak<sup>2</sup>; Shayne N. Hassler<sup>2</sup>; Kathia M. Johnson<sup>2</sup>; Norelle





## MONDAY POSTERS

- C. Wildburger<sup>1</sup>; Nicolas L. Young<sup>3,4</sup>; Alan G. Marshall<sup>3,4</sup>; Claire E. Hulsebosch<sup>2</sup>; Carol L. Nilsson<sup>1</sup>; <sup>1</sup>*Department of Pharmacology & Toxicology, UTMB, Galveston, TX*; <sup>2</sup>*Neuroscience and Cell Biology, UTMB, Galveston, TX*; <sup>3</sup>*Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*; <sup>4</sup>*Department of Chemistry and Biochemistry, FSU, Tallahassee, FL*
- MP 201 **Imaging and Profiling of Lipids in Human Tumors;** Roberto Fernández<sup>1</sup>; Antonio Veloso<sup>1</sup>; Silvia Terés<sup>2</sup>; Monica Higuera<sup>2</sup>; Daniel H Lopez<sup>2</sup>; Francisca Guardiola<sup>2</sup>; Xavier Busquets<sup>2</sup>; Pablo V. Escrivá<sup>2</sup>; Gwendolyn Barceló-Coblijn<sup>2</sup>; Jose A. Fernández<sup>1</sup>; <sup>1</sup>*University of Basque Country (UPV/EHU), Leioa, Spain*; <sup>2</sup>*University of the Balearic Islands, Palma, Spain*
- MP 202 **Identification Of Cancer Markers by Mass Spectrometry Imaging of Tissue Micro Arrays;** Marcus Wurlitzer<sup>1</sup>; Carina Borkowski<sup>2</sup>; Sinje Odinga Odinga<sup>2</sup>; Malte Buchholz Buchholz<sup>2</sup>; Christina Koop<sup>2</sup>; Maryam Omid<sup>1</sup>; Olga Kraus<sup>1</sup>; Michael Becker<sup>5</sup>; Matthias Witt<sup>5</sup>; Dennis Trede<sup>4</sup>; Maria Trusch<sup>6</sup>; Sarah Minner Minner<sup>2</sup>; Thorsten Schlomm<sup>3</sup>; Ronald Simon<sup>2</sup>; Guido Sauter<sup>2</sup>; Hartmut Schlüter<sup>1</sup>; <sup>1</sup>*UKE - Mass Spec Proteomics, Hamburg, Germany*; <sup>2</sup>*UKE - Institute of Pathology, Hamburg, Germany*; <sup>3</sup>*UKE - Martini-Clinic, Hamburg, Germany*; <sup>4</sup>*Steinbeis Innovation Center SCILS, Bremen, Germany*; <sup>5</sup>*Brüker Daltonik, Bremen, Germany*; <sup>6</sup>*University of Hamburg - Inst. of Organic Chemistry, Hamburg, Germany*
- MP 203 **Spatially Dependant Lipidomic Changes Associated with Non-alcoholic Fatty Liver Disease (NAFLD) Visualized by MALDI IMS;** Nick Bond<sup>1</sup>; Yajing Chu<sup>2</sup>; Scarlet Brockmoeller<sup>2</sup>; Julian Griffin<sup>1,2</sup>; Albert Koulman<sup>1</sup>; <sup>1</sup>*HNR MRC, Cambridge, England*; <sup>2</sup>*Dept. Biochemistry and CSBC, Uni. of Cambridge, Cambridge, England*
- MP 204 **A Novel Combined DESI MSI/MAS NMR Approach to the Diagnosis and Characterization of Breast Cancer Tissue;** Sabine Guenther<sup>1</sup>; Stefan Antonowicz<sup>1</sup>; Rathi Ramakrishnan<sup>1</sup>; Kirill A Veselkov<sup>1</sup>; Laura Muirhead<sup>1</sup>; Robert D Goldin<sup>1</sup>; Zoltan Takats<sup>1</sup>; *Imperial College London, London, UK*
- MP 205 **DESI-MS Imaging of Lipids and Metabolites in Cancers Activated by the MYC and RAS Oncogenes;** Livia S. Eberlin<sup>1</sup>; Emelyn H. Shroff<sup>1</sup>; Jialing Zhang<sup>1</sup>; David I. Bellovin<sup>1</sup>; Robert Tibshirani<sup>1</sup>; Dean W. Felsher<sup>1</sup>; Richard N. Zare<sup>1</sup>; *Stanford University, Stanford, CA*
- MP 206 **Biomarker Discovery and Validation: Coupling MALDI Imaging to Proteomic Expression and Metabolite Quantitation to Characterize Radiation-Induced Tissue Damage;** Jace W. Jones<sup>1</sup>; Alison J. Scott<sup>1</sup>; Young Ah Goo<sup>1</sup>; Artur Plett<sup>2</sup>; Christie M. Orschell<sup>2</sup>; David R. Goodlett<sup>1</sup>; Robert K. Ernst<sup>1</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*Indiana University, School of Medicine, Indianapolis, IN*
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- MP 208 **Statistical Analysis of MALDI-ToF Mass Spectra from Different Blood Components;** Rory T. Steven<sup>1</sup>; Alan M. Race<sup>1</sup>; Andrew D. Palmer<sup>1</sup>; Joscelyn Sarsby<sup>1</sup>; Rian L. Griffiths<sup>1</sup>; Ata Kaban<sup>1</sup>; G. Ed. Rainger<sup>1</sup>; Josephine Bunch<sup>1</sup>; *University of Birmingham, Birmingham, UK*
- MP 209 **MALDI-MS Imaging of Cardiolipins in Rat Organ Sections;** Hay-Yan J. Wang<sup>1</sup>; Hsuan-Wen Wu<sup>1</sup>; Ping-Ju Tsai<sup>2</sup>; Cheng Bin Liu<sup>1,3</sup>; <sup>1</sup>*National Sun Yat-Sen University, Kaohsiung, Taiwan*; <sup>2</sup>*Yuan's General Hospital, Kaohsiung, Taiwan*; <sup>3</sup>*Veterans General Hospital-Kaohsiung, Kaohsiung, Taiwan*
- MP 210 **A Simple MALDI MS-based Method to Detect Plasmalogens in Complex Lipid Mixtures - The Use of 2,4-Dinitrophenylhydrazine as Reactive Matrix;** Beate Fuchs<sup>1</sup>; Juergen Schiller<sup>1</sup>; *University of Leipzig, Leipzig, Germany*
- MP 211 **Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry Method for Lipid Profiling of Diabetic Rats Treated with Hepatoselective Glucokinase Activators;** Nicholas B. Vera<sup>1</sup>; *Pfizer, Cambridge, MA*
- MP 212 **Imaging Lipidomics by Microextraction Shotgun MS and nano-LCMS of Brain Tissue Sections ;** Reinaldo Almeida<sup>1</sup>; Zane Berzina Berzina<sup>1</sup>; Hans Kristian Hannibal-Bach<sup>1</sup>; Christer Ejnsing<sup>1</sup>; *University of Southern Denmark, Odense, Denmark*
- MP 213 **Sphingolipid Profiling of Adipose Tissue: Specific Overexpression of Ceramidase Improves Whole Body Glucose and Lipid Metabolism;** William L. Holland<sup>1,2</sup>; Yukiko Miyauchi<sup>1,2</sup>; Ruth Gordillo<sup>1,2</sup>; Philipp E. Scherer<sup>1,2</sup>; <sup>1</sup>*UTSouthwestern Medical Center, Dallas, TX*; <sup>2</sup>*Touchstone Diabetes Center, Dallas, TX*
- MP 214 **Lipids Analysis by 2 Dimensional LC Coupled to Triple Quadrupole Mass Spectrometer;** Liling Fang<sup>1</sup>; Taku Tsukamoto<sup>2</sup>; Jing Dong<sup>2</sup>; Keiko Yamabe<sup>2</sup>; Takashi Suzuki<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Inc., Columbia, MD*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- MP 215 **High Throughput Data Independent Approach for Qualitative and Quantitative Lipidomic Analysis;** Xu Wang<sup>1</sup>; Michael Kiebish<sup>2</sup>; Brigitte Simons<sup>1</sup>; John McNamara<sup>1</sup>; Christie Hunter<sup>1</sup>; <sup>1</sup>*AB SCIEX, Framingham, MA*; <sup>2</sup>*Berg Diagnostics, Natick, MA*
- MP 216 **Targeted Lipidomics Identifies Interaction of Sphingolipid Metabolism and Fatty Acid Elongation In The Development of Diabetic Retinopathy;** Todd A. Lydic<sup>1</sup>; Matthew Faber<sup>1</sup>; Svetlana Bozack<sup>1</sup>; Louis Glazer<sup>1</sup>; Susanne Mohr<sup>1</sup>; Julia V. Busik<sup>1</sup>; Gavin E. Reid<sup>1</sup>; *Michigan State University, East Lansing, MI*
- MP 217 **Robust Lipid Fragmentation Modeling to Identify Global Lipid Changes during Epithelial-Mesenchymal Transition (EMT);** Brendan Coutu<sup>1</sup>; Kristin Alexander<sup>1</sup>; Marc Hansen<sup>1</sup>; John Prince<sup>1</sup>; *Brigham Young University, Provo, UT*
- MP 218 **Metabolism and Protein Adduction of a Cyclooxygenase-2/15-prostaglandin Dehydrogenase Derived Product from Arachidonic Acid;** Nathaniel W. Snyder<sup>1</sup>; Alejandro D. Arroyo<sup>1</sup>; Xiaojing Liu<sup>1</sup>; Suhong Zhang<sup>1</sup>; Ian A. Blair<sup>1</sup>; *University of Pennsylvania, Philadelphia, PA*
- MP 219 **Profiling of Triacylglycerides Present in Edible Oils Consumed in India Using LC/MS/MS;** Deepthi Bhandarkar<sup>1</sup>; Shruti Raju<sup>1</sup>; Shailesh Damale<sup>1</sup>; Shailendra Rane<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India*
- MP 220 **Optimization of Supercritical Fluid Chromatography Coupled to Mass Spectrometry for Lipid Analysis;** Marie Méjean<sup>1</sup>; Alain Brunelle<sup>1</sup>; David Touboul<sup>1</sup>; *ICSN, CNRS, Gif-sur-Yvette, France*
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- MP 221 **Surface Oxidation under Ambient Air - A Fast and Economical Method to Identify Double Bond Positions in Unsaturated Lipids;** Hyejung Park<sup>1</sup>; Ying Zhou<sup>1</sup>; Philseok Kim<sup>2</sup>; Yan Jiang<sup>1</sup>; Catherine Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Harvard University, Cambridge, MA*
- MP 222 **One-step Reversed Phase Liquid Chromatography Coupled to ESI Mass Spectrometry for Separation, Detection of Polar Lipids Associated with Prion Proteins;** Ying Zhou<sup>1</sup>; Holger Wille<sup>2</sup>; Hyejung Park<sup>1</sup>; Julian



- ollesch<sup>2</sup>; Catherine E Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Ruhr-Universitaet Bochum, Bochum, Germany; <sup>3</sup>University of Alberta, Edmonton, Alberta, Canada
- MP 223 **Enabled by Speed of Analysis: Multidimensional LC-MS-Based Lipidomics**; Susanne Brodessa<sup>1</sup>; Axel Besa<sup>2</sup>; <sup>1</sup>CECAD Lipidomics Facility, Cologne, Germany; <sup>2</sup>AB SCIEX Europe, Darmstadt, Germany
- MP 224 **New Retroactive Approach for Global Lipidomics Analysis by Data Independent Acquisition**; Kazutaka Ikeda; Sanae Yamanaka; Masaru Tomita; Tomoyoshi Soga; Keio University, Tsuruoka, Japan
- MP 225 **Ultra-High Resolution Analysis of Triacylglycerol in Seed Oils Using a High-Performance Orbitrap Hybrid and Automated Data Processing Software**; Jeffrey Gilbert<sup>1</sup>; Debbie Schwedler<sup>1</sup>; Scott Greenwalt<sup>1</sup>; Brita McNew<sup>1</sup>; Daniel Gachotte<sup>1</sup>; Mary Evenson<sup>1</sup>; Yasuto Yokoi<sup>2</sup>; Tim Stratton<sup>3</sup>; David Peake<sup>3</sup>; <sup>1</sup>Dow AgroSciences, Indianapolis, IN; <sup>2</sup>Mitsui Knowledge Industry, Tokyo, Japan; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- MP 226 **Analysis of Isoleuglandin/Isoketal Lysine Adducts Using a Traveling Wave Ion Mobility Time-of-Flight Mass Spectrometer**; Lin Huang; Jaewoo Choi; Samanthi Wickramasekara; Claudia Maier; Oregon State University, Corvallis, OR
- MP 227 **Identification and Characterization of Endogenous and Novel Cardiolipins in Human Serum**; Elizabeth W. Kahuno; Feng-Ying C. Lin; Alfred L. Yergey; Peter S. Backlund; NICHD, NIH, Bethesda, MD
- MP 228 **A Shotgun Lipidomics Approach Coupled with Charge Switch Derivatization Applied to Identification and Quantitation of Fatty Acid Double Bond Isomers**; Kui Yang; Beverly Gibson Dilthey; Richard W. Gross; Washington University School of Medicine, St. Louis, MO
- MP 229 **Rapid Characterization of Phospholipid Isomeric Mixtures from Sample Arrays and Tissue Sections By Sequential Collision-Induced Dissociation and Ozone-Induced Dissociation**; Rachel L. Kozłowski; Todd W. Mitchell; Stephen J. Blanksby; University of Wollongong, Wollongong, Australia
- MP 230 **Analysis of Phosphocholines Using Metastable Atom Activated Dissociation Mass Spectrometry (MAD-MS) and Collision Induced Dissociation (CID)**; Robert E. Deimler<sup>1</sup>; Madlen Sander<sup>2</sup>; William D. Hoffmann<sup>1</sup>; Glen P. Jackson<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV; <sup>2</sup>Leipzig University, Leipzig, Germany
- MP 231 **High Resolution 193 nm UVPD-MS for the Top-down Structural Characterization of Lipid A and Lipopolysaccharides**; John O'Brien; Brittany Needham; Jeremy Henderson; M. Stephen Trent; Jennifer Brodbelt; University of Texas, Austin, TX
- MP 232 **Characterization and localization of d18:2 Sphingadienine Based Sulfatides in Rat Cerebellum Using 2D Offline LC-HRMS and MALDI Imaging**; Benoit Colsch<sup>1</sup>; Samia Boudah<sup>1,3</sup>; Christophe Junot<sup>1</sup>; Amina S. Woods<sup>2</sup>; <sup>1</sup>CEA, DSV/IBiTec-S/SPI/LEMM, Gif sur Yvette, France; <sup>2</sup>NIDA/NIH, Baltimore, MD; <sup>3</sup>GlaxoSmithKline, Centre de recherche F. Hyafil, Villebon-sur-Yvette, France
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- MP 234 **A Mass Spectrometry-based Method for the Identification of Novel G-Quadruplex-binding Proteins**; Preston Williams; Xiaoli Dong; Yinsheng Wang; University of California, Riverside, CA
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- MP 288 **Detection of a Low-Volatility Analyte Vapor Permeating a Polymer Membrane;** Bruce Salter<sup>1</sup>; Derek Lovingood<sup>3</sup>; Jeffery Owens<sup>2</sup>; <sup>1</sup>Universal Technology Corporation, Tyndall AFB, FL; <sup>2</sup>Air Force Research Laboratory, Tyndall AFB, FL; <sup>3</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN
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- MP 316 **Ion Mobility Measurements within Fourier Transform Ion Cyclotron Resonance Cells and Orbitraps;** Yi Xin<sup>1</sup>; Yu Chen<sup>1</sup>; Xiang Fang<sup>2</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>*Beijing Institute of Technology, Beijing, China*; <sup>2</sup>*National Institute of Metrology, Beijing, China*
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- MP 322 **Multi-Turn Time-of-Flight Mass Analyzers with Rotational Symmetry and Open Trajectories;** Vyacheslav Shchepunov; Roger Giles; Shimadzu Research Laboratory (Europe) Ltd.; *Manchester, UK*
- MP 323 **Advancements in Multi Reflecting High Resolution TOF Mass Analyzers with Folded Flight Path;** Viatcheslav Artaev<sup>1</sup>; Mikhail Yavor<sup>2</sup>; Timofey Pomozev<sup>2</sup>; Anatoly Verenchikov<sup>3</sup>; <sup>1</sup>*LECO Corporation, St. Joseph, MI*; <sup>2</sup>*Institute for Analytical Instrumentation RAS, St. Petersburg, Russia*; <sup>3</sup>*MSC-CG, Bar, Montenegro*
- MP 324 **Multiple-Reflection Time-of-Flight Mass Spectrometers for the Research With Exotic Nuclei and for Analytical Mass Spectrometry;** Wolfgang Plass<sup>1,2</sup>; Timo Dickel<sup>1</sup>; <sup>2</sup>; Jens Ebert<sup>1</sup>; Johannes Lang<sup>1</sup>; Samuel Ayet<sup>2</sup>; Emma Haettner<sup>1</sup>; Hans Geissel<sup>1,2</sup>; Christian Jesch<sup>1</sup>; Wayne Lippert<sup>1</sup>; Martin Petrick<sup>1</sup>; Christoph Scheidenberger<sup>1</sup>; <sup>2</sup>; Mikhail Yavor<sup>3</sup>; <sup>1</sup>*Justus-Liebig-Universität Gießen, Gießen, Germany*; <sup>2</sup>*GSI Helmholtzzentrum für*

- Schwerionenforschung, Darmstadt, Germany; <sup>3</sup>Institute for Analytical Instrumentation, RAS, St. Petersburg, Russia
- MP 325 **Optimization of Analytical Performances of Synchronized Dual-Polarity MALDI-TOF Mass Spectrometer for Fundamental Analysis;** Hsun Lee; Chih-Hao Hsiao; Yi-Sheng Wang; *GRC, Academia Sinica, Taipei, Taiwan*
- MP 326 **MS with 3D-reflective IO Subsystem;** Yerbol Sapargaliyev; Igor Spivak-Lavrov; Aldan Sapargaliyev; *REB, Almaty, Kazakhstan*
- MP 327 **Development of a Portable Mass Spectrometer for Operation at 1 Torr;** Feng Jin<sup>1</sup>; William D. Hoffmann<sup>1</sup>; Guido F. Verbeck<sup>2</sup>; Glen P. Jackson<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV; <sup>2</sup>Department of Chemistry, University of North Texas, Denton, TX
- MP 328 **The New Vienna parallel DMA – An Ion Mobility Analyzer System for High Molecular Mass Ions/Particles with Improved Resolution;** Peter Kallinger<sup>1</sup>; Victor Weiss<sup>2</sup>; Günter Allmaier<sup>2</sup>; Wladyslaw Szymanski<sup>1</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Vienna University of Technology, Vienna, Austria
- MP 329 **Simulation of a Novel Two-Dimensional Mass Separation Method Based on CCD Imaging of Spiral Ion Patterns;** Jens Langejuergen; Christian R. Raddatz; Stefan Zimmermann; *Leibniz University Hannover, Hannover, Germany*
- Ambient Ionization: Instrumentation, 330 - 356**
- MP 330 **Development and Performance Characterization of a Personal Mass Spectrometry System;** Linfan Li<sup>1</sup>; Yue Ren<sup>1</sup>; Tsung-Chi Chen<sup>1</sup>; Ziqing Lin<sup>1</sup>; R. Graham Cooks<sup>2</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Biomedical Engineering, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Chemistry, Purdue University, West Lafayette, IN
- MP 331 **A Miniature Mass Spectrometer for in-situ and Real-time Chemical Analysis;** Paul I. Hendricks<sup>1</sup>; Jacob T. Shelley<sup>1,2</sup>; Jon K. Dalgleish<sup>1</sup>; Jason S. Duncan<sup>3</sup>; Matt T. McNicholas<sup>4</sup>; Linfan Li<sup>5</sup>; Tsung-Chi Chen<sup>5</sup>; Zheng Ouyang<sup>3,5</sup>; R. Graham Cooks<sup>1,3</sup>; <sup>1</sup>Dept. Chemistry Purdue University, West Lafayette, IN; <sup>2</sup>University of Muenster, Muenster, Germany; <sup>3</sup>Center for Analytical Instrument Development, West Lafayette, IN; <sup>4</sup>Department of Electrical and Computer Engineering, West Lafayette, IN; <sup>5</sup>Weldon School of Biomedical Engineering, West Lafayette, IN
- MP 332 **Electrospray/Plasma Ionization Mass Spectrometry for Simultaneously Characterizing Polar and Nonpolar Compounds;** Sy-Chyi Cheng; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 333 **Detecting Polar and Nonpolar Compounds by Impacting Sample Surfaces with Reactive Species from Both ESI and Plasma-APCI;** Siou-Sian Jhang; Sy-Chyi Cheng; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 334 **Laser Desorption Combined with Electrospray/Plasma Ionization Mass Spectrometry for the Analysis of Polymers and Proteins;** Siou-Sian Jhang; Sy-Chyi Cheng; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 335 **Electrospray Ionization Mass Spectrometry Combined with High-Flow Fast Gas Chromatography for Characterizing Mixtures of Organic Compounds;** Chu-Nian Cheng; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 336 **Increasing Efficiency of Surface Acoustic Wave Nebulization with an Ion Funnel;** Mikhail Belov<sup>4</sup>; Yue Huang<sup>1</sup>; Lucas Monkonnen<sup>1</sup>; Scott Heron<sup>1,2</sup>; J. Scott Edgar<sup>3</sup>; Sung Hwan Yoon<sup>1,2</sup>; David R. Goodlett<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Maryland, Baltimore, MD; <sup>3</sup>Deurion LLC, Seattle, WA; <sup>4</sup>Spectrograph LLC, Richland, WA
- MP 337 **Simply Applying Heat and/or Vacuum for Ionization of Small and Large Nonvolatile Molecules for Use in MS and Its Applications;** Beixi Wang; Sarah Trimpin; *Wayne State University, Detroit, MI*
- MP 338 **Open Probe Supersonic Fast GC-MS – Real Time Analysis with Separation;** Alexander Fialkov; Aviv Amirav; Uri Keshet; Mati Morag; Eli Flaxer; Tal Alon; *Tel-Aviv University, Tel-Aviv, Israel*
- MP 339 **Development of Sheath-Flow Probe Electrospray Ionization (SF-PESI);** Kenzo Hiraoka<sup>1</sup>; Md. Obaidur Rahman<sup>1</sup>; Mridul Kanti Mandal<sup>1</sup>; Yasuo Shida<sup>1</sup>; Lee Chuin Chen<sup>1</sup>; Satoshi Ninomiya<sup>1</sup>; Hiroshi Nonami<sup>2</sup>; <sup>1</sup>University of Yamanashi, Kofu, Japan; <sup>2</sup>Ehime University, Matsuyama, Japan
- MP 340 **Fully Automated Liquid Microjunction Surface Sampling-HPLC-MS/MS Analysis of Drugs and Metabolites in Whole-Body Thin Tissue Sections;** Vilmos Kertesz<sup>1</sup>; Gary J. Van Berkel<sup>1</sup>; Paul Moench<sup>2</sup>; Alexandre Catoire<sup>2</sup>; Adam Bentley<sup>2</sup>; Jimmy Flarakos<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>Novartis Institutes for BioMedical Research, East Hanover, NJ
- MP 341 **Continuous Flow Liquid Microjunction Surface Sampling Probe Connected On-line with HPLC/MS for Spatially Resolved Analysis of Small Molecules and Proteins;** Gary J. Van Berkel; Vilmos Kertesz; *Oak Ridge National Laboratory, Oak Ridge, TN*
- MP 342 **Implementation of Ambient Ionization Sources on a Low Cost GC/MSD and Assessment of Its Performance;** Joseph Tice<sup>1</sup>; Michael Festa<sup>1</sup>; Taylor Feraco<sup>1</sup>; Brian D. Musselman<sup>1</sup>; Randy Pedder<sup>2</sup>; John Mazock<sup>2</sup>; <sup>1</sup>IonSense, Inc., Saugus, MA; <sup>2</sup>Ardara Technologies, Ardara, PA
- MP 343 **Ultra-fast Analysis of Synthetic Organic Compounds Using APGC without the CI;** Peter Stokes; David Parker; Jackie Mosely; *University of Durham, Durham, UK*
- MP 344 **Low Temperature Plasma Ionization Mass Spectrometry for Real-Time Analysis of Size-Selected Organic Aerosol Particles;** Sandra Spencer; Gary Glish; *Univ. of North Carolina at Chapel Hill, Chapel Hill, NC*
- MP 345 **Towards Micro Plasma Devices for Use in Ambient Mass Spectrometry and 2D Chemical Imaging;** Andrew Bowfield; *University of Liverpool, Liverpool, UK*
- MP 346 **A Compact, Robust and Light Weight Surface Ionization Source;** Vladimir Romanov; Jan Hendrikse; *Smiths Detection, Mississauga, Canada*
- MP 347 **Ultra-low Detection Limits for Trace Gas Analysis Using a Tunable Non-radioactive Electron Emitter in APCI-MS;** Jens Langejuergen; Stefan Zimmermann; *Leibniz University Hannover, Hannover, Germany*
- MP 348 **Direct, Real-Time Vapor Detection of Low Volatility Explosives;** Robert Ewing; David Atkinson; Brian H. Clowers; *Pacific Northwest National Laboratory, Richland, WA*
- MP 349 **Development of a Piezoelectric Inkjet Dopant Introduction Device for Atmospheric Pressure Photoionization and Its Performance in Analysis Polycyclic Aromatic Hydrocarbons;** Ma'an Amad; Salim Sioud; Erqiang Li; Sigurdur Thoroddsen; *King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*
- MP 350 **Detection of Naturally Occurring Flame Ions Using a High-Temperatureatmospheric Pressure Interface;** Thomas Bierkandt<sup>1</sup>; Erdal Akyildiz<sup>1</sup>; Tina Kasper<sup>1</sup>; Stefan Kaesdorf<sup>2</sup>; Ioannis Orfanopoulos<sup>3</sup>; Dimitris Papanastasiou<sup>3</sup>; <sup>1</sup>University of Duisburg-Essen, Duisburg, Germany; <sup>2</sup>Kaesdorf, Munich, Germany; <sup>3</sup>Fasmatech, Athens, Greece





## MONDAY POSTERS

- MP 351 **Development of a New DIP-APCI Ion Source;** Sonja Krieger; Oliver J. Schmitz; *University of Duisburg-Essen, Essen, Germany*
- MP 352 **Atmospheric Pressure Laser Evaporation Ionization of Levitated Droplets;** Jens Riedel; Arne Stindt; Ulrich Panne; *BAM Federal Institute for Materials, Berlin, Germany*
- MP 353 **Analysis of Biomolecules by Atmospheric Pressure Visible-Wavelength MALDI-ion trap-MS in Transmission Geometry;** Raymond West; Eric Findsen; Dragan Isailovic; *University of Toledo, Toledo, OH*
- MP 354 **Enhanced Direct Analysis of Biomedical Samples by Laser Ablation Electrospray Ionization with Ion Mobility Separation and Mass Spectrometry;** Bindesh Shrestha; Akos Vertes; *George Washington University, Washington, DC*
- MP 355 **Laser Ablation Electrospray Ionization Mass Spectrometry of Plant Cells in Transmission Geometry;** Rachelle Jacobson; Bindesh Shrestha; Akos Vertes; *George Washington University, Washington, DC*
- MP 356 **Peptides and Proteins Signal Enhancement in Electrospray-Assisted Laser Desorption/Ionization Mass Spectrometry by Black Oxide (Fe<sub>3</sub>O<sub>4</sub>) Coated Target;** Alexey Kononikhin<sup>1,3</sup>; Min-Zong Huang<sup>2</sup>; Igor Popov<sup>3,4</sup>; Alexey Boldyrev<sup>4</sup>; Evgeny Kukaev<sup>3,4</sup>; Alexander Spassky<sup>1</sup>; Ilya Leipunsky<sup>1</sup>; Jentaie Shiea<sup>2</sup>; Eugene Nikolaev<sup>1,3</sup>; <sup>1</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russia*; <sup>2</sup>*National Sun Yat-Sen University, Kaohsiung, Taiwan*; <sup>3</sup>*Emanuel Institute of Biochemical Physics, Moscow, Russia*; <sup>4</sup>*Moscow Institute of Physics and Technology, Moscow, Russia*
- Informatics: General, 357 - 373**
- MP 357 **GOAT: A Simple MS/MS Gradient Optimization and Analysis Tool;** David Trudgian<sup>1</sup>; Roman Fischer<sup>2</sup>; Xiaofeng Guo<sup>1</sup>; Hamid Mirzaei<sup>1</sup>; <sup>1</sup>*UT Southwestern Medical Center, Dallas, TX*; <sup>2</sup>*University of Oxford, Oxford, UK*
- MP 358 **New Plug-ins for Freely Available Mass++ Software to Identify Biomolecules;** Kentaro Morimoto<sup>1</sup>; Takashi Nishikaze<sup>1</sup>; Satoshi Tanaka<sup>1</sup>; Masaki Murase<sup>1</sup>; Shin-ichi Utsunomiya<sup>1</sup>; Shigeki Kajihara<sup>1</sup>; Tsuyoshi Tabata<sup>2</sup>; Ken Aoshima<sup>2</sup>; Yoshiya Oda<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Eisai Product Creation Systems, Eisai Corp., Tsukuba, Japan*
- MP 359 **Novel Preprocessing Method to Align Retention Time of LC-MALDI and New Implemented Functions in Mass++ for Differential Analysis;** Yuichiro Fujita<sup>1</sup>; Natsumi Funakoshi<sup>1</sup>; Yoshihiro Yamada<sup>1</sup>; Satoshi Tanaka<sup>1</sup>; Shin-ichirou Kawabata<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Shinichi Utsunomiya<sup>1</sup>; Shigeki Kajihara<sup>1</sup>; Tsuyoshi Tabata<sup>2</sup>; Ken Aoshima<sup>2</sup>; Yoshiya Oda<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Eisai Product Creation Systems Eisai Co., Ltd, Tsukuba, Japan*
- MP 360 **Mass++: A Platform for Mass Spectrometry to Construct Suitable Software to Achieve User's Own Purposes;** Shin-ichi Utsunomiya<sup>1</sup>; Satoshi Tanaka<sup>1</sup>; Masaki Murase<sup>1</sup>; Shigeki Kajihara<sup>1</sup>; Tsuyoshi Tabata<sup>2</sup>; Ken Aoshima<sup>2</sup>; Yoshiya Oda<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Eisai Product Creation Systems, Eisai Corp., Tsukuba, Japan*
- MP 361 **A Software Solution for Rapid Characterization of Biologics;** Xu Guo<sup>1</sup>; Robert Deutschman<sup>2</sup>; Byung-Hee Shin<sup>3</sup>; Eric Johansen<sup>2</sup>; <sup>1</sup>*AB SCIEX, Canada, Concord, ON*; <sup>2</sup>*AB SCIEX, USA, Foster City, CA*; <sup>3</sup>*AB SCIEX, South Korea, Seoul, South Korea*
- MP 362 **Building Proteomic Application Platforms for Cloud Computing Environments with CloudBioLinux;** John Chilton<sup>1</sup>; Roman Zenka<sup>2</sup>; Pratik Jagtap<sup>1</sup>; Benjamin Lynch<sup>1</sup>; Robert (Bob) Bergen<sup>2</sup>; Timothy Griffin<sup>3</sup>; <sup>1</sup>*University of Minnesota Supercomputing Institute, Minneapolis, MN*; <sup>2</sup>*Mayo Clinic, Rochester, MN*; <sup>3</sup>*University of Minnesota, Minneapolis, MN*
- MP 363 **Proteomics Pipeline Tracer Bullets;** Roman Zenka; Surendra Dasari; Carrie J. Heppelmann; Kenneth L. Johnson; H. Robert Bergen, III; *Mayo Clinic, Rochester, MN*
- MP 364 **Definitions of Terms Relating To Mass Spectrometry;** Kermit K. Murray<sup>1</sup>; Robert K. Boyd<sup>2</sup>; Marcos N. Eberlin<sup>3</sup>; G. John Langley<sup>4</sup>; Liang Li<sup>5</sup>; Yasuhide Naito<sup>6</sup>; <sup>1</sup>*Louisiana State University, Baton Rouge, LA*; <sup>2</sup>*National Research Council, Ottawa, Canada*; <sup>3</sup>*Thomson Lab Unicamp, Campinas, Brazil*; <sup>4</sup>*University of Southampton, Southampton, UK*; <sup>5</sup>*University of Alberta, Edmonton, Canada*; <sup>6</sup>*GPI, Hamamatsu, Japan*
- MP 365 **A Flexible Platform for Automating Mass Spectrometry Data Processing for Biotherapeutic Characterization;** Joe Shambaugh<sup>1</sup>; Alessio Ceroni<sup>1</sup>; Jessica Qi<sup>1</sup>; Jens Hoefkens<sup>1</sup>; Steven Pomerantz<sup>2</sup>; <sup>1</sup>*Genedata Inc, Lexington, MA*; <sup>2</sup>*Janssen Research and Development, Radnor, PA*
- MP 366 **Sample Reproducibility and Statistical Significance in a Nascent Microbial Community Proteomics Experiment;** Erik Hendrickson; Tony Wang; Murray Hackett; *University of Washington, Seattle, WA*
- MP 367 **Gene-based Protein Identification;** Honglan Li<sup>1</sup>; Seungjin Na<sup>2</sup>; Eunok Paek<sup>2</sup>; <sup>1</sup>*Soongsil University, Seoul, South Korea*; <sup>2</sup>*Hanyang University, Seoul, South Korea*
- MP 368 **Web Services for the Online NIST Libraries of Peptide Tandem Mass Spectra;** Niksa Blonder<sup>1</sup>; Manor Askenazi<sup>2</sup>; Dmitrii Tchekhovskoi<sup>1</sup>; Yuri Mirokhin<sup>1</sup>; Paul Rudnick<sup>1</sup>; Stephen Stein<sup>1</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*; <sup>2</sup>*The Ionomix Initiative, Arlington, MA*
- MP 369 **BRAIN 2.0: Time and Memory Quasi-Constant Algorithm for Calculating the Isotopic Distribution;** Piotr Dittwald<sup>1</sup>; Dirk Valkenborg<sup>2,3</sup>; <sup>1</sup>*University of Warsaw, Warszawa, Poland*; <sup>2</sup>*VITO, Mol, Belgium*; <sup>3</sup>*I-Biostat, Hasselt University, Diepenbeek, Belgium*
- MP 370 **Galaxy-P: Transforming MS-based Proteomic Informatics via Innovative Workflow Development, Dissemination, Standardization and Transparency;** Timothy Griffin<sup>1</sup>; John Chilton<sup>2</sup>; James Johnson<sup>2</sup>; Ebbing de Jong<sup>1</sup>; Getiria Onsongo<sup>2</sup>; Pratik Jagtap<sup>2</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*University of Minnesota Supercomputing Institute, Minneapolis, MN*
- MP 371 **Statistical Model for Alignment of Open Platform Proteomics Data - Incorporating Ion Mobility Separation and Product Ions;** Ashlee Benjamin; Will Thompson; Erik Soderblom; M Arthur Moseley; Joseph Lucas; *Duke University, Durham, NC*
- MP 372 **Molecular Isotopic Distribution Analysis (MIDAs) with Adjustable Mass Accuracy;** Gelio Alves; Aleksey Ogurtsov; Yi-Kuo Yu; *National Center for Biotechnology Information, NLM, Bethesda, MD*
- MP 373 **Trans-Proteomic Pipeline Tools for the Analysis of MS/MS Proteomics Data in Conjunction with Matching RNA-seq Data;** Eric W. Deutsch; Zhi Sun; Luis Mendoza; David Shteynberg; Joseph Slagel; Michael Hoopmann; Terry Farrah; Robert L. Moritz; *Institute for Systems Biology, Seattle, WA*
- Informatics: Workflow and Data Management, 374 - 386**
- MP 374 **Proteogenomics for the ENCODE Project: Investigating Genome-Wide Translation;** John Wrobel<sup>1,2</sup>; Harsha P. Gunawardena<sup>1</sup>; Jainab Khatun<sup>2</sup>; Brian Risk<sup>2</sup>; Yanbao Yu<sup>1</sup>; Morgan C. Giddings<sup>2</sup>; Xian Chan<sup>1</sup>; <sup>1</sup>*University of North Carolina at Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*Boise State University, Boise, ID*



- MP 375 **Peptide Tracker: A Software Tool for the Management of Peptides Used in MRM Based Assays;** Derek Smith<sup>1</sup>; Andrew Chambers<sup>1</sup>; Andrew Percy<sup>1</sup>; Dominik Domanski<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria Genome-BC Proteomics Centre, Victoria, BC Canada; <sup>2</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada
- MP 376 **User Friendly MS Analysis by Taking the Galaxy Environment to the Cloud;** Jorrit Boeke<sup>1,2</sup>; Janne Lehtio<sup>1,2</sup>; Lukas Käll<sup>1,3</sup>; <sup>1</sup>Science for Life Laboratory, Solna, Sweden; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>KTH Royal Institute of Technology, Stockholm, Sweden
- MP 377 **Customized Real-Time Control of Benchtop Orbitrap MS;** Andreas Kuehn<sup>1</sup>; Florian Grosse-Coosmann<sup>1</sup>; Thomas Rietpietsch<sup>1</sup>; Jan-Peter Hauschild<sup>1</sup>; Katja Tham<sup>1</sup>; Tim Stratton<sup>2</sup>; Derek Bailey<sup>1</sup>; Robert Malek<sup>1</sup>; Markus Kellmann<sup>1</sup>; Christoph Henrich<sup>1</sup>; Oliver Lange<sup>1</sup>; Andreas Wiegand<sup>1</sup>; Stevan Horning<sup>1</sup>; Alexander Makarov<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen), Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific (San Jose), San Jose, CA
- MP 378 **Reproducible Proteomic Workflows Using Extensions to the Galaxy Framework;** James Johnson; John Chilton; Pratik Jagtap; Ben Lynch; Tim Griffin; University of Minnesota, Minneapolis, MN
- MP 379 **A Novel Two-Pass Feature Extraction Workflow for the Statistical Profiling of Mass Spectrometric Data;** Norton Kitagawa<sup>1</sup>; Abhijit Rane<sup>2</sup>; Steven M. Fischer<sup>1</sup>; Joe Roark<sup>1</sup>; Maithilee Samant<sup>1</sup>; Theodore Sana<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Persistent Systems, Ltd., Pune, India
- MP 380 **MASSIVE: Mass Spectrometry Interactive Virtual Environment for Data Sharing in Proteomics;** Jeremy Carver; Ian Kaufman; Claudiu Farcas; Vineet Bafna; Nuno Bandeira; UCSD, La Jolla, CA
- MP 381 **Metabolomics Data Analysis Framework – Database and Web Portal for Curation and Analysis of Mass-Spectrometry Based Metabolomics Data;** Alexander Raskind; Anupama Janga; University of Michigan, Ann Arbor, MI
- MP 382 **Sharing Targeted Proteomics Assays Using Skyline and Panorama;** Vagisha Sharma<sup>1</sup>; Josh Eckels<sup>2</sup>; Brendan MacLean<sup>1</sup>; Shannon A. Joyner<sup>3</sup>; Jacob D. Jaffe<sup>4</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>LabKey Corp., Seattle, WA; <sup>3</sup>Carnegie Mellon University, Pittsburgh, PA; <sup>4</sup>The Broad Institute, Cambridge, MA
- MP 383 **ProteomicsDB: A Protein Centric Database and Repository for LC-MS/MS Data Sets;** Mathias Wilhelm<sup>1</sup>; Judith Schlegel<sup>2</sup>; Amin Moghaddas Gholami<sup>1</sup>; Hannes Hahne<sup>1</sup>; Joos-Hendrik Boese<sup>2</sup>; Marcus Lieberenz<sup>2</sup>; Mikhail Savitski<sup>3</sup>; Yuval Morad<sup>2</sup>; Lars Butzmann<sup>2</sup>; Emanuel Ziegler<sup>2</sup>; Anton Niadzelka<sup>2</sup>; Eyk Kny<sup>2</sup>; Helmut Cossmann<sup>2</sup>; Siegfried Gessulat<sup>2</sup>; Marcus Bantscheff<sup>3</sup>; Anja Gerstmair<sup>2</sup>; Franz Faerber<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>Technical University Munich, Freising, Germany; <sup>2</sup>SAP AG Germany, Walldorf, Germany; <sup>3</sup>Cellzome, Heidelberg, Germany
- MP 384 **A Common Analysis Pipeline for Interpretation of Data from the Clinical Proteomics Tumor Analysis Consortium (CPTAC);** Paul Rudnick<sup>1</sup>; Niksa Blonder<sup>1</sup>; Nathan Edwards<sup>2</sup>; Yuri Mirokin<sup>1</sup>; Dmitrii Tchekovskoi<sup>1</sup>; Xinjin Yan<sup>1</sup>; Stephen Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>Georgetown University, Washington, DC
- MP 385 **Solving the Bioinformatics Bottlenecks of Massive Storage & Data Distribution, Huge Computational Needs, and Flexible and Fast Reporting;** Gautam Saxena<sup>1</sup>; Christine Jellinek<sup>3</sup>; Vidya Venkat<sup>3</sup>; Rafael Dugarte<sup>1</sup>; Scott Kuzdzal<sup>2</sup>; Jennifer Van Eyk<sup>3</sup>; <sup>1</sup>Integrated Analysis, Bethesda, MD; <sup>2</sup>Shimadzu Scientific, Columbia, MD; <sup>3</sup>Johns Hopkins Medical School, Baltimore, MD
- MP 386 **A Workflow for Novel Image-Based Differential Analysis of LC/MS Experiments;** Hanqing Liao<sup>1</sup>; Emmanouil Moschidis<sup>1</sup>; Isabel Riba-Garcia<sup>1</sup>; Richard Unwin<sup>1</sup>; Warwick Dunn<sup>2</sup>; Jeffrey Morris<sup>3</sup>; Jim Graham<sup>1</sup>; Andrew Dowsey<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>University of Birmingham, Birmingham, UK; <sup>3</sup>UT MD Anderson Cancer Center, Houston, TX
- Informatics: Crosslinking and Structure Analysis, 387 - 392**
- MP 387 **Analyses of Yeast mRNPs by the Use of the Photo-Reactive Nucleobase 4-thio-uracil and Mass Spectrometry;** Uzma Zaman<sup>1</sup>; Kum-Loong Boon<sup>1</sup>; Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Oliver Kohlbacher<sup>2</sup>; Reinhard Lührmann<sup>1</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>Max Planck Institute for Biophysical chemistry, Goettingen, Germany; <sup>2</sup>University of Tuebingen, Tuebingen, Germany
- MP 388 **Development of a Bioinformatics Toolbox to Support Protein Cross-Linking Mass Spectrometry Analyses;** Mathieu Courcelles; Mike Tyers; IRIC/Université de Montréal, Montréal, Canada
- MP 389 **IMS, HCD, and ETD for Improved Chemical Cross-linking Mass Spectrometry;** Eric Merkley<sup>1</sup>; Erin Baker<sup>1</sup>; Kevin Crowell<sup>1</sup>; Daniel Orton<sup>1</sup>; Thomas Taverner<sup>2</sup>; Charles Ansong<sup>1</sup>; Yehia Ibrahim<sup>1</sup>; Meagan Burnet<sup>1</sup>; John Cort<sup>1</sup>; Gordon Anderson<sup>1</sup>; Richard Smith<sup>1</sup>; Arnab Mukherjee<sup>3</sup>; Kyle Miner<sup>3</sup>; Ambika Bhagi<sup>3</sup>; Yi Lu<sup>3</sup>; Joshua Adkins<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Mango Solutions, Chippenham, UK; <sup>3</sup>University of Illinois Urbana-Champaign, Urbana, IL
- MP 390 **ICC-CLASS Software for Automated Data Analysis of LC-MS MS/MS Crosslinking Data;** Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada
- MP 391 **MS-based Characterization of Endogenous Protein Complexes and Interactomes Using Global Glutaraldehyde Stabilization in the Cellular Milieu;** Roman Subbotin; Júlio Padovan; Brian Chait; The Rockefeller University, New York, NY
- MP 392 **Tissue Transglutaminase is a Negative Regulator of Monomeric Lactrin Bioactivity and Lactrin Crosslink Sites Identification by Mass Spectrometry;** Kari Green<sup>1</sup>; Liwen Zhang<sup>1</sup>; Gordon Laurie<sup>2</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>University of Virginia, Charlottesville, VA
- Crosslinking, 393 - 412**
- MP 393 **The Effect of Chemical Cross-Linking on Protein Structure and Function;** Daniel Rozbesky<sup>1,2</sup>; Josef Chmelik<sup>1</sup>; Zdenek Kukacka<sup>1,2</sup>; Petr Man<sup>1,2</sup>; Petr Novak<sup>1,2</sup>; <sup>1</sup>Institute of Microbiology, Prague, Czech Republic; <sup>2</sup>Charles University, Prague, Czech Republic
- MP 394 **Structure Characterization: Chemical Cross-Linking Combined with Mass Spectrometry, Dealing with Impure Protein Sample;** Li Peng<sup>1</sup>; Morten Rasmussen<sup>1</sup>; Gunnar Houen<sup>2</sup>; Peter Højrup<sup>1</sup>; <sup>1</sup>The University of Southern Denmark, Odense, Denmark; <sup>2</sup>Statens Serum Institut, Copenhagen, Denmark
- MP 395 **Charge State Profiles and CID versus ETD Fragmentation Features of Lys-Lys Cross-Linked Peptides Using Diimidoester-Based Cross-Linkers;** Hector Koolen; Alexandre Gomes; Fabio Gozzo; UNICAMP, Campinas, Brazil
- MP 396 **Expanding the Nuclease Toolkit for Middle-Down Characterization of Chemically Modified or Crosslinked RNA;** Matteo Scalabrini; Papa Nii Asare-Okai; Sugyan



## MONDAY POSTERS

- Dixit; John Mangrum; Will McIntyre; Rebecca Rose; Maria Basanta Sanchez; Daniele Fabris; *University at Albany, The RNA Institute, Albany, NY*
- MP 397 **A Novel Protein Cross-linker for Mass Spec Analysis: >95% Enrichment of Cross-linked Peptides in a "Minimalist Style";** Dan Tan<sup>1</sup>; Qiang Li<sup>1</sup>; Xiangke Li<sup>1</sup>; Sheng-Bo Fan<sup>2</sup>; Kun Zhang<sup>2</sup>; Hao Chi<sup>2</sup>; Li Tao<sup>1</sup>; Bing Yang<sup>1</sup>; Yue-He Ding<sup>1</sup>; Pan Zhang<sup>1</sup>; Xiaohui Liu<sup>3</sup>; Si-Min He<sup>2</sup>; Meng-Qiu Dong<sup>1</sup>; Xiaoguang Lei<sup>1,3</sup>; <sup>1</sup>*National Institute of Biological Sciences, Beijing, China*; <sup>2</sup>*ICT, Chinese Academy of Sciences, Beijing, China*; <sup>3</sup>*Tianjin University, Tianjin, China*
- MP 398 **Extending the Cross-Linking/MS Strategy: Investigation of Nidogen-1 Complexes by Incorporated Photo-Amino Acids and Photo-Cross-Linking;** Philip Lössl<sup>1</sup>; Knut Köbel<sup>1</sup>; Dirk Tänzler<sup>1</sup>; Christian Ihling<sup>1</sup>; Manuel Keller<sup>2</sup>; Frank Zaucke<sup>2</sup>; Jens Meiler<sup>3</sup>; Andrea Sinz<sup>1</sup>; <sup>1</sup>*Martin Luther University Halle, Halle, Germany*; <sup>2</sup>*Medical Faculty, University of Cologne, Cologne, Germany*; <sup>3</sup>*Vanderbilt University, Nashville, TN*
- MP 399 **Integrative Approach (Chemical Cross-linking and Hydrogen Deuterium Exchange) Reveals Differences between Crystal and Solution Structure of FimX-PilZ Complex;** Mariana Fioramonte<sup>1</sup>; Cristiane R. Guzzo<sup>2</sup>; Shaker Chuck Farah<sup>2</sup>; Fabio C. Gozzo<sup>1</sup>; <sup>1</sup>*University of Campinas, Campinas, Brazil*; <sup>2</sup>*University of São Paulo, São Paulo, Brazil*
- MP 400 **Impact of Crosslinker Chemistry on Peptide Fragmentation Spectra of Crosslinked Peptides;** Randy J. Arnold; Suraj Saraswat; Chao Ji; Haixu Tang; Predrag Radivojac; James P. Reilly; *Indiana University, Bloomington, IN*
- MP 401 **Structural Models of Lymphocyte Receptor NKR-P1C Revealed by Mass Spectrometry and Molecular Modeling;** Daniel Rozbesky<sup>1,2</sup>; Petr Man<sup>1,2</sup>; Zdenek Kukacka<sup>1,2</sup>; Zofie Sovova<sup>3,4</sup>; Rudiger Ettrich<sup>3,4</sup>; Julien Marcoux<sup>5</sup>; Carol V. Robinson<sup>5</sup>; Petr Novak<sup>1,2</sup>; <sup>1</sup>*Institute of Microbiology, Prague, Czech Republic*; <sup>2</sup>*Faculty of Sciences, Charles University, Prague, Czech Republic*; <sup>3</sup>*Institute of Nanobiology and Structural Biology, Nove Hrad, Czech Republic*; <sup>4</sup>*Faculty of Sciences, University of South Bohemia, Nove Hrad, Czech Republic*; <sup>5</sup>*Department of Chemistry, University of Oxford, Oxford, UK*
- MP 402 **Gas-Phase Intra- and Inter-Molecular Cross-Linking of Protein and Protein Complexes via Ion/Ion Reactions;** Ian Webb; Yang Gao; Scott McLuckey; *Purdue University, Lafayette, IN*
- MP 403 **Negative Ion Chemical Cross-linking Coupled With Ion Mobility Mass Spectrometry for Improved Structural Analysis of Protein Assemblies;** Antonio Calabrese; Deanna Carmen; Denise Tran; Danielle Williams; Yanqin Liu; Tara Pukala; *University of Adelaide, Adelaide, Australia*
- MP 404 **Development of Stable Isotope-Labeled CID-cleavable Cross-linkers for Structural Characterization of Protein Complexes;** Clinton Yu; Wynne Kandur; Athit Kao; Scott Rychnovsky; Lan Huang; *University of California, Irvine, CA*
- MP 405 **Zero-Length Crosslinking of Protein Heterodimers Using <sup>15</sup>N- Metabolically Labeled Monomers;** Karl Makepeace<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; James Bardwell<sup>2</sup>; Shu Quan<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*Dept of Mol., Cell., and Dev. Biology, U Michigan, Ann Arbor, MI*; <sup>3</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*
- MP 406 **Novel isotopically-Coded Photoreactive Heterobifunctional Short-Range Crosslinkers for Studying Protein Structure;** Karl Makepeace<sup>1</sup>; Nicholas Brodie<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*
- MP 407 **Mapping Cross-Links Introduced by bis(succinimidyl)-3-azidomethyl Glutarate in Complex Protein Samples;** Hansuk Buncherd; Behrad Ghavim; Winfried Roseboom; Leo J. de Koning; Chris G. de Koster; Luitzen de Jong; *University of Amsterdam, Amsterdam, Netherlands*
- MP 408 **Crosslinking Study of the Malaria Pathogen Surface Protein Complex Pf12-Pf41;** Michelle Tonkin<sup>1</sup>; Karl Makepeace<sup>2</sup>; Jason Serpa<sup>2</sup>; Evgeniy Petrotchenko<sup>2</sup>; Martin Boulanger<sup>1</sup>; Carol Parker<sup>2</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*; <sup>2</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*
- MP 409 **Evaluating the Potential of an MS/MS-Cleavable Cross-Linker for 3D-Structure Analysis of Protein Complexes;** Jens Pettelkau<sup>1</sup>; Romy Fritzsche<sup>1</sup>; Christian H. Ihling<sup>1</sup>; Mathias Müller<sup>3</sup>; Mathias Schäfer<sup>2</sup>; Andrea Sinz<sup>1</sup>; <sup>1</sup>*Martin-Luther-Universität Halle-Wittenberg, Halle, Germany*; <sup>2</sup>*Universität zu Köln, Köln, Germany*; <sup>3</sup>*ThermoFisher Scientific, Bremen, Germany*
- MP 410 **Quantitative Proteomics of the Prokaryotic Immune Defense System Including the Analysis of protein-RNA Interactions within the CRISPR/Cas System;** Kundan Sharma<sup>1</sup>; Britta Stoll<sup>2</sup>; Anita Marchfelder<sup>2</sup>; Hagen Richter<sup>3</sup>; Lennart Randau<sup>3</sup>; Henning Urlaub<sup>1,4</sup>; <sup>1</sup>*Max-Planck-Institut für Biophysikalische Chemie, Göttingen, Germany*; <sup>2</sup>*Universität Ulm, Ulm, Germany*; <sup>3</sup>*Max-Planck-Institut für terrestrische Mikrobiologie, Marburg, Germany*; <sup>4</sup>*Universitätsmedizin Göttingen, Göttingen, Germany*
- MP 411 **Probing the Human 26S Proteasome Structure by In vivo Cross-linking and Mass Spectrometry;** Athit Kao<sup>1</sup>; Xiaorong Wang<sup>1</sup>; Yingying Yang<sup>1</sup>; Anthony Burke<sup>2</sup>; Scott Rychnovsky<sup>2</sup>; Pierre Baldi<sup>3,4</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>*Dept. Phys. & Biophys., University of California, Irvine, CA*; <sup>2</sup>*Dept. of Chemistry, University of California, Irvine, CA*; <sup>3</sup>*Dept. of Comp. Sci., University of California, Irvine, CA*; <sup>4</sup>*Inst. for Genom. and Bioinf., Univ. of California, Irvine, CA*
- MP 412 **Investigating the Binding Site of the Psb28 Protein in Cyanobacterial Photosystem II Using Cross-Linking, GEE Labeling, and LC-MS/MS;** Daniel A. Weisz; Hao Zhang; Haijun Liu; Michael L. Gross; Himadri B. Pakrasi; *Washington University in St. Louis, St. Louis, MO*
- H/D Exchange: Protein Structure/Function, 413 - 440**
- MP 413 **Hydrogen/Deuterium Exchange Mass Spectrometry Reveals the Binding Interfaces Between Proliferating Cell Nuclear Antigen (PCNA) and SPIP;** Richard Yu-Cheng Huang<sup>1,2</sup>; Zhuo Li<sup>2</sup>; Zvi Kelman<sup>1,2</sup>; Jeffrey Hudgens<sup>1,2</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*; <sup>2</sup>*IBBR, Rockville, MD*
- MP 414 **Structural Changes of HIV-1 Nef upon Lipid Membrane Association;** Gregory Pirrone<sup>1</sup>; Michael S. Kent<sup>2</sup>; Xiaomeng Shi<sup>1</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Sandia National Laboratories, Albuquerque, NM*
- MP 415 **H/DX Mass Spectrometry Studies for the Stability of WT Apolipoprotein E and its Interaction with Amyloid-β 1-42;** Hanliu Wang; Kanchan Garai; Carl Frieden; Michael Gross; *Washington University in St. Louis, St. Louis, MO*
- MP 416 **Characterize the Local Conformational Effects of Chemical Degradation in Recombinant rhDNase by Hydrogen/Deuterium Exchange Mass spectrometry;** Jian Cao; Jin Li; Justin Jeong; Viswanatham Katta; Jennifer Zhang; *Protein Analytical Chemistry, Genentech Inc., South San Francisco, CA*



- MP 417 **Mechanism of Calmodulin-Induced Activation of Calcineurin Revealed Using Hydrogen/Deuterium Exchange Mass Spectrometry**; Mohammed Al-Naqshabandi; David Weis; *University of Kansas, Lawrence, U.S.*
- MP 418 **Structural Study of Redox Sensitive Protein, Nm23 by HDX**; Jae Jin Lee; Jaeho Jeong; In-Kang song; Jin-Hwan Cho; Kong-Joo Lee; *College of Pharmacy, Ewha Womans Univ., Seoul, South Korea*
- MP 419 **HXMS Investigation of Activation Segment Dynamics in the Tec-family Tyrosine Kinase Btk**; Thomas E. Wales<sup>1</sup>; Raji E. Joseph<sup>2</sup>; Amy H. Andreotti<sup>2</sup>; John R. Engen<sup>1</sup>; *<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Iowa State University, Ames, IA*
- MP 420 **Assessment of Protein Structural Differences by Hydrogen/Deuterium Exchange Mass Spectrometry**; Kai Zhang; Jon Fitchett; Bryan E. Jones; *Lilly Biotechnology Center, San Diego, CA*
- MP 421 **Locating Zn-bound Histidines in Metalloproteins Using Hydrogen-Deuterium Exchange Mass Spectrometry**; Jia Dong; Nicholas Borotto; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- MP 422 **LysRS Novel Function with Phosphorylated Thr52 Revealed by H/D Exchange FT-ICR Mass Spectrometry**; Qian Zhang<sup>1</sup>; Pengfei Fang<sup>2</sup>; Min Guo<sup>2</sup>; Nicolas Young<sup>3</sup>; Alan Marshall<sup>1,3</sup>; *<sup>1</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL; <sup>2</sup>The Scripps Research Institute, Scripps Florida, Jupiter, FL; <sup>3</sup>Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*
- MP 423 **Single Residue Level Hydrogen/Deuterium Exchange Kinetics Studied by Top-Down Mass Spectrometry to Probe Protein Solution Structure**; Yining Huang; Don Rempel; Weidong Cui; Michael Gross; *Washington University, St. Louis, MO*
- MP 424 **Higher-Order Structural Characterization of Post-Translationally Modified Proteins by Top-Down HDX-MS with Electron Capture Dissociation**; Jingxi Pan<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; *<sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*
- MP 425 **Structural Analysis of human RXR Homotetramer by use of Hydrogen Deuterium Mass Spectrometry**; Jennifer Cushing; Emily Cowart; LeeAnn Boerma; Gang Xia; Donald D. Muccio; Matthew B. Renfrow; *University of Alabama at Birmingham, Birmingham, AL*
- MP 426 **Analysis of Huntington's Disease Related Protein Aggregates by HDX-ETD-MS**; James Arndt; Justin Legleiter; Kathleen Burke; Stephen Valentine; *West Virginia University, Morgantown, WV*
- MP 427 **H/DX and Mass Spectrometry Reveal the pH Dependence Conformational Changes of Diphtheria Toxin T Domain**; Jing Li<sup>1</sup>; Mykola Rodnin<sup>2</sup>; Alexey Ladokhin<sup>2</sup>; Michael Gross<sup>1</sup>; *<sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>University of Kansas Medical Center, Kansas city, KS*
- MP 428 **Exploring the Effects of ATP Binding on the  $\epsilon$  Subunit of Bacterial  $F_0F_1$ -ATPase Using Hydrogen-Deuterium Exchange Mass Spectrometry**; Antony D. Rodriguez; Stanley D. Dunn; Lars Konermann; *The University of Western Ontario, London, Canada*
- MP 429 **Antibody-Antigen Interactions Investigated by Hydrogen/Deuterium exchange Mass Spectrometry**; Başak Kükrer; Cristina Puchades Garcia; Otto Diefenbach; Eveline Sneekes-Vriese; Adrian Apetri; *Crucell Vaccine Institute, Leiden, Netherlands*
- MP 430 **Hydrogen/Deuterium Exchange Coupled with Mass Spectrometry to Measure the Affect of Transition Metals on  $\beta$ -2 Microglobulin**; Nicholas Borotto; Jia Dong; Richard W. Vachet; *University of Massachusetts, Amherst, MA*
- MP 431 **Microfluidic H/DX MS Analysis of Recombinant Glycoproteins**; Gregory O. Staples<sup>1</sup>; Craig D. Wenger<sup>1</sup>; Reid A. Brennen<sup>1</sup>; Yunan Miao<sup>3</sup>; Terry D. Lee<sup>3</sup>; Debbie Ritchey<sup>1</sup>; Arpad Horvath<sup>1</sup>; Hongfeng Yin<sup>1</sup>; Kevin Killeen<sup>1</sup>; Julie Cichelli<sup>2</sup>; *<sup>1</sup>Agilent Laboratories, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Little Falls, DE; <sup>3</sup>City of Hope, Duarte, CA*
- MP 432 **Probing Human FXR LBD – Prenylflavonoid Interactions by Hydrogen/Deuterium Exchange Mass Spectrometry**; Liping Yang; David Broderick; Yuan Jiang; Yan Campbell; Adrian Gombart; Jan Stevens; Victor Hsu; Claudia Maier; *Oregon State University, Corvallis, OR*
- MP 433 **NEDD8ylation Induced Conformational Changes in Cullin Scaffold Protein Studied by Hydrogen Deuterium Exchange Mass Spectrometry**; Sasidhar N Nirudodhi<sup>1</sup>; Yuan Jiang<sup>3</sup>; Haibin Mao<sup>2</sup>; Ning Zheng<sup>2</sup>; Claudia S. Maier<sup>1</sup>; *<sup>1</sup>Dept. of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Dept. of Pharmacology, University of Washington, Seattle, WA; <sup>3</sup>Dept. of Statistics, Oregon State University, Corvallis, OR*
- MP 434 **Investigating Catalysis-Linked Dynamics in Yeast Alcohol Dehydrogenase by Measuring Kinetic Isotope Effects Using Time-Resolved ESI-MS with H/D Exchange**; Peter Liuni; Derek Wilson; *York University Department of Chemistry, Toronto, Canada*
- MP 435 **Studies of Changes in STAT3 Dynamics upon Interaction with Novel Small Molecule Dimerization Inhibitors by TRESI-MS/HDX**; Diana Resetca; Derek Wilson; *York University, Toronto, Canada*
- MP 436 **Hydrogen/Deuterium Exchange Reveals the Conformational Changes of Human  $\alpha$ 1-Acid Glycoprotein upon Glycosylation**; Richard Yu-Cheng Huang<sup>1,2</sup>; Jeffrey Hudgens<sup>1,2</sup>; *<sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>IBBR, Rockville, MD*
- MP 437 **Probing Protein Conformation of Cellobiose Dehydrogenase by Hydrogen/Deuterium Exchange Mass Spectrometry**; Petr Halada<sup>1</sup>; Alan Kadek<sup>1,2</sup>; Petr Novak<sup>1,2</sup>; Roland Ludwig<sup>3</sup>; Petr Man<sup>1,2</sup>; *<sup>1</sup>Institute of Microbiology of ASCR, v.v.i., Prague, Czech Republic; <sup>2</sup>Department of Biochemistry, Charles University, Prague, Czech Republic; <sup>3</sup>Food Biotechnology Laboratory, BOKU University, Vienna, Austria*
- MP 438 **Probing Conformational Changes in Amyloid Beta Aggregation by Pulsed Hydrogen/Deuterium Exchange Mass Spectrometry**; Ying Zhang<sup>1</sup>; Don Rempel<sup>1</sup>; Jun Zhang<sup>2</sup>; Anuj Sharma<sup>1</sup>; Liviu Mirica<sup>1</sup>; Michael Gross<sup>1</sup>; *<sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Department of Drug Product Development, Amgen Inc., Seattle, WA*
- MP 439 **Study of Protein Folding/Unfolding Structure Mechanism of Staphylococcal Nuclease Wild Type and Its Mutant V66W by PEPS-HDX-ESI-MS**; Rohana Liyanage; Derek Derek Pyland; Jennifer Gidden; Wesley Stites; Jackson Jackson O. Lay Jr; *University of Arkansas, Fayetteville, AR*
- MP 440 **Probing Conformational Dynamics of Estrogen Receptor  $\alpha$  (ER $\alpha$ ) Co-Activator PGC-1 by H/D Exchange Coupled with FT-ICR MS**; Yeqing Tao<sup>1</sup>; Sepideh Khorasanizadeh<sup>2</sup>; Qian Zhang<sup>1</sup>; Nicolas Young<sup>3</sup>; Fraydoon Rastinejad<sup>2</sup>; Alan Marshall<sup>1,3</sup>; *<sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>Sanford Burnham Medical Research Institute, Orlando, FL; <sup>3</sup>National High Magnetic Field Laboratory, Tallahassee, FL*



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- MP 441 **Characterization of Novel Polyketide Synthase Activity by the Measurement of Intact Protein and Proteolytic Products at Amino Acid Level Resolution;** Michaela M. Hinks; Shan M. Randall; Irina Koryakina; Gavin J. Williams; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- MP 442 **Limited Proteolytic Cleavage - Mass Spectrometry Driven Epitope Mapping of IL13ra2;** Maria Christina Malinao; Rebecca Carroll; Claudia Guevara; James Song; David Tae; Vladimir Kery; *Agensys, Inc., Santa Monica, CA*
- MP 443 **Epitope Structure and Binding Affinity of Single Chain Llama anti- $\beta$ -amyloid Antibodies Revealed by Proteolytic Excision Affinity-Mass Spectrometry;** Paraschiv Gabriela Ioana<sup>1</sup>; Cecile Vincke<sup>2</sup>; Paulina Czaplowska<sup>3</sup>; Marilena Manea<sup>1</sup>; Serge Muyldermans<sup>2</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*University of Konstanz, Konstanz, Germany*; <sup>2</sup>*Vrije Universiteit Brussel, Brussel, Belgium*; <sup>3</sup>*University of Gdańsk, Gdańsk, Poland*
- MP 444 **M+320 Da Ions in the Electrospray Ionization (ESI) Mass Spectra Of Proteins: Double Glycation or Something Completely Different?** Georg Drabner; Isabel Hermann; Verena Niggeloh; *Roche Diagnostics GmbH, Penzberg, Germany*
- MP 445 **Mapping the Binding Sites of New Photoactivatable Anticancer Complexes to Proteins via FT-ICR MS;** Christopher Wootton; Ilaria Finazzi; Mark Barrow; Peter B. O'Connor; Peter J. Sadler; *University of Warwick, Coventry, UK*
- MP 446 **Proteomic Identification of the BACE1 Cleavage Sites;** Nicole Heinks; Erik Carlson; Joseph Johnson; *University of Minnesota, Duluth, Duluth, MN*
- MP 447 **Protein Quantitation in Industrial Fermentation;** Barbara S. Larsen; Timothy Snow; Andrew Eliot; *The DuPont Company, Wilmington, DE*
- MP 448 **Degradation Processes of Archaeological Silk Proteins to Remind in Mass Spectrometry;** Kazuki Kawahara<sup>1</sup>; Mayumi Yamada<sup>2</sup>; Fumio Okada<sup>3</sup>; Miho Muguruma<sup>1</sup>; Atsuko Miyaji<sup>1</sup>; Yoshiaki Matsuo<sup>1</sup>; Takashi Nakazawa<sup>1</sup>; <sup>1</sup>*Nara Women's University, Nara, Japan*; <sup>2</sup>*Biosys Technologies, Inc., Tokyo, Japan*; <sup>3</sup>*Kyoto University of Art and Design, Kyoto, Japan*
- MP 449 **Stress Response in *Daphnia pulex*;** Aaron Steevens<sup>1</sup>; Roland Vergilino<sup>1</sup>; Melania Cristescu<sup>2</sup>; Panayiotis Vacratis<sup>1</sup>; <sup>1</sup>*University of Windsor, Windsor, Canada*; <sup>2</sup>*McGill University, Montreal, Canada*
- MP 450 **Intact Protein Supercharging and Characterization;** Ravi Kumar Krovvidi<sup>1</sup>; Arunkumar Padmanaban<sup>1</sup>; Vadiraja Bhat<sup>2</sup>; <sup>1</sup>*Agilent Tech, Bangalore, India*; <sup>2</sup>*Agilent, Little Falls*
- MP 451 **Rapid Mass Spectrometric Analysis of Disulfide-Containing Proteins Following Online Digestion, Online Electrolytic Reduction and DESI Analysis;** Qiuling Zheng<sup>1</sup>; Hao Zhang<sup>2</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>*Ohio University, Athens, OH*; <sup>2</sup>*Washington University, St. Louis, MO*
- MP 452 **Investigating Redox Regulation in the Apoptotic Pathway using High Resolution Mass Spectrometry;** Sophie Thurlow<sup>1</sup>; David Clarke<sup>1</sup>; Jenna Scotcher<sup>2</sup>; Colin Campbell<sup>1</sup>; C. Logan Mackay<sup>1</sup>; Patrick Langridge-Smith<sup>1</sup>; <sup>1</sup>*Edinburgh University, Edinburgh, UK*; <sup>2</sup>*NHMFL, Florida State University, Tallahassee, FL*
- MP 453 **Characterization of Redox-Labile Disulfide Bonds in Protein Using Differential Alkylation with O16/O18 Labeled Iodoacetic Acid;** Shunhai Wang; Igor Kaltashov; *University of Massachusetts, Amherst, MA*

- MP 454 **Online Electrochemical Reduction of the Disulfide Bond(s) in Oxytocin and Heptidin Results in Different CID and ETD Fragmentation Spectra;** Martin A. Giera<sup>1</sup>; Simone Nicolardi<sup>1</sup>; Pieter Kooijman<sup>1</sup>; Agnieszka Kraj<sup>2</sup>; Jean-Pierre Chervet<sup>2</sup>; André M. Deelder<sup>1</sup>; Yuri E.M. van der Burg<sup>1</sup>; <sup>1</sup>*Leiden University Medical Center, Leiden, Netherlands*; <sup>2</sup>*Antec, Zoeterwoude, Netherlands*
- MP 455 **An Enrichment Approach Using a Highly Selective Aptamer Modified PS-DVB Microbeads for Subpicomole Level Lysozyme Detection by Mass Spectrometry;** Ülkü Güler; Ömür Çelikbıçak; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- MP 456 **Identification of Gamma Carboxylation of Human Gas6 by Tandem Mass Spectrometry;** Li Zhang<sup>1</sup>; Kevin Xiao<sup>2</sup>; Faye Fang<sup>1</sup>; <sup>1</sup>*R&D Systems Inc, Minneapolis, MN*; <sup>2</sup>*Dept of Medicine, Duke University Medical Center, Durham, NC*
- MP 457 **Evaluation of Expressed Sequence Tags for the Identification of *Taenia solium* Metacestode Excretion/Secretion Proteins;** Björn Victor<sup>1</sup>; Pierre Dorny<sup>1</sup>; Kirezi Kanobana<sup>1</sup>; Katja Polman<sup>1</sup>; Johan Lindh<sup>2,3</sup>; André M. Deelder<sup>4</sup>; Magnus Palmblad<sup>4</sup>; Sarah Gabriël<sup>1</sup>; <sup>1</sup>*Institute of Tropical Medicine, Antwerpen, Belgium*; <sup>2</sup>*Karolinska Institutet, Stockholm, Sweden*; <sup>3</sup>*Swedish Institute for Communicable Disease Control, Solna, Sweden*; <sup>4</sup>*Leiden University Medical Center, Leiden, The Netherlands*
- MP 458 **Enhancing Peptide Identification by Combining an Efficient Protein Extraction Procedure with Dynamic Inclusion/Exclusion Lists in Data-Dependent LC-MS/MS Acquisition Mode;** Ying Zhang<sup>1</sup>; Dario Bottinelli<sup>1</sup>; Aivett Bilbao<sup>1,2</sup>; Bandar Alghanem<sup>1</sup>; Frédéric Nikitin<sup>2</sup>; Markus Müller<sup>2</sup>; Frédérique Lisacek<sup>2</sup>; Jeremy Luban<sup>3</sup>; Caterina Strambio De Castillia<sup>3</sup>; Emmanuel Varesio<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>*University of Geneva, Geneva, Switzerland*; <sup>2</sup>*Swiss Institute of Bioinformatics, Geneva, Switzerland*; <sup>3</sup>*University of Massachusetts, Worcester, MA*
- MP 459 **"MELD": A Bottom-Up Method to Fully de novo Sequence Purified Proteins;** Gabriel Mazzucchelli<sup>1</sup>; Tyler Zimmerman<sup>2</sup>; Marie-Alice Meuwis<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>*University of Liege, MS Lab - GIGA, Liege, Belgium*; <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- MP 460 **Optimization of a Broad Specificity Protease for Routine Bottom-Up Protein and Post-Translational Modification Identification;** Mike Naldrett; Ellen Marsh; Sophie Alvarez; *Donald Danforth Plant Science Center, St Louis, MO*
- MP 461 **Extent of Urea-Induced Protein Carbamylation during Sample Preparation;** Laxmikanth Kollipara; René Zahedi; *Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
- MP 462 **High-throughput Scheduled MRM for Multiplexed Quantitation of Chemical Probe Labeled Enzymes in Human Cells;** Song Li<sup>1</sup>; Pamela Diego<sup>1</sup>; Santosh Keshipeddy<sup>1</sup>; Bekim Bajrami<sup>1</sup>; Vahid Farrokhi<sup>1</sup>; Adam McShane<sup>1</sup>; Ying Wai Lam<sup>2</sup>; Bin Deng<sup>2</sup>; Reza Nemat<sup>1</sup>; Amy Howell<sup>1</sup>; Xudong Yao<sup>1</sup>; <sup>1</sup>*University of Connecticut, Storrs, CT*; <sup>2</sup>*University of Vermont, Burlington, VT*

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- MP 463 **Improving SWATH by Overlapped Windows;** David Cox; Sandra Chu; Stephen Tate; Ron Bonner; *AB SCIEX, Concord, Canada*
- MP 464 **Improved Peptide Fractionation Efficiency in Ion-Mobility Based Data-Independent Acquisition Enables the Identification of >4400 Proteins Using an Optimized 1D-nanoUPLC-IMS-MS<sup>E</sup> Workflow;** Ute Distler; Jörg

- Kuharev; Stefan Tenzer; *UMC of the Johannes Gutenberg University Mainz, Mainz, Germany*
- MP 465 **The Iterative Data Analysis towards the Unfractionated SWATH Data through Expansion of Ion Library**; Shenyang Zhang<sup>1,2</sup>; Bo Wen<sup>1</sup>; Shaohang Xu<sup>1</sup>; Baojin Zhou<sup>1</sup>; Zhen Chen<sup>2</sup>; Quanhui Wang<sup>1,2</sup>; Xiaomin Lou<sup>2</sup>; Haidan Sun<sup>2</sup>; Liang Lin<sup>1</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>BGI-Shenzhen, Shenzhen, China; <sup>2</sup>Beijing Institute of Genomics, CAS, Beijing, China
- MP 466 **Exploring Transition from SWATH Acquisition to MRM Analysis for Quantitative Proteomics**; Sahana Mollah; Christie Hunter; *AB SCIEX, Foster City, CA*
- MP 467 **Using Fractionation and Labeling with Data Independent Acquisition**; Sean L. Seymour; Christie L. Hunter; *AB SCIEX, Foster City, CA*
- MP 468 **Can We Use Conserved Domains to Reveal Unique Protein Functions Present in Hydrothermal Vent Plume Microbial Communities?** Brook Nunn<sup>1</sup>; Timothy Mattes<sup>2</sup>; Sonia Ting<sup>1</sup>; Giora Proskurovski<sup>1</sup>; Michael MacCoss<sup>1</sup>; Deborah Kelley<sup>1</sup>; David Goodlett<sup>3</sup>; Robert Morris<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Iowa, Iowa City, IA; <sup>3</sup>University of Maryland, Baltimore, MD
- MP 469 **Developing Peptide Library for SWATH™ Based Proteomic Profiling**; Melinda Wojtkiewicz; Jessica Winkler; Jayme Wiederin; Lance Villeneuve; Kelly Stauch; Howard S. Fox; Pawel Ciborowski; *University of Nebraska Medical Center, Omaha, NE*
- MP 470 **Understanding the Role of Proteolytic Digestion on Discovery – and Targeted-Proteome Measurements Using LC-MS/MS**; Philip Loziuk; *North Carolina State University, Raleigh, NC*
- MP 471 **Combining Pulsed-SILAC Labeling and Click-Chemistry to Probe Rapid Proteome and Secretome Dynamics – Application to Macrophage Activation**; Katrin Eichelbaum; Jeroen Krijgsveld; *EMBL Heidelberg, Heidelberg, Germany*
- MP 472 **Quantitative Degradomics Using an Isotope Labeled Mass Tag**; Kazutaka Shimbo<sup>1,2</sup>; Sami Mahrus<sup>2</sup>; Robert Chalkley<sup>2</sup>; James Wells<sup>2</sup>; <sup>1</sup>Ajinomoto CO., INC, Kawasaki-Shi, Japan; <sup>2</sup>University of California, San Francisco, CA
- MP 473 **Proteomic Analysis Identifies Differentially Expressed Proteins after Red Propolis Extract Treatment in Hep-2 Cells**; Mariana Roesch-Ely<sup>1</sup>; Sidnei Moura<sup>1</sup>; Caroline Olivieri da Silva Frozza<sup>1</sup>; Tanara da Silva Ribeiro<sup>1</sup>; Paulo Marcos Pinto<sup>2</sup>; Francine Ferreira Padilha<sup>3</sup>; João Antonio Pêgas Henriques<sup>1</sup>; <sup>1</sup>University of Caxias do Sul, Caxias do Sul, Brazil; <sup>2</sup>Federal University of Pampa, São Gabriel, Brazil; <sup>3</sup>Tiradentes University, Aracaju, Brazil
- MP 474 **Quantitative Analysis of the C2C12 and Mouse Skeletal Muscle Proteomes Using a Multiplexing Strategy**; Michelle Henderson; John Chilton; Getiria Onsongo; Pratik Jagtap; Edgar Arriaga; *U of M, Minneapolis, MN*
- MP 475 **Coping with the Trade-Off between Comprehensive Identification and Accurate Quantitation Using Stable Isotope Dimethyl Labeling**; Masaki Wakabayashi; Naoyuki Sugiyama; Yasushi Ishihama; *Kyoto University, Kyoto, Japan*
- MP 476 **High Throughput Quantitative p-SILAC in Niche Model Organisms**; Mario Looso<sup>1</sup>; Christian Michel<sup>1</sup>; Marc Bruckskotten<sup>1</sup>; Jens Preussner<sup>1</sup>; Panagiotis Tsonis<sup>2</sup>; Marcus Krueger<sup>1</sup>; Thomas Braun<sup>1</sup>; <sup>1</sup>Max-Planck-Institute for Heart and Lung Research, Bad Nauheim, Germany; <sup>2</sup>TREND, University of Dayton, Dayton, OH
- MP 477 **Depolarization Dependent Spatial Localization of Proteins in Nerve Terminals**; María Ibáñez-Vea; Sanah Shah; Alistair Edwards; Lene Jakobsen; Martin R. Larsen; *University of Southern Denmark, Odense, Denmark*
- MP 478 **Identification of Targets of c-Src Tyrosine Kinase by Chemical Complementation and Phosphoproteomics. Exploring the Mechanism of Activation of Rap1GEF (C3G)**; Isabel Martinez Ferrando<sup>1</sup>; Raghothama Chaerkady<sup>1</sup>; Jun Zhong<sup>1</sup>; Henrik Molina<sup>2</sup>; Harrys Jacobs<sup>1</sup>; Katie Herbst-Robinson<sup>3</sup>; Beverley Dancy<sup>1</sup>; Vikram Katju<sup>4</sup>; Ron Bose<sup>5</sup>; Jin Zhang<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; Cole Philip<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>Rockefeller University, New York City, US; <sup>3</sup>University of Pennsylvania, Philadelphia, US; <sup>4</sup>M.D. Anderson Cancer Center, University of Texas, Houston, US; <sup>5</sup>Washington University School of Medicine, Saint Louis, US
- MP 479 **Quantitative Proteomic and Proteogenomic Comparison of hESC and Neurons**; Harsha P. Gunawardena<sup>1</sup>; John Wrobel<sup>1</sup>; Jainab Khatun<sup>2</sup>; Brian Risk<sup>2</sup>; Morgan C. Giddings<sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Boise State University, Boise, ID
- MP 480 **Identification and Validation of PRP4 Kinase Substrates with Integrated Proteomics Approaches**; Qiang Gao; Nayanara Kothari; Zhuyan Guo; Huang Shih-Min A; Hong Cheng; Bailin Zhang; *Sanofi Oncology, Cambridge, MA*
- MP 481 **Synthesis of d-Labeled and Unlabeled Ethyl Succinic Anhydride and Application to Quantitative Analysis of Peptides by Isotope Differential Mass Spectrometry**; Satomi Niwayama; Masoud Zabet-Moghaddam; Aarif Shaikh; *Texas Tech University, Lubbock, TX*
- MP 482 **Application of CESI-MS on SILAC-based Quantitative Proteomics**; Herbert H. Lindner<sup>1</sup>; Klaus Faserl<sup>1</sup>; Leopold Kremser<sup>1</sup>; Martin Mueller<sup>2</sup>; David Teis<sup>2</sup>; Bettina Sarg<sup>1</sup>; <sup>1</sup>Biocenter, Division of Clinical Biochemistry, Innsbruck, Austria; <sup>2</sup>Biocenter, Division of Cell Biology, Innsbruck, Austria
- MP 483 **In-Source Fragmentation and the Sources of Partially Tryptic Peptides in Shotgun Proteomics**; Jong-Seo Kim<sup>1,2</sup>; Matthew E. Monroe<sup>1</sup>; David G. Camp II<sup>1</sup>; Richard D. Smith<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>Institute for Basic Science, Seoul National Univ., Seoul, Korea
- MP 484 **Faster Protein Identification with Surface Acoustic Wave Nebulization in Place of Infusion-based ESI**; Sung Hwan Yoon<sup>1,2</sup>; Young Ah Goo<sup>1,2</sup>; Michael Wilson<sup>1,2</sup>; Yue Huang<sup>1</sup>; J. Scott Edgar<sup>3</sup>; Scott Heron<sup>1,2</sup>; David R. Goodlett<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Maryland, Baltimore, MD; <sup>3</sup>Deurion LLC, Seattle, WA
- MP 485 **193 nm Ultraviolet Photodissociation for High Throughput Middle-Down Proteomics**; Joe R. Cannon; Jennifer S. Brodbelt; *Univ. of Texas at Austin, Austin, TX*
- MP 486 **Increased Peptide and Protein Identification Rate for Proteomics Samples by Controlling Peptide Charge States Generated by Captive Spray**; Stephanie Kaspar; Stuart Pengelley; Thorsten Ledertheil; Ralf Hartmer; Wolfgang Jabs; Carsten Baessmann; *Bruker Daltonik, Bremen, Germany*
- MP 487 **Characterization and Optimization of a High Field Orbitrap for Proteome Analysis**; Fiona Pachi; Bernhard Kuster; *Technical University Munich, Freising, Germany*
- MP 488 **Deep Proteome Mapping of HeLa and U2OS Human Cancer Cell Lines**; Cristian Ruse<sup>1</sup>; Samantha Peacock<sup>1</sup>; Vadiraja B Bhat<sup>2</sup>; <sup>1</sup>Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; <sup>2</sup>Agilent Technologies, Wilmington, DE
- MP 489 **Travelling Wave Ion Mobility Assisted Duty Cycle Enhancements for Targeted and Non-Targeted Proteomics Experiments**; Christopher J Hughes; Johannes PC Vissers; James Langridge; *Waters, Manchester, UK*



- MP 490 **Large Scale Targeted Protein Quantification Using HR/AM Selected Ion Monitoring with MS/MS Confirmation on A Novel Hybrid, Q-OT-qIT Mass Spectrometer;** Reiko Kiyonami<sup>1</sup>; Michael Senko<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Jarrett Egerton<sup>2</sup>; Sonia Ting<sup>2</sup>; Michael MacCoss<sup>2</sup>; Andreas Hühner<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>University of Washington, Seattle, WA
- MP 491 **Characterization of Proteomics Performance of a Novel Collision Cell for Ultrahigh Resolution Time of Flight Mass Spectrometers (UHR-TOF);** Markus Lubeck; Ralf Hartmer; Oliver Raether; Carsten Baessmann; *Bruker Daltonik GmbH, Bremen, Germany*
- MP 492 **Protein Separation and Identification Using Capillary Isoelectric Focusing (cIEF) Coupled to Mass Spectrometry;** Sunil Adav; Siu-Kwan Sze; *Nanyang Technological University, Singapore, SG*
- MP 493 **Reproducibility of SWATH™ MS Analysis and Implications for System Biology Studies;** Yang Kang; Stephen Tate; Christie Hunter; Suyu Liu; Ron Bonner; *AB Sciex, Concord, Canada*

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- MP 494 **Intact 20kDa Extracellular Domain of APO2L/TRAIL Bioanalysis by HRMS: A Potential Cancer Therapeutic Protein;** Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Quebec, Canada*
- MP 495 **Iodine-129 Microdosing for Protein and Peptide Drug Development;** Robert-Jan Lamers<sup>1</sup>; José Maria López-Gutiérrez<sup>2</sup>; Jose Manuel Gómez-Guzmán<sup>2</sup>; Peter Boshuis<sup>3</sup>; <sup>1</sup>Abundanz B.V., Woerden, The Netherlands; <sup>2</sup>Universidad de Sevilla, CNA, Sevilla, Spain; <sup>3</sup>Ducares, Utrecht, The Netherlands
- MP 496 **Quantitative Analysis of Blood Coagulation Factor VIII Therapeutics in Plasma Using UPLC/MS;** Hiroya Miura<sup>1</sup>; Taiji Kawase<sup>2</sup>; Kenji Hirose<sup>2</sup>; <sup>1</sup>Japanese Blood Products Organization, Tokyo, Japan; <sup>2</sup>Nihon Waters K.K., Tokyo, Japan
- MP 497 **Mass Spectrometry-Based Protein Quantification for Improved Definition of Therapeutic Targets;** Juergen Kast<sup>1</sup>; Martin Barnes<sup>1</sup>; Robert Boyd<sup>1</sup>; Jason Allen<sup>1</sup>; Amanda Anderson<sup>1</sup>; Jim Ackroyd<sup>1</sup>; Ludmila Bozhenok<sup>1</sup>; Lindsey Hudson<sup>1</sup>; Xiaohong Yu<sup>1</sup>; Jonathan Terrett<sup>2</sup>; Christian Rohlf<sup>1</sup>; <sup>1</sup>Oxford BioTherapeutics Ltd, Milton Park, Abingdon, UK; <sup>2</sup>Oxford BioTherapeutics Inc, San Jose, CA
- MP 498 **NTCB Cleavage of Proteins: First Application for Protein Therapeutics Quantitative Analysis in Mass Spectrometry;** Barbara Marsiglia; Luca Genovesi; Marina Ferroggio; Luca Barbero; *Merck Serono, Colleretto Giacosa, Italy*
- MP 499 **On the Feasibility of Using Non-Ferrous Metals as Tracers of Transferrin-Based Therapeutics in Clinical Samples;** Hanwei Zhao; Shunhai Wang; Cedric E. Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- MP 500 **Development of a Quantitative Mass Spectrometric Method to Measure the Protein Components in Virus Like Particles Used for Vaccination;** Michael D. Ward<sup>1</sup>; Ernst E. Brueggemann<sup>1</sup>; Lisa H. Cazares<sup>2</sup>; Sina Bavari<sup>1</sup>; <sup>1</sup>USAMRIID, Ft. Detrick, MD; <sup>2</sup>Geneva Foundation/USAMRIID, Frederick, MD
- MP 501 **Development and Application of a Comprehensive Isotope-labeled Peptide Library to Quantify the Twelve Signal Transduction Pathways of Carcinogenesis;** Lisa A Vasicsek<sup>1</sup>; Kelly A. Conrads<sup>1</sup>; Yutaka Shoji<sup>2</sup>; Brian L. Hood<sup>1</sup>; Amol Prakash<sup>3</sup>; Scott Peterman<sup>3</sup>; Joel Louette<sup>3</sup>; Chad A. Hamilton<sup>1,4</sup>; G. Larry Maxwell<sup>1,5</sup>; John I. Risinger<sup>2</sup>;

- Thomas P. Conrads<sup>1</sup>; <sup>1</sup>Women's Integrated Research Center at Inova Health, Annandale, VA; <sup>2</sup>Michigan State University, Grand Rapids, MI; <sup>3</sup>ThermoFisher Scientific, Inc., BRIMS, Cambridge, MA; <sup>4</sup>Walter Reed National Military Medical Center, Bethesda, MD; <sup>5</sup>INOVA Fairfax Hospital, Falls Church, VA
- MP 502 **Identification and Quantification of Low Abundant Proteins in Biotherapeutics by a Sensitive and Universal LC-High Resolution MS Based Assay;** Hongxia (Jessica) Wang; Zhiqi Hao; Yi Zhang; David Horn; Patrick Bennett; *Thermo Fisher Scientific, San Jose, CA*
- MP 503 **Integrated Targeted Quantitation Method for Insulin and Its Therapeutic Analogs;** Eric E. Niederkofer<sup>1</sup>; Tara Schroeder<sup>2</sup>; Dobrin Nedelkov<sup>1</sup>; Urban A. Kiernan<sup>1</sup>; David A. Phillips<sup>1</sup>; Kemmons A. Tubbs<sup>1</sup>; Scott Peterman<sup>3</sup>; Bryan Krastins<sup>3</sup>; Amol Prakash<sup>3</sup>; Mary Lopez<sup>3</sup>; <sup>1</sup>Tempe Thermo Fisher Scientific, Tempe, AZ; <sup>2</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>3</sup>BRIMS Thermo Fisher Scientific, Boston, MA
- MP 504 **Quantitation of a Therapeutic Protein in Rat Plasma by a Validated UPLC/MS/MS and Its Application to a GLP Toxicokinetic Study;** Bailuo Ren; Yan Mao; David Roos; John Yu; Jeffrey Duggan; *Boehringer Ingelheim Pharma, Ridgefield, CT*
- MP 505 **Development and Validation of an Assay for Quantitation of a Therapeutic Protein in Human Urine Using an LC/MS/MS Method;** David Roos; John Yu; Jeffrey Duggan; Lin-Zhi Chen; Elsy Philip; *Boehringer Ingelheim, Ridgefield, CT*
- MP 506 **LC/MS/MS Assays for Biotherapeutic Protein Quantitation in Biological Matrixes – Regulatory Considerations, Validation Procedures and Results;** David Roos; John Yu; Jeffrey Duggan; Lin-Zhi Chen; Shirin Pagels; *Boehringer Ingelheim, Ridgefield, CT*
- MP 507 **Quantification of Human mAbs in Mouse Tissues Using Generic Immunocapture and LC-MS/MS;** Bogdan Slecza<sup>1</sup>; John T. Mehl<sup>1</sup>; Katherine Lewis<sup>2</sup>; Robin Moore<sup>1</sup>; Ragini Vuppugalla<sup>1</sup>; Celia D'Arienzo<sup>1</sup>; Tim Olah<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb (Zymogenetics), Seattle, WA
- MP 508 **SPE Cleanup of Background Peptides for the LC-MS/MS Bioanalysis of a Monoclonal Antibody in Monkey Serum;** Long Yuan; Qin Ji; Anne-Françoise Aubry; *Bristol-Myers Squibb, Princeton, NJ*
- MP 509 **High-sensitivity Quantitative Analysis of Therapeutic Monoclonal Antibodies in Human Serum Using Q Exactive Selected Ion Monitoring NanoLC-MS;** Haibo Qiu<sup>1</sup>; Hongxia Wang<sup>2</sup>; Patrick Bennett<sup>2</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 510 **Strategies for Calibration and Signature Peptide Selection are Critical for Accurate Absolute Quantification of Therapeutic Monoclonal Antibodies in Pharmaceutical Matrices;** Ming Zhang; Haoying Yu; Eslam Nouri-Nigjeh; Jun Qu; *University at Buffalo, Buffalo, NY*
- MP 511 **Comparison of Methods for Quantitating Tryptic Digests of Monoclonal Antibodies using Q-TOF and QQQ Mass Spectrometry;** Caroline S. Chu; Alex Zhu; Ning Tang; *Agilent Technologies, Santa Clara, CA*
- MP 512 **Determination of Contaminant Bacterial Host Cell Proteins in Recombinant Proteins Expressed in E. coli by LC-MS/MS;** Oscar Potter; Yanan Yang; Hongfeng Yin; Kevin Killeen; *Agilent Technologies, Santa Clara, CA*
- MP 513 **Quantification of Large Peptides in Human Serum Using High Resolution Dual Ion Funnel LC-QTOF;** Anne E Blackwell; Rory Doyle; Alex Zhu; Vadiraja B. Bhat; *Agilent*



Technologies, Wilmington, DE

- MP 514 **Quantitative Analysis of a Therapeutic Monoclonal Antibody in Human Plasma by Accelerated Trypsin Digestion and LC-MS/MS;** Jianshuang Wang; Fumin Li; Douglas Fast; Covance, Madison, WI
- MP 515 **Low ng/ml Bioanalysis of Monoclonal Antibody Therapeutics Using nano-UPLC Coupled to HRMS;** William Douglas Van Dongen; Frédérique Van Holthoorn; Richard Bas; Anne Kleinnijenhuis; TNO Triskelion, Zeist, Netherlands
- MP 516 **Simultaneous Quantitative Peptide Mapping and Host Cell Protein Detection in an IgG1 Monoclonal Antibody Preparation using Data-Independent Acquisition;** Eric Johansen; Kelli Jonakin; Christie Hunter; AB SCIEX, Foster City, CA
- MP 517 **Accurate Quantitation of Deamidated Peptides by Spectral Accuracy;** Darryl Davis<sup>1</sup>; Ming Gu<sup>2</sup>; <sup>1</sup>Johnson and Johnson, Radnor, PA; <sup>2</sup>Cerno Bioscience, Norwalk, CT
- MP 518 **Simultaneous Quantitation of a Monoclonal Antibody and Two Proteins in Human Plasma by High Resolution and Accurate Mass Measurements;** Paul-Gerhard Lassahn<sup>1</sup>; Kai Scheffler<sup>2</sup>; Myriam Demant<sup>3</sup>; Nathanael Delmotte<sup>1</sup>; Winfried Wagner-Redeker<sup>1</sup>; Guenter Boehm<sup>4</sup>; <sup>1</sup>Swiss BioAnalytics AG, Basel, CH; <sup>2</sup>Thermo Fisher Scientific, Dreieich, Germany; <sup>3</sup>ThermoFisher Scientific, Reinach, CH; <sup>4</sup>CTC Analytics AG, Zwingen, CH
- MP 519 **Quantification of Biotherapeutics in DMPK Studies Using Accurate Mass MS/MS;** Joanne Mather<sup>1</sup>; Robert S. Plumb<sup>2</sup>; Gordon Fujimoto<sup>1</sup>; Jonathan R. Kheller<sup>3</sup>; Matthew E. Szapacs<sup>3</sup>; Christopher Evans<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Imperial College, London, UK; <sup>3</sup>GSK, King of Prussia, PA
- MP 520 **Development of an Immunoprecipitation and LC-MS/MS Based Method for Quantifying the 105 kDa Recombinant Protein SXN101959 in Plasma;** Steve Pleasance<sup>1</sup>; Richard Kay<sup>1</sup>; David Griffiths<sup>1</sup>; Aimee Cossins<sup>2</sup>; Andrew Splevins<sup>2</sup>; Alberto Martinez<sup>2</sup>; Helen Ludlow<sup>2</sup>; <sup>1</sup>Quotient Bioresearch Ltd, Fordham, England; <sup>2</sup>Syntaxin Ltd, Abingdon, England
- MP 521 **Improved Identification and Quantitation of Host Cell Proteins in Protein Therapeutics using 2D-LC and Ion Mobility;** Martha Stapels; Catalin Doneanu; Keith Fadgen; Waters Corporation, Milford, MA

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- MP 522 **Targeted Proteomics Workflow for Biomarker Analysis by Nano LCMS;** Jorge Smith<sup>1</sup>; Jeremy Post<sup>1</sup>; Rachel Lieberman<sup>1</sup>; Nataliya Bulayeva<sup>2</sup>; Kevin Rosenblatt<sup>2</sup>; Ben Figard<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Inst., Houston, TX; <sup>2</sup>UT-Health Science Center at Houston, Houston, TX
- MP 523 **Targeted Quantification of Proteins at Sub-nanogram/ mL Levels in Human Plasma by MRM-MS without the Need for Fractionation;** Michael Burgess; Hasmik Keshishian; D.R. Mani; Michael Gillette; Steven Carr; Broad Institute, Cambridge, MA
- MP 524 **Analysis of Serum Myostatin and Its Inhibitors N-terminal Pro-protein, GASP-1 and FLRG Simultaneously in Human Serum by LC-MS/MS;** Patrick Vanderboom; Olga Bondar; Linda Benson; Nathan LeBrasseur; Sundeep Khosla; Robert Bergen; Mayo Clinic, Rochester, MN
- MP 525 **Immunoaffinity Enrichment and Quantification of Serum Proteins Using Stable Isotope Labeled Proteins as Internal Standards;** Kevin Ray; Jim J. Walters; Melissa R. Radabaugh; Sigma-Aldrich, St. Louis, MO

- MP 526 **Characterization of Heavy Recombinant Proteins for Use as Internal Standards in Quantitative MS Workflows;** Gordon R. Nicol; Pegah Jalili; Mark Angeles; David Rhee; Kevin Ray; Sigma, St Louis, MO
- MP 527 **MRMcubed (MRM3) Optimization for Direct Quantification of Low Abundance Protein in Biological Fluids : Application to Plasma Biomarkers;** Jeremy Jeudy; Arnaud Salvador; Romain Simon; Aurore Jaffuel; Catherine Fonbonne; Jerome Lemoine; Institut des Sciences Analytiques, Villeurbanne, France
- MP 528 **Development and Validation of a Sensitive LC/MS/MS Assay for Fibrinogen Peptide A Quantitation in Human Plasma Using Nano-flow LC with Trizaic Tile;** Mingxiang Lin; Michael Lassman; Russell Weiner; Omar Laterza; Merck Research Laboratories, Rahway, NJ
- MP 529 **Quantification of Fibrin D-dimer by Peptide Immunoaffinity Enrichment and Tandem Mass Spectrometry;** Weixun Wang<sup>1</sup>; Bernard Choi<sup>1</sup>; Nykia Walker<sup>1</sup>; Li-ji Zhu<sup>1</sup>; Weizhen Wu<sup>1</sup>; Ge Lan<sup>1</sup>; David E. Gutstein<sup>1</sup>; Nathan A. Yates<sup>2</sup>; Ronald C. Hendrickson<sup>3</sup>; Martin L. Ogletree<sup>1</sup>; Michele Cleary<sup>1</sup>; Gregory J. Opitck<sup>1</sup>; Zhu Chen<sup>1</sup>; Lucinda H. Cohen<sup>1</sup>; <sup>1</sup>Merck Research Labs, Rahway, NJ; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Memorial Sloan-Kettering Cancer Center, New York, NY
- MP 530 **Pyroglutamylyl apelin-13 Identified as the Major Apelin Isoform in Human Plasma;** Eugene Y. Zhen; Richard E. Higgs; Jesus A. Gutierrez; Eli Lilly & Company, Indianapolis, IN
- MP 531 **Ultra-sensitive Immunoaffinity-UPLC/MS/MS Quantitation of Oxytocin in Rat Plasma;** Sarah Osgood; Angela Doran; Kari Fonseca; Thomas McDonald; Yanhua Zhang; Hongying Gao; Pfizer, Groton, CT
- MP 532 **Ultrasensitive Quantification Assay for Oxytocin in Human Plasma Using a LC/MS Microfluidic Platform;** Catalin Doneanu; Paul Rainville; Waters Corporation, Milford, MA
- MP 533 **High Sensitivity and Simultaneous Quantitation Method for Arginine Vasopressin and Desmopressin in Human Plasma Determined by LC-MS/MS/MS;** Yasuko Tsukazaki<sup>1</sup>; Naoto Senda<sup>1</sup>; Shigeru Yamada<sup>3</sup>; Kinya Kubo<sup>2</sup>; Yasuhiro Kazuki<sup>2</sup>; Mitsuo Oshimura<sup>2</sup>; <sup>1</sup>Mitsubishi Chemical Medience Co., Tsukuba, Ibaraki, Japan; <sup>2</sup>Chromosome Engineering Research Center, Tottori University, Yonago, Tottori, Japan; <sup>3</sup>K.K.AB SCIEX, Shinagawa, Tokyo, Japan
- MP 534 **Surrogate Matrix and Surrogate Analyte Approaches for the Quantitation Amyloid  $\beta$  Peptide Biomarkers in Human Cerebrospinal Fluid via LC-MS/MS;** William R. Mylott; Junlong Shao; Moucun Yuan; Bruce Hidy; Rand Jenkins; PPD, Richmond, VA
- MP 535 **Mass Spectrometry Quantification of Amyloid Precursor Protein Isoforms to Study Alzheimer's disease by QconCAT Strategy;** Junjun Chen; Illarion V. Turko; IBBR, Rockville, MD
- MP 536 **MRM-based Multiplexed Quantification of Progranulin and Granulin Peptides in Mouse Serum;** Toshiya Matsubara<sup>1,2</sup>; Tairo Ogura<sup>1</sup>; Ichiro Hirano<sup>1</sup>; Susumu Seino<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kobe University Graduate School of Medicine, Kobe, Japan
- MP 537 **Development of a Sensitive LC-MS/MS Assay for Quantitative Analysis of Hepcidin-25 in Human Urine;** Chaoran Ron Huang; Tao Ye; Liyu Yang; Biogen Idec, Cambridge, MA
- MP 538 **Mass Spectrometry-Based Approach for Absolute Quantitative Characterization and Validation of Neuronal-Glial Injury Biomarkers in Tissue and Biofluids;** Ahmed Moghieb; Nancy Denslow; Richard Yost; Kevin Wang; University of Florida, Gainesville, FL



- MP 539 **Quantitative Mass Spectrometry for Proteomic Screening of Potential Biomarkers in Alzheimer's Disease;** Sravani Musunuri; Kim Kultima; Martin Ingelsson; Lars Lannfelt; Jonas Bergquist; Magnus Wetterhall; Ganna Shevchenko; *Uppsala University, Uppsala, Sweden*
- MP 540 **Targeted Quantification of Low-Abundance TMPRSS2:ERG Fusion Proteins in Prostate Cancer Using a Highly Sensitive PRISM-SRM approach;** Jintang He<sup>1</sup>; Xuefei Sun<sup>1</sup>; Tujin Shi<sup>1</sup>; Athena A. Schepmoes<sup>1</sup>; Thomas L. Fillmore<sup>1</sup>; Vladislav A. Petyuk<sup>1</sup>; Fang Xie<sup>1</sup>; Rui Zhao<sup>1</sup>; Marina A. Gritsenko<sup>1</sup>; Feng Yang<sup>1</sup>; Naoki Kitabayashi<sup>2</sup>; Sung-Suk Chae<sup>2</sup>; Mark A. Rubin<sup>2</sup>; Javed Siddiqui<sup>2</sup>; John T. Wei<sup>3</sup>; Arul M. Chinnaiyan<sup>3</sup>; Wei-Jun Qian<sup>1</sup>; Richard D. Smith<sup>1</sup>; Jacob Kagan<sup>4</sup>; Sudhir Srivastava<sup>4</sup>; Tao Liu<sup>1</sup>; Karin D. Rodland<sup>1</sup>; David G. Camp, II<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Weill Cornell Medical College, New York, NY*; <sup>3</sup>*University of Michigan, Ann Arbor, MI*; <sup>4</sup>*National Cancer Institute, Rockville, MD*
- MP 541 **Prioritization of Plasma-Based Predictive Markers for Chemotherapy in Lung Cancer Using Fractionation and Targeted Mass Spectrometry;** Haizhen Zhang<sup>1</sup>; Jeffrey Whiteaker<sup>1</sup>; Chenwei Lin<sup>1</sup>; Pin Yan<sup>1</sup>; Yeoun Jin Kim<sup>2</sup>; Helen Ross<sup>3</sup>; Tony Tegeler<sup>4</sup>; Cheryl Selinsky<sup>4</sup>; Konstantinos Petritis<sup>4</sup>; Guy Berchem<sup>2</sup>; Bruno Domon<sup>2</sup>; Amanda Paulovich<sup>1</sup>; <sup>1</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>2</sup>*Luxembourg Clinical Proteomics Center, Luxembourg, Luxembourg*; <sup>3</sup>*Mayo Clinic, Scottsdale, AZ*; <sup>4</sup>*Translational Genomics Research Institute, Phoenix, AZ*
- MP 542 **Targeted Quantification of Low-Abundance Cancer-Related AGR2 Proteins in Clinical Prostate Cancer Specimens Using an Antibody-Free PRISM-SRM Assay;** Tujin Shi<sup>1</sup>; Yuguan Gao<sup>1</sup>; Dian Su<sup>1</sup>; Sue-Ing Quek<sup>2</sup>; Carrie Nicora<sup>1</sup>; Thomas L. Fillmore<sup>3</sup>; Athena A. Schepmoes<sup>1</sup>; Rui Zhao<sup>3</sup>; Ronald J. Moore<sup>1</sup>; Keqi Tang<sup>1</sup>; Karin D. Rodland<sup>1</sup>; Tao Liu<sup>1</sup>; Richard D. Smith<sup>1</sup>; David G. Camp<sup>1</sup>; Alvin Y. Liu<sup>2</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>*PNNL, Richland, WA*; <sup>2</sup>*Department of Urology, University of Washington, Seattle, WA*; <sup>3</sup>*Environmental Molecular Sciences Laboratory, PNNL, Richland, WA*
- MP 543 **MRM Analysis of Breast Adenocarcinomas Induced to Epithelial to Mesenchymal Transition;** Daniele Albuquerque<sup>1</sup>; Camila Palma<sup>1</sup>; Fernanda Melo<sup>2</sup>; Mariana Pinto<sup>2</sup>; Carolina Thome<sup>2</sup>; Gabriela Canchaya<sup>1</sup>; Vera Epifanio<sup>1</sup>; Dimas Covas<sup>1,2</sup>; Vitor Faça<sup>1</sup>; <sup>1</sup>*Fac. Medicina de Ribe. Preto - Univ. São Paulo, Ribeirão Preto-SP, Brazil*; <sup>2</sup>*Fund. Hemocentro de Ribe. Preto - Univ. São Paulo, Ribeirão Preto-SP, Brazil*
- MP 544 **Verification Study of breast Cancer Biomarker Candidates in Plasma Using Highly Multiplexed Peptide immuno-MRM-MS;** Regine M. Schoenherr<sup>1</sup>; Thomas YK. Lau<sup>2</sup>; Michael A. Gillette<sup>2</sup>; Jeffrey R. Whiteaker<sup>1</sup>; Eric Kuhn<sup>2</sup>; Lola Fagbami<sup>2</sup>; Jennifer Ross<sup>2</sup>; ChenWei Lin<sup>1</sup>; Pei Wang<sup>1</sup>; Francisco J. Esteva<sup>3</sup>; Steven A. Carr<sup>2</sup>; Amanda G. Paulovich<sup>1</sup>; <sup>1</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>2</sup>*Broad Institute, Cambridge, MA*; <sup>3</sup>*The University of Texas MD Anderson Cancer Center, Houston, TX*
- MP 545 **Applicability of Label-Free Selected Reaction Monitoring for the Analysis of S100 Proteins in Cancer;** Juan Martinez-Aguilar<sup>1</sup>; Mark P. Molloy<sup>1,2</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*Australian Proteome Analysis Facility, Sydney, Australia*
- MP 546 **Urinary Exosomes; A Source Of Biomarkers And Novel Diagnostics For Polycystic Kidney Disease;** Christopher Ward; Kenneth Johnson; Marie Hogan; Roman Zenka; Cristine Charlesworth; H. Robert Bergen, III; *Mayo Clinic, Rochester, MN*
- MP 547 **Development of an UPLC-MRM Quantitation Method to Monitor Pgp Expression Levels;** Zhenlian Ke; Jocelyn Yabut; Rena Zhang; Weixun Wang; Kevin Bateman; Bonnie Howell; Christopher Gibson; Daniel Spellman; *PPDM, Merck Research Laboratories, West Point, PA*
- MP 548 **Comprehensive MS-based Quantification of Anthrax Toxins Following Exposure to *Bacillus anthracis*;** Adrian R Woolfitt<sup>1</sup>; Anne E Boyer<sup>1</sup>; Maribel Gallegos-Candela<sup>1</sup>; Judith Heitz<sup>2</sup>; Renato C Lins<sup>2</sup>; Katie Isbell<sup>1</sup>; Maria I Solano<sup>1</sup>; John R Barr<sup>1</sup>; <sup>1</sup>*CDC, Atlanta, GA*; <sup>2</sup>*Battelle Institute, Atlanta, GA*
- MP 549 **Successful Implementation of Multiple Reaction Monitoring for the Validation of Tuberculosis Biomarkers;** Nicole Kruh-Garcia<sup>1</sup>; Gustavo Diaz<sup>1</sup>; Luke Davis<sup>2</sup>; Jolynn Trout<sup>1</sup>; Angelo Izzo<sup>1</sup>; Karen Dobos<sup>1</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*UCSF Pulmonary & Critical Care Medicine, San Francisco, CA*

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- MP 550 **Identification of Proteins Associated with Activation of Metastasis after Removal of Primary Tumor Using Murine Ehrlich Carcinoma;** Victoria Shender<sup>1</sup>; Rustam Ziganshin<sup>1</sup>; Fedor Donenko<sup>2</sup>; Georgij Arapidi<sup>1</sup>; Sergey Kovalchuk<sup>1</sup>; Vadim Govorun<sup>1</sup>; <sup>1</sup>*Institute of Bioorganic Chemistry, RAS, Moscow, Russian Federation*; <sup>2</sup>*N.N. Blokhin Russian Cancer Research Center, Moscow, Russian Federation*
- MP 551 **Imaging Mass Spectrometry to Uncover Proteomic Differences in Mantle Cell Lymphoma Subtypes;** Kristina Schwamborn<sup>1,2</sup>; Martina Rudelius<sup>1</sup>; Richard Caprioli<sup>2</sup>; <sup>1</sup>*Technical University Munich, Munich, Germany*; <sup>2</sup>*Department of Biochemistry, Vanderbilt University, Nashville, TN*
- MP 552 **Comparing Lung Protein Expression for Biomarkers within the Disease Phenotypes of COPD and Lung Cancer;** Brian Sandri; Chris Wendt; *University of Minnesota, Minneapolis, MN*
- MP 553 **Proteomic Profiling and Characterization of Human Endometrial Cancer Cell-Derived Extracellular Microvesicles;** Emma Arigi<sup>1</sup>; Gloria Polanco<sup>1</sup>; Clemente Aguilar-Bonavides<sup>1</sup>; Armando Varela-Ramirez<sup>1</sup>; Russell Broadus<sup>2</sup>; Igor Almeida<sup>1</sup>; <sup>1</sup>*University of Texas at El Paso, El Paso, TX*; <sup>2</sup>*University of Texas MD Anderson Cancer Center, Houston, TX*
- MP 554 **Identification of SRL Binding Receptors on human Colon Cancer Cells Using Micro-Fluidic Based LC System with an Advanced QTOF MS;** Ravindra Gudihai<sup>2</sup>; Sachin M. Eligar<sup>1,3</sup>; Srikanth Barkeer<sup>1</sup>; Jonathan M. Rhodes<sup>3</sup>; Lu-Gang Yu<sup>3</sup>; Bale M. Swamy<sup>1,3</sup>; Shashikala R. Inamdar<sup>1,3</sup>; <sup>1</sup>*Dept of Studies in Biochemistry, Karnatak Univ, Dharwad, India*; <sup>2</sup>*Agilent Technologies India Pvt. Ltd, Bangalore, India*; <sup>3</sup>*Department of Gastroenterology, Univ of Liverpool, Liverpool, UK*
- MP 555 **Proteomics Study of Synergistic Effects of Combinational Treatment for Pancreatic Cancer;** Jin-Gyun Lee; Kimberly Q. McKinney; Jean-Luc Mougeot; Herbert L. Bonkovsky; Sun-Il Hwang; *Carolinas Healthcare System, Charlotte, NC*
- MP 556 **Gastric Cancer Detection by Serum Glycan Signatures;** Sureyya Ozcan<sup>1</sup>; Cara Cooke<sup>2</sup>; Donald Barkauskas<sup>3</sup>; Hyun Joo An<sup>4</sup>; Serenus Hua<sup>4</sup>; Cynthia Williams<sup>1</sup>; Lauren Dimapasoc<sup>1</sup>; L. Renee Ruhaak<sup>1</sup>; Jae Han Kim<sup>4</sup>; David Rocke<sup>5</sup>; Javier Torres<sup>6</sup>; Carlito B Lebrilla<sup>1</sup>; Jay V Solnick<sup>2</sup>; <sup>1</sup>*UC Davis Chemistry Department, Davis, CA*; <sup>2</sup>*UC Davis, Center for Comparative Medicine, Davis, CA*; <sup>3</sup>*University of Southern California, Los Angeles, CA*; <sup>4</sup>*Chungnam National University, Daejeon, Korea*; <sup>5</sup>*University of California, Davis, CA*; <sup>6</sup>*Instituto Mexicano del Seguro Social, Mexico, Mexico*

- MP 557 **Functional Proteomic Analysis of KIAA1199 Overexpression in Breast Cancer;** Hong Peng<sup>1</sup>; Mohammad-Saeid Jami<sup>1</sup>; Jinxuan Hou<sup>2</sup>; Miao Liu<sup>1</sup>; Michelle Varney<sup>1</sup>; Rakesh Singh<sup>1</sup>; Shi-Jian Ding<sup>1</sup>; <sup>1</sup>Univ of Nebraska Med Center, Omaha, NE; <sup>2</sup>Zhongnan Hospital of Wuhan University, Wuhan, China
- MP 558 **Bladder Cancer Proteome: A Multiplexing Approach Using Online 2D RP-RP Chromatography Coupled with Data Independent Ion Mobility;** Lee A Gethings<sup>1</sup>; Zhuowei Wang<sup>2</sup>; Bo Wen<sup>3</sup>; Ju Zhang<sup>3</sup>; Quanhui Wang<sup>3</sup>; Liang Lin<sup>3</sup>; Chris Hughes<sup>1</sup>; Johannes P.C. Vissers<sup>1</sup>; James Langridge<sup>1</sup>; Siqi Liu<sup>3</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Waters (China), Beijing, China; <sup>3</sup>BGI, Beijing, China
- MP 559 **The Application of MALDI-TOF MS Plasma Protein Profiling for Discrimination of Patients with Gastric Cancer from Healthy Controls;** Natalia Arnotskaya; Valeriy Shevchenko; Elena Ogorodnikova; Mikhail M Davidov; Maksat Ibraev; Igor Turkin; Mikhail I Davidov; N. N. Blokhin Russian Cancer Research Center, Moscow, Russian Federation
- MP 560 **Identification of Candidate Lung Cancer Biomarkers by Proteomics Analysis of Conditioned Media of Two Lung Cancer Cell Lines;** Valeriy Shevchenko; Sergei Kovalev; Natalia Arnotskaya; Sergei Aushkap; Igor Kudryavtsev; N. N. Blokhin Russian Cancer Research Center, Moscow, Russian Federation
- MP 561 **Discovery of Glycoprotein Biomarkers for Differentiation of Pancreatic Cancer from Several Related Conditions by Lectin Array and Quantitative Mass Spectrometry;** Song Nie<sup>1</sup>; Andy Lo<sup>1</sup>; Mack T. Ruffin<sup>2</sup>; Kerby A. Shedden<sup>3</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>Department of Surgery, University of Michigan, Ann Arbor, MI; <sup>2</sup>Epidemiology Department, University of Michigan, Ann Arbor, MI; <sup>3</sup>Biostatistics Department, University of Michigan, Ann Arbor, MI
- MP 562 **A Label-Free Shotgun Proteomic Characterization of Multiple Myeloma Derived Extracellular Vesicles;** Sean W. Harshman; Alessandro Canella; Paul D. Ciarlariello; Kitty Agarwal; Tiffany Talabere; Michael E. Paulaitis; Don M. Benson, Jr; Flavia Pichiorri; Michael A. Freitas; Ohio State University, Columbus, OH
- MP 563 **GC/MS-based Metabolomic Profiling for Early Diagnosis of Pancreatic Cancer;** Masaru Yoshida; Takashi Kobayashi; Shin Nishiumi; Yoshihiro Izumi; Atsuki Matsubara; Takeshi Azuma; Kobe University, Kobe, Japan
- MP 564 **N-linked Glycoproteomic Landscape of Human Lymphoid Cancers;** Venkatesha Basrur; Delphine Rolland; Damian Fermin; Carla McNeil-Schwalm; Kevin Conlon; Thomas Wolfe; Chih-Chiang Tsou; Yoon-Kyung Jeon; Noah Brown; Dafydd Thomas; Nathanael Bailey; Gilbert Omenn; Alexey Nesvizhskii; Megan Lim; Kojo Elenitoba-Johnson; University of Michigan, Ann Arbor, MI
- MP 565 **Quantitative Proteomics Reveals Hypoxia Perturbed Pathways and Secretome that Promote Tumour Angiogenesis, Metastasis, and Therapy Resistance;** Siu Kwan Sze; Yan Ren; Bama Dutta; Nanyang Technological University, Singapore, Singapore
- MP 566 **Efforts Toward Molecular Classification of Prostate Cancer Tumors via Laser Capture Microdissection Coupled to LC MS/MS;** Michael Bereman; Martine Roudier; Lawrence True; Michael MacCoss; Univ of Washington, Seattle, WA
- MP 567 **Decreased Glucose-Regulated Protein 78 in Thioacetamide-Induced Liver Fibrosis Plays Crucially in the Development of Liver Fibrosis: A Proteomic Study;** Jungshan Chang<sup>1</sup>; Chun-Chia Cheng<sup>2</sup>; Fu-Der Mai<sup>1</sup>; Chun-Chao Chang<sup>3</sup>; <sup>1</sup>Taipei Medical University, Taipei City, Taiwan; <sup>2</sup>Institute of Nuclear Energy Research, Taoyuan, Taiwan; <sup>3</sup>Taipei Medical University Hospital, Taipei, Taiwan
- Immunology, 568 - 575**
- MP 568 **Multiplex Quantitative Proteomics Characterization of the Activation of Human CD4+ T-cells;** Robert Moulder; Tapio Lönnberg; Anne Rokka; Riitta Lahtesmaa; Turku Centre for Biotechnology, Turku, Finland
- MP 569 **Mechanistic Insights into E1B 55kDa-mediated Regulation of the Innate Immune Response;** George Hung<sup>1</sup>; Jasdave S. Chahal<sup>2</sup>; Caroline DeHart<sup>1</sup>; David H. Perlman<sup>3</sup>; S. J. Flint<sup>1</sup>; <sup>1</sup>Dept. of Molecular Biology, Princeton University, Princeton, NJ; <sup>2</sup>Whitehead Institute for Biomedical Research, MIT, Cambridge, MA; <sup>3</sup>Proteomics and Mass Spec. Core, Princeton Univ., Princeton, NJ
- MP 570 **Interleukin 6: A Deterrent or an Indicator of Mycobacterium Infection in the Endangered White-Winged Wood Duck;** Anita Iveljic; Pyi Saw; Jody M. Modarelli; Hiram College, Hiram, OH
- MP 571 **Characterization of Phagosomal Proteomes in Activated Macrophages;** Manman Guo<sup>1</sup>; Marek Gierlinski<sup>2</sup>; Brian Dill<sup>1</sup>; Matthias Trost<sup>1</sup>; <sup>1</sup>MRC-University of Dundee, Dundee, UK; <sup>2</sup>BCDD-University of Dundee, Dundee, UK
- MP 572 **Identification of Naturally Processed "Self" and HIV Derived MHC Class I Ligands Presented by Healthy and HIV-Infected Cells;** Marijana Ručević<sup>1</sup>; Mariko Shimada<sup>1</sup>; Georgio Kourjian<sup>1</sup>; Nicole Lai<sup>1</sup>; Carl Kadie<sup>2</sup>; David Heckerman<sup>2</sup>; Bruce D. Walker<sup>1,3</sup>; Sylvie LeGall<sup>1</sup>; <sup>1</sup>Ragon of MGH, MIT and Harvard, Boston, MA; <sup>2</sup>Microsoft Research, Los Angeles, CA; <sup>3</sup>Howard Hughes Medical Institute, Chevy Chase, MD
- MP 573 **Impact of Genomic Polymorphisms on the Human MHC Class I Immunoepitope;** Dev Sriranganadane<sup>1,4</sup>; Diana Paola Granados<sup>1,5</sup>; Céline Laumont<sup>1,5</sup>; Tariq Daouda<sup>1,2</sup>; Olivier Caron-Lizotte<sup>1</sup>; Antoine Zieger<sup>1,2</sup>; Sébastien Lemieux<sup>2</sup>; Claude Perreault<sup>1,3</sup>; Pierre Thibault<sup>1,4</sup>; <sup>1</sup>University of Montreal-IRIC, Montreal, Canada; <sup>2</sup>University of Montreal- IRIC Bioinformatics, Montreal, Canada; <sup>3</sup>Div. of Hematology Hôpital Maisonneuve-Rosemont, Montreal, Canada; <sup>4</sup>University of Montreal- Dept of Chemistry, Montreal, Canada; <sup>5</sup>University of Montreal- Dept of Medicine, Montreal, Canada
- MP 574 **Protein Composition, Stoichiometry, and Mass Estimation of the HHV-6B Z29 Viral Particle Using Label Free Quantitative Proteomics;** Scott A. Shaffer; Aniuska Becerra-Artiles; Karin M. Green; Stephanie A. Maniatis; J. Mauricio Calvo-Calle; Lawrence J. Stern; University of Massachusetts Medical School, Worcester, MA
- MP 575 **Optimizing the Multiplexing Strategy for Quantitative Proteomics Analysis of Immune Cell Subsets Using iTRAQ;** Parimal Samir; Kristen Hoek; Leigh Howard; Tara Allos; Xinnan Niu; Clarence Creech; Kathryn Edwards; Andrew Link; Vanderbilt University School of Medicine, Nashville, TN
- Molecular Systems Biology and Disease, 576 - 603**
- MP 576 **Breaking the Habit: A Comprehensive, Proteome-Wide Comparison of Chemical and Physical Synchronization of the Mammalian Cell Cycle;** Tony Ly; Angus Lamond; Wellcome Trust Centre for Gene Regulation and Expr, Dundee, UK



- MP 577 **Dynamic Changes in Protein and mRNA Expression Drive Functional Reprogramming during Osteoclast Development from Monocyte-Macrophage Lineage Cells;** Eunkyoung An; Manikandan Narayanan; Ronald Germain; Aleksandra Nita-Lazar; *NIH/NIAID/LSB, Bethesda, MD*
- MP 578 **Mass Spectrometric Strategies to Characterize and Understand Complex Microbial Biofilms - Applications to Fuel Degradation and to Biocorrosion;** Jan Sunner; Iwona Beech; Joe Sufliata; *University of Oklahoma, Norman, OK*
- MP 579 **Yeast on a Diet: Dextrose or Lactate, What's Your Favorite Carb?** Alejandro Cohen<sup>1</sup>; J. Pedro Fernandez-Murray<sup>2</sup>; Christopher McMaster<sup>2</sup>; <sup>1</sup>*Proteomics Facility, Dalhousie University, Halifax, Canada*; <sup>2</sup>*Dalhousie University, Halifax, Canada*
- MP 580 **System Wide Analysis of Lysine Acetylation in the Human Pathogen *Mycoplasma pneumoniae*;** Marco Hennrich; Vera van Noort; Peer Bork; Anne-Claude Gavin; *EMBL Heidelberg, Heidelberg, Germany*
- MP 581 **First Draft of the Human Proteome;** Mathias Wilhelm<sup>1</sup>; Judith Schlegel<sup>2</sup>; Amin Moghaddas Gholami<sup>1</sup>; Hannes Hahne<sup>1</sup>; Joos-Hendrik Boese<sup>2</sup>; Marcus Lieberenz<sup>2</sup>; Mikhail Savitski<sup>3</sup>; Yuval Morad<sup>2</sup>; Lars Butzmann<sup>2</sup>; Emanuel Ziegler<sup>2</sup>; Anton Nizdzelska<sup>2</sup>; Eyk Kny<sup>2</sup>; Helmut Cossmann<sup>2</sup>; Siegfried Gessulat<sup>2</sup>; Marcus Bantscheff<sup>3</sup>; Anja Gerstmaier<sup>2</sup>; Franz Faerber<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technical University Munich, Freising, Germany*; <sup>2</sup>*SAP AG, Walldorf, Germany*; <sup>3</sup>*Cellzome, Heidelberg, Germany*
- MP 582 **The First Draft of the Human Proteome Enables Systematic Analyses of Protein Expression;** Hannes Hahne<sup>1</sup>; Mathias Wilhelm<sup>1</sup>; Amin Moghaddas Gholami<sup>1</sup>; Judith Schlegel<sup>2</sup>; Joos-Hendrik Boese<sup>2</sup>; Marcus Lieberenz<sup>2</sup>; Mikhail Savitski<sup>3</sup>; Yuval Morad<sup>2</sup>; Lars Butzmann<sup>2</sup>; Emanuel Ziegler<sup>2</sup>; Anton Nizdzelska<sup>2</sup>; Eyk Kny<sup>2</sup>; Helmut Cossmann<sup>2</sup>; Siegfried Gessulat<sup>2</sup>; Marcus Bantscheff<sup>3</sup>; Anja Gerstmaier<sup>2</sup>; Franz Faerber<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technische Universität München, Freising, Germany*; <sup>2</sup>*SAP AG, Walldorf, Germany*; <sup>3</sup>*Cellzome, Heidelberg, Germany*
- MP 583 **A Comprehensive Characterization of the Pig Islet Proteome: PTMs, Amino Acid Substitutions and Novel Isoforms;** Ebbing de Jong; Bernhard Hering; Pratik Jagtap; John Chilton; Getiria Onsongo; Timothy Griffin; *University of Minnesota, Minneapolis, MN*
- MP 584 **Analysis of the Impact of a Perturbed Metabolism on Enzymes Controlling Adipocyte Metabolism;** William K. Russell; KyungOh Choi; Arul Jayaraman; *Texas A&M University, College Station, TX*
- MP 585 **Global Proteome Analysis of the NCI-60 Cell Line Panel;** Amin Moghaddas Gholami; Hannes Hahne; Zhixiang Wu; Florian Auer; Chen Meng; Mathias Wilhelm; Bernhard Kuster; *Technical University Munich, Freising, Germany*
- MP 586 **Global and Targeted Proteomics of Nonstandard Amino Acid Incorporation into Proteins and Proteomes;** Hans Rudolf Aerni<sup>1,2</sup>; Patrick O'Donoghue<sup>3</sup>; Svetlana Rogulina<sup>1,2</sup>; Mark Shifman<sup>4</sup>; Jesse Rinehart<sup>1,2</sup>; <sup>1</sup>*Yale Univ. School of Medicine, New Haven, CT*; <sup>2</sup>*Yale Systems Biology Institute, West Haven, CT*; <sup>3</sup>*Molecular Biophysics and Biochemistry, New Haven, CT*; <sup>4</sup>*Keck Biotechnology Resource Laboratory, New Haven, CT*
- MP 587 **System-wide Analysis of Protein Degradation Using Quantitative Proteomics;** Romain Christiano; Xiuling Guo; Tobias C. Walther; *Yale University, New Haven, CT*
- MP 588 **Progress towards Real-Time Cell Secretome Analysis by Mass Spectrometry;** Rafael Montenegro Burke<sup>1</sup>; Jeffrey Enders<sup>1</sup>; Kevin Seale<sup>2</sup>; John Wikswo<sup>3</sup>; John McLean<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Vanderbilt University, Nashville, TN*; <sup>2</sup>*Dep. Biomedical Engineering, Vanderbilt University, Nashville, TN*; <sup>3</sup>*Dept. Physics and Astronomy, Vanderbilt University, Nashville, TN*
- MP 589 **Molecular Characterization of Rough Endoplasmic Reticulum Subproteome in Pancreatic Beta Cells;** Xuequn Chen; Jin-sook Lee; Jingye Fang; *Wayne State University, Detroit, MI*
- MP 590 **The Proteomics of Dietary Restriction: Are Sex-Specific Fitness Effects Mediated by Differential Protein Expression?** Simin Maleknia; Elizabeth Cassidy; Russell Bonduriansky; *University of New South Wales, Sydney, Australia*
- MP 591 **Characterizing the Role of Caspases in Apoptosis Induced by Endoplasmic Reticulum Stress;** Veronica Anania; Han Li; Diana Jeon; Avi Ashkenazi; Jennie Lill; *Genentech, Inc., South San Francisco, CA*
- MP 592 **Effect of Western Diet on Lipoprotein Mediated Atherosclerosis. <sup>2</sup>H<sub>2</sub>O-metabolic Labeling Based Dynamic Proteomics Approach;** Ling Li<sup>1</sup>; Stephen Previs<sup>2</sup>; Arthur McCullough<sup>3</sup>; Belinda Willard<sup>1</sup>; Takhar Kasumov<sup>3</sup>; <sup>1</sup>*Department of Core Service, Cleveland Clinic, Cleveland, OH*; <sup>2</sup>*Case Western Reserve University, Cleveland, OH*; <sup>3</sup>*Department of Hepatology, Cleveland Clinic, Cleveland, OH*
- MP 593 **Identification of HLA-DR Presented Peptides in Synovial Fluid from a Patient with Antibiotic-refractory Lyme Arthritis;** Qi Wang<sup>1</sup>; Elise E. Drouin<sup>2</sup>; Allen C. Steere<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Massachusetts General Hospital, Boston, MA*
- MP 594 **Proteomic Investigation of the Tumor Differentiation Factor (TDF)-induced Cell Differentiation;** Armand Ngounou; Izabela Sokolowska; Pinguang Yang; Urmi Roy; Alisa Woods; Costel Darie; *Clarkson University, Potsdam, NY*
- MP 595 **Dissecting Ageing-Related Disease by Studying Protein Changes after Calorie Restriction;** Mark Laranca; Ehsan Pourkarimi; Anton Gartner; Angus Lamond; *University of Dundee, Dundee, UK*
- MP 596 **Global In-Depth Quantitative Proteomic Analysis of HIV Infected Cells Using a Novel Q-OT-qIT Mass Spectrometer;** Shannon Eliuk<sup>1</sup>; Jeffrey Johnson<sup>2</sup>; Leonard Chavez<sup>3</sup>; Vlad Zabrouskov<sup>1</sup>; Christopher Mullen<sup>1</sup>; Eric Verdin<sup>3</sup>; Nevan Krogan<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*UCSF, San Francisco, CA*; <sup>3</sup>*Gladstone Institute, San Francisco, CA*
- MP 597 **Proteomics and Glycomics of Glioma-Derived Stem-Like Cells Correlated to Gene Expression Data and Patient Outcomes;** Carol L. Nilsson<sup>1</sup>; Huiling Liu<sup>1</sup>; Cheryl F. Licht<sup>1</sup>; Mark R. Emmett<sup>1</sup>; Norelle C. Wildburger<sup>1</sup>; Alexander S. Shavkunov<sup>1</sup>; Huan He<sup>3</sup>; Alan G. Marshall<sup>5</sup>; Roger A. Kroes<sup>4</sup>; Joseph R. Moskal<sup>4</sup>; Erik P. Sulman<sup>2</sup>; Frederick F. Lang<sup>2</sup>; Charles A. Conrad<sup>2</sup>; <sup>1</sup>*UTMB, Galveston, TX*; <sup>2</sup>*The University of Texas M. D. Anderson Cancer Ctr, Houston, TX*; <sup>3</sup>*Ion Cyclotron Resonance Program, NIMH, Tallahassee, FL*; <sup>4</sup>*Falk Center for Molecular Therapeutics, Evanston, IL*; <sup>5</sup>*Department of Chemistry & Biochemistry, FSU, Tallahassee, FL*
- MP 598 **Proteomics Based Investigation of Cystic Fibrosis Cell-Line Models - A Step towards Understanding the Disease Process;** Navin Rauniyar; Vijay Gupta; William E. Balch; John R. Yates; *The Scripps Research Institute, La Jolla, CA*
- MP 599 **Multi-omic Analysis of ApoE Isoform Effects in AD-vulnerable Brain Regions;** Tal Nuriel; *Columbia University Medical Center, New York, NY*
- MP 600 **Quantitative Proteome Turnover in *C. elegans*;** Krishna Vukoti; John Feng; Masaru Miyagi; *Case Western Reserve University, Cleveland, OH*

- MP 601 **Analysis of BDNF-triggered Protein Translation Using BONCAT and SILAC;** Guoan Zhang; Heather Bowling; Eric Klann; Moses Chao; Thomas Neubert; *New York University, New York, NY*
- MP 602 **Strategies for Interactome Tracking and Scoring: How ProHits and SAINT Complement Strong Experimental Designs;** Guomin Liu<sup>1</sup>; Hyungwon Choi<sup>2</sup>; Jianping Zhang<sup>1</sup>; Zhen-Yuan Lin<sup>1</sup>; Brett Larsen<sup>1</sup>; Mike Tyers<sup>3</sup>; Brian Raught<sup>4</sup>; Alexey Nesvizhskii<sup>5</sup>; Anne-Claude Gingras<sup>1</sup>; <sup>1</sup>*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, Canada*; <sup>2</sup>*Saw Swee Hock School of Public Health, National University of Singapore, Singapore*; <sup>3</sup>*Université de Montréal, Montréal, Canada*; <sup>4</sup>*Ontario Cancer Institute, Toronto, Canada*; <sup>5</sup>*University of Michigan, Ann Arbor, MI*
- MP 603 **Application of Proteomics to the Characterization of Deformation of Nautilus Pompilius Shell in Captivity;** Timothy P. Cleland; Mehdi Moini; *Smithsonian Institution, Suitland, MD*
- Forensics, 604 - 628**
- MP 604 **Primate & Other Species Identification by Proteomic Analysis;** Heyi Yang; Bo Zhou; Mechthild Prinz; Donald Siegel; *Office of Chief Med Exam, New York, NY*
- MP 605 **Effect of Aging and Radiation on Museums' Proteinaceous Specimens at Molecular Levels;** Mehdi Moini; Raquel Fleskes; Christopher Rollman; *Smithsonian Institution, Suitland, MD*
- MP 606 **A Multi-Platform Strategy Applied to the Detection and Characterization of Falsified Artemisinin Combination Therapies;** Prabha Dwivedi<sup>1</sup>; Maria Julia Culzoni<sup>1</sup>; Mohamed El-Sherbiny<sup>2</sup>; Obinna Onwujekwe<sup>3</sup>; Ogochukwu Ezeoke<sup>3</sup>; Naiela Malik<sup>2</sup>; Ifeyinwa Fadeyi<sup>2</sup>; Harparkash Kaur<sup>2</sup>; Facundo M. Fernández<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*London School of Hygiene and Tropical Medicine, London, UK*; <sup>3</sup>*College of Medicine, University of Nigeria, Enugu, Nigeria*
- MP 607 **Identification and Attribution Profiling of Chemical Threat Agents Using Liquid Chromatography-Mass Spectrometry Applied to Amanita Toxins in Food;** Daniel Jansson; Sten-Åke Fredriksson; Calle Nilsson; *Swedish Defence Research Agency, Umeå, Sweden*
- MP 608 **Assessment of Decontamination Protocols on the Analysis of Hair by Multi-Modal Mass Spectrometry Imaging;** Bryn Flinders<sup>1</sup>; Tiffany Porta<sup>2</sup>; Emmanuel Varesio<sup>2</sup>; Gerard Hopfgartner<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, The Netherlands*; <sup>2</sup>*University of Geneva, Geneva, Switzerland*
- MP 609 **New Methods and Algorithms Using Allions-MS/MS Data for the Identification of Isomeric Drugs/Drug-Metabolites in Blood Samples by LC-MS/MS Accurate-Mass-Quadrupole-Time-Of-Flight-Mass-Spectrometry;** Martin Josefsson<sup>1</sup>; Bernhard Wuest<sup>2</sup>; Markus Roman<sup>1</sup>; <sup>1</sup>*National Board of Forensic Medicine, Linköping, Sweden*; <sup>2</sup>*Agilent Technologies GmbH, Waldbronn, Germany*
- MP 610 **Human Scent Differentiation;** Elizabeth Magnuson; Douglas J. Beussman; *St. Olaf College, Northfield, MN*
- MP 611 **Bulk versus LC-IRMS Amino-Acid-Specific Isotopic Analysis of Human Hair;** Yan An<sup>1</sup>; Ayat Bani Rashaid<sup>1</sup>; Glen P. Jackson<sup>2</sup>; <sup>1</sup>*Ohio University, Athens, OH*; <sup>2</sup>*West Virginia University, Morgantown, WV*
- MP 612 **Rapid LC-MS/MS Screening Method for Forty-Three Phosphodiesterase Type 5 Inhibitors and Six Flavone Drugs in Counterfeit Samples;** Philippe Lebel; Karen C. Waldron; Alexandra Furtos; *Université de Montréal, Montréal, Canada*
- MP 613 **Detection of Metabolites of Drugs in Wastewater of Lubbock, TX;** David Klein; *Texas Tech University, Lubbock, TX*
- MP 614 **The Detection of Pseudo-Endogenous Androgenic Anabolic Steroids in Sports by Isotope Ratio Mass Spectrometry: A Global Sample Purification Strategy;** Xavier De La Torre; Cristiana Colamonici; Davide Curcio; Francesco Molaioni; Francesco Botrè; *Laboratorio Antidoping FMSI, Rome, Italy*
- MP 615 **An Improved and Accurate Method for the Analysis of Testosterone Related Urinary Metabolites Using Gas Chromatography-Combustion-Isotope Ratio Mass Spectrometry;** Alexandre Ouellet; Nicolas LeBerre; Christiane Ayotte; *INRS-IAF-Doping Control Laboratory, Laval, Canada*
- MP 616 **Identification Tree Based on Fragmentation Rules for Structure Elucidation of Organophosphorus Esters by Electrospray Mass Spectrometry;** Adrián Schwarzenberg<sup>1</sup>; Farid Ichou<sup>1</sup>; Richard B. Cole<sup>1</sup>; Xavier Machuron-Mandard<sup>2</sup>; Christophe Junot<sup>3</sup>; Denis Lesage<sup>1</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>*UPMC/IPC, UMR-CNRS 7201, Paris, France*; <sup>2</sup>*CEA, Centre DAM/DIF Ile-de-France, Arpajon, France*; <sup>3</sup>*CEA, DSV/IBiTec-S, Saclay, France*
- MP 617 **High Resolution and Accurate Mass Forensic Toxicology Screening in Plasma/Blood Sample Using Q Exactive Mass Spectrometer;** Isabelle Morel<sup>2</sup>; Sylvie Lepage<sup>2</sup>; Benedicte Duret<sup>1</sup>; <sup>1</sup>*Thermo Fisher, Courtaboeuf, France*; <sup>2</sup>*Forensic and Toxicology Laboratory, Rennes, France*
- MP 618 **Identification of Dyes Directly From Textile Fibers Using Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Coupled to FT-ICR-MS;** Kristin H. Cochran; Jeremy A. Barry; Guillaume Robichaud; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- MP 619 **Differentiation of Cotton Fibers Using Isotope Ratio Mass Spectrometry;** Kristi Gangelhoff; Douglas J. Beussman; *St. Olaf College, Northfield, MN*
- MP 620 **Characterization of the Photodegradation of Crystal Violet by LDI-TOF-MS;** Megan Czerniejewski; Gary Kinsel; *Southern Illinois University, Carbondale, Illinois*
- MP 621 **Utilization of DART Ion Source Coupled with HR/AM Q-Orbitrap MS for Car Paint Component Identification for Traffic Accident Criminal Investigation;** Wei-Shun Lai<sup>1</sup>; Tai-Hung Chen<sup>2</sup>; Hsin-Hung Huang<sup>1</sup>; Shu-Hui Lee<sup>1</sup>; <sup>1</sup>*Mass Solutions Technology, New Taipei, Taiwan*; <sup>2</sup>*Criminal Investigation Brigade, Taipei, Taiwan*
- MP 622 **Using a Portable Mass Spectrometer for Direct Screening of Arson and Clandestine Drug Laboratory Evidence;** Seth E. Hall; Adam E. O'Leary; Kyle E. Vircks; Christopher C. Mulligan; *Illinois State University, Normal, IL*
- MP 623 **Beyond the Ridge Pattern - Multi Informative Analysis of Latent Fingermarks by MALDI Mass Spectrometry;** Robert Bradshaw<sup>1</sup>; Leesa Ferguson<sup>1</sup>; Rosalind Wolstenholme<sup>1</sup>; Malcolm Clench<sup>1</sup>; Wei Rao<sup>2</sup>; Stephen Bleay<sup>3</sup>; Simona Francese<sup>1</sup>; <sup>1</sup>*BMRC, Sheffield, UK*; <sup>2</sup>*University of Nottingham, Nottingham, UK*; <sup>3</sup>*CAST, Home Office, St Albans, UK*
- MP 624 **Towards a Versatile Mass Spectrometric Platform for Comprehensive Crime Scene Analytics;** Christopher Mulligan; Seth Hall; Adam O'Leary; Kyle Vircks; Jamie Wieland; *Illinois State University, Normal, IL*
- MP 625 **Detection, Quantification and Identification of Dermorphin in Equine Plasma and Urine by LC-MS/MS for Doping Control;** Fuyu Guan<sup>1,3</sup>; Cornelius Ubob<sup>2</sup>; Lawrence Soma<sup>1,3</sup>; Mary Robinson<sup>1,3</sup>; George Maylin<sup>4</sup>; Xiaoqing Li<sup>1,3</sup>; <sup>1</sup>*University of Pennsylvania, West Chester, PA*; <sup>2</sup>*Pennsylvania Equine Toxicology and Research Center, West Chester, PA*; <sup>3</sup>*University of Pennsylvania, Kennett Square, PA*; <sup>4</sup>*Morrisville College, Ithaca, NY*



- MP 626 **Detection of Efaproxiral (RSR13) and Its Metabolites in Equine by Liquid Chromatography Tandem Mass Spectrometry;** Rong Yi; Jasmeet Sandhu; Sarah Zhao; Geoffrey Lam; Devan Loganathan; Barbara Morrissey; MAXXAM Analytics, Burnaby, BC, Canada
- MP 627 **Development of a Broad Range Screen, Utilising UPLC-MS/MS, UPLC-Orbitrap and GC-MS/MS for Drug Detection in Equine Hair Samples;** Bob Gray; Jane Bright; Marjaana Viljanto; Suzanne Lister; Steve Maynard; HFL Sport Science, Fordham, UK
- MP 628 **Identification and Quantification of an Opioid Peptide (Dermorphin) in Biological Matrix Using Liquid Chromatography Tandem Mass Spectrometry;** Daniel McKemie; Scott Stanley; Heather Knych; University of California, Davis, CA

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- MP 629 **QTOF Analysis and Sample Profiling for Environmental Applications;** Sylvain Merel; Tarun Anumol; Ai Jia; Shane Snyder; University of Arizona, Tucson, Az,
- MP 630 **Comparative PCDD/F Analysis with GC-HRMS, GC-HRTOFMS and GCxGC-TOFMS: Discovery of Compounds Not Found in Environmental Analysis Guided by EPA 1613B;** Peter Gorst-Allman<sup>1</sup>; David E Alonso<sup>2</sup>; Jayne de Vos<sup>3</sup>; Jack Cochran<sup>4</sup>; Eric Reiner<sup>5</sup>; <sup>1</sup>Leco Africa, Kempton Park, Gauteng, RSA; <sup>2</sup>LECO Corporation, Saint Joseph, MI; <sup>3</sup>National Metrology Institute of South Africa, Pretoria, Gauteng, RSA; <sup>4</sup>Restek Corporation, Bellefonte, PA; <sup>5</sup>Ontario Ministry of the Environment, Toronto, Canada
- MP 631 **Non-Target and Post-Target Analysis of Emerging Halogenated Contaminants in American and European Eels by Gas Chromatography-High Resolution Time-of-Flight MS;** Jonathan Byer<sup>1</sup>; Grazina Pacepavicius<sup>2</sup>; Peter V. Hodson<sup>3</sup>; Claude Belpaire<sup>4</sup>; David E Alonso<sup>1</sup>; Joe Binkley<sup>1</sup>; Mehran Alaei<sup>2</sup>; <sup>1</sup>LECO Corporation, St. Joseph, MI; <sup>2</sup>Aquatic Contaminants Research, Environment Canada, Burlington, ON, Canada; <sup>3</sup>Queen's University, Kingston, ON, Canada; <sup>4</sup>Research Institute for Nature and Forest, Groenendaal-Hoeilaart, Belgium
- MP 632 **LC/MS/MS with Novel Online SPE Valving Solution for the Analysis of Sub-Parts-Per-Trillion Contaminants in Drinking Water;** Sheher Bano Mohsin; Michael Woodman; Agilent Technologies, Schaumburg, IL
- MP 633 **Determination of Sucralose and Acesulfame in Source, Tap and Bottled Waters;** Jessica M. Boyd; Minghuo Wu; Dylan Baustad-Thomas; Steve Hruday; Xing-Fang Li; University of Alberta, Edmonton, Canada
- MP 634 **Determination of Odor Compounds in Surface Water by Solid Phase Micro Extraction and Quadrupole Time Of Flight Gas Chromatograph Mass Spectrometer;** Keun-Joo Choi<sup>1</sup>; Yeanwoong You<sup>2</sup>; Seung-ju Yang<sup>2</sup>; <sup>1</sup>Seoul Waterworks Research Institute, Seoul, South Korea; <sup>2</sup>Agilent Technologies Korea, Ltd, Seoul, Korea
- MP 635 **GCMS Approach towards the Characterization of Metabolites Formed Due to Biodegradation of Nicotine by a New Strain Pseudomonas plecoglossicida TND35;** Gurusamy Raman<sup>1</sup>; Mohan Kasi<sup>2</sup>; Saravanan Subramaniyan<sup>2</sup>; Venkat Manohar<sup>2</sup>; Natarajan Sakthivel<sup>1</sup>; <sup>1</sup>Dept. of Biotechnology, Pondicherry University, Puducherry, India; <sup>2</sup>IICMS, Chennai, India
- MP 636 **Simultaneous Determination of Bisphenol A, Alkylphenols and Alkylphenol Ethoxylates in NIST SRM 2585 by GC/MS/MS;** Xinghua Fan; Cariton Kubwabo; Fang Wu; Health Canada, Ottawa, Canada

- MP 637 **The New Fast Approach for the Determination of Semi Volatile Organic Compounds According to EPA 8270D;** Ilaria Ferrante<sup>1</sup>; Daniele Recenti<sup>1</sup>; Luigi Motti<sup>2</sup>; Chiara Abate<sup>1</sup>; <sup>1</sup>DANI, Cologno Monzese, Italy; <sup>2</sup>DANI SA, Contone, Switzerland
- MP 638 **EPA 8260: Dynamic Headspace Purge & Trap GC/TOF-MS for VOCs Determination in Environmental Matrices;** Roberta Lariccia<sup>1</sup>; Ilaria Ferrante<sup>1</sup>; Daniele Recenti<sup>1</sup>; Luigi Motti<sup>2</sup>; <sup>1</sup>DANI, Cologno Monzese, Italy; <sup>2</sup>Dani SA, Contone, Switzerland
- MP 639 **Selective and Sensitive Detection and Quantification of Stockholm Convention POPs, Including Dioxins, Using Atmospheric Pressure Gas Chromatography MS/MS;** Kendon Graham<sup>1,2</sup>; Jody Dunstan<sup>1,2</sup>; Michael McCullagh<sup>1,2</sup>; Ingrid Ericson Jogsten<sup>3</sup>; Jessica Hagberg<sup>3</sup>; Bert van Bavel<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Manchester, UK; <sup>3</sup>MTM Research Centre, Orebro, Sweden
- MP 640 **In situ Detection of Ambient Aerosol in Jiangmen, China Using Single Particle Aerosol Mass Spectrometry;** Mei Li<sup>1</sup>; Li Zhang<sup>1</sup>; Lei Li<sup>1</sup>; Zhengxu Huang<sup>1</sup>; Wei Gao<sup>1</sup>; Ping Cheng<sup>1</sup>; Zhen Zhou<sup>1</sup>; Zhong Fu<sup>2</sup>; Huiqing Nian<sup>2</sup>; <sup>1</sup>Shanghai University, Shanghai, China; <sup>2</sup>Guangzhou Hexin Analytical Instrument Company, Guangzhou, China
- MP 641 **Air Quality Test Using Home-made Portable Membrane Inlet Single Photon Ionization Time-of-flight Mass Spectrometer;** Guobin Tan<sup>1</sup>; Wei Gao<sup>1</sup>; Zhengxu Huang<sup>1</sup>; Mei Li<sup>1</sup>; Ping Cheng<sup>1</sup>; Zhen Zhou<sup>1</sup>; Huiqing Nian<sup>2</sup>; Zhong Fu<sup>2</sup>; <sup>1</sup>Shanghai University, Shanghai, China; <sup>2</sup>Guangzhou Hexin Analytical Instrument Company, Guangzhou, China
- MP 642 **Screening of Pesticides in Water Using SPE On Line;** Stefano Lucini; Stefano Zaza; Shimadzu, Milano, Italy
- MP 643 **Method Development for Detection of Vinyl Chloride from Water using Solid Phase Micro-extraction (SPME) with Gas Chromatography/Mass Spectrometry (GC/MS);** Rachel Logemann; Christine N. Dalton; Carson-Newman College, Jefferson City, TN
- MP 644 **Preliminary Analysis of Athabasca Samples Using Gas Chromatography Atmospheric Pressure Chemical Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Mark Barrow<sup>1</sup>; Kerry Peru<sup>2</sup>; John Headley<sup>2</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Environment Canada, Saskatoon, Canada
- MP 645 **Use of Non-Targeted Environmetrics and GCxGC-TOF-MS to Assess the Sewage Treatment Plant Removal Efficiency of Emerging Contaminants;** Peter Haglund<sup>1</sup>; Ulrika Olofsson<sup>1</sup>; Kevin Siek<sup>2</sup>; David Alonso<sup>2</sup>; <sup>1</sup>Umea University, Department of Chemistry, Umea, Sweden; <sup>2</sup>Leco Corp. Life Science & Chemical Analysis Center, St Joseph, MI
- MP 646 **An Online VOCs Monitoring System Using Ion Trap Based Gas Chromatography Mass Spectrometry Technology;** Luhong Wen<sup>1</sup>; Jiancheng Yu<sup>1</sup>; Xiaoxu Li<sup>2</sup>; <sup>1</sup>Ningbo University, Ningbo, China; <sup>2</sup>Suzhou University, Suzhou, China
- MP 647 **Development of Methods on the Basis of Large-Volume-Injection Solid-Phase Extraction Hyphenated to Tandem Mass Spectrometry for the Determination of Hormones;** Norbert Wenkel<sup>2</sup>; Thorsten Teutenberg<sup>1</sup>; Jochen Türk<sup>1</sup>; Christoph Portner<sup>1</sup>; Linda Gehrmann<sup>1</sup>; Sandy-Dominic Freihoff<sup>1</sup>; <sup>1</sup>IUTA e.V., Duisburg, Germany; <sup>2</sup>Axel Semrau GmbH & Co. KG, Sprockhövel, Germany
- MP 648 **FT-ICR MS Analysis of complex Mixtures Produced by Pyrolysis of Plastics;** Justin Elliott<sup>1</sup>; Alan T. Taylor<sup>1</sup>; David Kilgour<sup>2</sup>; Meric Gursoy<sup>3</sup>; Pat Langridge Smith<sup>1</sup>; Peter O'Connor<sup>2</sup>; Ondrej Masek<sup>3</sup>; Logan Mackay<sup>1</sup>; <sup>1</sup>School of Chemistry, University of Edinburgh, Edinburgh, UK; <sup>2</sup>Department of Chemistry, University of Warwick, Coventry, UK; <sup>3</sup>University of Edinburgh, Edinburgh, UK



- MP 649 **Direct Analysis of Secondary Organic Aerosol Using the Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Mass Spectrometry source;** Martin Brüggemann; Thorsten Hoffmann; Johannes Gutenberg University, Mainz, Germany
- MP 650 **Elemental Composition Analysis of Biogenic Secondary Organic Aerosol by FTMS;** Jae-Eun Park<sup>1</sup>; Sun Jong Baek<sup>1</sup>; Hyun Sik Kim<sup>1</sup>; Jun-Hyun Park<sup>2</sup>; Woung Woo<sup>2</sup>; Ho-Jin Lim<sup>2</sup>; <sup>1</sup>Korea Basic Science Institute, Ochang-Myun Cheongwon-Gun, South Korea; <sup>2</sup>Kyungpook National University, Daegu, South Korea
- MP 651 **Combination of FTMS and DirectProbe(DIP) Analysis of Complex Cigarette Smoke;** Hu Nan<sup>1</sup>; Pu Hai<sup>1</sup>; Wu Yiqin<sup>2</sup>; <sup>1</sup>Brucker China, Beijing, China; <sup>2</sup>Yunnan Academy of Tobacco Science, Kunming, Yunnan, China
- MP 652 **Molecular Characterization of Sedimentary Organic Matter in the Estuary-Lagoon System Cananéia-Iguape (Brazil) by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Giovana Bataglion<sup>1</sup>; Clécio Klitzke<sup>1</sup>; Diego Senatore<sup>2</sup>; Roberto Barcellos<sup>3</sup>; Rolf Weber<sup>2</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>Unicamp, Campinas, Brasil; <sup>2</sup>USP, São Paulo, Brasil; <sup>3</sup>UFPE, Recife, Brasil
- Plant"omics", 653 - 671**
- MP 653 **Mass Spectrometry Analysis of Redox Proteins in Guard Cell Hormone Signaling;** Mengmeng Zhu<sup>1</sup>; Ning Zhu<sup>1</sup>; Wenyuan Song<sup>1</sup>; Alice Harmon<sup>1</sup>; Sarah Assmann<sup>2</sup>; Sixue Chen<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Pennsylvania State University, State College, PA
- MP 654 **Relative Mass Defect Filtering for Discovery of Conjugated Terpenoid Metabolites from Complex Plant Extracts;** E.A. Prabodha Ekanayaka; A. Daniel Jones; Michigan State University, East Lansing, MI
- MP 655 **Unusual Fragmentation Patterns of Ionized Lignin Model Compounds with  $\alpha$ -O-4 Linkages in (+)/(-)-ESI/ Tandem Mass Spectrometry;** Huaming Sheng; Purdue University, West Lafayette, IN
- MP 656 **Extraction Methodology and Metabolite Analysis by LC-MS of *Eucalyptus grandis*, Resistant and Susceptible to *Puccinia psidii*, Aiming for Identifying Resistance Biomarkers;** Thais Regiani; Felipe Garbelini Marques; Ilara Gabriela Frasson Budzinski; Fabricio Edgar de Moraes; Carlos Alberto Labate; Max Feffer Laboratory of Plant Genetics, Piracicaba, Brazil
- MP 657 **Comparative Metabolomic Studies on *Portulaca oleracea* L. Using GC-MS and LC-MS;** Li-Chun Liu; Qing Wang; Ying Wang; Ming-Quan Guo; Wuhan Botanical Garden, Chinese Academy of Science, Wuhan, China
- MP 658 **Atmospheric Pressure Photoionization Combined with UV Laser Desorption Mass Spectrometry;** Katie-Jo Galayda; Tim Anderson; Andrew Korte; Young-Jin Lee; R. S. Houk; Iowa State University, Ames, IA
- MP 659 **Application of Sub-2 $\mu$ m Particle CO<sub>2</sub>-based Chromatography Coupled to Mass Spectrometry for Chemical Profiling of Various Chamomiles;** Bharathi Avula<sup>1</sup>; Yan-Hong Wang<sup>1</sup>; Michael D Jones<sup>2</sup>; Larry Meeker<sup>2</sup>; Kate Yu<sup>2</sup>; Troy J. Smillie<sup>1</sup>; Ikhlal A. Khan<sup>1,3</sup>; <sup>1</sup>University of Mississippi, NCNPR, University, MS; <sup>2</sup>Waters, Milford, MA; <sup>3</sup>University of Mississippi, School of Pharmacy, University, MS
- MP 660 **Detecting Substances in Tea Leaves by Live Single-cell Mass Spectrometry;** Iwao Sakane<sup>1</sup>; Yuko M. Sagesaka<sup>1</sup>; Hajime Mizuno<sup>2</sup>; Naohiro Tsuyama<sup>2</sup>; Takanori Harada<sup>3</sup>; Tsutomu Masujima<sup>2</sup>; <sup>1</sup>ITO-EN LTD, Mckinhohara, Japan; <sup>2</sup>RIKEN Quantitative Biology Center (QBiC), Osaka, Japan; <sup>3</sup>Hiroshima Univ. Grad. Sch. Biomed. Sci, Hiroshima, Japan
- MP 661 ***Quercus ilex*: Protein Identification Strategies for an Orphan Tree Species;** Christof Lenz<sup>1</sup>; Henning Urlaub<sup>1</sup>; Jesús V. Jorrrin Novo<sup>2</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>University of Córdoba, Córdoba, Spain
- MP 662 **Characterization of Barley Chloroplast Proteins by Quantitative Proteomics Using Optimized 2D-LC Coupled to an LTQ-Orbitrap Velos Tandem Mass Spectrometer;** Jørgen Petersen<sup>1</sup>; Richard R. Sprenger<sup>1</sup>; Adelina Rogowska-Wrzesinska<sup>1</sup>; Pai Pedas<sup>2</sup>; Ken Krogholm<sup>2</sup>; Søren Husted<sup>2</sup>; Poul Erik Jensen<sup>2</sup>; Jan Kofod Schjoerring<sup>2</sup>; Ole Nørregaard Jensen<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense C, Denmark; <sup>2</sup>University of Copenhagen, Copenhagen, Denmark
- MP 663 **Comparative Characterization of Carotenoid Regulatory Network in Melon Using TMT-based Quantitative Proteomics Analysis;** Yong Yang<sup>1</sup>; Li Li<sup>1</sup>; Yongqiang Wang<sup>2</sup>; Theodore W. Thannhauser<sup>1</sup>; <sup>1</sup>USDA-ARS at Cornell University, Ithaca, NY; <sup>2</sup>Department of Plant Breeding and Genetics, Cornell, Ithaca, NY
- MP 664 **An Untargeted, Quantitative Comparison of Early ABA-induced Phosphoproteomic Changes Using Wildtype and Quadruple ABA Receptor Mutant A. Thaliana Strains;** Benjamin Minkoff; University of Wisconsin, Madison, WI
- MP 665 **Integrating Multiple 'omics' Analysis of Fruit Development in High-Yielding Oil Palm Mesocarp;** Huey Fang Teh; Sime Darby Technology Centre, Serdang, Malaysia
- MP 666 **Metabolite Profile of Sugarcane (*Saccharum*Spp) under Water Stress;** Simone Guidetti-Gonzalez; Ilara Gabriela Frasson Budzinski; Fabricio Edgar de Moraes; Carlos Alberto Labate; ESALQ/USP, Piracicaba, Brazil
- MP 667 **The Effect of Genetics and Environment on the Metabolome of Commercial Maize Hybrids Using LC/MS: A Multisite Study;** Vincent Asiago; Chris Vlahakis; Hamid Baniasadi; Jan Hazebroek; Cathy Zhong; DuPont Pioneer, Johnston, IA
- MP 668 **Characterization of Cytosolic Protein Complexes in Plants Using Multi-Step Chromatographic Separation and Quantitative Mass Spectrometry;** Uma Aryal<sup>1</sup>; Yi Xiong<sup>2</sup>; Eileen Mallery<sup>3</sup>; Mark Hall<sup>1</sup>; Jun Xie<sup>4</sup>; Daisuke Kihara<sup>2</sup>; Daniel Szymanski<sup>3</sup>; <sup>1</sup>Department of Biochemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Computer Science, Purdue University, West Lafayette, IN; <sup>3</sup>Department of Agronomy, Purdue University, West Lafayette, IN; <sup>4</sup>Department of Statistics, Purdue University, West Lafayette, IN
- MP 669 **Integrating Genomics, Transcriptomics, and Proteomics for the Identification of Protein Sequence Variants in the Genus *Populus*;** Paul Abraham<sup>1,2</sup>; Xiaojing Wang<sup>3</sup>; Priya Ranjan<sup>2</sup>; Bing Zhang<sup>3</sup>; Gerald Tuskan<sup>2</sup>; Robert Hettich<sup>2</sup>; <sup>1</sup>University of Tennessee, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>Vanderbilt University School of Medicine, Nashville, TN
- MP 670 **Stable Isotope Labeling of *Brachypodium distachyon* with Nitrogen 15 for Quantitative Mass Spectrometry;** David Shearer<sup>1</sup>; Victor Spicer<sup>1</sup>; Steve Haber<sup>2</sup>; Kenneth Standing<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Agriculture and Agri-Food Canada, Winnipeg, Canada
- MP 671 **Absolute Quantification of TIR1/AFB Proteins in Arabidopsis Using the QconCAT Strategy;** Kai-Ting Fan; Jerry D. Cohen; William M. Gray; Adrian D. Hegeman; University of Minnesota, Twin Cities, MN



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- MP 672 **Coupling Genetics and Molecular Biology with Mass Spectrometry Revealed Arboviruses Usurp Similar Transport Pathways in Insect Vectors and Hosts;** Michelle Cilia<sup>1,2</sup>; Michael Bereman<sup>3</sup>; Cecilia Tamborindeguy<sup>4</sup>; Qiaoxia Shang<sup>2,5</sup>; David Igwe<sup>2,6</sup>; Stacy Deblasio<sup>3</sup>; Theodore Thannhauser<sup>1</sup>; Stewart Gray<sup>1</sup>; Michael MacCoss<sup>3</sup>; <sup>1</sup>USDA-Agricultural Research Service, Ithaca, NY; <sup>2</sup>Plant Pathology, Cornell University, Ithaca, NY; <sup>3</sup>Genome Sciences, University of Washington, Seattle, WA; <sup>4</sup>Entomology, Texas A&M University, College Station, TX; <sup>5</sup>Beijing University of Agriculture, Beijing, China; <sup>6</sup>International Institute of Tropical Agriculture, Ibadan, Nigeria
- MP 673 **Coupling a Simple, ELISA-based Co-Immunoprecipitation Technique with Tandem Mass Spectrometry to Characterize a Plant-Virus Interactome;** Stacy Deblasio<sup>1</sup>; Michael Bereman<sup>2</sup>; Jaclyn Mahoney<sup>3</sup>; Theodore Thannhauser<sup>1</sup>; Stewart Gray<sup>1,3</sup>; Michael MacCoss<sup>2</sup>; Michelle Cilia<sup>1,3</sup>; <sup>1</sup>USDA-Agricultural Research Service, Ithaca, NY; <sup>2</sup>Genome Sciences, University of Washington, Seattle, WA; <sup>3</sup>Plant Pathology, Cornell University, Ithaca, NY
- MP 674 **Quantitation of Antiviral Drugs in Chicken Samples by Ultra-High Performance Liquid Chromatography Tandem Triple Quadrupole Mass Spectrometry with Triggered MRM;** Jianzhong Li; Tao Bo; Cuiling Wu; Wei Chen; Zhixu Zhang; *Agilent Technologies(China), Beijing, China*
- MP 675 **Comparison of Proteomes from Escherichia coli Strains that cause Transient and Persistent Intramammary Infections;** John Lippolis<sup>1</sup>; Timothy Reinhardt<sup>1</sup>; Randy Sacco<sup>1</sup>; Brian Nonnecke<sup>1</sup>; Belgin Dogan<sup>2</sup>; Kenneth Simpson<sup>2</sup>; Ynte Schukken<sup>2</sup>; <sup>1</sup>USDA ARS - Nat'l Animal Disease Ctr., Ames, IA; <sup>2</sup>Cornell University, College of Veterinary Medicine, Ithaca, NY
- MP 676 **Fragmentation Patterns of Monomeric and Oligomeric Wine Stilbenoids by UHPLC-ESI-QTOF MS;** Ryan Moss<sup>1</sup>; Qunyong Mao<sup>2</sup>; Dennis Taylor<sup>1,2</sup>; Cédric Saucier<sup>1,2</sup>; <sup>1</sup>University of British Columbia, Kelowna, Canada; <sup>2</sup>University of Adelaide, Adelaide, SA
- MP 677 **Proteomic Analysis of the Effect of Pre-Sound Wave Stimulation on Botrytis cinerea-infected Arabidopsis;** Yeong-Sang Kwon<sup>1</sup>; Sung Woo Jeong<sup>1</sup>; Hanhong Bae<sup>2</sup>; Sung Chul Shin<sup>1</sup>; Mi-Jeong Jeong<sup>3</sup>; Soo-Chul Park<sup>3</sup>; Dong-Won Bae<sup>1</sup>; <sup>1</sup>GyeongSang National University, Jinju, South Korea; <sup>2</sup>Yeungnam University, Gyeongsan, Korea; <sup>3</sup>National Academy of Agricultural Science, Suwon, Korea
- MP 678 **Distribution of Metabolites and Biosynthesis in a Cell of a Plant Tissue Analyzed by Live Single-cell Mass Spectrometry;** Shuichi Mastuda<sup>1</sup>; Satomi Hatano-Saga<sup>2</sup>; Sachiko Date<sup>2</sup>; Hajime Mizuno<sup>2</sup>; Naohiro Tsuyama<sup>1</sup>; Tsutomu Masujima<sup>1,2</sup>; <sup>1</sup>Graduate School of Biomedical, Hiroshima University, Hiroshima, Japan; <sup>2</sup>Quantitative Biology Center (QBiC), RIKEN, Suita, Japan
- MP 679 **Analysis of Various Deoxynivalenol (DON) LC-MS Methods without Acetate in the Mobile Phase;** Sheldon M. Williams; Yoko S. Johnson; Treeske Ehresmann; Michele M. Swarbrick; *Minnesota Department of Agriculture, St Paul, MN*
- MP 680 **Stable Isotope Tracer Guided LC-MS Metabolomics to Elucidate Biochemical Mechanisms of Temperature Dependent Anthocyanin Degradation in Grapes Cultured in vitro;** Alexander Chassy<sup>1</sup>; Christoph Büschel<sup>2</sup>; Hye-Young Lee<sup>1</sup>; Larry Lerno<sup>1</sup>; Anita Oberholster<sup>1</sup>; Daniela Barile<sup>1</sup>; Rainer Schuhmacher<sup>2</sup>; Andrew Waterhouse<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>University of Natural Resources and Life Sciences, Vienna, Austria

- MP 681 **Muscle, Marbling, maXis and Mascot - Meat Quality Phenotyping;** Stefan Clerens<sup>1</sup>; Santanu Deb-Choudhury<sup>1</sup>; Anita Grosvenor<sup>1</sup>; Stephen Haines<sup>1</sup>; Ancy Thomas<sup>1</sup>; Peter Dobbie<sup>2</sup>; Chris McMahon<sup>2</sup>; Monica Senna-Salerno<sup>2</sup>; Gina Nicholas<sup>2</sup>; Shelley Falconer<sup>2</sup>; Katja Rosenvold<sup>2</sup>; <sup>1</sup>AgResearch Lincoln Research Centre, Christchurch, New Zealand; <sup>2</sup>AgResearch Ruakura Research Centre, Hamilton, New Zealand
- MP 682 **Quantitative Analysis of the Host-Pathogen Proteomics of Israeli Acute Paralysis Virus (IAPV) Infection in the Honey Bee (Apis mellifera);** Sarah Natrasany<sup>1</sup>; Humberto Boncristiani<sup>2</sup>; Leonard Foster<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada; <sup>2</sup>University of North Carolina, Greensboro, NC

## Natural Products, 683 - 714

- MP 683 **LC-MS/MS Study of Indian Ginseng Metabolism;** Manoj Pillai<sup>1,2</sup>; Takeo Sakuma<sup>1,2</sup>; Carmai Seto<sup>1,2</sup>; <sup>1</sup>AB SCIEX, Gurgaon, India; <sup>2</sup>AB SCIEX, Concord, Canada
- MP 684 **Unknowns Analysis of Natural Products Using GC/Q-TOF and GC/IonTrap in Positive Electron Impact and Positive Chemical Ionization Modes with MS/MS;** Ron Honnold; Rafael Acosta; *Agilent Technologies, Santa Clara, CA*
- MP 685 **Accurate Mass Retention Time Locked Flavor Database by GC/Q-TOF;** Susan E. Ebeler<sup>3</sup>; Sean LaFond<sup>3</sup>; Frank David<sup>2</sup>; Stephan Baumann<sup>1</sup>; Tim Conjelko<sup>1</sup>; Sofia Aronova<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Research Institute for Chromatography, Kortrijk, Belgium; <sup>3</sup>UC Davis Department of Viticulture and Enology, Davis, CA
- MP 686 **Mass Spectrometric Characterization of Pyrrolizidine Alkaloids in Black Cohosh;** Dejan Nikolic; Guannan Li; Tamara Cisowska; Tanja Goedecke; Shaon-Nong Chen; David Lankin; Guido Pauli; Richard van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- MP 687 **In-situ Measurement of the Defense Response of the Sea Anemone to Spatial Encroachment Stresses Using On-line LC/MS;** James Buchner; Ross Willoughby; James Buchner Jr; Robert Moskala; *BIOMICom, Inc., Allison Park, PA*
- MP 688 **Optimized Plant Extractions for Phytochemical Library Construction: Evaluating Solvent Systems Using Metabolomics Approaches;** Amanda C. Martin; Alison D. Pawlus; Erin Jewet; Stephen Brockman; Donald L. Wyse; Adrian D. Hegeman; *University of Minnesota, Saint Paul, MN*
- MP 689 **Identification of Antibacterial Component from Extract of Garcinia indica Fruit Rind Using LC/MS/MS;** Shailendra Rane<sup>1</sup>; Shailesh Damale<sup>1</sup>; Shruti Raju<sup>1</sup>; Rashi Kochhar<sup>1</sup>; Deepti Bhandarkar<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Manasi Kher<sup>2</sup>; Komal Barbade<sup>2</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India; <sup>2</sup>G.N.I.R.D., G.N. Khalsa College, Matunga, Mumbai, Maharashtra, India
- MP 690 **Study of Antibacterial Activity of Essential Oil Components Obtained from Pericarp of Zanthoxylum rhetsa (Indian origin) Using HS-GCMS;** Durvesh Sawant<sup>1</sup>; Dheeraj Handique<sup>1</sup>; Ankush Bhone<sup>1</sup>; Prashant Hase<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Ajit Datar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Nital Patil<sup>2</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India; <sup>2</sup>G.N.I.R.D., G.N. Khalsa College, Matunga, Mumbai, Maharashtra, India
- MP 691 **Characterization of Flavonoids and Phytoestrogens in an Extract of Pueraria Mirifica by UHPLC-MS-MS;** Jeff Dahl<sup>1</sup>; Rocky Graziose<sup>2</sup>; Youssef W. Mirhom<sup>2</sup>; Frank S. D'Amelio<sup>2</sup>; <sup>1</sup>Shimadzu, Columbia, MD; <sup>2</sup>Bio-Botanica, Hauppauge, NY



- MP 692 **Alkaloids Characterization of Tabernaemontana catharinensis by ESI-Orbitrap**; Sidnei Moura; Flávio Marinho; Carla Nicola; Mariana Roesch-Ely; *Caxias do Sul University, Caxias do Sul, Brazil*
- MP 693 **Fragmentation Study and Comprehensive Profiling of Escin, a Mixture of Triterpene Saponins from Aesculus Hippocastanum, by LC-MS/MS**; Antonio Triolo<sup>1</sup>; Elisa Libralesso<sup>1</sup>; Serena Staccioli<sup>2</sup>; Fabiana Tavani<sup>2</sup>; <sup>1</sup>*Menarini Ricerche Spa, Firenze, ITALY*; <sup>2</sup>*A. Menarini Manufacturing Logistics and Services, Firenze, Italy*
- MP 694 **High Resolution UPLC-TOF Mass Spectrometric Characterization of an Herbal Preparation of Senna**; Tiffany A. Freed<sup>1</sup>; Melanie A. Rehder Silinski<sup>1</sup>; James C. Blake<sup>1</sup>; Megan Grabenauer<sup>1</sup>; Reshan A. Fernando<sup>1</sup>; Veronica G. Robinson<sup>2</sup>; Suramya Waidyanatha<sup>2</sup>; <sup>1</sup>*RTI International, Research Triangle Park, NC*; <sup>2</sup>*Division of National Toxicology Program, NIEHS, Research Triangle Park, NC*
- MP 695 **Characterization of Commercially Available Stevia-derived Sweeteners Using Liquid Chromatography-High Resolution Time of Flight Mass Spectrometry and Advanced Data Processing**; Juergen Wendt<sup>1</sup>; Norbert Helle<sup>2</sup>; Jutta Lintelmann<sup>3</sup>; Jeffrey S. Patrick<sup>4</sup>; <sup>1</sup>*LECO European LSCA Centre, Moechengladbach, Germany*; <sup>2</sup>*TeLA GmbH, Bremerhaven, Germany*; <sup>3</sup>*Helmholtz Zentrum München, Neuherberg, Germany*; <sup>4</sup>*LECO Corporation, Separation Sciences Division, St. Joseph, MI*
- MP 696 **Quality-by-Design UHPLC Method Development with High Resolution MS<sup>E</sup> for Biomarker Identification of Phyllanthus Species**; Amadeu Iglesias<sup>1</sup>; Ricardo Sprenger<sup>2</sup>; Fernando de Paula<sup>1</sup>; Tiago Campos<sup>1</sup>; Michael Murgu<sup>1</sup>; Quezia Cass<sup>2</sup>; <sup>1</sup>*Waters Corporation, Barueri, Brazil*; <sup>2</sup>*Universidade Federal de São Carlos - UFSCar, São Carlos, SP, Brazil*
- MP 697 **Structural Elucidation of Iridoids from the Leaves of Vitex negundo Linn. by Liquid Chromatography-Tandem Mass Spectrometry**; Lolita A. Lagurin<sup>1</sup>; Maria Cristina A. Dancel<sup>2</sup>; Jodie V. Johnson<sup>2</sup>; Fabian M. Dayrit<sup>1</sup>; <sup>1</sup>*Ateneo de Manila University, Quezon, Philippines*; <sup>2</sup>*University of Florida, Gainesville, FL*
- MP 698 **Mapping the "Known Metabolome" Using SciFinder Scholar for More Efficient HPLC-PDA-HRMS Dereplication of Crude Plant Extracts**; Andrew Newsome; Elizabeth Martinez; Richard van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- MP 699 **Analysis of Red Propolis Samples by UPLC-MS**; Begoña Gimenez-Cassina; Alexandra C.H.F. Sawaya; *BTPB - Institute of Biology - Unicamp, Campinas, Brazil*
- MP 700 **Analysis of Bioactive Loline Alkaloids in Achnatherum robustum and Lolium pratense by High Resolution Mass Spectrometry**; Scott Jarmusch<sup>1</sup>; Mario Figueroa<sup>1</sup>; Brandie Ehrmann<sup>1</sup>; Tatsiana Shymanovich<sup>1</sup>; Stanley Faeth<sup>1</sup>; Jonathan Scheerer<sup>2</sup>; Nadja Cech<sup>1</sup>; <sup>1</sup>*University of North Carolina Greensboro, Greensboro, NC*; <sup>2</sup>*College of William and Mary, Williamsburg, VA*
- MP 701 **Rapid Screening of Herbal Extracts by Thin Layer Chromatography-Information Dependent Acquisition-High Resolution Mass Spectrometry (TLC-IDA-HRMS)**; Jeffrey Morré<sup>1</sup>; Jeremiah Kelley<sup>1</sup>; Nora Gray<sup>2</sup>; Amala Soumyanath<sup>2</sup>; Jan F. Stevens<sup>1</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*Oregon Health and Science University, Portland, OR*
- MP 702 **Imaging Metabolite Distributions in Hypericum Plants**; Zhihong Song<sup>1,2</sup>; Matthew C. Crispin<sup>1</sup>; Eve Syркиn Wurtele<sup>1</sup>; Andrew R. Korte<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; Basil J. Nikolau<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*The Ames Laboratory of US DOE, Ames, IA*
- MP 703 **Use of t-BDMS Derivatization for Enhanced Gas Chromatography-Mass Spectrometry Analysis of Hydroxy Terpenes in Essential Oils**; Deborah Chance; Thomas Mawhinney; *University of Missouri, Columbia, MO*
- MP 704 **Determination of Vanillin in Natural Vanilla Bean Extracts from Different Geographic Regions Using LC/TOF**; Avinash Dalmia; Daniel Pentek; Robert Packer; George Perkins; *Perkinelmer, Shelton, CT*
- MP 705 **Differentiation of Positional Carotenoid Glucoside Isomers (Crocins) and Detection of a New Aglycon Moiety in Crocus Sativus L**; Nikolaos Stavros Koulakiotis<sup>1,2</sup>; Ernst Pittenauer<sup>3</sup>; Guenter Allmaier<sup>3</sup>; Anthony Tsarbopoulos<sup>1,4</sup>; <sup>1</sup>*The Goulondris Natural History Museum, Kifissia, Greece*; <sup>2</sup>*University of Patras, Pharmacy Department, Patras, Greece*; <sup>3</sup>*Vienna University of Technology, Vienna, Austria*; <sup>4</sup>*University of Athens Medical School, Pharmacology, Athens, Greece*
- MP 706 **Quantitative Proteomics Analysis for the Effects of Garlic Extracts on Neuroinflammation**; Hui Zhou<sup>1,3</sup>; Zhe Qu<sup>1,3</sup>; Dineo L Nkholise<sup>1,3</sup>; Jilong Li<sup>4</sup>; Jianlin Cheng<sup>4</sup>; C. Michael Greenleaf<sup>5</sup>; Valeri V. Mossine<sup>2</sup>; Thomas Mawhinney<sup>2</sup>; Paula N Brown<sup>7</sup>; Kevin L. Fritsche<sup>6</sup>; Dennis B. Lubahn<sup>2</sup>; Grace Y. Sun<sup>2,3</sup>; Zezong Gu<sup>1,3</sup>; <sup>1</sup>*University of Missouri School of Medicine Pathology, Columbia, MO*; <sup>2</sup>*Biochemistry, Columbia, Mo*; <sup>3</sup>*Center for Translational Neuroscience, University, Columbia, MO*; <sup>4</sup>*Department of Computer Science, Informatics Insti, Columbia, Mo*; <sup>5</sup>*Chemistry, Columbia, Mo*; <sup>6</sup>*Division of Animal Sciences, Columbia, Mo*; <sup>7</sup>*British Columbia Institute of Technology, Vancouver, BC, Canada*
- MP 707 **Discovering Peptidic Natural Products by Computational Mass Spectrometry and Genome Mining**; Hosein Mohimani<sup>1</sup>; Roland Kersten<sup>1</sup>; Wei Ting Liu<sup>1</sup>; Mingxun Wang<sup>1</sup>; Samuel O. Purvine<sup>2</sup>; Si Wu<sup>2</sup>; Heather M. Brewer<sup>2</sup>; Ljiljana Pasa-Tolic<sup>2</sup>; Bradley S. Moore<sup>1</sup>; Pieter C. Dorrestein<sup>1</sup>; Pavel A. Pevzner<sup>1</sup>; <sup>1</sup>*University of California, San Diego, La Jolla, CA*; <sup>2</sup>*PNNL, Richland, WA*
- MP 708 **Identification of Bioactive Compounds in Gentiana by UHPLC tandem QTOF Mass Spectrometry**; Wei Du; Xiaorong Ran; Tao Bo; Wei Chen; *Agilent Technologies(China) Co. Ltd., Beijing, China*
- MP 709 **Rapid Identification of Major Active Constituents in Traditional Chinese Medicine Using UHPLC/ High Resolution Q-TOF Mass Spectrometry and Database Searching**; Xiaorong Ran; Tao Bo; Wei Chen; Zhixu Zhang; *Agilent Technologies (China), Beijing, China*
- MP 710 **Rapid Accurate Mass Technology for Comparative Metabolism Study of Isoimperatorin and Imperatorin in Liver Microsomes of Five Species**; Kerong Zhang<sup>1</sup>; Xiaomei Zhuang<sup>2</sup>; Yuhuan Zhong<sup>2</sup>; Ping Du<sup>1</sup>; Jiehui Hu<sup>1</sup>; Ting Liu<sup>1</sup>; Jingchao Lin<sup>1</sup>; Yongming Xie<sup>1</sup>; Hua Li<sup>2</sup>; <sup>1</sup>*AB SCIEX, Beijing, China*; <sup>2</sup>*Beijing Institute of Pharmacology and Toxicology, Beijing, China*
- MP 711 **Identification and Confirmation of Ginsenosides in Panax Extract Using a hybrid Triple Quadrupole Linear Ion Trap System**; Dandan Si; Ting Liu; Jiehui Hu; Xiaoyan Xu; Ping Du; Yongming Xie; *AB SCIEX, Shanghai, CN*
- MP 712 **Specific Drug Target Identification with Quantitative Chemical Proteomics**; Jigang Wang<sup>1</sup>; Xing Fei Tan<sup>1</sup>; Van Sang Nguyen<sup>1</sup>; Peng Yang<sup>2</sup>; Jing Zhou<sup>1</sup>; Mingming Gao<sup>3</sup>; Zhengjun Li<sup>4</sup>; Teck Kwang Lim<sup>1</sup>; Yingke He<sup>5</sup>; Chye Sun Ong<sup>6</sup>; Yifei Lay<sup>1</sup>; Jianbin Zhang<sup>1</sup>; Guili Zhu<sup>5</sup>; Yu Keung Mok<sup>1</sup>; Han-Ming Shen<sup>1</sup>; Qingsong Lin<sup>1</sup>; <sup>1</sup>*National University of Singapore, Singapore, Singapore*; <sup>2</sup>*School of Pharmacy, University of Pittsburgh, Pittsburgh, PA*; <sup>3</sup>*University of Maryland, Rockville, MD*; <sup>4</sup>*NUS Environmental Research Institute, Singapore, Singapore*; <sup>5</sup>*Duke-NUS Graduate Medical School, Singapore, Singapore*; <sup>6</sup>*Singapore Polytechnic, Singapore, Singapore*



- MP 713 **Identification of Complex Constituents in Herba Sarcandrae Using High Speed Accurate Mass Technology;** Guoliang Xu<sup>1</sup>; Yu Lei<sup>2</sup>; Ting Liu<sup>2</sup>; Qiyun Zhang<sup>1</sup>; Guangbin Shang<sup>1</sup>; Xiaoyan Xu<sup>2</sup>; Ping Du<sup>2</sup>; Yongming Xie<sup>2</sup>; Xilan Tang<sup>1</sup>; <sup>1</sup>*Jiangxi University of Traditional Chinese Medicine, Nanchang, Jiangxi Province, China*; <sup>2</sup>*AB SCIEX Asia Pacific Application Support Center, Shanghai, China*
- MP 714 **Development of Qualitative Method for Marker Compounds of Bang-poong-tong-sung-san by Iontrap Hybrid Time Of Flight (IT-TOF) Mass Spectrometer;** Unyong Kim; Han Young Eom; Joon Hyuk Suh; Sang Beom Han; *Chung Ang Univ., Seoul, South Korea*

#### Astrobiology & Atmospheric Chemistry, 715 - 720

- MP 715 **Astrobiologically-Relevant Ions in the Gas Phase;** Callie Cole<sup>1</sup>; Nadine Wehres<sup>1,2</sup>; Jennifer Reece<sup>1</sup>; Nicholas Demarais<sup>1</sup>; Theodore Snow<sup>2,3</sup>; Veronica Bierbaum<sup>1,2</sup>; <sup>1</sup>*University of Colorado at Boulder, Boulder, CO*; <sup>2</sup>*Center for Astrophysics and Space Astronomy, Boulder, CO*; <sup>3</sup>*Department of Astrophysical and Planetary Sciences, Boulder, CO*
- MP 716 **Characterization of Heavy Ion Radiation-Induced Changes of Lipid Biochemistry in the Liver by MALDI Imaging Mass Spectrometry;** Alexander S. Shavkunov<sup>1</sup>; Huiling Liu<sup>1</sup>; Norelle C. Wildburger<sup>1,2</sup>; Maureen McCarthy<sup>3,4</sup>; Yongjia Yu<sup>3,4</sup>; Lauren N. Macias<sup>3,4</sup>; Astrid D. Corbitt<sup>3,4</sup>; Daniel Olivares<sup>3,4</sup>; Robert L. Ullrich<sup>3,4</sup>; Carol L. Nilsson<sup>1,4</sup>; <sup>1</sup>*Department of Pharmacology and Toxicology, UTMB, Galveston, TX*; <sup>2</sup>*Department of Neuroscience and Cell Biology, UTMB, Galveston, TX*; <sup>3</sup>*Department of Radiation Oncology, UTMB, Galveston, TX*; <sup>4</sup>*UTMB Cancer Center, Galveston, TX*
- MP 717 **Characterization of Biogenic Secondary Organic Aerosol using Ultrahigh-Resolution FT-ICR Mass Spectrometry;** Lynn Mazzoleni; Yunzhu Zhao; Megan Dalbec; *Michigan Technological University, Houghton, MI*
- MP 718 **In situ Analysis of Mars Analog Samples Containing Perchlorate by the MOMA Linear Ion Trap Mass Spectrometer;** Ricardo Arevalo Jr.<sup>1</sup>; Veronica Pinnick<sup>2</sup>; Xiang Li<sup>2</sup>; Friso van Amerom<sup>3</sup>; Ryan Danell<sup>4</sup>; William Brinckerhoff<sup>1</sup>; Paul Mahaffy<sup>1</sup>; <sup>1</sup>*NASA Goddard Space Flight Center, Greenbelt, MD*; <sup>2</sup>*University of Maryland Baltimore County, Baltimore, MD*; <sup>3</sup>*SRI International, Inc., St. Petersburg, FL*; <sup>4</sup>*Danell Consulting, Inc., Greenville, NC*
- MP 719 **Miniature Two-Step Laser Time-of-Flight Mass Spectrometer for in situ Planetary Missions;** Xiang Li<sup>1</sup>; Stephanie Getty<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Timothy Cornish<sup>3</sup>; Scott Ecelberger<sup>3</sup>; Melissa Floyd<sup>2</sup>; <sup>1</sup>*University of Maryland, Baltimore County, Baltimore, MD*; <sup>2</sup>*NASA Goddard Space Flight Center, Greenbelt, MD*; <sup>3</sup>*C&E Research, Inc., Columbia, MD*
- MP 720 **Micro-Ion Trap Mass Spectrometers for (Pre)-Biotic Organic Compound Analysis on Comets;** Friso Van Amerom<sup>1</sup>; Ashish Chaudhary<sup>1</sup>; Timothy Short<sup>1</sup>; Patrick Roman<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Daniel Glavin<sup>2</sup>; Paul Mahaffy<sup>2</sup>; <sup>1</sup>*SRI International, St. Petersburg, Florida*; <sup>2</sup>*NASA Goddard Space Flight Center, Greenbelt, MD*

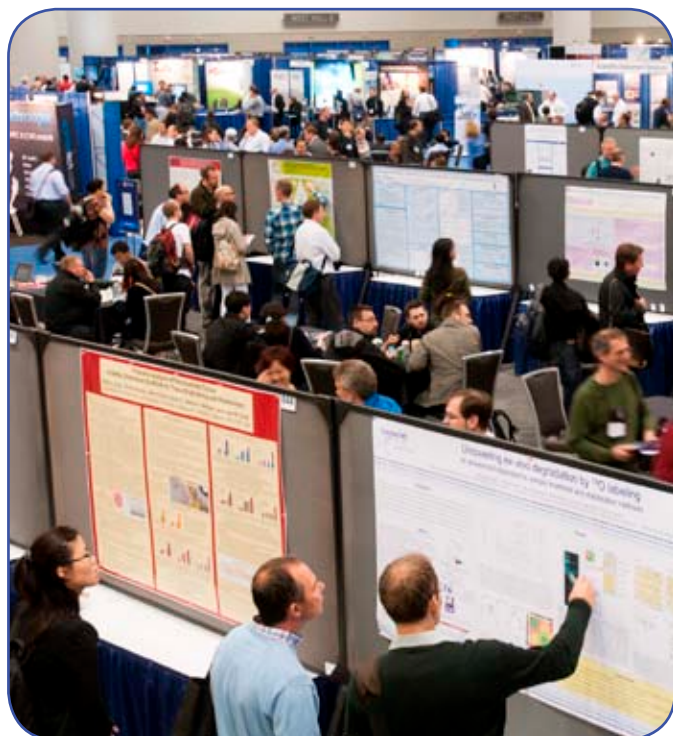
#### Polymers, 721 - 749

- MP 721 **The NIST Synthetic Polymer MALDI Recipes Database: Current Status and Future Prospects;** William E. Wallace; Janiel J. Reed; Charles M. Guttman; *National Institute of Standards & Technology, Gaithersburg, MD*

- MP 722 **In situ Characterisation of Microbicidal Agents within Polymer-Based Surface Coatings by Liquid Extraction Surface Analysis Mass Spectrometry;** Martin R. L. Paine<sup>1</sup>; Tran T. Hyunh<sup>2</sup>; Mike J. Manefield<sup>2</sup>; Philip J. Barker<sup>3</sup>; Scott A. Rice<sup>2</sup>; Stephen J. Blanksby<sup>1</sup>; <sup>1</sup>*University of Wollongong, Wollongong, Australia*; <sup>2</sup>*University of New South Wales, Sydney, Australia*; <sup>3</sup>*BlueScope Steel Research, Port Kembla, Australia*
- MP 723 **Using Ion Mobility for 'Shape-Selective' Characterization of Polymers;** Kirsten Craven<sup>1</sup>; Julien De Winter<sup>2</sup>; Pascal Gerbaux<sup>2</sup>; <sup>1</sup>*Waters, Manchester, UK*; <sup>2</sup>*University of Mons, Mons, Belgium*
- MP 724 **Characterization of Oligomeric Polyethylene Monoiodides by MALDI-ToF Mass Spectrometry Following Derivatization;** Roman Borisov; Nikolai Polovkov; Vladimir Zaikin; Alexei Vinogradov; Alexei Ivaniuk; *Topchiev Institute of Petrochemical Synthesis, Moscow, Russian Federation*
- MP 725 **Mass Spectrometry and Tandem Mass Spectrometry Analysis of Alkyl Polyglycoside (APG) Surfactants;** Ahlam Alalwiat; Chrys Wesdemiotis; *The University of Akron, Akron, U.S.A*
- MP 726 **Tandem Mass Spectrometry of Polyethers - Size and Collision Energy Effects;** Nadrah Alawani; Lydia Cool; Chrys Wesdemiotis; *University of Akron, Akron, OH*
- MP 727 **Copolyesters – Influence of End-Capping and Main Chain Sterics on Biodegradation;** Lydia Cool; Chrys Wesdemiotis; *The University of Akron, Akron, OH*
- MP 728 **Multidimensional Mass Spectrometry Studies on Dendritic Calibrants;** Aleer M. Yoi<sup>1</sup>; Scott M. Grayson<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH*; <sup>2</sup>*Tulane University, New Orleans, LA*
- MP 729 **Characterization of Poly(ε-caprolactone)-b-poly(ethylene glycol) Copolymers by Mass Spectrometry Techniques;** Marisa Carchedi<sup>1,2</sup>; Chrys Wesdemiotis<sup>2</sup>; Bartolo Gabriele<sup>1</sup>; Alessia Fazio<sup>1</sup>; Giovanni Sindona<sup>1</sup>; <sup>1</sup>*University of Calabria, Rende (CS), Italy*; <sup>2</sup>*University of Akron, Akron, OH*
- MP 730 **Tandem Mass Spectrometry of Glycopolymers;** Xiumin Liu; Lydia Cool; Chrys Wesdemiotis; *The University of Akron, Akron, OH*
- MP 731 **Quantitative Analysis of Fibre Mixture by Matrix Assisted Laser Desorption/Ionization Coupled Time of Flight Mass Spectrometer (MALDI-TOF MS);** Ssu-Hsueh Sun; Tsung-Ming Huang; *Bureau of Standards, Metrology and Inspection, Taipei, Taiwan*
- MP 732 **Effectiveness of Tertiary Ionic Liquid Matrix in the MALDI Analysis of PEG Polymers;** Taehee Kim; Jihyeon Lee; Jeongkwon Kim; *Chungnam National University, Daejeon, South Korea*
- MP 733 **High Throughput Characterization of Biopolyol Using DART-MS with Ultra-Fast Polarity Switching;** Christopher Gilles<sup>1</sup>; Keiko Matsumoto<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; Jun Watanabe<sup>2</sup>; Mariko Yoshioka<sup>4</sup>; Nobuo Shiraishi<sup>5</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Inc., Columbia, MD*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*; <sup>4</sup>*Kyoto University, Kyoto, Japan*; <sup>5</sup>*Shiraishi Biomass Co., Ltd., Kyoto, Japan*
- MP 734 **Completely Elucidating Soft Matter: Sequencing Linear Copolymers;** Martin S. Engler<sup>1</sup>; Sarah Crotty<sup>1</sup>; Christian Pietsch<sup>1</sup>; Kerstin Scheubert<sup>1</sup>; Ulrich S. Schubert<sup>1,2</sup>; Sebastian Boecker<sup>1,2</sup>; <sup>1</sup>*Friedrich Schiller University, Jena, Germany*; <sup>2</sup>*Jena Center for Soft Matter, Jena, Germany*
- MP 735 **Location of Cations Adducted to PEO-PAMAM Hybrid Molecules: A Combined MS/MS and Ion Mobility Study;** Christophe Chendo; Aura Tintaru; Qi Wang; Ling Peng; Laurence Charles; *Aix-Marseille University, Marseille, FR*

- MP 736 **Advantages of Mass Spectrometric Detection for Polymers Separated by UltraPerformance Convergence Chromatography;** Oliver Burt<sup>1</sup>; Baiba Cabovska<sup>2</sup>; Michael O'Leary<sup>2</sup>; Peter Hancock<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Waters, Milford, MA
- MP 737 **MALDI-TOF MS of Hyperbranched Polymers Aided by Liquid Chromatography Separation;** Jessica N. Hoskins<sup>1</sup>; Hans R. Kricheldorf<sup>2</sup>; Steffen M. Weidner<sup>1</sup>; Jana Falkenhagen<sup>1</sup>; <sup>1</sup>Fed. Institute for Materials Research and Testing, Berlin, Germany; <sup>2</sup>Institute for Technical and Macromolecular Chem., Hamburg, Germany
- MP 738 **Analysis of Ethylene Oxide and Propylene Oxide Random Copolymer by Using LC-MALDI-SpiralTOF MS;** Yoshiyuki Itoh<sup>1</sup>; Masahiro Hashimoto<sup>1</sup>; Bram van der Meer<sup>2</sup>; Akihiko Kusai<sup>1</sup>; <sup>1</sup>JEOL Ltd., Akishima, Japan; <sup>2</sup>JEOL (Europe) B.V., Nieuw-Vennep, The Netherlands
- MP 739 **Fragmentation of Deprotonated Polyethylene Glycol;** Daniel Goebbert; Thomas Hester; The University of Alabama, Tuscaloosa, AL
- MP 740 **Quantitation of ppm-ppb Level Oligomeric Surfactants for Contact Lens Wear Clinical Studies Using HR/AM-MS and Low Resolution Chromatography;** William Nichols<sup>1</sup>; Andrew J. Hotelling<sup>2</sup>; <sup>1</sup>Mass2Charge Consulting LLC, Newark, NY; <sup>2</sup>Bausch+Lomb, Rochester, NY
- MP 741 **Evaluating the Use of Ion Mobility-Mass Spectrometry for Polymer End Group Characterization Using Polydimethyl Siloxane as a Model;** Andrew J. Hotelling<sup>1</sup>; Eleanor Riches<sup>2</sup>; <sup>1</sup>Bausch + Lomb, Rochester, NY; <sup>2</sup>Waters Corporation, Manchester, UK
- MP 742 **Characterization of Polymer Extracts by Gas Chromatography-High Resolution Time-Of-Flight Mass Spectrometry with Electron Impact and Chemical Ionization Strategies;** Nick Hall; David Alonso; Joe Binkley; Leco Corporation, St. Joseph, MI
- MP 743 **MALDI-ToF MS Analysis for Confirmation of Polymer End Groups;** Brittany Myers; Boyu Zhang; Scott M. Grayson; Tulane University, New Orleans, LA
- MP 744 **Versatile Dendritic Calibrants for the Improved Accuracy of Mass Determination for High Molecular Weight Analytes;** Scott M. Grayson; Joseph Giesen; Brittany Myers; Tulane University, New Orleans, LA
- MP 745 **An Integrated Systems Approach to Identifying Extractables From Single Use Materials: "Closing the Gap on Total Organic Content (TOC).";** Catherine E Petersen; Sarah Robinson; Trent Volz; Ray Colton; Validation Resources, Bend, OR
- MP 746 **End-Group Cleavage during MALDI of ATRP Made Polystyrene: The Problem is in the Solution;** Laurence Charles; Aura Tintaru; Christophe Chendo; Trang Phan; Marion Rollet; Laurent Giordano; Stéphane Viel; Didier Gigmes; Aix-Marseille University, Marseille Cedex 20, France
- MP 747 **Identification of Defective Structures of PAMAM Dendrimer Using Various Separation Methods Coupled with Mass Spectrometry: LC-MS, CE-MS and TLC-MS;** Emma-Dune Leriche<sup>1</sup>; Marie Hubert-Roux<sup>1</sup>; Martin Grosselet<sup>2</sup>; Catherine Lange<sup>1</sup>; Carlos Afonso<sup>1</sup>; Corinne Loutelier-Bourhis<sup>1</sup>; <sup>1</sup>Normandie Univ UMR 6014, FR 3038; Univ Rouen; CNRS, Mont-St-Aignan, France; <sup>2</sup>University of Southampton, School of chemistry, Southampton, UK
- MP 748 **Identification and Quantitation of Plastics Additives in Medicine and Containers by HR LCMS and Triple Quadrupole GCMS;** Ekong Bassey; Kate Comstock; Thermofisher Scientific, San Jose, CA

- MP 749 **Characterization of Trace Organic Impurities in Purified Terephthalic Acid (PTA) by Using UPLC Q-TOF MS for Process Optimization;** Yuhong Zhang<sup>1</sup>; Chuan Wang<sup>1</sup>; Zhenlei Peng<sup>1</sup>; Yidan Guo<sup>1</sup>; Kejun Qian<sup>2</sup>; Xiaomei Huang<sup>2</sup>; Peter Lee<sup>3</sup>; <sup>1</sup>SINOPEC SRIPT, Shanghai, China; <sup>2</sup>Waters Technologies (Shanghai) Limited, Shanghai, China; <sup>3</sup>Waters Cooperation, Milford, MA





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

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Photoionization: Instrumentation & Applications.....	049-053
Instrumentation: New Developments in Ionization and Sampling .....	054-087
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Peptides: Ion Activation/Dissociation Strategies.....	124-128
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Metabolomics: General.....	357-382
Metabolomics: Untargeted Metabolite Profiling Applications.....	383-419
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Diagnostic Clinical Chemistry: Small Molecules I.....	557-577
Environmental Analysis: Pharmaceuticals and Pesticides .....	578-607
Elemental Analysis .....	608-618
Ion Mobility Applications .....	619-661
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Glycoproteins I.....	715-737
Food Safety .....	738-772

### Ion Activation/Dissociation, 001 – 020

- TP 001 **Investigation into UV Photon Induced Fragmentation in a RF confined Ion Guide using a Vacuum UV Ionisation Lamp;** Martin Green; Keith Richardson; Jeff Brown; Paul Murray, *Waters Corporation, Manchester, United Kingdom*
- TP 002 **UV Photodissociation within an Axially Illuminated Stacked Ring Ion Guide of an Ion Mobility Enabled Q-ToF;** Jeff Brown<sup>1</sup>; Mike Morris<sup>1</sup>; Kevin Giles<sup>1</sup>; Richard Chapman<sup>1</sup>; Paul Murray<sup>1</sup>; Emmy Hoyes<sup>1</sup>; Christopher Jones<sup>1</sup>; Jakub Ujma<sup>2</sup>; Bruno Bellina<sup>3</sup>; Isabelle Compagnon<sup>3</sup>; Perdita Barran<sup>2</sup>, <sup>1</sup>*Waters Corporation, Manchester, UK*; <sup>2</sup>*The University of Edinburgh, Edinburgh, UK*; <sup>3</sup>*CNRS et Université Lyon, Lyon, France*
- TP 003 **Hybrid UVPD Activation of N- and C-Terminal Fixed Charge Peptides;** Dustin Holden; Jennifer Brodbelt; *University of Texas Chemistry, Austin, TX*
- TP 004 **Fragmentation of Fluorescence Dye Labels Activated by Collisions or Photons;** Jonathan Peters; Claus Gernert; Martin Clemen; Tassilo Muskat; Jürgen Grottemeyer; *Inst. f. Phys. Chemie, Christian-Albrechts-Uni, Kiel, Germany*
- TP 005 **Sequential Losses of HONO, CO and HCN from Deprotonated ortho-Nitrobenzenesulfonylglycine (Ns-Gly) Upon ESI(-)MS/MS;** Robert L. White; Tara E. Tovstiga; Elizabeth A.L. Gillis; J. Stuart Grossert; *Dalhousie University, Department of Chemistry, Halifax, Canada*
- TP 006 **Diastereomeric Quantification of O-diglycosyl Flavonoids by a Complex-Free Kinetic Method Using ESI/QToF Mass Spectrometry;** Yong-Ill Lee; Kuangcai Chen; Jae-Min Lim; *Changwon National University, Changwon, Korea*
- TP 007 **Characterization of Temperature-Dependent Peptide Bond Cleavage Using Low- and High-Mass Quantitation Signals from Amine-Reactive N-Acetyl Dipeptide Tags;** Jongcheol Seo; Hye-Joo Yoon; Seung Koo Shin; *Postech, Pohang, South Korea*
- TP 008 **Fragmentation of Trans-Membrane Helices in Gaseous Protein Ions;** Owen Skinner; Adam Catherman; Kenneth Durbin; Bryan Early; Paul Thomas; Neil Kelleher; *Northwestern University, Evanston, IL*
- TP 009 **Metastable Atom-Activated Dissociation of Phosphocoline Lipids in Protonated, Sodiated, and Potassiated Forms;** William D. Hoffmann<sup>1</sup>; Robert E. Deimler<sup>1</sup>; Madlen Sander<sup>2</sup>; Glen P. Jackson<sup>1</sup>; <sup>1</sup>*West Virginia*

*University, Morgantown, WV*; <sup>2</sup>*Leipzig University, Leipzig, Germany*

- TP 010 **Focused Proteomics Through Selective Modification of Tryptophan or Arginine Residues;** Dustin Klein; Sylvester Greer; Jennifer Brodbelt; *University of Texas, Austin, TX*
- TP 011 **Fragmentation of Protonated Nitromethane;** Thomas Hester; Daniel Goebbert; *The University of Alabama, Tuscaloosa, AL*
- TP 012 **Comparison between Surface-Induced Dissociation (SID) and Collision-Induced Dissociation (CID) of Ion-Mobility (IM)-Separated Detergent Clusters;** Yun Zhang; Mowei Zhou; Xin Ma; Vicki H. Wysocki; *The Ohio State University, Columbus, OH*
- TP 013 **Optimization of Surface Induced Dissociation (SID) Effect in Intermediate Vacuum Ion Guides;** Zoltán Takáts<sup>2</sup>; Tamás Karancsi<sup>1</sup>; Dániel Szalay<sup>1</sup>; Andor Rozsnyai<sup>1</sup>; <sup>1</sup>*Medimass Ltd., Budapest, Hungary*; <sup>2</sup>*Imperial College London, London, Egyesült Királyság*
- TP 014 **Dipolar Direct Current Driven Collision Induced Dissociation in Digital Ion Trap;** Liang Wang; Fuxing Xu; Chuan-Fan Ding; *Fudan University, Shanghai, China*
- TP 015 **Hydration Energies of First-Row Transition Metal Dications Determined by Collision Induced Dissociation and Density Functional Theory;** Rebecca Thomas; Theresa Hofstetter; Peter Armentrout; *University of Utah, Salt Lake City, UT*
- TP 016 **Gas-Phase Fragmentation of Cationic Metal Adducts of Oxalate Salts;** Robert Hale; Carl Weisbecker; Chang-Ching Chan; Athula Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- TP 017 **Structures and Activation Energies for Glycosidic Bond Cleavage of Protonated Nucleosides: A Synergy of Theory and Threshold Collision-Induced Dissociation Experiments;** Mary T. Rodgers; Ranran Wu; *Wayne State University, Detroit, MI*
- TP 018 **Nazarov Cyclization and Six-Membered Cyclization of Chalcones Catalyzed by the Naked Silver Cation in Gas Phase;** Hezhi Sun; Yunfeng Chai; Lin Wang; Yuanjiang Pan; *Zhejiang University, Hangzhou, China*
- TP 019 **Second Generation Electron Transfer Dissociation (ETD) on a Novel Hybrid Instrument with Improved Functionality, Increased Speed, and Robustness of Data;** Christopher Mullen<sup>1</sup>; Lee Earley<sup>1</sup>; Jean-Jacques Dunyach<sup>1</sup>; John E.P. Syka<sup>1</sup>; Philip Daniel Compton<sup>2</sup>; Jeffrey



- Shabanowitz<sup>3</sup>; Donald F. Hunt<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Northwestern University, Evanston, IL; <sup>3</sup>University of Virginia, Charlottesville, VA
- TP 020 **Comparison of MALDI-MS and High-Energy CID Using a Spiral-Trajectory Time-Of-Flight Mass Spectrometer;** Masaaki Ubukata<sup>1</sup>; John Dane<sup>1</sup>; Robert B. Cody<sup>1</sup>; Ayumi Kubo<sup>2</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA; <sup>2</sup>JEOL Ltd., Tokyo, Japan
- Ion/Molecule, Ion/Ion, Ion/Electron Interactions, 021 - 048**
- TP 021 **Distinguishing Amorphous and Crystalline Ices by Ultra-Low Energy Collisions of Reactive Ions;** Radha Gobinda Bhuin; Soumabha Bag; T. Pradeep; *Indian Institute of Technology, Madras, Chennai, India*
- TP 022 **Experimental Evidence and Characterization of Cobalt(II) Complexes Relevant in Regioselective Diels-Alder Reactions. A Gas Phase Study;** Lukas Fiebig<sup>1</sup>; Julian Kuttner<sup>2</sup>; Martin C. Schwarzer<sup>2</sup>; Gerhard Hilt<sup>2</sup>; Gernot Frenking<sup>2</sup>; Hans-Günther Schmalz<sup>1</sup>; Mathias Schaefer<sup>1</sup>; <sup>1</sup>University Cologne, Department of Chemistry, Koeln, Germany; <sup>2</sup>Philipps University, Department of Chemistry, Marburg, Germany
- TP 023 **Computational Studies of Ion-neutral Reactions of Astrochemical Relevance: Formation of Hydrogen Peroxide and Amino Acetonitrile;** Zhibo Yang; *University of Oklahoma, Norman, OK*
- TP 024 **Chiral Selectivity of Copper Di-imine Catalysts in the Gas Phase;** Mark Davis; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- TP 025 **Synthesis, Characterization, and Reactivity of Gold Carbenes in the Gas Phase;** Christopher Swift; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- TP 026 **The Flipper: New MS Technology for the Generation of Highly Charged Anionic Reagents for Gas-Phase Purification;** Rebeca Pinhancos; Catherine E. Vincent; Michael S Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- TP 027 **Electrochemical-Assistance for Electron Transfer Dissociation Ion Mobility MS of Peptides and Proteins;** Jonathan P. Williams; Christopher Hughes; Jeffery Brown; *Waters, Manchester, UK*
- TP 028 **The Use of Reagent Clusters in Ion/ion Reactions for Multiple Gas-phase Covalent Modifications of Peptides and Proteins;** Boone Prentice; John Stutzman; Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 029 **Characterization of Gas-Phase Esterification of Various Doubly Deprotonated Analytes;** Joshua D. Gilbert; Boone M. Prentice; John R. Stutzman; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 030 **Lithium Cation Basicity: Revisiting the High Basicity Range by Experiment and Theory;** Charly Mayeux<sup>1</sup>; Peeter Burk<sup>1</sup>; Jean-François Gal<sup>2</sup>; Tõiv Haljasorg<sup>1</sup>; Ivari Kaljurand<sup>1</sup>; Ivo Leito<sup>1</sup>; <sup>1</sup>University of Tartu, Tartu, Estonia; <sup>2</sup>University of Nice-Sophia Antipolis (UMR CNRS 7272), Nice, France
- TP 031 **A Custom Mass Spectrometer to Probe Ion-Ion Reaction Products Through Infrared Spectroscopy;** Nathan Roehr; Corey Stedwell; Nick Polfer; Kerim Gulyuz; *University of Florida, Gainesville, FL*
- TP 032 **Gas-Phase Synthesis of Copper Carbene Complexes and Evaluation of Their Structure and Reactivity;** Jamal Aldajaei; *Virginia Commonwealth Uni., Richmond, VA*
- TP 033 **Electron Detachment Dissociation of Anion-Adducted Peptides;** Tao Jiang; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- TP 034 **Gas-Phase Chemistry of Polycyclic Aromatic Hydrocarbon Cations and Their Nitrogen Containing Analogues;** Nicholas Demarais; Theodore Snow; Veronica Bierbaum; *U of Colorado, Boulder, CO*
- TP 035 **Gas-Phase Organic Reactions of the Atomic Oxygen Radical Cation;** Charles Nichols<sup>1</sup>; Zhibo Yang<sup>2</sup>; Veronica Bierbaum<sup>1</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>University of Oklahoma, Norman, OK
- TP 036 **Gas-Phase Studies of Radical Migration within Tryptophan-Containing Peptides;** Andrii Piatkivskyi; Victor Ryzhov; *Northwestern University, Dekalb, IL*
- TP 037 **A Bracketing Method for Proton Affinity Measurements for Pyridine Radicals and Biradicals;** Guannan Li; Vanessa Gallardo; John Nash; Anyin Li; Hilka Kenttämää; *Purdue University, West Lafayette, IN*
- TP 038 **A Comparison of the Reactions of N-Methyl-3-dehydropyridinium Cation with Adenine, Cytosine, Thymine and Uracil in Gas Phase and Aqueous Solution;** Ashley Wittig; Hilka Kenttämää; *Purdue University, West Lafayette, IN*
- TP 039 **Steric Effects in the Characterization of Proton Affinities of N,N'-Diamidocarbenes;** Mu Chen<sup>2</sup>; Christopher Bielawski<sup>1</sup>; Jeehiun K. Lee<sup>2</sup>; <sup>1</sup>The University of Texas at Austin, Austin, TX; <sup>2</sup>Rutgers University-New Brunswick-Chemistry, Piscataway, NJ
- TP 040 **Formation of Hydroxymethyl Radicals and Their Reactions with Cysteine Peptides in NanoESI Plume;** Craig Stinson; Yu Xia; *Purdue University, West Lafayette, IN*
- TP 041 **Characterization of Gas-Phase Ion-Molecule Reagent Complexes In Support of Trace Explosives Detection Using API-MS;** Kerin Gregory; Alla Ostrinskaya; Roderick Kunz; *MIT Lincoln Laboratory, Lexington, MA*
- TP 042 **Ion/Ion Reactions to Extend Peptides in the Gas Phase: A Route to Gas Phase Peptide Synthesis;** William M. McGee; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 043 **Probing the Reactivity and Radical Nature of Oxidized Transition Metal-Thiolate Complexes by Mass Spectrometry;** Mei Lu<sup>1</sup>; Larry Campbell<sup>2</sup>; Rajat Chauhan<sup>3</sup>; Craig Grapperhaus<sup>3</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Ohio University, Athens, OH; <sup>2</sup>AB Sciex, Concord, Ontario; <sup>3</sup>University of Louisville, Louisville, Kentucky
- TP 044 **High-Temperature Mass Spectrometric Study of the System Csl-Cel;** Dmitry Ivanov; Anatoly Dunaev; Dmitry Sergeev; Lev Kudin; *Ivanovo State University of Chemistry and Technology, Ivanovo, Russia*
- TP 045 **Analysis Method for Competitive CAD-ETD Gas Phase Reaction with Kinetic Energy Measurement of Ionic and Neutral Fragments;** Masataka Ohkubo<sup>1</sup>; Shigetomo Shiki<sup>1</sup>; Masahiro Ukibe<sup>1</sup>; Shigeo Tomita<sup>2</sup>; Shigeo Hayakawa<sup>3</sup>; <sup>1</sup>AIST, RIIF, Tsukuba, Japan; <sup>2</sup>University of Tsukuba, Tsukuba, JP; <sup>3</sup>Osaka Prefecture University, Osaka, JP
- TP 046 **Oxidation of CO by Molecular Oxygen Catalyzed with Y<sub>3</sub>O<sub>6</sub><sup>-</sup> Cluster Anions;** Yan-Xia Zhao; Zi-Yu Li; Xun-Lei Ding; Sheng-Gui He; *State Key Laboratory for Structural Chemistry of U, Beijing, China*
- TP 047 **Etoricoxib as a Tool for the Detection of Low Levels of Oxygen in Mass Analyzers;** Freneil Jariwala; John Hibbs; Athula Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- TP 048 **Energy-Resolved Collision-Induced Dissociation Studies of 1,10-Phenanthroline Complexes of the Late First-Row Divalent Transition Metal Cations: Determination of the Binding Energies;** Holliness Nose; Mary Rodgers; *Wayne State University, Detroit, MI*

## Photoionization: Instrumentation &amp; Applications, 049 – 053

- TP 049 **Capture of Tunneling Electrons and Dissociation of Organic Molecules Initiated by Unpaired Electrons;** Hongying Zhong; Lulu Huang; *Central China Normal University, Wuhan, China*
- TP 050 **Mass Spectrometry Analysis of Volatile Nitro-Substituted Explosives by Laser Ionization under Ambient Conditions;** Evgeny Kukaev<sup>1,4</sup>; Alexey Kononikhin<sup>1,2</sup>; Igor Popov<sup>1,4</sup>; Konstantin Nagornov<sup>2,3</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Inst of Radio-engin., Electronics and Automation, Moscow, Russia; <sup>4</sup>Moscow Institute of Physics and Technology, Moscow, Russia
- TP 051 **Photoionization Mass Spectrometry of Thermolabile Biomolecules at the French National Synchrotron Facility SOLEIL;** David Touboul<sup>1</sup>; Marie Méjean<sup>1</sup>; François Gaie-Levrel<sup>2</sup>; Gustavo Garcia Macias<sup>3</sup>; Laurent Nahon<sup>3</sup>; Lionel Poisson<sup>4</sup>; Martin Schwell<sup>5</sup>; Majdi Hochlaf<sup>6</sup>; Alexandre Giuliani<sup>7</sup>; Alain Brunelle<sup>1</sup>; <sup>1</sup>CNRS, Institut de Chimie des Substances Naturelles, Gif-sur-Yvette, France; <sup>2</sup>National Metrology Institute and Testing, Paris, France; <sup>3</sup>Synchrotron SOLEIL, DESIRS beamline, Gif-sur-Yvette, France; <sup>4</sup>Laboratoire Francis PERRIN, Gif-sur-Yvette, France; <sup>5</sup>LISA UMR 7583, Créteil, France; <sup>6</sup>Université Paris-Est, MSME, Maren-la-Vallée, France; <sup>7</sup>Synchrotron SOLEIL, DISCO beamline, Gif-sur-Yvette, France
- TP 052 **The Use of Isoprene as a New Dopant in Negative Ion Atmospheric Pressure Photo Ionization (NI-APPI) Mass Spectrometry;** Faezeh Dousty; Rob O'Brien; *University of British Columbia, Okanagan Campus, Kelowna, Canada*
- TP 053 **Online Quantification of Tobacco by Soft Photo Ionization Time of Flight Mass Spectrometry;** Matthias Bente-Von Frowein; Andreas Walte; Thomas Gröger; Mohammad Reza Saraji-Bozorgzad; *Photonion, Schwerin, Germany*

## Instrumentation: New Developments in Ionization and Sampling, 054 – 087

- TP 054 **Study of an ESI Source Which Uses a Vacuum Insulated Tube to Increase Ionization Efficiency and Operates at Subambient Pressure;** Steve Schachterle; Zicheng Yang; Maurizio Splendore; Stephen Zanon; Roy Moeller; Felician Muntean; *Bruker Daltonics, Fremont, CA*
- TP 055 **Evaluation of Amine-Containing Polymer Brushes and Polymer Thin Films for Biomolecular Mixture Fractionation Prior to MALDI MS;** Stephanie Eastwood; Bojan Mitrovic; Venney Wong; Joshua Pogue; Colleen Scott; Gary Kinsel; *Southern Illinois University, Carbondale, IL*
- TP 056 **Flow Characteristics of a Laminar Flow Interface for LC-MS/MS;** Serguei Savtchenko; Charles Joliffe; Heather Gamble; Lisa M. Cousins; Hui Quao; *IONICS Mass Spectrometry Group, Inc., Bolton, Canada*
- TP 057 **Coupling High Performance Ion Mobility Spectrometers to Common Mass Spectrometers;** Robert Jackson; Mark Osgood; Eugenie Hainsworth; Jianglin Wu; Ching Wu; *Excellims Corporation, Acton, MA*
- TP 058 **Static Electricity and Novel Spray Ionization Methods;** Abdil Ozdemir<sup>2</sup>; Jung-Lee Lin<sup>1</sup>; Kent J. Gillig<sup>1</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Sakarya University, Adapazari, Turkey
- TP 059 **Velocity Map Imaging Spectrometer: An Off-the-Shelf System for Gas-Phase Chemistry and Laser Physics Experiments;** Orla Kelly<sup>1,2</sup>; Panos Kapetanopoulos<sup>1</sup>; Michael NR Ashfold<sup>2</sup>; <sup>1</sup>Photek Ltd, St Leonards On Sea, UK; <sup>2</sup>School of Chemistry, University of Bristol, Bristol, UK

- TP 060 **An UV-AP-MALDI Source and Liquid UV-MALDI Samples Enable the Formation of Multiply Charged Peptides and Proteins and Their High-Sensitivity Analysis;** Rainer Cramer<sup>1</sup>; Alex Pirkel<sup>2</sup>; Franz Hillenkamp<sup>2</sup>; Klaus Dreisewerd<sup>2</sup>; <sup>1</sup>University of Reading, Reading, UK; <sup>2</sup>University of Muenster, Muenster, Germany
- TP 061 **Novel Soft Electron Ionisation for Mass Spectrometers;** Nick Bukowski<sup>1</sup>; Pierre Schanen<sup>2</sup>; Gerhard Horner<sup>2</sup>; <sup>1</sup>ALMSCO International, Llantrisant, UK; <sup>2</sup>five technologies GmbH, Munich, Germany
- TP 062 **Solvent Assisted Inlet Ionization (SAIL): Perspectives on Source Design, Application, and Ionization Mechanism;** Vincent S. Pagnotti; Sarah J. Saylor; Shubhashis Chakrabarty; Charles N. McEwen; *University of the Sciences, Philadelphia, PA*
- TP 063 **Enhancing Ionization Efficiency in ESI by a Novel Nebulizer Design;** Anneli Kruve; Ivo Leito; Rünno Lõhmus; Asko Laaniste; Hanno Evard; Kristo Kleemann; Jaanus Liigand; Vahur Toss; Koit Herodes; Ants Lõhmus; *University of Tartu, Tartu, Estonia*
- TP 064 **Optimization of Surface Acoustic Wave Nebulizer Designs for Proteomics;** Scott Heron<sup>1,2</sup>; J. Scott Edgar<sup>3</sup>; Yue Huang<sup>1</sup>; Young Ah Goo<sup>1,2</sup>; Michael Wilson<sup>1,2</sup>; Sung Hwan Yoon<sup>1,2</sup>; David R. Goodlett<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Maryland, Baltimore, MD; <sup>3</sup>Deurion LLC, Seattle, WA
- TP 065 **A Closer Look at the Sensitivity Enhancement Observed with Capillary and Nanoflow UPLC for Both Small and Large Molecules;** James Murphy; Jay Johnson; Paul Rainville; *Waters Corporation, Milford, MA*
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- TP 067 **Development of a Soft Ionization Discharge Source for Gas Chromatography Used with a High Resolution Time of Flight Mass Spectrometer;** Lloyd Allen<sup>1</sup>; Alexander Kolosov<sup>2</sup>; Viatcheslav Artaev<sup>1</sup>; Anatoly Verenchikov<sup>2</sup>; *LECO Corp., Saint Joseph, MI; <sup>2</sup>MSC-GC, Bar, Montenegro*
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- TP 069 **An Elemental Ion Source for LC-MS: Halogen Detection;** Haopeng Wang<sup>1</sup>; Kaveh Kahan<sup>2</sup>; Ninghang Lin<sup>1</sup>; Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>Georgetown Univ., Washington, DC; <sup>2</sup>PerkinElmer Inc., Woodbridge, Canada
- TP 070 **Internal and External Ionization in a Mobile FTICR-MS;** Clotilde Le Vot<sup>1</sup>; Essyllt Louarn<sup>1</sup>; Helene Mestdag<sup>1</sup>; Michel Heninger<sup>1</sup>; Pierre Boissel<sup>2</sup>; Gérard Maucilaire<sup>2</sup>; Joel Lemaire<sup>1</sup>; <sup>1</sup>LCP CNRS - Université Paris Sud, Orsay, France; <sup>2</sup>AlyXan, Orsay, France
- TP 071 **Online High-Capacity Capillary Isoelectric-Point Fractionation Increases the Proteome Coverage of Human Cell Line in Shotgun LC-MS Proteomics Analysis;** Mohammad Pirmoradian Najafabadi; Konstantin Chinglin; Juan Astorga-Wells; Harshavardhan Budamgunta; Roman Zubarev; *Karolinska Institute, Solna, Sweden*



- TP 072 **SmartAGC: Precursor Mass and Charge Dependent Automatic Gain Control Improves Efficiency of Protein Identification;** Stefan K Maier<sup>1,2</sup>; Hannes Hahne<sup>1</sup>; Fiona Pacht<sup>1</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technische Universität München, Freising, Germany*; <sup>2</sup>*Helmholtz Zentrum München, Neuherberg, Germany*
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- TP 074 **Understanding the Effects of the Earth's Magnetic Field on Mobile Mass Spectrometry: Simulation, Experimentation and Solutions;** Ryan J. Bell<sup>5</sup>; Nicholas G. Davey<sup>1,5</sup>; Morten Martinsen<sup>2,5</sup>; Christian Collin-Hansen<sup>3</sup>; R. Timothy Short<sup>4</sup>; Erik T. Krogh<sup>1,5</sup>; Christopher G. Gill<sup>1,5</sup>; <sup>1</sup>*University of Victoria, Victoria, BC, Canada*; <sup>2</sup>*NTNU, Trondheim, Norway*; <sup>3</sup>*Statoil ASA, Trondheim, Norway*; <sup>4</sup>*SRI International, St. Petersburg, FL*; <sup>5</sup>*AERL, Vancouver Island University, Nanaimo, BC, Canada*
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- TP 076 **Laser LESA: Fully Automated Laser Ablation Sample Transfer to Solution for NanoESI Mass Spectrometry;** Matthias Lorenz; Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
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- TP 078 **Fabrication of Dense Polymer Nozzle Array on Microstructured Fibers for Multi-Electrospray Ionization;** Yueqiao Fu<sup>1</sup>; Graham Gibson<sup>1</sup>; Richard Oleschuk<sup>1</sup>; Tom Covey<sup>2</sup>; Bradley Schneider<sup>2</sup>; <sup>1</sup>*Queen's University, Kingston, ON, Canada*; <sup>2</sup>*AB Sciex, Concord, ON, Canada*
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- TP 081 **Miniature Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS) Probes for the Direct Measurement of Pharmaceuticals and Contaminants in Complex Samples;** Kyle D. Duncan<sup>1,2</sup>; Erik T. Krogh<sup>1,2</sup>; Christopher G. Gill<sup>1,2</sup>; <sup>1</sup>*University of Victoria, Victoria, BC, Canada*; <sup>2</sup>*AERL, Vancouver Island University, Nanaimo, BC, Canada*
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- TP 087 **Development of Laser Ablation and Droplet Capture (LADC) for in vivo Mass Spectrometry;** Benoit Fatou; Isabelle Fournier; Michael Ziskind; Maxence Wisztorski; Cristian Focsa; Michel Salzet; *University Lille 1, Villeneuve D'ascq, France*
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- TP 090 **Optimizing the Performance of a Miniaturized Linear Ion Trap: Adjusting RF and SWIFT Auxiliary Waveform Parameters;** Friso H.W. Van Amerom<sup>1</sup>; Veronica Pinnick<sup>2</sup>; Xiang Li<sup>2</sup>; Ricardo Arevalo<sup>2</sup>; Rayn Danell<sup>3</sup>; Paul Mahaffy<sup>2</sup>; Will Brinckerhoff<sup>2</sup>; <sup>1</sup>*SRI International, St Petersburg, FL*; <sup>2</sup>*Goddard Space Flight Center, Greenbelt, MD*; <sup>3</sup>*Danell Consulting Inc., Winterville, NC*
- TP 091 **Design of Portable Mass Spectrometers with Handheld Probes: An Aspect of Ion Introduction and Pumping System;** Tsung-Chi Chen<sup>1</sup>; Chien-Hsun Chen<sup>1</sup>; R. Graham Cooks<sup>1</sup>; Robert Kline-Schoder<sup>2</sup>; Paul Sorensen<sup>2</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Creare Inc., Hanover, NH*
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- TP 093 **Predictive Automatic Gain Control on a New Quadrupole Mass Filter-Orbitrap-Linear Ion Trap Platform;** Philip M Remes; Justin Blethrow; Vlad Zabrouskov; Michael Senko; *Thermo Fisher Scientific, San Jose, CA*
- TP 094 **Implementing UV and Visible Photodissociation in an Q-Exactive Mass Spectrometer;** Marion Girod<sup>1,2</sup>; Quentin Enjalbert<sup>1</sup>; Jérémy Jeudy<sup>1</sup>; Rodolphe Antoine<sup>1,2</sup>; Jerome Lemoine<sup>1</sup>; Philippe Dugourd<sup>1,2</sup>; <sup>1</sup>*Université Lyon 1, Villeurbanne, France*; <sup>2</sup>*CNRS, Villeurbanne, France*
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- TP 096 **Harnessing Q Exactive Multiplexing Capabilities for Improvements in Peptide Quantitation and Identification;** Jolene K. Diedrich<sup>1</sup>; Gregory A. Barding<sup>2</sup>; Xuemei Han<sup>1</sup>; Vlad Zabrouskov<sup>3</sup>; Michael W. Senko<sup>3</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>University of California, Riverside, CA; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- TP 097 **Design and Characterization of a Novel Hybrid-field Ion Guide as part of a Time-of-Flight Mass Spectrometry Platform;** Alexander Lekkas; Athanasios Zacharos; Diamantis Kounadis; Ioannis Orfanopoulos; Dimitris Papanastasiou; Emmanuel Raptakis; *Fasmatech, Athens, Greece*
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- TP 099 **Multiplexed Analysis of Steroid Hormones in Human Serum Using Novel Microflow Tile Technology and LC-MS/MS;** Carolyn Broccardo<sup>1</sup>; Kevin Schauer<sup>1</sup>; Wendy Kohrt<sup>2</sup>; Robert Schwartz<sup>2</sup>; James Murphy<sup>3</sup>; Jessica Prenni<sup>1</sup>; <sup>1</sup>Colorado State University, Ft Collins, CO; <sup>2</sup>University of Colorado Anschutz Medical Campus, Aurora, CO; <sup>3</sup>Waters Corporation, Milford, MA
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- TP 101 **Design of a High Throughput Atmospheric Pressure Interface with Improved Ion Transmission at High Pressure;** Eloy R. Wouters<sup>1</sup>; Satendra Prasad<sup>1</sup>; Alexander A. Makarov<sup>2</sup>; Jean-Jacques Dunyach<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
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- TP 109 **Duty Cycle-Based Isolation in Linear Quadrupole Ion Traps;** Peter TA Reilly<sup>1</sup>; Rachit Singh<sup>2</sup>; Vivek Jayaram<sup>2</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Pullman High School, Pullman, WA
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S  verine Zirah<sup>1</sup>; <sup>1</sup>National Museum of Natural History; UMR 7245, Paris, France; <sup>2</sup>Normandie Univ UMR 6014, FR 3038; Univ Rouen; CNRS, Mont-Saint-Aignan, France; <sup>3</sup>University Claude Bernard of Lyon; UMR 5579, Lyon, France; <sup>4</sup>University Pierre & Marie Curie; UMR 7201, Paris, France

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- TP 132 **The Effect of a Newly Redesigned Triple Quadrupole Mass Spectrometer on Targeted Peptide Quantitation;** Michael Bereman<sup>1</sup>; Richard Johnson<sup>1</sup>; Reiko Kiyonami<sup>2</sup>; Harald Oser<sup>2</sup>; Mary Blackburn<sup>2</sup>; Brendan MacLean<sup>1</sup>; Andy Hoofnagle<sup>1</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>Univ of Washington, Seattle, WA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
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- TP 137 **Increasing the Multiplexing of High Resolution Targeted Peptide Quantification Assays Using a Scheduled High Resolution MS/MS Workflow;** Mark Cafazzo; *AB SCIEX, Framingham, MA*
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- TP 140 **Advanced Use of High Resolution Mass Spectrometry (HRMS) to Overcome Triple Quadrupole Limitations in Large Molecules Quantification;** Louis-Philippe Morin; Jean-Nicholas Mess; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Quebec, Canada*
- TP 141 **Finding the Unexpected in SWATH<sup>TM</sup> Data Sets - Implications for Protein Quantitation;** Ron Bonner; Stephen Tate; Adam Lau; *AB SCIEX, Concord, Canada*
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- TP 143 **Universal Approach to Relative Quantitation of Proteomic Data Using a Novel Library of Peptide Standards;** Michael Heaven<sup>1</sup>; Archie Cobbs<sup>2</sup>; Landon Wilson<sup>1</sup>; Matthew Renfrow<sup>1</sup>; Stephen Barnes<sup>1</sup>; Michael Brenner<sup>1</sup>; Jeremy Norris<sup>3</sup>; <sup>1</sup>Univ. of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>Vulcan Analytical, Birmingham, AL; <sup>3</sup>Vanderbilt University, Nashville, TN
- TP 144 **Automated Protein Expression Analysis – A Procedure Robust to Experimental Variance;** Gordana Ivosev; Stephen Tate; Ron Bonner; Lyle Burton; *AB Sciex, Concord, Canada*

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- TP 146 **Peptide Peaks Growing Up in a Tough Chromatographic Neighborhood: Characterizing MRM Reproducibility and Robustness in Complex Microbial Samples;** Adam Martin<sup>1,2</sup>; Paul Abraham<sup>1,2</sup>; Rachel Adams<sup>1,2</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN
- TP 147 **Lessons Learned: What to Expect when Using MS1- and MS2-based Label Free Methods for Quantification;** Jan Muntel<sup>1</sup>; Sarah A. Boswell<sup>2</sup>; Waltraud Mair<sup>1</sup>; Judith A. J. Steen<sup>1</sup>; Michael Springer<sup>2</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Children’s Hospital Boston, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
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- TP 152 **Selectivity and Sensitivity Evaluation in Peptide Quantification by Using LC-SRM3 and LC-Differential Ion Mobility Spectrometry Approaches;** Bandar Alghanem<sup>1</sup>; Dario Bottinelli<sup>1</sup>; Ying Zhang<sup>1</sup>; Aivett Bilbao<sup>1,3</sup>; Frédéric Nikitin<sup>3</sup>; Markus Mueller<sup>3</sup>; Frédérique Lisacek<sup>3</sup>; Jeremy Luban<sup>2</sup>; Caterina Strambio De Castillia<sup>2</sup>; Emmanuel Varesio<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>University of Massachusetts, Worcester, MA; <sup>3</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland
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- TP 157 **Expression of Mutant Proteins as Reagents for LC-MRM Assay Development and Internal Standards for Quantification;** Elizabeth Remily-Wood<sup>1</sup>; Nicholas Woods<sup>1</sup>; Robin Hurst<sup>2</sup>; Michael Rosenblatt<sup>2</sup>; Alvaro Monteiro<sup>1</sup>; John Koomen<sup>1</sup>; <sup>1</sup>H. Lee Moffitt Cancer Center, Tampa, FL; <sup>2</sup>Promega, Madison, WI
- TP 158 **Proteomic Analysis of Mouse Macrophage (RAW264.7) Cells Infected with Burkholderia pseudomallei K96243;** Zhaojing Meng<sup>1</sup>; King Chan<sup>1</sup>; Ming Zhou<sup>1</sup>; David Deshazer<sup>2</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>USAMRIID, Frederick, MD
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- TP 161 **Quantitative Analysis of Human Progranulin and Granulin Peptides Using Multiple Reaction Monitoring;** Toshiya Matsubara<sup>1,2</sup>; Noriyuki Ojima<sup>1</sup>; Tairo Ogura<sup>1</sup>; Ichiro Hirano<sup>1</sup>; Susumu Seino<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kobe University Graduate School of Medicine, Kobe, Japan
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- TP 163 **New 2-Dimensional Image-Converted Analysis of Liquid Chromatography and Mass Spectrometry (2DICAL) Version with an Algorithm for High-Performance Mass Spectrometry Data;** Tomohiro Sakuma<sup>1</sup>; Miho Banno<sup>1</sup>; Masahiro Kamita<sup>2</sup>; Tesshi Yamada<sup>2</sup>; Masaya Ono<sup>2</sup>; <sup>1</sup>Mitsui Knowledge Industry Co.,Ltd., Tokyo, Japan; <sup>2</sup>National Cancer Center Research Institute, Tokyo, Japan
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- TP 166 **Structure of Histone H2A/H2B Dimer Analyzed by Ion Mobility Mass Spectrometry and Molecular Dynamics Simulation;** Kazumi Saikusa<sup>1</sup>; Sotaro Fuchigami<sup>1</sup>; Yuuki Asano<sup>1</sup>; Aritaka Nagadoi<sup>1</sup>; Hiroaki Tachiwana<sup>2</sup>; Hitoshi Kurumizaka<sup>2</sup>; Mitsunori Ikeguchi<sup>1</sup>; Yoshifumi Nishimura<sup>1</sup>; Satoko Akashi<sup>1</sup>; <sup>1</sup>Yokohama City Univ., Grad. Sch. of Nanobioscience, Yokohama, Japan; <sup>2</sup>Waseda Univ., Sch. of Adv. Sci. & Eng., Tokyo, Japan
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- TP 189 **On-line Generation of Reactive Intermediates by Electrochemistry as Approach for Differential Protein Labeling;** Lars Büter<sup>1</sup>; Helene Faber<sup>2</sup>; Kristina Wentker<sup>2</sup>; Uwe Karst<sup>2</sup>; <sup>1</sup>University of Münster-Graduate School of Chemistry, Münster, Germany; <sup>2</sup>University of Münster, Münster, Germany
- TP 190 **A New Label Free Approach for The Determination of Reaction Rates in Oxidative Footprinting Experiments;** Eduardo Pilau<sup>1</sup>; Amadeu Iglesias<sup>2</sup>; Fabio Gozzo<sup>3</sup>; <sup>1</sup>University of Maringá, Maringá, Brazil; <sup>2</sup>Waters Technology, São Paulo, Brazil; <sup>3</sup>University of Campinas, Campinas, Brazil
- TP 191 **Study of Terephthalic Acid as the Radical Dosimeter in Hydroxyl Radical Protein Footprinting;** Boer Xie; Complex Carbohydrate Research Center, UGA, Athens, GA
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A. Tarr<sup>2</sup>; Yang Cai<sup>1,2</sup>; <sup>1</sup>The Research Institute for Children, New Orleans, New Orleans, LA; <sup>2</sup>Department of Chemistry, University of New Orleans, New Orleans, LA

- TP 196 **Using Isotopically-Coded Hydrogen Peroxide as a Surface Modification Reagent for the Structural Characterization of Prion-Protein Aggregates;** Jason Serpa<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; David Wishart<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>University of Alberta, Alberta, Canada; <sup>3</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada
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Madison, WI; <sup>4</sup>Department of Cell and Regenerative Biology, SMPH, Madison, WI; <sup>5</sup>Department of Chemistry, UW-Madison, Madison, WI

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- TP 219 **Top-Down Analysis of Intact Antibodies Using Orbitrap Mass Spectrometry;** Eugen Damoc; Eduard Denisov; Alexander Makarov; *Thermo Fisher Scientific, Bremen, Germany*
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- TP 222 **Top-down Assisted Bottom-up Method for Avian Hemoglobin Sequencing;** Yang Stella Song<sup>1</sup>; Ü nige A. Laskay<sup>2</sup>; Alan G. Barbour<sup>3</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*; <sup>2</sup>*The University of Arizona, Tucson, AZ*; <sup>3</sup>*University of California, Irvine, CA*
- TP 223 **A Front-End ETD Modified Orbitrap-Velos with Ion-Ion Proton Transfer Reactions and Multiple Fills Provides Near-Complete Sequence Coverage of Intact Proteins;** A. Michelle English; Lissa C. Anderson; Weihang Wang; Dina L. Bai; Jeffrey Shabanowitz; Donald F. Hunt; *University of Virginia, Charlottesville, VA*
- TP 224 **Preferential N-terminal Conjugation as a Strategy to Sequence N-terminus by ISD-MALDI Top Down Sequencing Alone;** Gomathinayagam Ponniah; Adam Lucka; Bruce Andrien; *Alexion Pharmaceuticals, Cheshire, CT*
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- TP 225 **An Integrated Cross-Platform Workflow for Detecting Low-Abundance Sequence Variants;** Hangtian Song; Wei Wu; Yunping Huang; Richard Ludwig; Li Tao; *Bristol-Myers Squibb, Hopewell, NJ*
- TP 226 **New Approaches for MALDI MS-based Biopharmaceutical Characterization;** Marion Rohmer<sup>1</sup>; Dominic Baeumlisberger<sup>1,2</sup>; Ute Bahr<sup>1</sup>; Michael Karas<sup>1</sup>; <sup>1</sup>*Goethe University, Frankfurt Am Main, Germany*; <sup>2</sup>*SunChrom GmbH, Friedrichsdorf, Germany*
- TP 227 **Optimized HDX-MS Workflow for Analyzing the Conformation of Therapeutic Antibodies;** Pernille Foged Jensen<sup>1</sup>; Maximiliane Hilger<sup>2</sup>; Kasper D. Rand<sup>1</sup>; <sup>1</sup>*University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Roche Diagnostics GmbH, Penzberg, Germany*
- TP 228 **Contribution of the Interchain Disulfide Bonds to the Conformation and Stability of Immunoglobulin as Revealed by HDX MS;** Jing Fang; Jason Richardson; Zhongqi Zhang; *Amgen, Thousand Oaks, CA*
- TP 229 **Sheathless Capillary Electrophoresis Mass Spectrometry as a Versatile and Very Powerful Tool for the Characterization of Monoclonal Antibodies;** Anna Lou<sup>1</sup>; Jean-Marc Busnel<sup>1</sup>; Zhiqi Hao<sup>2</sup>; Dona Neloni Wijeratne<sup>1</sup>; David Horn<sup>2</sup>; Elsa Wagner<sup>3</sup>; Alain Beck<sup>3</sup>; Patrick Bennett<sup>2</sup>; <sup>1</sup>*Beckman Coulter, Brea, CA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Centre d'Immunologie Pierre Fabre, Saint-Julien-En-Genevois, FR*
- TP 230 **Characterization of Lower Molecular Weight Fragments of Recombinant Monoclonal IgG1 Antibodies Using Non-Reducing SDS-PAGE and Mass Spectrometry;** Chong-Feng Xu; Li Zang; Yi Zang; Andrew Weiskopf; *Biogen Idec, Cambridge, MA*
- TP 231 **Characterization of Heterogeneous Therapeutics by Mass Spectrometry Utilizing Charge Reduction;** Cedric E. Bobst<sup>1</sup>; Ruth Frenkel<sup>2</sup>; Damian Houde<sup>2</sup>; Andrew Weiskopf<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*Biogen IDEC, Cambridge, MA*
- TP 232 **Characterization and Comparison of O-glycosylation between the Innovator and a Biosimilar of Etanercept;** Stephane Houel<sup>1</sup>; Ying Qing Yu<sup>1</sup>; Jonathan P. Williams<sup>2</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corp., Milford, MA*; <sup>2</sup>*Waters Corp, Manchester, UK*
- TP 233 **Glycoform Profiling from Therapeutic Antibodies at the Protein, Peptide and Cleaved Glycan Level Using Mass Spectrometry;** Chris Hosfield<sup>1</sup>; Marjeta Urh<sup>1</sup>; Michael Rosenblatt<sup>1</sup>; Richard Jones<sup>2</sup>; Michael Ford<sup>2</sup>; Ravi Amunugama<sup>2</sup>; Dave Allen<sup>2</sup>; <sup>1</sup>*Promega, Madison, WI*; <sup>2</sup>*MS Bioworks, Ann Arbor, MI*
- TP 234 **Ion Mobility-Mass Spectrometry Enables the Facile Characterization of Stapled Peptide Crosslink Configuration;** Eric (Xiangguo) Shi; Vincent Guerlavais; Krzysztof Darlak; Jim Horstick; Scott Lentini; D. Allen Annis; *Aileron Therapeutics, Cambridge, MA*
- TP 235 **Isomer-specific LC/MS/MS Characterization of Biopharmaceutically-Relevant Glycans and Glycan Modifications;** Serenus Hua<sup>1</sup>; Myung Jin Oh<sup>1</sup>; Ha Neul Jeong<sup>1</sup>; Bum Jin Kim<sup>1</sup>; Gregory Staples<sup>2</sup>; Rudolf Grimm<sup>1,2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*Chungnam National University, Daejeon, Korea*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- TP 236 **In-Depth Characterization of a Q $\beta$  Virus-like Particle Using High Resolution Mass Spectrometry;** Justin B. Sperry<sup>1</sup>; John H. A. Amery<sup>1</sup>; James A. Carroll<sup>1</sup>; Jason C. Rouse<sup>2</sup>; <sup>1</sup>*Analytical R&D, Pfizer, Chesterfield, MO*; <sup>2</sup>*Pfizer, Andover, MA*
- TP 237 **Characterizing Glycosylation in Therapeutic Antibodies;** Maria Lorna A. De Leoz<sup>1,2</sup>; Xinjian Yan<sup>1</sup>; Xiaoyu Yang<sup>1</sup>; Yuxue Liang<sup>1</sup>; Lisa Kilpatrick<sup>1</sup>; Yamil Simon<sup>1</sup>; Michael J. Tarlov<sup>1</sup>; Stephen E. Stein<sup>1</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*; <sup>2</sup>*University of Maryland, College Park, MD*
- TP 238 **LC-MS/MS Analysis of Site-Specific Glycosylation and Site-Occupancy of Glycoproteins Containing Multiple N-linked and O-linked Glycosylation Sites;** Hongwei Xie; Song Klappoetke; Jeremy Woods; Linda Yi; Tyler Davis; *KBI Biopharma, Durham, NC*
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- TP 239 **The Lambda Scoring Framework: a Bayesian Posterior Probability Model to Improve Identification and Characterization of Top-Down Proteomic Results;** Ryan T. Fellers<sup>1</sup>; Richard D. LeDuc<sup>2</sup>; Bryan P. Early<sup>1</sup>; Paul M. Thomas<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Indiana University, Bloomington, IN*
- TP 240 **Algorithm for Identification and Sequencing of Protein Variants Using Top-Down MS Data;** Christian Heckendorf; Roger Theberge; Jean L. Spencer; Catherine E. Costello; Mark E. McComb; *Boston University School of Medicine, Boston, MA*
- TP 241 **MIND: A Soft-Sensor to Improve Mass Accuracy in High-Resolution Top-Down Proteomics;** Piotr Dittwald<sup>3</sup>; Frederik Lermite<sup>2,4</sup>; Frank Sobott<sup>2,4</sup>; Ania Gambin<sup>3</sup>; Dirk Valkenborg<sup>1,2</sup>; <sup>1</sup>*Applied Bio & Molecular Systems, VITO, Mol, Belgium*; <sup>2</sup>*Center for Proteomics, University of Antwerp, Antwerp, Belgium*; <sup>3</sup>*Computational Biology Group, University of Warsaw, Warsaw, Poland*; <sup>4</sup>*Biomolec. Mass Spectrometry, University of Antwerp, Antwerp, Belgium*
- TP 242 **Identification of Ultramodified Proteins Using Top-Down Mass Spectra;** Xiaowen Liu<sup>1</sup>; Shawna Hengel<sup>2</sup>; Si Wu<sup>2</sup>; Nikola Tolic<sup>2</sup>; Ljiljana Pasa-Tolic<sup>2</sup>; Pavel Pevzner<sup>3</sup>; <sup>1</sup>*IUPUI, Indianapolis, IN*; <sup>2</sup>*PNNL, Richland, WA*; <sup>3</sup>*UCSD, San Diego, CA*
- TP 243 **Sequencing Antibodies from Top-Down Spectra;** Mikhail Dvorkin<sup>1</sup>; Sonya Alexandrova<sup>1</sup>; Xiaowen Liu<sup>2</sup>; Si Wu<sup>3</sup>; Ljiljana Paša-Tolić<sup>3</sup>; Nikola Tolić<sup>3</sup>; Lennard Dekker<sup>4</sup>; Martijn Vanduijn<sup>4</sup>; Theo Luider<sup>4</sup>; Pavel Pevzner<sup>1,5</sup>; Kira Vyatkina<sup>1</sup>



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- TP 244 **Autopilot: An Acquisition Control System with Fragmentation Reanalysis Informed by Online Database Searching to Optimize Top Down Proteome Analysis;** Ken Durbin; Philip Compton; Ioanna Ntai; Adam Catherman; Ryan Fellers; Neil Kelleher; *Northwestern University, Evanston, IL*

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- TP 245 **Comparative Study of Global Protein Turnover in Tissues and Cell Lines;** Martin Damsbo; Jacob Poder; Erik Nielsen; Christian Ravnsborg; Alexandre Podtelejnikov; *Thermo Fisher Scientific, Odense, Denmark*
- TP 246 **Quantitative In-Depth Analysis of the Vascular Smooth Muscle Proteome in a Model of Angiotensin-II Mediated Hypertrophy;** Fernando J. García-Marqués; Elena Bonzón Kulichenko; Jesus Vazquez Cobos; *CNIC, Madrid, Spain*
- TP 247 **An Automated Program for Protein Turnover Calculations from LC/MS Shotgun Proteomics Data Resulting from Partial Metabolic Labelling Experiments;** David Lyon; *Molecular Systems Biology, Vienna, Austria*
- TP 248 **An Integrated Systems Biology Platform for Complete Proteogenomic Analysis;** Pratik Jagtap<sup>1</sup>; John Chilton<sup>1</sup>; Ebbing de Jong<sup>2</sup>; James Johnson<sup>1</sup>; Joel Kooren<sup>2</sup>; Getiria Onsongo<sup>1</sup>; Sricharan Bandhakavi<sup>3</sup>; Timothy Griffin<sup>2</sup>; <sup>1</sup>Minnesota Supercomputing Institute, UMN, Minneapolis, MN; <sup>2</sup>University of Minnesota, Minneapolis, MN; <sup>3</sup>Bio-Rad Laboratories, Hercules, CA
- TP 249 **Scoring Protein Interactions Using CRAPome – A Contaminant Repository for Affinity Purification Mass Spectrometry Data;** Dattatreya Mellacheruvu<sup>1</sup>; Zachary Wright<sup>1</sup>; Anne-Claude Gingras<sup>2,3</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>University of Toronto, Toronto, Canada; <sup>3</sup>Samuel Lunenfeld Research Institute, Toronto, Canada
- TP 250 **Analysis of the STAT3 Interactome Using *in-situ* Biotinylation and SILAC;** Stefan Kalkhof<sup>1</sup>; Conny Blumert<sup>2</sup>; Riccardo Brumm<sup>3</sup>; Dirk Labudde<sup>3</sup>; Friedemann Horn<sup>2</sup>; Martin von Bergen<sup>1</sup>; <sup>1</sup>Helmholtz-Centre UFZ, Leipzig, Germany; <sup>2</sup>University Leipzig, Leipzig, Germany; <sup>3</sup>University of applied sciences, Mittweida, Germany
- TP 251 **IsoMS: A High-Throughput Data Analysis Software for Extracting Quantitative Information from Data Generated by Differential Isotope Labeling LC-MS;** Ruokun Zhou; Chiao-Li Tseng; Liang Li; *Department of Chemistry, University of Alberta, Edmonton, Canada*
- TP 252 **A Novel Algorithm for Protein Profiling Based on Cross-Run Correlations Implemented in the Spectronaut Software;** Oliver M. Bernhardt<sup>1</sup>; Roland M. Bruderer<sup>1,2</sup>; Tejas P. Gandhi<sup>1</sup>; Saša M. Miladinović<sup>1,2</sup>; Reto Ossola<sup>1</sup>; Yulia Butscheid<sup>1</sup>; Oliver Rinner<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys, Schlieren, Switzerland; <sup>2</sup>ETH Zurich, Zurich, Switzerland
- TP 253 **Identification of More than 8000 Proteins in Single-Runs in Cancer Cell Lines Using Rigorous, FDR-controlled Matching between Runs;** Nagarjuna Nagaraj; Jürgen Cox; Matthias Mann; *MaxPlanck Institute of Biochemistry, Martinsried, Germany*
- TP 254 **Mass Spectrometry and Ribosome Profiling, a Perfect Combination towards a More Comprehensive Identification Strategy of True *in vivo* Protein Forms;** Gerben Menschaert<sup>1</sup>; Petra Van Damme<sup>1,2</sup>; Jeroen Crappé<sup>1</sup>;

Alexander Koch<sup>1</sup>; Sandra Steyaert<sup>1</sup>; Wim Van Crielinge<sup>1</sup>; <sup>1</sup>Ghent University, Gent, Belgium; <sup>2</sup>VIB-Flanders Institute for Biotechnology, Ghent, Belgium

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- TP 255 **Comparison of Long-term-non-progressors vs. Normal-progressors among HIV-1 Infected Patients Using Extensive Ion-Current-Based Proteomic Expression Profiling Revealed Novel Virus Control Mechanisms;** Xiaomeng Shen<sup>1</sup>; Xiaosheng Jiang<sup>1,2</sup>; Jun Li<sup>1,2</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>NY CoE in Bioinformatics and Life Sciences, Buffalo, NY
- TP 256 **Differential Proteomics of Monosodium Urate Crystal Induced Inflammatory Response in Dissected Murine Air Pouch Membranes by iTRAQ Technology;** Chih-Wei Chiu<sup>1</sup>; Ying-Chu Shih<sup>2</sup>; Sung-Fang Chen<sup>1</sup>; <sup>1</sup>National Taiwan Normal University, Taipei, Taiwan; <sup>2</sup>Industrial Technology Research Institute, Hsinchu, Taiwan
- TP 257 **Tandem Affinity Depletion Coupled with Large-Scale, Extensive Ion Current Based Profiling Revealed Interesting Plasma Biomarkers Predicting Sudden Cardiac Arrest;** Chengjian Tu<sup>1,2</sup>; Jun Li<sup>1,2</sup>; James Fallavollita<sup>1</sup>; Rebecca Young<sup>1</sup>; Xiaomeng Shen<sup>1,2</sup>; Bo An<sup>1,2</sup>; John M. Canty<sup>1</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>NY CoE in Bioinformatics and Life Sciences, Buffalo, NY
- TP 258 **Biomarkers of Western Diet Induced Metabolic Disorder in Mouse Heart;** Stephen A. Whelan; Chunxiang Yao; Jessica B. Behring; Jean L. Spencer; Deborah A. Siwick; Wilson S. Colucci; Richard A. Cohen; Catherine E. Costello; Markus M. Bachschmid; Mark E. McComb; *Boston University School of Medicine, Boston, MA*
- TP 259 **Detection of Endothelial Cell Surface Proteins Following Irradiation as Potential Targets for Brain Arteriovenous Malformations;** Margaret Simonian<sup>2</sup>; Nalaka Runnulu<sup>1</sup>; Rachel Ogorzalek Loo<sup>2,1</sup>; Joseph Loo<sup>1</sup>; Marcus Stoodley<sup>2</sup>; Mark Molloy<sup>3</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>Australian School of Advanced Medicine, Sydney, Australia; <sup>3</sup>Australian Proteomics Analysis Facility, Sydney, Australia
- TP 260 **Quantitative Proteomic Analysis of Saliva in Periodontal Health, Gingivitis, Mild and Severe Periodontitis, and Following Periodontal Treatment;** Andrew Creese<sup>1</sup>; Melissa Grant<sup>1</sup>; Marcelo Aspiras<sup>2</sup>; Marko de Jager<sup>2</sup>; Helen Cooper<sup>1</sup>; Iain Chapple<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>Philips Oral Healthcare, Bothell
- TP 261 **Quantitative Proteomic Mapping of Gingival Crevicular Fluid From Dogs Progressing from Mild Gingivitis to Periodontitis;** Andrew W. Jones<sup>1</sup>; Andrew J. Creese<sup>1</sup>; Ian Davis<sup>2</sup>; Iain L. C. Chapple<sup>1</sup>; <sup>1</sup>College of Medical & Dental Sciences, University of Birmingham, Birmingham, UK; <sup>2</sup>Waltham Centre for Pet Nutrition, Waltham-on-the-Wolds, Melton Mowbray, UK
- TP 262 **Application of Multi-omic and Functional Network Analysis for Paediatric Patients Diagnosed with Idiopathic Nephrotic Syndrome;** Lee A Gethings<sup>1</sup>; Johannes P.C. Vissers<sup>1</sup>; John Shockcor<sup>2</sup>; Stephen McDonald<sup>2</sup>; Sandra Kraljević Pavlič<sup>3</sup>; Mirela Sedici<sup>3</sup>; Maja Lemac<sup>4</sup>; Danica Batinić<sup>4</sup>; James Langridge<sup>1</sup>; Olga Vasieva<sup>5</sup>; Keith Compson<sup>1</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>Waters Corp, Milford, MA; <sup>3</sup>University of Rijeka, Rijeka, Croatia; <sup>4</sup>University of Zagreb, Zagreb, Croatia; <sup>5</sup>University of Liverpool, Liverpool, UK
- TP 263 **Proteomic Profiling for Peritoneal Dialysate: Differential Display Analysis for the Protein Expression between Diabetes Mellitus and Chronic Glomerulonephritis;** Yi-Ling Chen<sup>1</sup>; Ming-Hui Yang<sup>2</sup>; Yu-Chang Tyan<sup>3</sup>; <sup>1</sup>Kaohsiung

Medical University Hospital, Kaohsiung, Taiwan; <sup>2</sup>National Yunlin University of Science & Technology, Yunlin, Taiwan; <sup>3</sup>Kaohsiung Medical University, Kaohsiung, Taiwan

- TP 264 **Characterization of the Secretome of Vascular Smooth Muscle Cells in Response to TGF- $\beta$ /Smad3 by Label-free MS<sup>E</sup> Quantification;** Chenxi Yang; Di Ma; Xudong Shi; K. Craig Kent; Lingjun Li; *University of Wisconsin, Madison, WI*
- TP 265 **Protein Profile Analysis of Kidney Transplant: Value in Prognosis of Kidney Failure;** Matthew Wroblewski; William Oetting; Gary Nelsestuen; *University of Minnesota, Minneapolis, MN*
- TP 266 **Nicotine Alters the Proteome of Pancreatic Cell Lines: Implications in Pancreatic Disease;** Joao A. Paulo; Steven P. Gygi; *Harvard Medical School, Boston, MA*
- TP 267 **Proteomic Analysis of Matched Normal and Diseased Formalin-Fixed Paraffin-Embedded Human Breast Tissues;** Fayun Che; Jennifer T aguilan; Edward Nieves; Abdissa Negassa; Ruth H Angeletti; Thomas E Rohan; *Albert Einstein College of Medicine, Bronx, NY*
- TP 268 **Protein and Post-Translational Modification Markers in Sickle Cell Disease;** Stephen A Whelan; Roger Theberge; Jean L Spencer; Paula Griffin; Chuanhua Xing; Martin H Steinberg; Catherine E Costello; Elizabeth S Klings; Mark E. McComb; *Boston University School of Medicine, Boston, MA*
- TP 269 **Interference of Protease Inhibitors with Peptidomic Biomarker Discovery and Peptide Identification;** Diana Klingler<sup>1</sup>; Markus Hardt<sup>2</sup>; <sup>1</sup>*Boston Biomedical Research Institute, Watertown, MA*; <sup>2</sup>*The Forsyth Institute, Cambridge, MA*
- TP 270 **Direct MALDI Analysis of Naturally Cleaved Human Saliva Samples: Mapping to a Series of KPQ-terminated Peptides from Small Salivary Proteins;** Kenneth Parker<sup>1</sup>; Na Tian<sup>2</sup>; Frank Oppenheim<sup>2</sup>; Eva Helmerhorst<sup>2</sup>; <sup>1</sup>*SimulTOF/ VIC Instruments, Sudbury, MA*; <sup>2</sup>*Boston University School of Dental Medicine, Boston, MA*
- TP 271 **Identification of Novel Serum Biomarkers for Preeclampsia with High Predictive Sensitivity;** Swati Anand; *BYU, Provo, UT*
- TP 272 **Proteomic Profiling of Bronchopulmonary Dysplasia in Preterm Infants;** Lindsay Schambeau<sup>1</sup>; Lewis Pannell<sup>1</sup>; John Benjamin<sup>2</sup>; Chadi Eltah<sup>3</sup>; <sup>1</sup>*USA Mitchell Cancer Institute, Mobile, AL*; <sup>2</sup>*Vanderbilt University Medical Center, Nashville, TN*; <sup>3</sup>*University of South Alabama, College of Medicine, Mobile, AL*
- TP 273 **Global Quantitative Proteomics of Irradiated Nrf2 Knockout Mus for Biomarker Discovery;** Joseph Capri; Puneet Souda; Upendra Kar; Chris Ryan; William McBride; Andrew Norris; Julian Whitelegge; *UCLA DGSOM, Los Angeles, CA*
- TP 274 **Mass Spectrometry Based Quantitative Proteomics for Discovery of Plasma Protein Biomarkers at Different Phases of Atherosclerosis;** Linhong Jing<sup>1</sup>; Zhu-qiu Jin<sup>1</sup>; Wei Xie<sup>1</sup>; Shuaipeng Zhang<sup>2</sup>; <sup>1</sup>*South Dakota State University, Brookings, SD*; <sup>2</sup>*Vanderbilt University, Nashville, Tennessee*
- TP 275 **SWATH MS Quantification of Human Urine from ICU Patients Applied to the Quest for Predictive Biomarkers in Acute Kidney Injury;** Peter Pichler<sup>1</sup>; Ludwig Wagner<sup>2</sup>; Christian Baumann<sup>3</sup>; Michael Schutzbier<sup>1</sup>; Volker Kruff<sup>3</sup>; Karl Mechtler<sup>1</sup>; <sup>1</sup>*IMP Vienna, Vienna, Austria*; <sup>2</sup>*Medical University of Vienna, Vienna, Austria*; <sup>3</sup>*AB SCIEX, Darmstadt, Germany*
- TP 276 **Developing a High-Throughput Clinical Assay Using Selected Reaction Monitoring-Mass Spectrometry to Diagnose Parkinson's Disease;** Christine Jelinek<sup>1</sup>; Liana Rosenthal<sup>1</sup>; Rachel Lieberman<sup>2</sup>; Kevin Meyers<sup>3</sup>; Ted Dawson<sup>1</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>*Johns Hopkins School of Medicine, Baltimore, MD*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*; <sup>3</sup>*Perfinity Biosciences, Inc, West Lafayette, IN*
- TP 277 **Identification of Age Dependent Periodontitis Associated Changes in the Proteome of Whole Human Saliva By Mass Spectrometric Analysis;** Manuela Gesell Salazar; Annette Murr; Elke Hammer; Nico Jehmlich; Vishnu Mukund Dhople; Birte Holtfreter; Thomas Kocher; Uwe Völker; *University Medicine Greifswald, Greifswald, Germany*
- TP 278 **Identification of Novel Serum Biomarkers for Alzheimer's Disease Using an Integrated Serum Proteomics Method;** Dipti Shah; Frederick Rohlfing; Jesse Cobell; MeiHwa Tanielle Bench Alvarez; John Kauwe; Steven Graves; *Brigham Young University, Provo, UT*
- TP 279 **Characterization and Quantitation of Alpha-Synuclein and Subspecies in Human CSF as Candidate Biomarkers for Parkinson's Disease;** Bekim Bajrami; Cheryl Lu; Sri Laxmanan; Jaya Goyal; Juan Chavez; Bernard Ravina; Joleen White; Teresa Compton; Ru Wei; *Biogen Idec, Cambridge, MA*
- TP 280 **Characterization of the C-terminal End of Soluble Amyloid Precursor Protein in Human Cerebrospinal Fluid;** Gunnar Brinkmalm<sup>1</sup>; Ann Brinkmalm<sup>1</sup>; Philippe Bourgeois<sup>2</sup>; Rita Persson<sup>1</sup>; Oskar Hansson<sup>3,4</sup>; Erik Portelius<sup>1</sup>; Marc Mercken<sup>5</sup>; Ulf Andreasson<sup>1</sup>; Stéphane Parent<sup>2</sup>; Francesco Lipari<sup>2</sup>; Annika Öhrfelt<sup>1</sup>; Maria Bjerke<sup>1</sup>; Lennart Minthon<sup>3,4</sup>; Henrik Zetterberg<sup>1,6</sup>; Kaj Blennow<sup>1</sup>; Magdalena Nutu<sup>1</sup>; <sup>1</sup>*University of Gothenburg, Mölndal, Sweden*; <sup>2</sup>*PerkinElmer Biosignal, Inc., Montreal, Canada*; <sup>3</sup>*Lund University, Malmö, Sweden*; <sup>4</sup>*Skåne University Hospital, Malmö, Sweden*; <sup>5</sup>*Janssen Research and Development, Beerse, Belgium*; <sup>6</sup>*UCL Institute of Neurology, London, UK*
- TP 281 **Comprehensive Analysis of Glycosylation Patterns of Human Plasma Clusterin - A Putative PTM Marker of Alzheimer's Disease;** Hui-Chung Liang<sup>1</sup>; Claire Russell<sup>1</sup>; Ray Chung<sup>2</sup>; Abdul Hye<sup>2</sup>; Chantal Bazenet<sup>2</sup>; Simon Lovestone<sup>2</sup>; Ian Pike<sup>1</sup>; Malcolm Ward<sup>1</sup>; <sup>1</sup>*Proteome Sciences plc, London, UK*; <sup>2</sup>*King's College London, London, UK*
- TP 282 **Quantitative Proteomic Analysis of Amyotrophic Lateral Sclerosis-linked Cellular Stress Response with Tandem Mass Tags;** Kristin J. Boggio; John D. Leszyk; Scott A. Shaffer; Daryl A. Bosco; *University of Massachusetts Medical School, Worcester, MA*
- TP 283 **Disease Biomarkers for Schizophrenia Reverted by Antipsychotic Drug Administration: Six-Plex Quantitative Phosphoproteomics of Prefrontal Cortex Synaptosomes;** Marianne Danielsen<sup>1</sup>; Kamilla Sofie Pedersen<sup>1</sup>; Nadia Taouatas<sup>1</sup>; Jens D Mikkelsen<sup>2</sup>; Henrik H Hansen<sup>3</sup>; Majbrit M Jensen<sup>2</sup>; Hans Christian Beck<sup>4</sup>; <sup>1</sup>*Danish Technological Institute, Aarhus, DK*; <sup>2</sup>*Neurobiology Research Unit, Rigshospitalet, Copenhagen, DK*; <sup>3</sup>*NeuroSearch A/S, Ballerup, DK*; <sup>4</sup>*Centre for Clinical Proteomics, OUH, Odense, DK*
- TP 284 **Validation of Disease Markers in Secretin-Stimulated Duodenal Juice Using Selected Reaction Monitoring;** Yngvild Bjorlykke<sup>1</sup>; Erling Tjora<sup>1</sup>; Fiona E. McAllister<sup>3</sup>; Frode



- Berven<sup>4</sup>; Helge Raeder<sup>2</sup>; <sup>1</sup>University of Bergen, Department of Medicine, Bergen, Norway; <sup>2</sup>University of Bergen, Department of Pediatrics, Bergen, Norway; <sup>3</sup>Department of Cell Biology, Harvard Medical School, Boston, MA; <sup>4</sup>Proteomics Unit (PROBE), University of Bergen, Bergen, Norway
- TP 285 **Systematic Characterization of Human Platelets in Arterial Vascular Disorders by Quantitative Proteomics;** Julia M. Burkhart<sup>1</sup>; Marc Vaudel<sup>1</sup>; Kristin Becker<sup>1</sup>; Lennart Martens<sup>2</sup>; Albert Sickmann<sup>1</sup>; Rene P. Zahedi<sup>1</sup>; <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; <sup>2</sup>VIB Department of Medical Protein Research, Gent, Belgium
- TP 286 **Taking Control: Human Cytomegalovirus Invades Host Cellular Organelles for Virion Assembly, Maturation, and Release;** Rommel Mathias; Todd Greco; Ileana M. Cristea; Princeton University, Princeton, NJ
- TP 287 **Quantitative Analysis of the Parotid Salivary Proteome in Patients with Primary Sjögren's Syndrome;** Stephen Swatkowski<sup>1</sup>; Kiran Ambatipudi<sup>2</sup>; James Melvin<sup>2</sup>; Marjan Gucek<sup>1</sup>; <sup>1</sup>NIH/NHLBI, Bethesda, MD; <sup>2</sup>NIH/NIDCR, Bethesda, MD
- TP 288 **Finding Invasive Aspergillosis Protein Biomarkers in Patient Bronchoalveolar Lavage Fluid;** Chengsi Huang<sup>1,2</sup>; Jason W. McCarthy<sup>3</sup>; Yun Zhang<sup>1</sup>; Carmen Luraschi-Monjagatta<sup>2</sup>; Donna Wolk<sup>2</sup>; KS Knox<sup>2</sup>; Marta Feldmesser<sup>3</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>The University of Arizona, Tucson, AZ; <sup>3</sup>Albert Einstein CoM, Yeshiva University, Bronx, NY
- TP 289 **Identification of Plasma Protein and Glycoprotein Markers of Intestinal Fibrosis Using Lectin Enrichment, cystTMT Labeling, and LC/MS;** Andy Lo; Ryan W. Stidham; David M. Lubman; University of Michigan, Ann Arbor, MI
- TP 290 **Glycomic Profiling and IgG Quantification of HIV-Infected Plasma;** Cynthia Williams; Anne Fenton; Lauren Nagy; Qiuting Hong; L.Renee Ruhaak; Satya Dadenkar; Carlito Lebrilla; UC Davis, Davis, CA
- TP 291 **Valley Fever: MS Based Diagnostics and Potential Vaccine Characterization;** Andrew VanSchoiack<sup>1</sup>; Tao Peng<sup>1</sup>; Lourdes Lewis<sup>1</sup>; John Galgiani<sup>1</sup>; Vicki Wysocki<sup>2</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>The Ohio State University, Columbus, OH
- TP 292 **Unique Protein Signature of Circulating Microparticles in Systemic Lupus erythematosus;** Ole Østergaard<sup>1</sup>; Christoffer T. Nielsen<sup>1</sup>; Line V. Iversen<sup>1</sup>; Julia T. Tanassi<sup>1</sup>; Steen Knudsen<sup>2</sup>; Søren Jacobsen<sup>3</sup>; Niels H. H. Heegaard<sup>1</sup>; <sup>1</sup>Statens Serum Institut, Copenhagen, Denmark; <sup>2</sup>Medical Prognosis Institute, Copenhagen, Denmark; <sup>3</sup>Rigshospitalet, Copenhagen University Hospital, Copenhagen, Denmark
- TP 293 **Analysis of Key Methionine Oxidation in ADAMTS13 from Human Plasma by nanoLC-ESI-MS/MS;** Yi Wang<sup>1</sup>; Junmei Chen<sup>1</sup>; William E. Hobbs<sup>1</sup>; José A. López<sup>1,2</sup>; Dominic W. Chung<sup>1,2</sup>; Xiaoyun Fu<sup>1,2</sup>; <sup>1</sup>Puget Sound Blood Center, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- TP 294 **Improvement of a Targeted MS Method used to Compare Enzyme Levels versus Enzyme Activity as Tools for Diagnosing Liver Disease;** Julie Weisz; Christine Wu; University of Pittsburgh, Cell Biology, Pittsburgh, PA
- TP 295 **A Novel Hybrid Targeted/Unbiased LC/MS/MS Method Using Isotopic TMT Enables Superior Peptide Selection for Clinical MS Assay Development;** Christopher Löfner<sup>1</sup>; Stephan Jung<sup>1</sup>; Emma Lahert<sup>2</sup>; Hans Dieter Zucht<sup>1</sup>; Stefan Selzer<sup>1</sup>; Ian Pike<sup>2</sup>; Malcolm Ward<sup>2</sup>; <sup>1</sup>Proteome Sciences R&D GmbH & Co. KG, Frankfurt, Germany; <sup>2</sup>Proteome Sciences plc, London, UK
- TP 296 **Evaluation of a Multiplexed Mass Spectrometry-Based Method for Measuring Candidate Peptide Biomarkers in Alzheimer's Disease Neuroimaging Initiative (ADNI) CSF;** Daniel S. Spellman<sup>1</sup>; Kristin R. Wildsmith<sup>2</sup>; Lee Honigberg<sup>2</sup>; Angus C. Nairn<sup>3</sup>; Judith A. Siuciak<sup>4,7</sup>; Mitchel A. Kling<sup>5</sup>; Howard Schulman<sup>6</sup>; Michael Schirm<sup>6</sup>; Daniel Chelsky<sup>6</sup>; William Z. Potter<sup>4,7</sup>; Alzheimer's Disease Neuroimaging Initiative<sup>7</sup>; Biomarkers Consortium CSF Proteomics Project Team<sup>4</sup>; <sup>1</sup>Merck and Co., Inc., West Point, PA; <sup>2</sup>Genentech, Inc., South San Francisco, CA; <sup>3</sup>Yale University School of Medicine, New Haven, CT; <sup>4</sup>Foundation of the National Institutes of Health, Bethesda, MD; <sup>5</sup>University of Pennsylvania, Philadelphia, PA; <sup>6</sup>Capriom Proteome, Inc., Montreal, Canada; <sup>7</sup>Alzheimer's Disease Neuroimaging Initiative (ADNI), Bethesda, MD
- TP 297 **Simultaneous Analysis of Tryptophan, Kynurenines and Several Amino Acids Using GC/Q-TOF in Negative Chemical Ionization Mode;** Anthony Macherone<sup>1,2</sup>; Rafael Acosta<sup>1</sup>; David Graham<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- New Technologies in Biomarker Discovery, 298 – 305**
- TP 298 **Screening of 13-HPODE-derived Protein Modifications by Orbitrap Mass Spectrometry with Isotope Data Dependent Scan;** Ryo Takahashi; Seon Hwa Lee; Takaaki Goto; Tomoyuki Oe; Tohoku University, Sendai, Japan
- TP 299 **New Analytical Platform Based on MS Technologies for Investigation of Exhaled Breath Condensate (EBC) for Medical Diagnostics;** Igor Popov<sup>1,5</sup>; Alexey Kononikhin<sup>2,3</sup>; Konstantin Nagornov<sup>2</sup>; Nataliia Starodubtseva<sup>2,3</sup>; Anna Ryabokon<sup>1</sup>; Maria Indeykina<sup>1,2</sup>; Evgeny Kukaev<sup>1,5</sup>; Viktoria Kurova<sup>1</sup>; Alexander Spassky<sup>1,2</sup>; Stanislav Pekov<sup>2</sup>; Irina Larina<sup>4</sup>; Sergei Varfolomeev<sup>1,6</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Research Center for Obstetrics, Gynecology, Moscow, Russia; <sup>4</sup>Institute for Biomedical Problems, Moscow, Russia; <sup>5</sup>Moscow Institute of Physics and Technology, Moscow, Russia; <sup>6</sup>Lomonosov Moscow State University, Moscow, Russia
- TP 300 **Optimization of LCMS for Analysis of Small Peptide and Disulfide Molecules;** Usha Mishra; Minnmass(Minnesota Mass Spec), Minneapolis Mn, MN
- TP 301 **Rapid Analysis of Endogenous Steroids Using Convergence Chromatography Coupled with Mass Spectrometric Detection;** Christopher J. Hudalla<sup>1</sup>; Stuart Chadwick<sup>2</sup>; Fiona Liddicoat<sup>2</sup>; Andrew Peck<sup>1</sup>; Kenneth J. Fountain<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation (UK), Manchester, UK
- TP 302 **Accelerated Protein Biomarker Discovery with Microwave & Magnetic (M<sup>2</sup>) Proteomics;** David Black<sup>1</sup>; Linda Nagore<sup>1</sup>; Anjali Purkar<sup>1</sup>; Swetha Mahesula<sup>1</sup>; Itay Raphael<sup>1</sup>; Jonathan Gelfond<sup>2</sup>; Stephen Bach<sup>1</sup>; Thomas Forsthuber<sup>1</sup>; William Haskins<sup>1,2</sup>; <sup>1</sup>University of Texas, San Antonio, TX; <sup>2</sup>University of Texas HSC, San Antonio, TX
- TP 303 **Over-Representation of Proteins Identified as Disease Biomarkers and Their Relation to Post-Mortem Events;** Ulla Sollenberg<sup>1</sup>; Kim Kultima<sup>2</sup>; Mats Borén<sup>1</sup>; Marcus Söderquist<sup>1</sup>; Karl Sköld<sup>1</sup>; <sup>1</sup>Denator AB, Gothenburg, Sweden; <sup>2</sup>Uppsala University, Uppsala, Sweden
- TP 304 **Calcyclin Levels Determined by High-Throughput SRM in Serum Samples of Pre-Eclampsia Patients;** Coskun Güzel<sup>2</sup>; Johannes PC Vissers<sup>1</sup>; Lennard Dekker<sup>2</sup>; Gerda G Zeeman<sup>3</sup>; Eric AP Steegers<sup>3</sup>; Theo M Luider<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>ErasmusMC, Department of Neurology, Rotterdam, The Netherlands; <sup>3</sup>ErasmusMC, Department of Gynaecology, Rotterdam, The Netherlands



- TP 305 **The Role of GC/Q-TOF in Exposomics**; Anthony Macherone<sup>1,2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- Proteomics: Plasma and Tissue, 306 – 341**
- TP 306 **Absolute Quantitation of Vitellogenin Using microLC-SRM to Determine Reproductive Status of Breeding Leatherback Turtles, a Non-Sequenced Organism**; Marine Plumel<sup>1</sup>; Virginie Plot<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Christine Carapito<sup>1</sup>; Jean-Yves Georges<sup>2</sup>; Fabrice Bertile<sup>1</sup>; <sup>1</sup>DSA, IPHC, Strasbourg, France; <sup>2</sup>DEPE, IPHC, Strasbourg, France
- TP 307 **Plasma Proteome Kinetics in Nonhuman Primates: Probing Lipoprotein Synthesis with <sup>2</sup>H<sub>2</sub>O and Targeted Proteomics**; Haihong Zhou; David McLaren; Ablatt Mahsut; Yi Pan; Ying Chen; Kathy Bierlo; Dan Xie; Steve Stout; Kithsiri Herath; Keiana Dunn; Alison Kulick; Rui Tang; Ray Rosa; Marcie Donnelly; Cesaie Gai; Andrew Gewain; Harmony Lederman; Jose Castro-Perez; Doug Johns; Michelle Cleary; Stephen Previs; Thomas Roddy; *Merck & Co., Inc., Kenilworth, NJ*
- TP 308 **Serum Proteomics for Biomarker Discovery Before and After Antidepressant Treatment of Major Depressive Disorder**; JiYeong Lee<sup>1</sup>; Hee-Joung Lim<sup>2</sup>; Jong-Moon Park<sup>3</sup>; Kyu Young Lee<sup>4</sup>; Ju Eun Yi<sup>4</sup>; HooKeun Lee<sup>3</sup>; Jong-Hoon Kim<sup>2</sup>; Eun-Jeong Joo<sup>4</sup>; Hee-Gyoo Kang<sup>1</sup>; <sup>1</sup>Eulji University, Seongnam, Korea; <sup>2</sup>Korea University, Seoul, Korea; <sup>3</sup>Lee Gil Ya Cancer and Diabetes Institute, Incheon, Korea; <sup>4</sup>School of Medicine Eulji University, Seoul, Korea
- TP 309 **Improving Label-Free Quantitation of Plasma and Serum Proteins Using a High-Resolution Hybrid Orbitrap Mass Spectrometer**; Maryann S. Vogelsang<sup>1</sup>; Amol Prakash<sup>1</sup>; David A. Sarracino<sup>1</sup>; Scott Peterman<sup>1</sup>; Bryan Krastins<sup>1</sup>; Jennifer N. Sutton<sup>1</sup>; Gregory Byram<sup>1</sup>; Gouri Vadali<sup>1</sup>; Shadab Ahmad<sup>1</sup>; Bruno Darbouret<sup>2</sup>; Mary F. Lopez<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, BRIMS Center, Cambridge, MA; <sup>2</sup>Thermo Fisher Scientific, CD Biomarkers, Nimes, France
- TP 310 **Variability in Individual Plasma Protein Profiles over Time Using SWATH acquisition**; Saša M. Miladinović<sup>1,2</sup>; Reto Ossola<sup>1</sup>; Jasmin van den Heuvel<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Yulia Butscheid<sup>1</sup>; Oliver Bernhardt<sup>1</sup>; Lukas Reiter<sup>1</sup>; Ruedi Aebersold<sup>2</sup>; Johan Malmström<sup>1,3</sup>; Oliver Rinner<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland; <sup>2</sup>ETH Zurich, Zurich, Switzerland; <sup>3</sup>Lund University, Lund, Sweden
- TP 311 **Comparative Proteomic and Metabolomic Analyses to Study the Effects of Nanoparticle Exposure**; Greg Donohoe; Hossein Maleki; Tim Nurkiewicz; Stephen Valentine; *West Virginia University, Morgantown, WV*
- TP 312 **Hexafluoroisopropanol as a Novel Reagent for Plasma Proteomic Analysis**; Jon Reed; Ariel Hart; Robert Pelot; Gogce Crynen; James Evans; Laila Abdulla; Fiona Crawford; *Roskamp Institute, Sarasota, FL*
- TP 313 **QconCATs for Cholesterol-Related Proteins in Alzheimer's Disease**; Meiyao Wang; Illarion V. Turko; *IBBR, Rockville, MD*
- TP 314 **Easy Access to Mass Spectrometry at Multiple Core Facilities Operating TripleTOF 5600 and Orbitrap Elite/Velos Pro/Q Exactive Instruments**; Anthony Yeung<sup>1</sup>; Kelly Jones<sup>1</sup>; Phillip Kim<sup>1</sup>; Bhavinkumar Patel<sup>1</sup>; Kelsen Steven<sup>2</sup>; Alan Braverman<sup>2</sup>; Derrick Swinton<sup>3</sup>; Philip Gafken<sup>4</sup>; Lisa Nader Jones<sup>4</sup>; William Lane<sup>5</sup>; John Neveu<sup>5</sup>; Hon-Chiu Leung<sup>6</sup>; Scott Shaffer<sup>7</sup>; John Leszyk<sup>7</sup>; Bruce Stanley<sup>8</sup>; Todd Fox<sup>8</sup>; Anne Stanley<sup>8</sup>; Michael Hall<sup>1</sup>; Heather Hampel<sup>9</sup>; Albert de la Chapelle<sup>9</sup>; Christopher South<sup>9</sup>; Randall Burt<sup>10</sup>; David Jones<sup>10</sup>; Levy Kopelovich<sup>11</sup>; <sup>1</sup>Fox Chase Cancer Center, Philadelphia, PA; <sup>2</sup>Temple University School of Medicine, Philadelphia, PA; <sup>3</sup>Lincoln University, Lincoln, PA; <sup>4</sup>Fred Hutchinson Cancer Center, Seattle, WA; <sup>5</sup>Harvard University, Cambridge, MA; <sup>6</sup>Baylor College of Medicine, Houston, TX; <sup>7</sup>University of Massachusetts Medical School, Worcester, MA; <sup>8</sup>Penn State College of Medicine, Hershey, PA; <sup>9</sup>The Ohio State University, Columbus, OH; <sup>10</sup>The U. of Utah, Salt Lake City, UT; <sup>11</sup>National Cancer Institute, Bethesda, MD
- TP 315 **Effects of Chronic Ethanol Consumption on Protein Expression in Rat Amygdala Studied by Quantitative Proteomics Using Dimethyl or 18O Labeling**; Bill Huang<sup>1</sup>; Zheng-Ming Ding<sup>2</sup>; William McBride<sup>2</sup>; Hee-Yong Kim<sup>1</sup>; <sup>1</sup>NIAAA/NIH, Rockville, MD; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- TP 316 **Quantitative Proteomic Study of Nucleus Accumbens in Response to Cocaine Self-Administration in Environmentally Enriched and Isolated Rats**; Cheryl F. Lichti; Robert D. English; Xiuzhen Fan; Thomas Green; *University of Texas Medical Branch, Galveston, TX*
- TP 317 **Effect of Chronic Methamphetamine Exposure on the Proteomics of Different Mouse Brain Tissues**; Rui Zhu<sup>1</sup>; Tianjiao Yang<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Kevin Wang<sup>2</sup>; Mark Gold<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>University of Florida, Gainesville, FL
- TP 318 **In vivo Quantitative Proteomics of Somatosensory Cortical Synapses Shows Which Protein Levels are Modulated by Sensory Deprivation**; Jeffrey Savas<sup>1</sup>; Margaret Butko<sup>2</sup>; Beth Friedman<sup>2</sup>; Claire Delahunty<sup>1</sup>; Ford Ebner<sup>3</sup>; Roger Tsien<sup>2</sup>; John Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>University of California at San Diego, La Jolla, CA; <sup>3</sup>Vanderbilt University, Nashville, TN
- TP 319 **Postsynaptic Density Protein Composition is Altered in Behaviorally Depressed Adult Female Cynomolgus Macaques**; Stephanie L. Willard<sup>1</sup>; Karin E. Borgmann-Winter<sup>1,2</sup>; Matthew L. MacDonald<sup>1</sup>; Carol A. Shively<sup>3</sup>; Chang-Gyu Hahn<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Dept of Psychiatry, Philadelphia, PA; <sup>2</sup>Childrens Hospital of Philadelphia, Philadelphia, PA; <sup>3</sup>Wake Forest School of Medicine, Dept of Pathology, Winston-Salem, NC
- TP 320 **Constellation of Synaptic Proteins at the Postsynaptic-Density Differentiates Schizophrenia from Normal Controls**; Matthew L. Macdonald<sup>1</sup>; Nathan Yates<sup>2</sup>; Robert Sweet<sup>1</sup>; <sup>1</sup>Univ. of Pittsburgh, Dept of Psychiatry, Pittsburgh, PA; <sup>2</sup>Univ. of Pittsburgh, Genomics and Proteomics Core, Pittsburgh, PA
- TP 321 **Study of Cerebral Proteomics Expression of Hippocampal Region from Rats Exposed to Stress Induced by Forced Swimming Using 2D-SDS-PAGE and MALDI-TOF/TOF**; Victor Alfonso Hernández; Enrique Mejía-Ospino; Nasser Guerrero; Rodrigo Torres-Saez; Carlos Conde; *Universidad Industrial de Santander, Bucaramanga, Colombia*
- TP 322 **The Sex Biased Phosphoproteome: A Novel Approach Towards Understanding The Molecular Basis for Sex Differences in Neuropsychiatric Diseases**; Rita J. Valentino; Debra A. Bangasser; Zach Plona; Christopher McKennan; Hua Ding; Steven H. Seeholzer; *Children's Hospital of Philadelphia, Philadelphia, PA*
- TP 323 **Targeted mass Spectrometry Based Quantification and Characterization of SNARE Complex proteins from Human Brain Tissue**; Ann Brinkmalm<sup>1</sup>; Gunnar Brinkmalm<sup>1</sup>; Henrik Zetterberg<sup>1</sup>; Rita Persson<sup>1</sup>; Jenny Ho<sup>2,3</sup>; Martin Hornshaw<sup>2,3</sup>; Madalina Oppermann<sup>2,3</sup>; William G Honer<sup>4</sup>; Kaj Blennow<sup>1</sup>; Annika Öhrfelt<sup>1</sup>; <sup>1</sup>University of Gothenburg, Molndal, Sweden; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, UK; <sup>3</sup>Thermo Fisher Scientific, Kungens kurva, Sweden; <sup>4</sup>University of British Columbia, Vancouver, Canada

- TP 324 **Quantitative Phosphoproteomic Analysis of Postmortem Brain Tissues from Healthy and HIV-Infected Individuals;** Lerna Uzasci<sup>1</sup>; Avindra Nath<sup>2</sup>; Robert Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>National Institute of Health, Bethesda, MD
- TP 325 **Effects of Developmental Exposure to a Commercial PBDE Mixture (DE-71) on Protein Networks in the Rat Cerebellum and Hippocampus;** Witold M Winnik<sup>1</sup>; Joyce E. Royland<sup>1</sup>; Cristina Osorio<sup>2</sup>; Oscar Alzate<sup>2</sup>; Prasada Rao S. Kodavanti<sup>1</sup>; <sup>1</sup>U.S. Environmental Protection Agency, Research Triangle Park, NC; <sup>2</sup>Systems Proteomics Center, UNC, Chapel Hill, NC
- TP 326 **Data-Independent Acquisition with Ion Mobility (HDMSE) for Analysis of the Mouse Synaptosome Proteome;** Lewis M. Brown; Guomei Tang; Ryan M. Colligan; David Sulzer; *Columbia University, New York, NY*
- TP 327 **Global Proteome Analysis of Wild-Type and FoxJ1 Knock-Out Mouse Brain Tissues Using a Quadrupole Orbitrap Mass Spectrometer;** Radiance J. Gibson; Angelito I. Nepomuceno; Nagendran Muthusamy; Shan M. Randall; Philip L. Loziuk; H. Troy Ghashghaei; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- TP 328 **Absolute Quantification of the Lignin Biosynthesis Pathway Proteins and Metabolites in Transgenic Populus trichocarpa;** Zhichang Yang; Jie Liu; Quanzi Li; Ronald Sederoff; Vincent L. Chiang; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- TP 329 **Mass Spectrometry-Based Proteome Characterization of Laser Microdissected Ovary and Oviduct Tissues from Chickens with Ovarian Cancer;** Angelito I. Nepomuceno<sup>1</sup>; Adam M. Hawkridge<sup>2</sup>; James N. Petitte<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Virginia Commonwealth University, Richmond, VA
- TP 330 **In-depth Proteomic Analysis of Rhesus Macaque Testis;** Jing Wang; Yankai Xia; Gaigai Wang; Yueshuai Guo; Tao Zhou; Yujie Sun; Xuejiang Guo; Zuomin Zhou; Jiahao Sha; *Nanjing Medical University, Nanjing, China*
- TP 331 **Qualitative and Quantitative Expression Status of the Human Chromosome 20 Genes in Cancer Tissues and the Representative Cell Lines;** Quanhui Wang<sup>1</sup>; Bo Wen<sup>1</sup>; Shaohang Xu<sup>1</sup>; Dahai Jiang<sup>1</sup>; Liang Lin<sup>1</sup>; Jin Zi<sup>1</sup>; Xiaomin Lou<sup>2</sup>; Haidan Sun<sup>2</sup>; Chuangbin Chen<sup>1</sup>; Fengji Tan<sup>1</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>BGI-Shenzhen, Shenzhen, China; <sup>2</sup>Beijing Institute of Genomics, Beijing, China
- TP 332 **A Streamlined Proteomic Workflow from Global Analysis through Parallel Reaction Monitoring with SID MS for Breast Cancer Tumor Tissue;** Matthew Meyer<sup>1</sup>; Kelly V. Ruggles<sup>2</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Robert Kitchens<sup>1</sup>; Jacqueline Snider<sup>1</sup>; Jeremy Hoog<sup>1</sup>; Shunqiang Li<sup>1</sup>; Jeanne Rumsey<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>1</sup>; David Fenyo<sup>2</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO; <sup>2</sup>New York University, New York, NY
- TP 333 **Development of an SRM Assay for the Quantification of HER2 in FFPE Tissue from Breast Cancer;** Carine Steiner<sup>1,2</sup>; Pierre Lescuyer<sup>1,3</sup>; Jean-Christophe Tille<sup>3</sup>; Thomas McKee<sup>3</sup>; Marlene Thomas<sup>4</sup>; Miro Venturi<sup>4</sup>; Laura Rubbia-Brandt<sup>3</sup>; Denis Hochstrasser<sup>1,3</sup>; Paul Cutler<sup>2</sup>; Alexander Scherl<sup>3</sup>; Axel Ducret<sup>2</sup>; <sup>1</sup>University Hospital Geneva, Geneva, Switzerland; <sup>2</sup>F. Hoffmann-La Roche, Basel, Switzerland; <sup>3</sup>University of Geneva, Geneva, Switzerland; <sup>4</sup>Roche Pharma Research, Penzberg, Germany
- TP 334 **An MRM-based Approach for Quantifying Microheterogeneity in Cancer Tissues;** Jeffrey Whiteaker; Richard Ivey; Lei Zhao; Regine Schoenherr; Jacob Kennedy; Chenwei Lin; Ping Yan; Amanda Paulovich; *Fred Hutchinson Cancer Research Center, Seattle, WA*
- TP 335 **The Detection of Breast Cancer Using Mass Spectrometry Based Targeted Proteomics;** Yun Chen; *Nanjing Medical University, Nanjing, China*
- TP 336 **Proteomic Investigation of the Mechanism of Infection of Hepatitis B Virus (HBV) in HepaRG Cells;** Catalina Petrareanu<sup>1</sup>; Izabela Sokolowska<sup>2</sup>; Alina Macovei<sup>1</sup>; Alisa G Woods<sup>2</sup>; Costel C. Darie<sup>2</sup>; Norica Branza-Nichita<sup>1</sup>; <sup>1</sup>Institute of Biochemistry, Bucharest, Romania; <sup>2</sup>Clarkson University, Potsdam, NY
- TP 337 **An Extensive and Reproducible Ion-Current-Based Method Enabled Large-Scale Pharmacoproteomic Assessment of Corticosteroid Treatment in 60 Animals;** Eslam Nouri-nigjeh; Siddharth Sukumaran; Chengjian Tu; Jun Li; Haoying Yu; Debra C. DuBois; Richard R. Almon; William Jusko; Jun Qu; *University at Buffalo, Buffalo, NY*
- TP 338 **Quantitative Mitochondrial Proteomics Revealed an Intimate Connection between Insulin Signaling, Mitochondrial Metabolism, and Aging;** Chun-Qing Song<sup>1,2</sup>; En-Zhi Shen<sup>1,2</sup>; Mei-Jun Zhang<sup>2</sup>; Hanqing Zhao<sup>3</sup>; Yu-Xin Li<sup>2</sup>; Wen-Hong Zhang<sup>2</sup>; Liping Wei<sup>2,3</sup>; Meng-Qiu Dong<sup>1,2</sup>; <sup>1</sup>College of Biological Sciences, CAU, Beijing, China; <sup>2</sup>National Institute of Biological Sciences, Beijing, China; <sup>3</sup>Center for Bioinformatics, Peking University, Beijing, China
- TP 339 **Heat Inactivation Enables Reliable Measurement of Tissue Proteome;** Charlotta Göransson; Marcus Söderquist; *Denator AB, Gothenburg, Sweden*
- TP 340 **Identification of Proteomic Differentiation Factors in Beta Cell Development;** Christopher Moss<sup>1</sup>; Holger Russ<sup>2</sup>; Roger Higdon<sup>1</sup>; Matthias Hebrok<sup>2</sup>; Eugene Kolker<sup>1</sup>; <sup>1</sup>Seattle Children's Research Institute, Seattle, WA; <sup>2</sup>University of California, San Francisco, CA
- TP 341 **Protein Profiling of Animal Tissues Using Laser Ablation Electrospray Mass Spectrometry (LAESI-MS);** Trust Razunguzwa; Gregory Boyce; Pamela Williams; Callee Walsh; Holly Henderson; Brent Reschke; Matthew Powell; *Protea Biosciences, Morgantown, WV*
- Epigenetic Modifications/Histones, 342 – 356**
- TP 342 **WCX-HILIC Coupled to Middle-Down ECD Mass Spectrometry for Histone Post-Translational Modifications Analysis;** Annie Moradian<sup>1</sup>; Michael Sweredoski<sup>1</sup>; Anastasia Kalli<sup>2</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, CA; <sup>2</sup>Children's Hospital Los Angeles, Los Angeles, CA
- TP 343 **Quantitative Histone Proteoform Dynamics with Top and Middle Down FT-ICR Mass Spectrometry;** Xibei Dang; Yeqing Tao; Jenna Scotcher; Nicolas L. Young; *NHMFLL / FSU, Tallahassee, FL*
- TP 344 **Dynamic Changes in Histone Post-Translational Modifications During the Cell Cycle by Top-Down MS/MS Analysis;** Xibei Dang<sup>1,2</sup>; Jenna Scotcher<sup>1</sup>; Yeqing Tao<sup>1,2</sup>; Takayo Sasaki<sup>2</sup>; David M. Gilbert<sup>2</sup>; Alan G. Marshall<sup>1,2</sup>; Nicolas L. Young<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University, Tallahassee, FL
- TP 345 **Investigations of Histone H2B Isoform Function Using Top and Middle-down Mass Spectrometry;** Rosalynn Molden<sup>1</sup>; Anna Arnaudo<sup>1</sup>; Nicolas Young<sup>2</sup>; Benjamin Garcia<sup>3</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>University of Pennsylvania, Philadelphia, PA
- TP 346 **Novel Somatic Mutations in Histone H3 are Associated with Global Histone PTM Changes in Human Pediatric Glioblastomas;** Shu Lin<sup>1</sup>; Peter Lewis<sup>2</sup>; Manuel Müller<sup>3</sup>; Matthew Koletsky<sup>2</sup>; Francisco Cordero<sup>4</sup>; Laura Banaszynski<sup>2</sup>; Tom Muir<sup>3</sup>; Oren Becher<sup>4</sup>; C. David Allis<sup>2</sup>; Benjamin Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>The Rockefeller University, New York, NY; <sup>3</sup>Princeton



University, Princeton, NJ; <sup>4</sup>Duke University Medical Center, Durham, NC

- TP 347 **Development of a Click-Chemistry Based Method to Quantitatively Study Propagation of Histone Post-Translational Modifications on Newly Synthesized Nucleosomes;** Anna Arnaudo<sup>1,2</sup>; Peter DiMaggio<sup>3</sup>; A James Link<sup>1</sup>; Benjamin Garcia<sup>2</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Imperial College, London, UK
- TP 348 **Quantification of Lysine Crotonylation during *in vitro* Human Myogenic Differentiation;** Natarajan Bhanu; Leila Afjehi-Sadat; Benjamin A Garcia; University of Pennsylvania, Philadelphia, PA
- TP 349 **An *in vitro* Enzymatic Assay for Quantification of Immediate-Early Histone Modifications in Compartmentalized Cell Extracts via Mass Spectrometry;** Tobias Maile<sup>1</sup>; Laura-Mae Britton<sup>2</sup>; Tom Januario<sup>1</sup>; Bob Yauch<sup>1</sup>; Benjamin Garcia<sup>3</sup>; David Arnott<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Princeton University, Princeton, NJ; <sup>3</sup>University of Pennsylvania, Philadelphia, PA
- TP 350 **A New Strategy for Bottom-Up Analysis of Histone Posttranslational Modifications Improves Detection and Quantification of H3K4 Di- and Tri-Methyl Marks;** Anita Izrael-Tomasevic<sup>1</sup>; Tobias Maile<sup>1</sup>; Victoria Pham<sup>1</sup>; Robert Pitti<sup>1</sup>; Alexandre Masselot<sup>1</sup>; Eric Chan<sup>2</sup>; Patrick Trojer<sup>2</sup>; Marie Classon<sup>1</sup>; David Arnott<sup>1</sup>; <sup>1</sup>Genentech, Inc., S. San Francisco, CA; <sup>2</sup>Constellation Pharmaceuticals, Cambridge, MA
- TP 351 **High-Resolution Accurate Mass and Intelligent Acquisition-Enabled Global Discovery and Quantification of Histones, PTMs and Modification Enzymes in Mesenchymal Stem Cells;** Amol Prakash<sup>1</sup>; Maryann Vogelsang<sup>1</sup>; David Sarracino<sup>1</sup>; Scott Peterman<sup>1</sup>; Victoria Lunyak<sup>2</sup>; James Tollervey<sup>2</sup>; Benny Blackwell<sup>2</sup>; Shadab Ahmad<sup>1</sup>; Gregory Byram<sup>1</sup>; Bryan Krastins<sup>1</sup>; Mary F Lopez<sup>1</sup>; <sup>1</sup>ThermoFisher, Cambridge, MA; <sup>2</sup>Buck Institute, Novato, CA
- TP 352 **A Direct LC-MRM Measurement of Histone H3K27 Di-, Tri-Methylation and Acetylation without Lysine Propionylation;** Lei Wang; Yasuhiro Funahashi; Mark Matijevic; Yoshiya Oda; *Eisai Inc, Andover, MA*
- TP 353 **Quantifying the Effects of FLASH Knockdown On Regulation of Histone Synthesis by LC-MS/MS;** Joshua A Reavis; Kerry M Bauer; Susan B Skube; Evan S Merryman; Amanda B Hummon; University of Notre Dame, Notre Dame, IN
- TP 354 **Systems Analysis of Epigenetic Domains – Deducing the Interactome of Modified Chromatin Using Quantitative Mass Spectrometry;** Miroslav Nikolov<sup>1</sup>; Nadin Zimmermann<sup>1</sup>; Alexandra Stützer<sup>1</sup>; Efrat Shema<sup>2</sup>; Mahmood Haj-Yahya<sup>3</sup>; Ashraf Brik<sup>3</sup>; Moshe Oren<sup>2</sup>; Henning Urlaub<sup>1,4</sup>; Wolfgang Fischle<sup>1</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; <sup>2</sup>Weizmann Institute of Science, Rehovot, Israel; <sup>3</sup>Ben-Gurion University, Beer-Sheva, Israel; <sup>4</sup>University Medical Center, Göttingen, Germany
- TP 355 **Studying the Influence of DNA Methylation on a Translational Level in the DNMT Double Knockout (DKO) HCT116 Model;** Alexander Koch<sup>1</sup>; Gerben Menschaert<sup>1</sup>; Petra Van Damme<sup>1,2</sup>; Jolien Hollebeke<sup>1,2</sup>; Wim Van Criekinge<sup>1</sup>; <sup>1</sup>Ghent University, Gent, Belgium; <sup>2</sup>VIB-Flanders Institute for Biotechnology, Ghent, Belgium
- TP 356 **Absolute Quantification of Histone Deacetylase Isoforms Using <sup>15</sup>N-labeled Quantification Concatamers as Internal Standards;** Kyle W. Anderson; Junjun Chen; Illarion V. Turko; *IBBR, Rockville, MD*

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- TP 357 **Off-line High-pH Low-pH 2D-LC Separation Combined with Isotope Labeling MS for Comprehensive Metabolome Profiling of Saliva, Serum and Urine Samples;** Tao Huan; Wei Han; Liang Li; University of Alberta, Edmonton, Canada
- TP 358 **Comprehensive Polar Metabolite Analysis in Two Minutes: Rapid CE-MS Separations Combined with Ultrafast, High Resolution Time-Of-Flight Mass Spectrometry;** Roza Wojcik; Matthew Giardina; Jeffrey S. Patrick; Viatcheslav Artaev; *LECO Corporation, St. Joseph, IN*
- TP 359 **Metabolite Profiling of Carbohydrates and Their Isomers with Improved Selectivity by Capillary Electrophoresis-Mass Spectrometry;** Naomi Kuehnbaum; Philip Britz-McKibbin; *McMaster University, Hamilton, Canada*
- TP 360 **An Automated Microfluidics System for Real-Time Measurement of Intracellular Metabolites;** Joshua Heinemann; Ece Topulzu; Brian Bothner; *Montana State University, Bozeman, MT*
- TP 361 **Collision-Cross Sections of Common Cellular Metabolites to Support Metabolomics Applications;** Giuseppe Paglia<sup>1</sup>; Giuseppe Astarita<sup>2,4</sup>; J. Will Thompson<sup>3</sup>; Jonathan P. Williams<sup>2,4</sup>; James Langridge<sup>2,4</sup>; Bernhard O. Palsson<sup>1,5</sup>; <sup>1</sup>Center for Systems Biology, University of Iceland, Reykjavik, Iceland; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Duke Proteomics Core Facility, Durham, NC; <sup>4</sup>Waters Corporation, Manchester, UK; <sup>5</sup>Systems Biology Research Group, UCSD, San Diego, CA
- TP 362 **Comparison and Refinement of UPLC-MS Based Broad Spectrum Metabolomics Methods;** Suraj Dhungana; Brian F. Thomas; Susan Sumner; *RTI RCMRC, RTI International, Durham, NC*
- TP 363 **Using Simultaneous Selective Ion Monitoring and Scan Data Collection to Streamline the Analysis of Untargeted Metabolomic Datasets Generated by GC-MS;** Joe Gummer<sup>1</sup>; Catherine Rawlinson<sup>1</sup>; Laura Grogan<sup>2</sup>; John Hewetson<sup>3</sup>; Robert Trengove<sup>1</sup>; <sup>1</sup>Murdoch University, Murdoch, Australia; <sup>2</sup>James Cook University, Townsville, Australia; <sup>3</sup>Shimadzu Scientific Instruments (Oceania), Sydney, Australia
- TP 364 **An IROA (Isotopic Ratio Outlier Analysis) Phenotypic Analysis of Field-Grown Corn Using High Resolution Accurate Mass;** Josef Ruzicka<sup>1</sup>; Mark Szewc<sup>1</sup>; Jan Hazebroek<sup>2</sup>; Chris Vlahakis<sup>2</sup>; Chris Beecher<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>DuPont Pioneer, Johnston, IA; <sup>3</sup>NextGen Metabolomics, Ann Arbor, MI
- TP 365 **Chemoselective Capture of Carbonyl-Containing Metabolites for Stable Isotope Resolved Metabolomic Analysis of Crude Cell Extracts by FTICR-MS;** Pawel K. Lorkiewicz<sup>1,2</sup>; Richard M. Higashi<sup>1,2</sup>; Stephanie J. Mattingly<sup>2</sup>; Michael H. Nantz<sup>2</sup>; Hunter N. B. Moseley<sup>1,2</sup>; Andrew N. Lane<sup>1,3</sup>; Teresa W-M. Fan<sup>1,2</sup>; <sup>1</sup>CREAM, University of Louisville, Louisville, KY; <sup>2</sup>Department of Chemistry, University of Louisville, Louisville, KY; <sup>3</sup>J.G. Brown Cancer Center, University of Louisville, Louisville, KY
- TP 366 **Protein Sensor for Discrimination of Complex Metabolite Samples;** Timothy Hamerly<sup>1</sup>; Joshua Heinemann<sup>1</sup>; Monika Tokmina-Lukaszewska<sup>1</sup>; Elizabeth R. Lusczek<sup>2</sup>; Kristine E. Mulier<sup>2</sup>; Greg Beilman<sup>2</sup>; Brian Bothner<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Department of Surgery - University of Minnesota, Minneapolis, MN



- TP 367 **A Novel Strategy for Quantification of Primary Amine-Containing Metabolites Using N,N-Dimethyl Leucine Reagents via Capillary Electrophoresis-Electrospray Ionization-Mass Spectrometry;** Ling Hao; Hui Ye; Xuefei Zhong; Tyler Greer; Dustin Frost; Zhidan Liang; Lingjun Li; *University of Wisconsin, Madison, WI*
- TP 368 **Material-oriented Tandem MS Libraries for Metabolomics and Other “-omics” Technologies;** Yamil Simón-Manso<sup>1</sup>; Kelly H. Telu<sup>1</sup>; John Halket<sup>2</sup>; Yuri Mirokhin<sup>1</sup>; Stephen E. Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>King's College London and Imperial College London, London, UK
- TP 369 **Construction of a Plant Natural Products Tandem Mass Spectral Library;** Zhentian Lei<sup>1</sup>; Li Jing<sup>2</sup>; Hua Zhang<sup>2</sup>; David Huhman<sup>1</sup>; Zhiqin Zhou<sup>2</sup>; Lloyd Sumner<sup>1</sup>; <sup>1</sup>The Samuel Roberts Noble Foundation, Ardmore, OK; <sup>2</sup>Southwest University, Chongqing, China
- TP 370 **Understanding Environmental Tobacco Smoke Exposure and Effects in Asthmatic Children through Determination of Urinary Cotinine and Targeted Metabolomics of Plasma;** Denise K. MacMillan; R. Dan Zehr; Barbara Jane George; James L. Crooks; Jane E. Gallagher; *USEPA/NHEERL, Durham, NC*
- TP 371 **Metabolic Alterations in Breast Cancer Cells and Mitochondria;** Haiwei Gu<sup>1</sup>; Daciana Margineantu<sup>2</sup>; Danijel Djukovic<sup>1</sup>; George Rogers<sup>3</sup>; David Hockenbery<sup>2</sup>; Daniel Raftery<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>3</sup>Seahorse Bioscience, North Billerica, MA
- TP 372 **Xenobiotic Control of Lung Cancer Metabolism by activation of the Aryl Hydrocarbon Receptor (AhR);** Sonnet Davis; Alexander Patent; Kylie Mitchell; Arvind Ramanathan; *Buck Institute for Research on Aging, Novato, CA*
- TP 373 **A Nutritional Urinary Metabolomics Approach to Investigate the Effect of Pulse-Based Diets in an Spontaneously Hypertensive Rat (SHR) Model;** Matthew Hanson<sup>2,3</sup>; Carla G Taylor<sup>1,3</sup>; Peter Zahradka<sup>2,3</sup>; Michel Aliani<sup>1,3</sup>; <sup>1</sup>Human Nutritional Sciences, University of Manitoba, Winnipeg, MB, Canada; <sup>2</sup>Dept Physiology, University of Manitoba, Winnipeg, MB, Canada; <sup>3</sup>CCARM, St. Boniface Hospital Research Centre, Winnipeg, MB, Canada
- TP 374 **Metabolic Rebalancing of CR6 Interaction Factor 1-Deficient Mouse Embryonic Fibroblasts; A Mass Spectrometry-Based Analysis;** Surender Tadi<sup>1,2</sup>; Soung Jung Kim<sup>2</sup>; Min Jeong Ryu<sup>2</sup>; Tae Seong Park<sup>3</sup>; Ji-Seon Jeong<sup>1</sup>; Young Hwan Kim<sup>3</sup>; Gi Ryang Kweon<sup>2</sup>; Minho Shong<sup>2</sup>; Yong-Hyeon Yim<sup>1</sup>; <sup>1</sup>KRISS, Daejeon, South Korea; <sup>2</sup>Chungnam National University, School of Medicine, Daejeon, Korea; <sup>3</sup>Korea Basic Science Institute, Cheongwon-gun, Korea
- TP 375 **Regulation of Oligodendrocyte Lipid Composition by mTOR and Metabolomic Profiling of Its Variables;** Richard Schneider<sup>1</sup>; Caroline Reiss<sup>2</sup>; Hebe Guardiola-Diaz<sup>3</sup>; <sup>1</sup>Pfizer Global R&D, Groton, CT; <sup>2</sup>Yale University, New Haven, CT; <sup>3</sup>Trinity College, Hartford, CT
- TP 376 **Application of nanoLC-MS/MS in a Metabolomics Study of Acute Kidney Injury in Mice;** Stephen Barnes<sup>1</sup>; Landon Wilson<sup>1</sup>; Ali Arabshahi<sup>1</sup>; Wei Wu<sup>2</sup>; Sanjay Niggam<sup>2</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of California-San Diego, La Jolla, CA
- TP 377 **On-line Detection of Human Stress by Real Time Mass Spectrometric Monitoring of Skin Volatiles;** Ernesto Criado-Hidalgo<sup>1</sup>; Guillermo Vidal-de-Miguel<sup>1</sup>; Rafael Borrajo-Pelaez<sup>1,2</sup>; <sup>1</sup>SEADM S. L., Boecillo, Spain; <sup>2</sup>University of California, Irvine, CA
- TP 378 **Finding Potential Biologically Significant Metabolites in C. Elegans Media Using Global Metabolomics;** Yaoling Long; Puneet Chowdhary; Rebecca Butcher; Nicolas Polfer; David Powell; *Department of Chemistry, University of Florida, Gainesville, FL*
- TP 379 **A Metabolomic Analysis of the Effects of Environmental Stress on Deinococcus radiodurans using LC-MS;** Jingyueh Jeng<sup>1</sup>; Chunain Cheng<sup>2</sup>; Kuan-lin Yu<sup>1</sup>; <sup>1</sup>Chia Nan Univ of Pharmacy & Science, Tainan, Taiwan; <sup>2</sup>National Sun Yat-sen University, Kaohsiung, Taiwan
- TP 380 **High Resolution Peptidomics Links Drug Resistance to Impaired Hemoglobin Metabolism in the Malaria Parasite Plasmodium falciparum;** Ian A. Lewis; Katelynn S. Baska; David H. Perlman; Manuel Llinas; *Princeton University, Princeton, NJ*
- TP 381 **Method for Analysis of Wine and Origin Grape Juice Properties;** Julie Lin<sup>1</sup>; Michael Athanas<sup>1</sup>; Mark Dreyer<sup>1</sup>; Rose Herbold<sup>1</sup>; Paul Tarr<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>California Institute of Technology, Pasadena, CA
- TP 382 **Untargeted Metabolomics Workflow Using UHPLC/Quadrupole Orbitrap Mass Spectrometer and SIEVE 2.1;** Junhua Wang; David Peake; Yingying Huang; *Thermo Fisher Scientific Inc, San Jose, CA*
- Metabolomics: Untargeted Metabolite Profiling Applications, 383 – 419**
- TP 383 **Evaluating the Effects of Penicillin Treatment on the Urine and Plasma Metabolomes of Sprague-Dawley Rats;** Jinchun Sun<sup>1</sup>; Laura Schnackenberg<sup>1</sup>; Sangeeta Khare<sup>1</sup>; Xi Yang<sup>1</sup>; James Greenhaw<sup>1</sup>; William Salminen<sup>2</sup>; Donna Mendrick<sup>1</sup>; Richard Beger<sup>1</sup>; <sup>1</sup>NCTR / USFDA, Jefferson, AR; <sup>2</sup>PAREXEL International, Boston, MA
- TP 384 **UPLC-MS Metabolic Profiling Reveals Involvement of Novel Biological Pathways in the Progression of Atherosclerosis;** Panagiotis Vorkas<sup>1</sup>; Joseph Shalhoub<sup>2</sup>; Giorgis Isaac<sup>3</sup>; Elizabeth Want<sup>1</sup>; Jeremy Nicholson<sup>1</sup>; Alun Davies<sup>2</sup>; Elaine Holmes<sup>1</sup>; <sup>1</sup>Biomolecular Medicine, Imperial College, London, UK; <sup>2</sup>Section of Vascular Surgery, Imperial College, London, UK; <sup>3</sup>Waters Corporation, Milford, MA
- TP 385 **Determination of SIRT-3 Dependent Metabolic Changes in Diabetic Nephropathy Using Novel Metabolomic Approaches;** Suma Ramagiri<sup>1</sup>; Hari Kosanam<sup>2</sup>; Kerri Thai<sup>3</sup>; Dave Cox<sup>1</sup>; Lyle Burton<sup>1</sup>; Eva Duchoslav<sup>1</sup>; Ron Bonner<sup>1</sup>; Andrew Advani<sup>3</sup>; Richard Gilbert<sup>3</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>Mt. Sinai Hospital, Dept of Pathology and Lab Med, Toronto, Canada; <sup>3</sup>St. Michael's Hospital, Dept of Medicine, Toronto, Canada
- TP 386 **Multi-platform Metabolomic Study of Burn Injury in a Rat Model using NMR Spectroscopy and HILIC and Reverse Phase LC-MS/MS;** Sam Li<sup>1</sup>; Anna Karen Carrasco Laserna<sup>1</sup>; Siong Chun Foo<sup>1</sup>; Shabbir Mochhala<sup>2</sup>; <sup>1</sup>National University of Singapore, Singapore, Singapore; <sup>2</sup>DSO, Singapore
- TP 387 **Direct Analysis of Serum Lipids from Zucker Rats using High Performance TOFMS – Resolution, Mass Accuracy and Unsaturation;** Jeffrey Patrick; Lucas Smith; Kevin Siek; Stephanie Amaya; Joe Binkley; *LECO Corporation, St. Joseph, MI*
- TP 388 **Metabolomics of Opiate-Induced Changes in Murine Brain by GC/Q-TOF;** Manhong Wu<sup>1</sup>; Peyman Sahbaei<sup>1</sup>; Ming Zheng<sup>1</sup>; David Clark<sup>1</sup>; Gary Peltz<sup>1</sup>; Sofia Aronova<sup>2</sup>; Stephan Baumann<sup>2</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA

- TP 389 **High Accuracy Prostate Cancer Detection Using Human Blood Sera Metabolomic Profiling;** Xiaoling Zang<sup>1</sup>; Christina Jones<sup>1</sup>; Tran Long<sup>1</sup>; Maria Monge<sup>1</sup>; Manshui Zhou<sup>1</sup>; L. DeEtte Walker<sup>1</sup>; Alexander Gray<sup>1</sup>; John McDonald<sup>1</sup>; Nikhil Shah<sup>2</sup>; Rajesh Laungani<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Piedmont Hospital, Atlanta, GA
- TP 390 **Metabolomic Profiling of Human Breast Cancer Tissues by UPLC-IM-MS;** Kelly Hines<sup>1</sup>; Billy Ballard<sup>2</sup>; Dana Marshall<sup>2</sup>; John McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, Tennessee; <sup>2</sup>Meharry Medical College, Nashville, Tennessee
- TP 391 **Metabolomic Response of Human Breast Cancer Lines after Exposure to Estradiol;** Liang Zhao; Shelly Odwin-DaCosta; Mounir Bouhifd; Helena Hogberg; Lena Smirnova; Andre Kleensang; James D. Yager; Thomas Hartung; School of Public Health, Johns Hopkins University, Baltimore, MD
- TP 392 **Metabolite Phenotypes Predictive of Non-Small Cell Lung Cancers;** Ji-Won Park<sup>1</sup>; Hyobin Jeong<sup>2</sup>; Sujin Kim<sup>1</sup>; Byeongsoo Kang<sup>2</sup>; Hark Kyun Kim<sup>3</sup>; Daehee Hwang<sup>2</sup>; Tae Geol Lee<sup>1</sup>; <sup>1</sup>KRISS, Daejeon, South Korea; <sup>2</sup>postech, Pohang, South Korea; <sup>3</sup>NCC, Goyang, South Korea
- TP 393 **Biomarkers of Pancreatic Cancer;** Suhong Zhang<sup>4</sup>; Maya Khezam<sup>1,4</sup>; Nathaniel Snyder<sup>2,4</sup>; Clementina Mesaros<sup>2,4</sup>; Kenneth Yu<sup>3,4</sup>; Ian Blair<sup>2,4</sup>; <sup>1</sup>Centers for Excellence in Environmental Toxicology, Philadelphia, PA; <sup>2</sup>Cancer Pharmacology, University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Memorial Sloan-Kettering Cancer Center, New York, NY; <sup>4</sup>Philadelphia, PA
- TP 394 **Metabolomics Investigation of Ovarian Cancer Progression in a Dicer-Pten Double Knockout Mouse Model;** Christina Jones<sup>1</sup>; Maria Monge<sup>1</sup>; Jaeyeon Kim<sup>2</sup>; Martin Matzok<sup>2</sup>; John McDonald<sup>1</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Baylor College of Medicine, Houston, TX
- TP 395 **Metabolic Profiling of Gottingen Minipig Plasma Using GC-MS and LC-MS;** Jeffrey McGuire; US Army ECBC, Aberdeen Proving Ground, MD
- TP 396 **Mass Spectrometry Metabolomics to Identify Novel Diet-Dependent Plasma Metabolites;** Masoumeh Karimpour<sup>1</sup>; Izabella Surowiec<sup>1</sup>; Johan Trygg<sup>1</sup>; Angela Zivkovic<sup>2</sup>; Malin Nording<sup>1</sup>; <sup>1</sup>Department of Chemistry, Umea University, Umea, Sweden; <sup>2</sup>University of California, Davis, CA
- TP 397 **Effect of Exercise on Fatty Acid Metabolism in Aging Brain;** Nataliya Chorna; Ivan Santos; Sandra Pena de Ortiz; University of Puerto Rico, San Juan, PR
- TP 398 **Untargeted Metabolite Profiling of Porcine Urine Samples: Individual's Response to Stress During Hemorrhage, Shock and Recovery;** Monika Tokmina-Lukaszewska<sup>1</sup>; Navid Movahed<sup>1</sup>; Kristine Mulier<sup>2</sup>; Nancy Witowski<sup>2</sup>; Greg Beilman<sup>2</sup>; Brian Bothner<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Medical School, University of Minnesota, Minneapolis, MN
- TP 399 **Metabolite Profiling of Wild Yeast Strains for Brewing Makgeolli Depending on the Strains and the *in vitro* Physiological Activities;** HyeRyun Kim; Jang-Eun Lee; Jae Ho Kim; Byung Hak Ahn; Korea Food Research Institute, Seongnamsi, Asia/Pacific Region
- TP 400 **Expanding Metabolic Pathways in the Ovarian Tissues Using Metal-assisted SIMS (Meta-SIMS);** Tae Geol Lee<sup>1</sup>; Ji-Won Park<sup>1</sup>; Su Jin Kim<sup>1</sup>; Byeongsoo Kang<sup>2</sup>; Hyobin Jeong<sup>2</sup>; Hark Kyun Kim<sup>3</sup>; DaeHee Hwang<sup>2</sup>; <sup>1</sup>KRISS, Daejeon, South Korea; <sup>2</sup>Postech, Pohang, South Korea; <sup>3</sup>NCC, Goyang, South Korea
- TP 401 **Fecal Metabolomics of the Mouse Digestive Tract to Determine the Effect of Host Antimicrobial Peptides;** Samanthi I. Wickramasekara<sup>1</sup>; Chunxiao Guo<sup>1</sup>; Fereshteh Zandkarimi<sup>1</sup>; Jeffrey Morré<sup>1</sup>; Richard L. Gallo<sup>2</sup>; Adrian F. Gombart<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>University of California, San Diego, CA
- TP 402 **Exploration of Ethanol-induced Liver disease using High Performance GC-TOF-MS and Robust Statistical Analysis;** Jeffrey Patrick<sup>1</sup>; Joe Binkley<sup>1</sup>; John Heim<sup>1</sup>; Jens Hoefkens<sup>2</sup>; <sup>1</sup>LECO Corporation, St. Joseph, MI; <sup>2</sup>Genedata (USA), Lexington, MA
- TP 403 **Untargeted Metabolomics Reveals Alteration of the Sphinganine-Ceramide Pathway in Spinal Cord Injury;** Jaewoo Choi; Debbie J. Mustacich; Wendy I. Baltzer; Jan F. Stevens; Oregon State University, Corvallis, OR
- TP 404 **Analysis of Cerebrospinal Fluid to Investigate the Effect of Iron Deficiency Anemia on the Central Nervous System Metabolome;** Farbod Fazlollahi<sup>1</sup>; Christopher Coe<sup>2</sup>; Gabriele Lubach<sup>2</sup>; Kym Faull<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>University of Wisconsin, Madison, WI
- TP 405 **Metabolomic Profiling of Obese Pig Colon Mucosa and Fecal Samples to Study the Effect of Consuming Anthocyanin-rich Color-fleshed Potatoes;** Lavanya Reddivari<sup>1</sup>; Sridhar Radhakrishnan<sup>1</sup>; Sumit Shah<sup>2</sup>; Jairam Vanamala<sup>1,3</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Agilent Technologies, Inc, Wakefield, MA; <sup>3</sup>University of Colorado Cancer Center, Aurora, CO
- TP 406 **Untargeted Metabolomics Identifies Putrescine as a Candidate Predictive Biomarker of L-Asparaginase Response and as an Additive for Possible Combination Therapy;** Leslie Silva; Philip Lorenzi; David Hawke; John Weinstein; MD Anderson Cancer Center, Houston, TX
- TP 407 **Metabolomics of Asbestos Exposure;** Clementina Mesaros; Nathaniel W. Snyder; Anil Vachani; Ian A. Blair; University of Pennsylvania, Philadelphia, PA
- TP 408 **The Metabolomics of Oxidative Stress: Investigating the Impact of a Sod1-null Mutant and Paraquat Induced Stress Using Liquid Chromatography/Mass Spectrometry;** Jose M. Knee<sup>1</sup>; Teresa Z. Rzezniczak<sup>1</sup>; Kevin K. Guo<sup>3</sup>; Aiko Barsch<sup>2</sup>; Gabriela Zurek<sup>2</sup>; Thomas J. S. Merritt<sup>1</sup>; <sup>1</sup>Dept. Chemistry & Biochemistry Laurentian University, Sudbury, Ontario, Canada; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Bruker Daltonics Inc., Billerica, MA
- TP 409 **Untargeted Metabolomics for Profiling Multiple Auxotrophic Yeast Strains by LC-QqTOF;** Lekha Sleno<sup>1</sup>; Audrey Ste-Rose<sup>1</sup>; Guri Giaever<sup>2</sup>; Corey Nislow<sup>2</sup>; <sup>1</sup>UQAM, Montreal, Canada; <sup>2</sup>UBC, Vancouver, CA
- TP 410 **Comprehensive Metabolomic Profiling of Lotus Seeds from Different Cultivars Using GC-MS and LC-MS;** Ming-Zhi Zhu; Sha Chen; Shao-Hua Li; Ming-Quan Guo; Wuhan Botanical Garden, Chinese Academy of Science, Wuhan, China
- TP 411 **Metabolomic Analysis of a Staphylococcus Variant SG1 Cultured in the Absence and Presence of Butanol;** Feifei Fu; Yiman Wu; Victor Cheng; Joel Weiner; Liang Li; University of Alberta, Edmonton, Canada
- TP 412 **Untargeted Metabolomic Analysis of UV Stress Response in Chlamydomonas reinhardtii Using GC-QTOF and GC-TOF Mass Spectrometry;** Zipora Tietel; Kohei Takeuchi; Mine Palazoglu; Oliver Fiehn; UC Davis Genome center, Metabolomics, Davis, CA
- TP 413 **Untargeted Metabolomic Study on the Effect of *in vitro* Mineral Nutrition on Raspberry (Rubus idaeus) Growth;** Soyoun Ahn<sup>1,2</sup>; Sukalya Poonthong<sup>2</sup>; Barbara Reed<sup>2,3</sup>; Claudia Maier<sup>1,2</sup>; <sup>1</sup>EHSC Oregon State University, Corvallis, OR; <sup>2</sup>Department of Horticulture Oregon State University, Corvallis, OR; <sup>3</sup>USDA-ARS, Corvallis, OR



- TP 414 **Metabolomics of Hermaphroditic *C. elegans* via Isotopic Ratio Outlier Analysis Using High-Resolution Accurate Mass LC/MS/MS**; Kevin J. McHale<sup>1</sup>; Mark Szewc<sup>1</sup>; Gregory S. Stupp<sup>2</sup>; Chaevien Clendinen<sup>2</sup>; Ramadan Ajredini<sup>2</sup>; Arthur S. Edison<sup>2</sup>; Chris Beecher<sup>3</sup>; <sup>1</sup>*Thermo Fisher, Somerset, NJ*; <sup>2</sup>*University of Florida, Gainesville, FL*; <sup>3</sup>*NextGen Metabolomics, Ann Arbor, MI*
- TP 415 **Natural Products Drug Discovery from Marine Invertebrate-Associated Bacteria: Strain Selection Using Principle Component Analysis of LC/MS Data**; Gregory A. Ellis<sup>1</sup>; Yanpeng Hou<sup>2</sup>; Thomas P. Wyche<sup>1</sup>; Doug R. Braun<sup>1</sup>; Navid Adnani<sup>1</sup>; Emmanuel Vazquez-Rivera<sup>1</sup>; Tim S. Bugni<sup>1</sup>; <sup>1</sup>*University of Wisconsin School of Pharmacy, Madison, WI*; <sup>2</sup>*PepsiCo, New Haven, CT*
- TP 416 **Untargeted Metabolomics for the Discovery of Small Molecule Regulators of Thermogenesis**; Jay Kirkwood; Cristobal Miranda; Fred Stevens; *Oregon State University, Corvallis, OR*
- TP 417 **Metabolomics Study or Model Systems for Microbially**; Vincent Bonifay<sup>1</sup>; Whitney Smith<sup>1</sup>; Iwona Beech<sup>2</sup>; Jan Sunner<sup>1</sup>; <sup>1</sup>*Oklahoma University, Norman, OK*; <sup>2</sup>*University of Portsmouth, Portsmouth, UK*
- TP 418 **Bacterial Nutritional Growth and Responses to Varying Nitrogen Sources by IROA Protocol**; Chris Beecher<sup>1</sup>; Peng Jiang<sup>2</sup>; Alex Ninf<sup>2</sup>; <sup>1</sup>*NextGen Metabolomics, Ann Arbor, MI*; <sup>2</sup>*University of Michigan Medical School, Ann Arbor, MI*
- TP 419 **Metabolomics of Carbon Fixing Mutants of Cyanobacteria by GC/Q-TOF**; Dong hee Chung<sup>1</sup>; Christine Rabinovitch-Deere<sup>1</sup>; Shota Atsumi<sup>1</sup>; Sofia Aronova<sup>2</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- Drug Metabolism: Quantitative Analysis, 420 – 451**
- TP 420 **Investigating the Importance of Resolution and Scan Speed for Qualitative/Quantitative Bioanalysis Using a Benchtop HR/AM Orbitrap Mass Spectrometer**; Brad Yuska<sup>1</sup>; Ragu Ramanathan<sup>1</sup>; Tim Stratton<sup>2</sup>; Hongxia Wang<sup>2</sup>; Frank Morris<sup>1</sup>; Patrick Bennett<sup>2</sup>; <sup>1</sup>*QPS, LLC, Newark, DE*; <sup>2</sup>*ThermoFisher, San Jose, CA*
- TP 421 **Analysis of Pharmaceutical Small Molecules Using a Prototype Microfluidics Tandem Quadrupole LCMS System**; Yun W. Alelyunas<sup>1</sup>; Mark D. Wrona<sup>1</sup>; Catalin Doneanu<sup>1</sup>; Stephen McDonald<sup>1</sup>; Paul D. Rainville<sup>1</sup>; Philip Tiller<sup>2</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*RMI laboratories, North Wales, PA*
- TP 422 **Development of Ultrasensitive Nanoscale LC/MS Techniques for Quantification of an HIV-1 Integrase Inhibitor in Human Plasma**; Miaoqing Shen<sup>1</sup>; Li Sun<sup>2</sup>; Kevin Bateman<sup>2</sup>; Jack Henion<sup>1</sup>; <sup>1</sup>*Advion Bioanalytical Lab, a Quintiles company, Ithaca, NY*; <sup>2</sup>*Merck Research Laboratories, West Point, PA*
- TP 423 **Parallel-Micro Liquid Chromatography - Mass Spectrometry for the Quantification of Pharmaceuticals using Dried Blood Spot Tube-based Sample Collection Format**; Kyoko Watanabe<sup>1,3</sup>; Emmanuel Varesio<sup>1</sup>; Neil Loftus<sup>2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>*Université de Genève, Genève, Switzerland*; <sup>2</sup>*Shimadzu Corporation, MS/BU, Manchester, UK*; <sup>3</sup>*Shimadzu Corporation, GADC, Kyoto, Japan*
- TP 424 **Electrochemistry Coupled to LC-ICP-MS for the Elucidation and Quantitative Assessment of the Oxidation Pathway of Selected Isatins**; Daniel Melles<sup>1</sup>; Christoph A. Wehe<sup>2</sup>; Panupun Limpachayaporn<sup>1</sup>; Günter Haufe<sup>2</sup>; Uwe Karst<sup>2</sup>; <sup>1</sup>*University of Münster-Graduate School of Chemistry, Münster, DE*; <sup>2</sup>*University of Münster, Münster, DE*
- TP 425 **A Novel Direct Analysis in Real Time (DART) Mass Spectrometry Method for Determination of Imatinib in Human Plasma**; Kumari Ubhayasekera; Warunika Aluthgedara; Tommy Lewander; Jonas Bergquist; *Uppsala University, Uppsala, Sweden*
- TP 426 **Evaluation of Centroid and Profile Mode Data Collection Methods for High Resolution Mass Spectrometry Based Integrated Qualitative and Quantitative Bioanalysis**; Eldho Raju; Dil Ramanathan; *Kean University, Union, NJ*
- TP 427 **SWATH – A High Resolution Data Independent Acquisition Approach to Pharmaceutical/ Biotherapeutic Quantitation and Retrospective Qualitative Interrogation**; Loren Olson<sup>1,2</sup>; Paul Clemens<sup>1,2</sup>; Eva Duchoslav<sup>1,2</sup>; Gary Impey<sup>1,2</sup>; <sup>1</sup>*AB SCIEX, Foster City, CA*; <sup>2</sup>*AB SCIEX, Toronto, Canada*
- TP 428 **SWATH Based Pharmacokinetic Quantification to Increase Selectivity, Specificity and Signal-to-Noise Ratio with the Benefits of Non-Targeted Approach on UHPLC-HRMS**; Ragu Ramanathan<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Brad Yuska<sup>1</sup>; Frank Morris<sup>1</sup>; Jiye Wang<sup>1</sup>; Anthony Srnka<sup>1</sup>; Yves LeBlanc<sup>2</sup>; Gary Impey<sup>2</sup>; Loren Olson<sup>2</sup>; Helen Shen<sup>1</sup>; <sup>1</sup>*QPS, LLC, Newark, DE*; <sup>2</sup>*AB SCIEX, Concord, Ontario, Canada*
- TP 429 **Parameter-Free Peak Area Integration for Multiple Batches of LC/MS/MS Data**; Yongdong Wang; Hongliang (Leo) Xu; Ming Gu; *Cerno Bioscience, Norwalk, CT*
- TP 430 **Pragmatic Approaches to Determine the Exposures of Drug Metabolites in Pre-Clinical and Clinical Subjects**; Johanna Haglund<sup>1,2</sup>; Åsa Brunnström<sup>1,2</sup>; Göran Eklund<sup>1,2</sup>; Antti Kautiainen<sup>1,2</sup>; Anna Sandholm<sup>1,3</sup>; Magnus Halldin<sup>1</sup>; Suzanne Iverson Hemberg<sup>1</sup>; <sup>1</sup>*AstraZeneca AB, Södertälje, Sweden*; <sup>2</sup>*MetaSafe AB, Södertälje, Sweden*; <sup>3</sup>*Scandinavian Development Services AB, Stockholm, Sweden*
- TP 431 **Evaluate and Overcome the Impact of Hemolysis on the Quantitation Using LC-MS/MS - Is "Revising SOP" the Solution?** Jing Ke; Yijin Xiao; Kelly Lam; Harry Zhao; Zhongping (John) Lin; *Frontage Laboratories, Inc, Exton, PA*
- TP 432 **Automated, Empirical Method Development for Solid-Phase Extraction of Pharmaceuticals from Biological Fluids for LC-MS/MS Analysis**; Kc Van Home<sup>1</sup>; Phil Dimson<sup>1</sup>; Luigi Chanco<sup>1</sup>; Bruce Redmond<sup>1</sup>; Jacob Christ<sup>2</sup>; David Hall<sup>1</sup>; <sup>1</sup>*SPEware Corporation, Baldwin Park, CA*; <sup>2</sup>*ProLinear/Pontech, Inc., Rancho Cucamonga, CA*
- TP 433 **Quantitation of Amino Acids in Response to L-Asparaginase Treatment in Ovarian Cancer**; Preeti Purwaha; Philip L. Lorenzi; David Hawke; John N. Weinstein; *MD Anderson Cancer Center, Houston, TX*
- TP 434 **UPLC-ESI+-MS/MS Method for Quantitation of Circulating Levels of 13 Opiate and Opioid Analgesics from Dried Blood Spot Samples**; Melissa Goggin; Richard Lundberg; Karla Walker; Gregory Janis; *MedTox Laboratories, New Brighton, MN*
- TP 435 **An LC-MS/MS Method for Quantification of Debrisoquine and OH-debrisoquine in Dried Blood Spots**; Jason Barricklow; Hongying Gao; *Pfizer, Groton, CT*
- TP 436 **A Sensitive and Selective Liquid Chromatography-Tandem Mass Spectrometry Method for Quantitative Analysis of Efavirenz in Human Dried Blood Spots**; Praveen Srivastava<sup>1</sup>; Ganesh Moorthy<sup>1</sup>; Vu Nguyen<sup>1</sup>; Robert Gross<sup>2</sup>; Jeffrey Barrett<sup>1</sup>; <sup>1</sup>*The Children's Hospital of Philadelphia, Philadelphia, PA*; <sup>2</sup>*University of Pennsylvania, Philadelphia, PA*
- TP 437 **Quantitative Acetylation Analysis of Mitochondrial Proteins in Type 2 Diabetic Mice and Treatment of Metformin**; Xiaolu Zhao<sup>1</sup>; Jie Dai<sup>2</sup>; Jianshuang Li<sup>1</sup>; Xiujuan Zhu<sup>1</sup>; Ling Zheng<sup>1</sup>; Ole Nørregaard Jensen<sup>2</sup>; Lin Guo<sup>1</sup>;



- <sup>1</sup>Wuhan University, Wuhan, P.R.China; <sup>2</sup>University of Southern Denmark, Odense, Denmark
- TP 438 **Determination of Norgestrel and Norgestimate in Human Plasma by LC/MS-MS**; Hongkun Liang; crystal Nguyen; Angel Tseng; Vi Dan; Yuan-Chek Chen; Kumar Ramu; QPS, LLC., Newark, DE
- TP 439 **An LC-MS/MS Assay for Simultaneous Quantitation of Docetaxel and its Prodrug-Conjugate for Pharmacokinetic Studies of PRINT-Lipidized-Docetaxel Nanoparticles in Mice**; Allison N. Schorzman; Kevin Chu; Matthew Finniss; Charles Bowerman; Jennifer Kuijer; Andrew Madden; Joseph DeSimone; William Zamboni; UNC, Chapel Hill, NC
- TP 440 **Characterization of Xylazine Metabolism in Rat Liver Microsomes by HPLC-QqLIT MS**; David St-Germain Lavoie<sup>1</sup>; Floriane Pailleux<sup>1,2</sup>; Pascal Vachon<sup>1</sup>; Francis Beaudry<sup>1</sup>; <sup>1</sup>Université de Montréal, Saint-Hyacinthe, Canada; <sup>2</sup>Université de Lyon, Villeurbanne, France
- TP 441 **Validation of the Trans Stereoisomer Enclomiphene in Human Serum by LC/MS/MS API5000**; Adlai Niggebrugge; Mario Pellerin; Ardeshtir Khadang; PRACS Institute, Fargo, ND
- TP 442 **Simultaneous Determination of Pinitol and its metabolites (Chiro-, Myo-inositol) in Rat Plasma by LC-MS/MS**; Yun Kyoung Choi<sup>1</sup>; In Young Choi<sup>1</sup>; Ji Hoon Jeoung<sup>2</sup>; Hohyun Kim<sup>1</sup>; <sup>1</sup>Korea Medicine Research Institute, Inc., Seoungnam, South Korea; <sup>2</sup>College of Medicine, Chung-Ang University, Seoul, South Korea
- TP 443 **Quantitation of Praziquantel and Its Metabolites in Mouse Plasma Using Ultra-Performance Liquidchromatography- Tandem Mass Spectrometry**; Amy Qiu Wang; Edward Kerns; Xin Xu; Gurmit Grewal; Philip Sanderson; John Shen; John McKew; NCATS, NIH, Rockville, MD
- TP 444 **Study of the Brain-Uptake of a Non-Radioactive Pseudo-Carrier for [<sup>18</sup>F]-AV-133 by Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry**; Xue Zhou<sup>1</sup>; Ai-Fang Deng<sup>1</sup>; Jinping Qiao<sup>1</sup>; Xian-Ying Wu<sup>1</sup>; Yan Zhang<sup>1</sup>; Wei Yin<sup>1</sup>; Lin Zhu<sup>1</sup>; Hank Kung<sup>2</sup>; <sup>1</sup>Beijing Normal University, Beijing, China; <sup>2</sup>Department of Radiology, University of Pennsylvania, Philadelphia, PA
- TP 445 **Highly Sensitive Determination of Desmopressin in Human Plasma by UPLC-MS/MS**; Yun Kyoung Choi<sup>1</sup>; Jae Geun Lee<sup>1</sup>; Ji Hoon Jeoung<sup>2</sup>; Hohyun Kim<sup>1</sup>; <sup>1</sup>Korea Medicine Research Institute, Inc., Seoungnam, South Korea; <sup>2</sup>Chung-Ang University, Seoul, South Korea
- TP 446 **A Simplified Method for Quantification of Gemcitabine with LC-MS from Tissue Applied to Research on the Surgical Delivery of Chemotherapy**; Preston Sparks<sup>1</sup>; Michael Roach<sup>1</sup>; Jesse Hines<sup>2</sup>; <sup>1</sup>Eisenhower Army Medical Center, Fort Gordon, GA; <sup>2</sup>Perkin Elmer, Waltham, MA
- TP 447 **Mometasone Furoate in Human Plasma by LC/MS/MS with Column Switch**; Allan Xu; Xiaohua Li; Vince Windisch; Keystone Bioanalytical, North Wales, PA
- TP 448 **A Sensitive and Robust Assay for Determination of Clonidine in Human Plasma Using Derivatization and LC-MS/MS Techniques**; Yansheng Liu; Marsha Luna; Julie Showalter; Rochelle Burke; Moo-Young Kim; KCAS LLC, Shawnee, KS
- TP 449 **The "Double edge sword" of Hydroxypropyl-beta-Cyclodextrin on the Quantitative Analysis of a Lipoglycopeptide and its Hydroxylated Metabolites by LC-MS/MS**; Moucyun Yuan; James Waltrip; Song Zhao; William R. Mylott; Bruce Hidy; Rand Jenkins; PPD, Richmond, VA
- TP 450 **Determination of CTP-499 and Its Major Metabolites in Dog, Rat and Rabbit Plasma by LC-MS/MS**; Xiaonan Tang<sup>1</sup>; Jing Ke<sup>1</sup>; Halil Erol<sup>1</sup>; Chih Hsien Lin<sup>1</sup>; Harry Zhao<sup>1</sup>; Zhongping (John) Lin<sup>1</sup>; Changfu Cheng<sup>2</sup>; <sup>1</sup>Frontage Laboratories, Inc., Exton, PA; <sup>2</sup>CoNCERT Pharmaceuticals, Inc., Lexington, MA
- TP 451 **Diastereomeric Separation of Chiral Metabolites Utilizing SFC-MS/MS; A Powerful Tool to Investigate Stereoselective Metabolism?** Chester L. Bowen<sup>1</sup>; Hermes Licea-Perez<sup>1</sup>; Tom DePhillipo<sup>2</sup>; Denise Heyburn<sup>2</sup>; Paul Rainville<sup>2</sup>; Robert Plumb<sup>2</sup>; Christopher Evans<sup>1</sup>; <sup>1</sup>GlaxoSmithKline, King Of Prussia, PA; <sup>2</sup>Waters, Milford, MA
- Small Molecules: Quantitative Analysis II, 452 – 477**
- TP 452 **Detailed Characterization of Conjugation Pathways of the Tetrahydro-Reduced Metabolites of Glucocorticoids by Rat and Human Liver Fractions Using LC/ESI-MS/MS**; Kuniko Mitamura<sup>1</sup>; Mami Kamibayashi<sup>1</sup>; Kanta Sato<sup>1</sup>; Sachi Fujioka<sup>1</sup>; Rika Satoh (née Okihara)<sup>2</sup>; Takashi Iida<sup>2</sup>; Shigeo Ikegawa<sup>1</sup>; <sup>1</sup>Kinki University, Higashi-Osaka, Japan; <sup>2</sup>Nihon University, Tokyo, Japan
- TP 453 **Quantitation of Testosterone and Nandrolone Using Dried Blood Spots (DBS) for Steroid Pharmacological Study**; Gurmeet Kaur Surindar Singh<sup>1,2</sup>; Reena Desai<sup>1</sup>; Mark Jimenez<sup>1</sup>; David Handelsman<sup>1</sup>; <sup>1</sup>ANZAC Research Institute, University of Sydney, New South Wales, Sydney, Australia; <sup>2</sup>Faculty of Pharmacy, Universiti Teknologi MARA, Kuala Selangor, Selangor, Malaysia
- TP 454 **Quantitative Measurement of Fludarabine Incorporation in Cellular DNA by Enzymology and Mass Spectrometry**; Ye Feng<sup>1</sup>; Lan Li<sup>1</sup>; Lili Liu<sup>2</sup>; Stanton L. Gerson<sup>2</sup>; Yan Xu<sup>1,2</sup>; <sup>1</sup>Cleveland State University, Cleveland, OH; <sup>2</sup>Case Comprehensive Cancer Center, Cleveland, OH
- TP 455 **Neurotransmitter Analysis in Rat Brain Microdialysis Samples Using LC-MS/MS**; Changyu Quang; Michael V. Stoeling; William C. Nethero; Jonathan D. Toot; Eric S. Bodle; Spencer J. Carter; WIL Research, Ashland, OH
- TP 456 **Pharmacokinetic Studies of a Novel Thiazolidinedione mitoNEET Ligand, NL-1, Using a Quantitative LC-MS/MS Method in Dosed Mouse Serum and Brain**; Kiran Pedada<sup>1</sup>; Xiang Zhou<sup>1</sup>; Harini Jogiraju<sup>1</sup>; Richard Carroll<sup>2</sup>; Werner Geldenhuys<sup>2</sup>; Li Lin<sup>2</sup>; David Anderson<sup>1</sup>; <sup>1</sup>Cleveland State University, Cleveland, OH; <sup>2</sup>Northeast Ohio Medical University, Rootstown, OH
- TP 457 **Simultaneous LC-ESI-MSMS-MRM Quantification of Glutathione and Six Related Compounds**; Alexander Yoon; Stephen Shew; Joseph Watson; Kym Faull; University of California, Los Angeles, CA
- TP 458 **Comprehensive LC/MRM Assay for Determination of Nerve Agent Therapeutics in Guinea Pig Brain Microdialysate and African Green Monkey Plasma**; Benjamin Oyler; Tsung-Ming Shih; John McDonough; Benedict Capacio; USAMRICD, Aberdeen Proving Ground, MD
- TP 459 **Low-Level Quantitative Analysis of Prostaglandins in Human Serum and Urine by LC/MS/MS Utilizing Dual Ion Funnel Technology**; Yanan Yang; Kevin McCann; Anabel Fandino; Caroline Chu; Mark Sartain; Na Pi; Agilent Technologies, Inc, Santa Clara, CA
- TP 460 **Application of a Highly Sensitive LC/MS/MS Assay for the Comparison of Exposure to Nicotine and its Metabolites**; Kimberly Clark; Joshua Prey; Richard O'Connor; Mark Travers; Gerald Fetterly; Roswell Park Cancer Institute, Buffalo, NY

- TP 461 **Determination of Urinary Catecholamines and Metanephrines in a Single Run by LC/MS/MS for Clinical Research;** Linda Cote<sup>1</sup>; Christophe Deckers<sup>1</sup>; Kevin McCann<sup>2</sup>; <sup>1</sup>Agilent Technologies Canada, Saint-Laurent, Canada; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 462 **Quick Sample Preparation of Opiates from Urine for UHPLC/MS analysis;** Daniel Tran; *Agilent Technologies, Lake Forest, Ca, CA*
- TP 463 **High Throughput, Simultaneous Analysis, Separation and Validation of Eight Opioids and Metabolites in Human Urine by LC-MS/MS;** Jianmei Wang; Ramiro Cavazos; Toqueer Rizvi; *Texas Medical Toxicology, Houston, Texas*
- TP 464 **Fast and Sensitive Assay of Tobacco Specific Nitrosamines by UHPLC-MS/MS;** Mikael Levi; Maureen Ramero; Stéphane Moreau; *Shimadzu France, Noisiel, France*
- TP 465 **Quantifying Metformin in Mouse Serum Using Hydrophilic Interaction Liquid Chromatography and Stable Isotope Dilution-Assisted Multiple Reaction Monitoring Mass Spectrometry (HILIC-SID-MRM-MS);** Da-Qing Yang; Mikel R. Roe; Michael E. Grossmann; Nancy K. Mizuno; Adrian D. Hegeman; Margot P. Cleary; *University of Minnesota, Austin, MN*
- TP 466 **Small Molecule, Big Challenges: Development and Validation for the Determination of Mesalamine and Its Metabolite in Human Plasma by HILIC-MS/MS;** Jingguo Hou; Ravi Orugunt; Xiaodong Zhu; Melvin Tan; Thomas Horvath; Jing Zhou; Gregory Poch; Michael Sullivan; Edward Wells; Steve Unger; *WWCT, Austin, TX*
- TP 467 **Development and Validation of a HILIC Based UPLC-ESI-MS/MS Method for the Quantification of Free Carnitine in Human Plasma;** Tiffany Thomas; Roseann Zott; Danielle Awad; Dawn Hershman; Serge Cremers; *Columbia University, New York, NY*
- TP 468 **Quantitation of Glutathione and Related Thiols in Acid-Preserved Samples by Hydrophilic Interaction Chromatography-Mass Spectrometry;** Alan W. Taylor; Deborah Hobbs; Debbie J. Mustacich; Balz Frei; *Linus Pauling Institute, Oregon State University, Corvallis, OR*
- TP 469 **Simultaneous Quantification of Metanephrine, Normetanephrine, Histamine, Serotonin, and 3,4-dihydroxyphenylglycol in Dog plasma by LC-MS/MS;** Aihua Liu; Troy Voelker; Min Meng; *Tandem Labs, Salt Lake City, UT*
- TP 470 **Development of an Analytical Method for Hydroxyurea in Rat Plasma, Amniotic Fluid, and Fetus by HILIC-MS/MS;** Michael S. Gardner<sup>1</sup>; Melanie A. Rehder Silinski<sup>1</sup>; Reshan A. Fernando<sup>1</sup>; Veronica G. Robinson<sup>2</sup>; Suramya Waidyanatha<sup>2</sup>; <sup>1</sup>RTI International, Research Triangle Park, NC; <sup>2</sup>Division of National Toxicology Program, NIEHS, Research Triangle Park, NC
- TP 471 **Determination of S-ketamine in Rat Plasma by a Short-Run LC-MS/MS Method;** Qingtao (Mike) Huang<sup>1</sup>; Eric De Waal<sup>1</sup>; Naidong Weng<sup>1</sup>; Weimin Wang<sup>2,2</sup>; Chih Hsien Lin<sup>2,2</sup>; Hsiaoju Lin<sup>2</sup>; Zhongping (John) Lin<sup>2</sup>; Harry Zhao<sup>2</sup>; <sup>1</sup>Johnson & Johnson, Raritan, NJ; <sup>2</sup>Frontage Lab, Exton, PA
- TP 472 **Validation of (R,S)-Enantiomers of Amphetamine in Human Plasma by SOLA-CX LC/MS/MS API4000;** Adlai Niggebrugge; Laura Baum; Sarah Maasjo; Dan Pederson; David O'Connor; Mario Pellerin; Ardesir Khadang; *PRACS Institute, Fargo, ND*
- TP 473 **(S)-(+)-Vigabatrin Determination in Plasma by LC/MS with Two Methods: Chiral Column Without Derivatization and Non-Chiral Column with Pre-Column Derivatization;** Shan Jin; Eric Britton; Steven Wiltshire; *Agilux Laboratories, Worcester, MA*
- TP 474 **Analysis for Hydroxylated Polybrominated Diphenyl Ethers (OH-PBDEs);** Yan-Ping Lin<sup>1</sup>; Louis Maljers<sup>2</sup>; Helen Sun<sup>2</sup>; Isaac N. Pessah<sup>1</sup>; Birgit Puschner<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>Bruker Daltonics Inc., Fremont, CA
- TP 475 **Determination of Valproic Acid in Human Plasma Using Derivatization and LC-MS/MS Techniques;** Moo-Young Kim; Anika Pippin; Yu-Hui Ann Fu; Yansheng Liu; *KCAS, Shawnee, KS*
- TP 476 **A Novel LC-MS/MS Method for the Ultra-Sensitive Isolation and Detection of 1a,25(OH)2-Vitamin D3 and Its Common Metabolites in Serum Samples;** Adam Latawiec; Michael Jarvis; *AB SCIEX, Concord, Canada*
- TP 477 **Chemical Derivatization of d6-bisphenol A Increases Sensitivity in Trace Level Serum Evaluations;** Nathan C. Twaddle; Mona I. Churchwell; Daniel R. Doerge; *NCTR/ FDA, Jefferson, AR*
- Lipids: Quantitative Analysis, 478 – 497**
- TP 478 **High-speed Monitoring Method for Eicosanoids and Related Compounds Using Liquid Chromatography / Mass Spectrometry;** Masaki Yamada<sup>1,2</sup>; Yoshihiro Kita<sup>1</sup>; Suzumi Tokuoka<sup>1</sup>; Takahiro Kohira<sup>1,3</sup>; Takao Shimizu<sup>1</sup>; <sup>1</sup>The University of Tokyo, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Japanese Red Cross Society, Tokyo, Japan
- TP 479 **Global Analysis of Lipidome of Caenorhabditis elegans Based on Shotgun Lipidomics Strategy;** Tanxi Cai<sup>1</sup>; Jiaojiao Ma<sup>1</sup>; Charles C. Liu<sup>2</sup>; Fuquan Yang<sup>1</sup>; <sup>1</sup>Institute of Biophysics, CAS, Beijing, China; <sup>2</sup>ASPEC Technologies Limited, Beijing, China
- TP 480 **A Novel UHPLC-Q-TOF Method for the Detection and Quantification of Plasma Lipids;** Carlos Leon; William Wikoff; Tomas Cajka; Brian DeFelice; Dmitry Grapov; Oliver Fiehn; *UC Davis, Davis, CA*
- TP 481 **Differential Quantitation of TAG Isomers by Mathematical Modeling of Neutral Losses Of Fatty Acids;** Haowei Song; Jack Ladenson; Fongfu Hsu; John Turk; *Washington University in St. Louis, School of Medi, St. Louis, MO*
- TP 482 **Quantitative Analysis of Sulfatides in Mouse Plasma Membrane Using UHPLC-MS-MS;** Guannan Li<sup>1</sup>; Ana Lis Moyano<sup>2</sup>; Jan-Eric Mansson<sup>3</sup>; Maria Irene Givogri<sup>2</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>University of Illinois College of Medicine, Chicago, IL; <sup>3</sup>University of Gothenburg The Sahlgrenska Academy, Gothenburg, Sweden
- TP 483 **Quantitative Targeted Lipidomics in Urine: Phosphatidylserine by UPLC-MS/MS;** Sabrina Forni; Lawrence Sweetman; *Baylor Research Institute, Dallas, TX*
- TP 484 **Lipids Analysis in 9 Seconds Sample to Sample with Surface Improved Plates and Vaporization Enhancement Solution in LDTD-MS/MS;** Pierre Picard<sup>1</sup>; Gregory Blachon<sup>1</sup>; Serge Auger<sup>1</sup>; Réal Paquin<sup>2</sup>; <sup>1</sup>Phytronix Technologies, Quebec city, Canada; <sup>2</sup>Université Laval, Quebec City, Canada
- TP 485 **Comprehensive Lipid Profiling of Drosophila melanogaster (fruit fly) under Diverse Starvation Conditions Using Metabolic 13C Isotope Labeling;** Vinzenz Hofferek; *Max-Planck-Institute, Potsdam-Golm, Germany*
- TP 486 **Shotgun Lipidomics Analysis of Diacylglycerol Species in Biological Samples after One-step Derivatization;** Miao Wang; Huafeng Fang; Jacina Redden; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*

- TP 487 **Trimethylation Enhancement using Diazomethane (TrEnDi): Rapid Methylation of Phospholipids to Permit Quantitative Analysis Using Tandem Mass Spectrometry;** Karl Wasslen; Hyunmin Lee; Jeffrey Manthorpe; Jeffrey C. Smith; *Carleton University, Ottawa, Canada*
- TP 488 **Formation and the Use of [M+42]<sup>+</sup> Ion for the Identification and Quantitation of sphingosine-1-phosphate and Its Analogs after bis-Acetylation;** Irina Gorshkova; Evgeny Berdyshev; *University of Illinois at Chicago, Chicago, IL*
- TP 489 **LC-MS and MALDI-TOF Characterization of Glycolipid-bearing Liposomes;** Spiros Manolagos<sup>1,2</sup>; Theresa Evans-Nguyen<sup>1,2</sup>; Leila Albers<sup>1,2</sup>; James Comolli<sup>1,2</sup>; <sup>1</sup>*The Charles Stark Draper Laboratory, Tampa, FL*; <sup>2</sup>*The Charles Stark Draper Laboratory, Cambridge, MA*
- TP 490 **A Rapid Serum Free Fatty Acids Profiling by MALDI-FTICR MS;** Yaping Zhang; Yujie Liu; Shuai Guo; Hui Liu; Fenjie Li; Zhili Li; *IBMS, CAMS&PUMC, Beijing, China*
- TP 491 **Profiling Biochemical Effects of Osteopathic Manipulative Treatment on COPD Patients: Multi-Class Determination of Bioactive Lipids in Plasma Samples;** Chen Zhang; *Michigan State University, East Lansing, MI*
- TP 492 **Rapid Profiling of Oxylipins for Drug Discovery&Development, Nutritional and Clinical Research;** Roy Martin<sup>1</sup>; Katrin Strassburg<sup>2,3</sup>; Thomas Hankemeier<sup>3</sup>; Giorgis Isaac<sup>1</sup>; James Langridge<sup>1</sup>; Claude Mallet<sup>1</sup>; Rob Vreeken<sup>2,3</sup>; Giuseppe Astarita<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Netherlands Metabolomics Centre, Leiden, The Netherlands*; <sup>3</sup>*Analytical BioSciences, LACDR, Leiden, The Netherlands*
- TP 493 **Hydroxylated Metabolites of Docosahexaenoic Acid are Substrates for 15-Hydroxyprostaglandin Dehydrogenase (15-PGDH): Electrophile Formation and Anti-inflammatory Signaling Actions;** Stacy L. Gelhaus; Franca Golin-Bisello; Sally Wenzel; Fernando Holguin; Bruce A. Freeman; *School of Medicine, University of Pittsburgh, Pittsburgh, PA*
- TP 494 **Combined Proteomics and Lipidomics Analyses Enable the Characterization of Phagosome Maturation in Activated Macrophages;** Christina Bell<sup>1</sup>; Guanghou Shui<sup>2</sup>; Markus Wenk<sup>2</sup>; Michel Desjardins<sup>1</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*University of Montreal, Montreal, Canada*; <sup>2</sup>*National University of Singapore, Singapore*
- TP 495 **Quantification of Lipids in Human Cancer Cells and Culture Supernatants by LC-MS/MS;** Finnur Eiriksson<sup>2</sup>; Baldur Sigurdsson<sup>2</sup>; Sesselja Omarsdottir<sup>1</sup>; Kari Skulason<sup>1</sup>; Helga Ogmundsdottir<sup>1</sup>; Margret Thorsteinsdottir<sup>1,2</sup>; <sup>1</sup>*University of Iceland, Reykjavik, Iceland*; <sup>2</sup>*ArcticMass, Reykjavik, Iceland*
- TP 496 **Identification of Lipid Bio-Markers for Dry Eye Disease in Post-Menopausal Women Using Shotgun Electrospray Mass Spectrometry;** Mark Apsega<sup>1</sup>; Jianzhong Chen<sup>1</sup>; Kelly Nichols<sup>2</sup>; Jason J. Nichols<sup>2</sup>; Kari B. Green<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*; <sup>2</sup>*University of Houston, Houston, TX*
- TP 497 **Phosphatidylserine Effects on Platelet-Activating Factor Secretion from Platelets;** Audrey Meyer; Cecil Koseoglu; Yiwen Wang; Joseph Dalluge; Christy Haynes; *University of Minnesota, Minneapolis, MN*
- Informatics: Quantification/Validation, 498 – 528**
- TP 498 **Evaluation of Different Computational Algorithms for Label-Free Protein Quantitation by Mass Spectrometry;** Francesco Mattia Mancuso; Cristina Chiva; Mireia Ortega; Eduard Sabidó; *Proteomics Unit, CRG/UPF, Barcelona, Spain*
- TP 499 **Integration of mProphet Chromatogram Peak Identification Probability Model into Skyline;** Brendan Maclean<sup>1</sup>; Don Marsh<sup>1</sup>; Hannes Röst<sup>2</sup>; Lucia Espona Pernas<sup>2</sup>; George Rosenberger<sup>2</sup>; Ruedi Aebersold<sup>2</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>*Univ of Washington, Seattle, WA*; <sup>2</sup>*Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland*
- TP 500 **The Use of QCONCAT Labeled Peptides to Validate Label-Free Antigen Quantitation for Influenza Vaccines;** Daryl G.S. Smith; Genevieve Gingras; Yves Aubin; Terry D. Cyr; *Health Canada, Ottawa, Canada*
- TP 501 **PRiMe: Open Source Software for Visualization and Quantitation of Large Scale Targeted Proteomics Using Parallel Reaction Monitoring;** Michael R. Hoopmann; Samuel L. Bader; Robert L. Moritz; *Institute for Systems Biology, Seattle, WA*
- TP 502 **Tandem MS Epigenetics histones Analysis: A Novel Medium Throughput Approach for Identification, Labeled Quantification and Exploration;** Alexandre Masselot; Tobias Maile; Victoria Pham; Anita Izrael-Tomasevic; Robert Yauch; David Arnott; *Genentech Inc., South San Francisco, CA*
- TP 503 **X-Quant: A Transplantable Tool for Label-Free Quantification of Proteomics Based on MS/MS;** Bo Wen<sup>1</sup>; Haiyi Zhao<sup>1</sup>; Guilin Li<sup>1</sup>; Qiang Feng<sup>1</sup>; Quanhui Wang<sup>1,2</sup>; Siqi Liu<sup>1,2</sup>; Jun Wang<sup>1</sup>; <sup>1</sup>*BGI-Shenzhen, Shenzhen, China*; <sup>2</sup>*Beijing Institute of Genomics, CAS, Beijing, China*
- TP 504 **iPiG: Proteogenomic Data Integration in Genome Browsers;** Mathias Kuhring; Bernhard Renard; Robert Koch-Institute, Berlin, Germany
- TP 505 **MRM Protein Quantification and Serum Sample Classification;** Pascal Szacherski<sup>1</sup>; Laurent Gerfault<sup>1</sup>; Jean-François Giovannelli<sup>2</sup>; Audrey Giremus<sup>2</sup>; Pierre Mahé<sup>3,4</sup>; Tanguy Fortin<sup>3,4</sup>; Geneviève Choquet-Kastylevsky<sup>3,4</sup>; Amna Klich<sup>5</sup>; Catherine Mercier<sup>5</sup>; Pascal Roy<sup>5</sup>; Arnaud Salvador<sup>6</sup>; Jérôme Lemoine<sup>6</sup>; Jean-Philippe Charrier<sup>3,4</sup>; Bruno Lacroix<sup>3,4</sup>; Pierre Grangeat<sup>1</sup>; <sup>1</sup>*CEA Leti, MINATEC Campus, Grenoble, France*; <sup>2</sup>*Univ. Bordeaux, IMS, UMR 5218, Talence, France*; <sup>3</sup>*bioMérieux, Grenoble, France*; <sup>4</sup>*bioMérieux, Marcy l'Etoile, France*; <sup>5</sup>*HCL, Service de Biostatistique, Univ. Lyon I, CNRS, Lyon, France*; <sup>6</sup>*Institut des Sciences Analytiques, CNRS, Univ. Lyon, Lyon, France*
- TP 506 **Collisional Ion Trap Simulator (CITSIM) for Trajectory Computation for Unsteady Flow Conditions Ranging from Vacuum to Atmospheric Pressure;** Sorin Mitran; Bruno Coupier; J. Michael Ramsey; *University of North Carolina, Chapel Hill, NC*
- TP 507 **Detection and Correction of Interference in MS1 Quantitation of Peptides Using their Isotope Distributions;** Yifei Bao<sup>2</sup>; Jessica Chapman<sup>1</sup>; Joseph Glavy<sup>2</sup>; Beatrix Ueberheide<sup>1</sup>; Manor Askenazi<sup>3</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>*New York University Langone Medical Center, New York, NY*; <sup>2</sup>*Stevens Institute of Technology, Hoboken, NJ*; <sup>3</sup>*The Ionomix Initiative, Arlington, MA*
- TP 508 **Accurate Multiplexed Proteomics at the MS2-Level Using the Complement Reporter Ion Cluster;** Martin Wühr; Wilhelm Haas; Graeme C. McAlister; Leonid Peshkin; Ramin Rad; Marc W. Kirschner; Steven P. Gygi; *Harvard Medical School, Boston, MA*
- TP 509 **Protein Cluster Identification and Quantitation with Scaffold;** Caleb J. Emmons; Brian C. Searle; *Proteome Software, Portland, OR*
- TP 510 **Deconvolution of Overlapping Peptide Isotopic Peak Clusters with EM Algorithm for Label-free Quantification;** Lei Xin<sup>1</sup>; M. Ziaur Rahman<sup>1</sup>; Weiwu Chen<sup>1</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>*Bioinformatics Solutions Inc., Waterloo, Canada*; <sup>2</sup>*University of Waterloo, Waterloo, Ontario*



- TP 511 **RIPPER: A New Software Framework for Biomarker Discovery Using the Proportionality Paradigm and Proximity-based Intensity Normalization (PIN);** Susan K. Van Riper<sup>1</sup>; Kathryn J. Doroschak<sup>2</sup>; Ebbing P. de Jong<sup>2</sup>; LeeAnn Higgins<sup>2</sup>; Nelson L. Rhodus<sup>2</sup>; Frank G. Ondrey<sup>2</sup>; John V. Carlis<sup>2</sup>; Timothy J. Griffin<sup>2</sup>; <sup>1</sup>University of Minnesota Rochester, Rochester, MN; <sup>2</sup>University of Minnesota, Minneapolis, MN
- TP 512 **An Instrument Independent Demultiplexing Method for Computationally Improving the Specificity of Data Independent Acquisition;** Dario Amodei<sup>1</sup>; Jarrett Egerton<sup>2</sup>; Brendan McLean<sup>2</sup>; Richard Johnson<sup>2</sup>; Olga Vitek<sup>3</sup>; Michael MacCoss<sup>2</sup>; Parag Mallick<sup>1</sup>; <sup>1</sup>Stanford University, Palo Alto, CA; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Purdue University, West Lafayette, IN
- TP 513 **New Algorithm Utilizing All Ions MS/MS Data on TOF/Q-TOF and Accurate Mass MS/MS Libraries for Rapid Development of Quant/Qual Methods;** Frank Kuhlmann; Stephen Madden; Bernhard Wuest; Maithilee Samant; Hong Chen; Prerana Kapase; *Agilent Technologies, Santa Clara, CA*
- TP 514 **Automated Quantification and Analysis of SILAC-ITRAQ Dual-labeled Data;** Getiria Onsongo; John Chilton; Michelle Henderson; Timothy J. Griffin; Pratik Jagtap; Edgar Arriaga; *University of Minnesota, Minneapolis, MN*
- TP 515 **Refinements to Label-free Proteome Quantitation: Applying Spectral Counting Strategies to Parent Ion and Fragment Ion Intensities and Chromatographic Peak Area;** Ying Zhang; Zhihui Wen; Michael Washburn; Laurence Florens; *The Stowers Institute for Medical Research, Kansas City, MO*
- TP 516 **Label-Free Inter-Sample Replicate Similarity Metrics for LC-MS Data Using Intra-Sample Information;** Rob Smith; Dan Ventura; John Prince; *Brigham Young University, Provo, UT*
- TP 517 **A Simplified Method Development Interface for Routine Quantification Applications on High-Resolution, Accurate Mass Instrumentation;** David Brant<sup>1</sup>; Catharina Crone<sup>2</sup>; Tim Stratton<sup>1</sup>; Nick Duczak<sup>1</sup>; Patrick Bennett<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany
- TP 518 **ProDIA-id: An Automatic Tool to Extract MS/MS Spectra for Protein Identification in Proteomic Experiments Using Data-Independent Acquisition;** Hui-Yin Chang<sup>1</sup>; Nai-Yuan Chiang<sup>1</sup>; Chia-Feng Tsai<sup>2</sup>; Ya-Wen Tsai<sup>2</sup>; Ke-Shiuan Lynn<sup>1</sup>; Chia-Ying Cheng<sup>1</sup>; Yu-Ju Chen<sup>2</sup>; Ting-Yi Sung<sup>1</sup>; Wen-Lian Hsu<sup>1</sup>; <sup>1</sup>Institute of Information Science, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- TP 519 **A Qualitative and Quantitative Ion Mobility Enabled Data Independent SILAC Workflow;** Andrew JK Williamson<sup>1</sup>; Steven Ciavarini<sup>2</sup>; Scott J Geromanos<sup>2</sup>; Andrew Tudor<sup>3</sup>; Barry Dyson<sup>3</sup>; Lee Gethings<sup>3</sup>; Kelly McMahon<sup>3</sup>; Robert Tonge<sup>3</sup>; James I Langridge<sup>3</sup>; Anthony D Whetton<sup>1</sup>; Johannes PC Vissers<sup>3</sup>; <sup>1</sup>School of Cancer and Imaging Sciences, Manchester, UK; <sup>2</sup>Waters Corporation US, Milford, MA; <sup>3</sup>Waters Corporation UK, Manchester, UK
- TP 520 **Critical Assessment of Proteome-Wide Label-Free Absolute Quantification Strategies;** Erik Ahrné; Timo Glatzer; Lars Molzahn; Alexander Schmidt; *Proteomics Core Facility, Biozentrum, Basel, Switzerland*
- TP 521 **MS1Probe – Implementation of a Statistical Tool for MS1-based Quantitation in Skyline for High Throughput Quantitative Analysis;** Alexandria K. D'Souza<sup>1</sup>; Birgit Schilling<sup>1</sup>; Julian Chytrowski<sup>1</sup>; Brendan MacLean<sup>2</sup>; Daniel Broudy<sup>2</sup>; Nicholas J. Shulman<sup>2</sup>; Michael J. MacCoss<sup>2</sup>; Bradford W. Gibson<sup>1</sup>; <sup>1</sup>Buck Institute for Research on Aging, Novato, CA; <sup>2</sup>University of Washington, Seattle, Seattle, WA
- TP 522 **Validation of Label-Free Methods for Protein Quantitation and Their Application to the Characterization of the Exon Junction Complex;** John Leszyk; Guramrit Singh; Melissa J. Moore; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*
- TP 523 **THOR: an Algorithm for Determining the Variance Cutoff In Proteomics Count Data;** Scott Walmsley<sup>1</sup>; Damian Fermin<sup>1</sup>; Hyungwon Choi<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan Department of Pathology, Ann Arbor, MI; <sup>2</sup>National University of Singapore, Singapore, Singapore
- TP 524 **Automatic Reprocessing, Analysis and Reporting in High-Throughput Analytical Environments;** Manuel Perez Pacheco<sup>1</sup>; Carlos Cobas<sup>1</sup>; Felipe Seoane<sup>1</sup>; Santiago Dominguez<sup>1</sup>; Mike Bernstein<sup>1</sup>; Chen Peng<sup>1</sup>; Agustin Barba<sup>1</sup>; George Maydwell<sup>2</sup>; Scott Campbell<sup>2</sup>; <sup>1</sup>Mestrelab Research, Santiago De Compostela, Spain; <sup>2</sup>Sierra Analytics, Modesto, CA
- TP 525 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data;** Luis Mendoza<sup>1</sup>; David Shteynberg<sup>1</sup>; Joseph Slagel<sup>1</sup>; Michael Hoopmann<sup>1</sup>; Terry Farrah<sup>1</sup>; Zhi Sun<sup>1</sup>; Brian Pratt<sup>2</sup>; Henry Lam<sup>3</sup>; Jimmy K. Eng<sup>4</sup>; Alexey I. Nesvizhskii<sup>5</sup>; Eric W. Deutsch<sup>1</sup>; Robert L. Moritz<sup>1</sup>; <sup>1</sup>Institute For Systems Biology, Seattle, WA; <sup>2</sup>Insilicos, LLC, Seattle, WA; <sup>3</sup>Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong; <sup>4</sup>University of Washington, Seattle, WA; <sup>5</sup>University of Michigan, Ann Arbor, MI
- TP 526 **Capturing Multi-Dimensional Proteomes in an Online Encyclopedia;** Yasmeen Ahmad; Mark Larence; Tony Ly; Kathryn Kirkwood; Dalila Bensaddek; Arnel Nicolas; Angus I. Lamond; *Centre for Gene Regulation & Expression, University of Dundee, UK*
- TP 527 **MZDASoft™ Parallel Peak Extractor™: A Software Tool for LC/MS data Integration and Compression;** Nelson Ramirez; Zhiwei Wang; David M. Noriega; Yung Lai; Jianqiu (Michelle) Zhang; *UTSA, San Antonio, TX*
- TP 528 **Graph-based Time Alignment Algorithms for LC-MS Datasets with Large Retention-Time Drifts;** Jijie Wang; Henry H. N. LAM; *The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China*
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- TP 529 **High-Throughput Cotinine Determination in Human Plasma, Urine and Saliva Using LDTD-MS/MS in 8 Seconds Sample to Sample;** Sylvain Letarte<sup>1</sup>; Gregory Blachon<sup>1</sup>; Serge Auger<sup>1</sup>; Pierre Picard<sup>1</sup>; Sarah Demers<sup>2</sup>; <sup>1</sup>Phytronix Technologies, Québec, Canada; <sup>2</sup>Université Laval, Québec, Canada
- TP 530 **Cadmium Exposure Results in the Up-regulation of DDAH I&II in Human Fibroblast Cells as Revealed by SILAC-based Quantitative Proteomics;** John Prins; Yinsheng Wang; *University of California, Riverside, CA*
- TP 531 **Stable Isotope Dilution NanoLC-Nanospray Ionization Tandem Mass Spectrometry Analysis of Three Ethylated Thymidine Adducts in Human Salivary DNA;** Hauh-Jyun Candy Chen; Chin-Ron Lee; *National Chung Cheng Univ., Ming-Hsiung, Chia-Yi, Taiwan*
- TP 532 **High Throughput Liquid Chromatography-Tandem Mass Spectrometry Method for Analysis of 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL) and its Glucuronides in Human Urine;** Steven Carmella; Xun Ming; Andrea Yoder; Elizabeth Vielguth; Stephen S. Hecht; *Univ. of Minnesota Cancer Center, Minneapolis, MN*
- TP 533 **Liquid Chromatography-Tandem Mass Spectrometry Quantitation of DNA Adducts in Tissues of Rats Treated Chronically with Enantiomers of the Carcinogen N'-Nitrosomonicotine;** Lijiao Zhao; Silvia Balbo; Mingyao

- Wang; Peter Villalta; Pramod Upadhyaya; Stephen S. Hecht; *Univ. of Minnesota Cancer Center, Minneapolis, MN*
- TP 534 **Toxicological Analysis of Whole Blood Samples Using Automated SPE/HPLC/MS/MS; Ken Lewis<sup>1</sup>**; Robert Sears<sup>2</sup>; Kim Gamble<sup>3</sup>; <sup>1</sup>OpAns, LLC, Durham, NC; <sup>2</sup>South Carolina Law Enforcement Division, Columbia, SC; <sup>3</sup>ITSP Solutions, Hartwell, GA
- TP 535 **Comprehensive Toxicological Screening Using Generic MS/MS<sup>ALL</sup> Acquisition on a Q-TOF Tandem Mass Spectrometer; Michael J. Y. Jarvis**; Jesse Seegmiller; Jenny Moshin; Adrian Taylor; *AB SCIEX, Concord, Canada*
- TP 536 **Automated Direct Sample Analysis (DSA/TOF) for the Rapid Screening and Confirmation of Illicit Street Drugs; Sean Daugherty<sup>1</sup>**; Alun Huchings<sup>2</sup>; Mark Upton<sup>1</sup>; <sup>1</sup>PerkinElmer, Bucks, UK; <sup>2</sup>Cardiff Tox Lab, University Hospital Llandough, Cardiff, Wales
- TP 537 **Detection and Metabolic Characterization of the Hallucinogenic Compound 25I-NBOME in Biological Samples via LC-MS; David Le<sup>1</sup>**; An Nguyen<sup>1</sup>; Samuel J Stelpflug<sup>2</sup>; Gregory Janis<sup>1</sup>; <sup>1</sup>MedTox Laboratories, New Brighton, MN; <sup>2</sup>Regions Hospital Dept. of Emergency Medicine, Saint Paul, MN
- TP 538 **Chiral Separation and Quantification of Methamphetamine Stereoisomers by Capillary Electrophoresis/Triple Quadrupole Mass Spectrometry; Flaubert Mbeunkui**; Steven Cohen; Joseph Wiegel; Brent Dixon; *Physicians Choice Laboratory Services, Charlotte, NC*
- TP 539 **A Mixed Targeted and Untargeted LC-TOF Approach for Monitoring Emerging Drugs of Abuse in Biological Samples; An Nguyen**; Gregory Janis; *MedTox Laboratories, New Brighton, MN*
- TP 540 **Qualitative and Quantitative Analysis of Illicit Drugs in Biological Fluids by Turbulent-Flow LC Coupled to an Exactive benchtop Orbitrap MS; Jérémy Pinguet<sup>1,2</sup>**; Lucie Roche<sup>1</sup>; Pauline Herviou<sup>1</sup>; Damien Richard<sup>1,2</sup>; <sup>1</sup>CHU Clermont Ferrand, Clermont Ferrand, France; <sup>2</sup>UMR INSERM 1107 Neurodol, Université d'Auvergne, Clermont ferrand, France
- TP 541 **Determination of Barbiturates and 11-nor-9-carboxy- $\Delta^9$ -THC in Urine Using Automated Disposable Pipette Extraction (DPX) and LC/MS/MS; Oscar G. Cabrices**; Fred Foster; Edward Pfannkoch; *Gerstel Inc., Linthicum, MD*
- TP 542 **Development of an LC-NSI-HRMS/MS-PRM Method for Quantification of Attomole Levels of 7-Phenyl-Guanine to Determine the Mechanism of Benzene-Induced Cancer; Adam Zarth**; Silvia Balbo; Guang Cheng; Stephen Hecht; *University of Minnesota, Minneapolis, MN*
- TP 543 **Selective Inhibition of Cytochrome P450 Isoform of Hyperoside: Potent Effect on CYP2D6; Oh Kwang Kwon**; Miri Hong; Min Song; Sunju Kim; Ju Hee Sim; Jong-Sup Bae; Sangkyu Lee; *Kyungpook National University, Daegu, Korea*
- TP 544 **Pain Management Drug Monitoring in Urine Using HPLC/MS-MS; Jill Volken**; Thomas Doran; Paula Smith; Anita Iwanski; Don Wiebe; *University of Wisconsin Hospital and Clinics, Madison, WI*
- TP 545 **An Improved Immunosuppressant Drug Research Method based on a Novel SPLC-MS/MS System; Joseph Di Bussolo**; Christopher Esposito; Francois Espourteille; *Thermo Fisher Scientific, Franklin, MA*
- TP 546 **Comprehensive Clinical Toxicology Screening by a Novel Ion Trap MSn Workflow; Markus Meyer<sup>1</sup>**; Christoph Gebhardt<sup>1</sup>; Birgit Schneider<sup>1</sup>; Sebastian Götz<sup>1</sup>; Laura M. Huppertz<sup>2</sup>; Susanne Vogt<sup>2</sup>; Jürgen Kempf<sup>2</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Institute of Legal Medicine, University Freiburg, Freiburg, Germany
- TP 547 **High Throughput Analysis of the Polycyclic Aromatic Hydrocarbon Metabolite Phenanthrene Tetraol in Human Urine by Gas Chromatography-Tandem Mass Spectrometry; Natalie Olvera**; Claire Brookmeyer; Steven Carmella; Stephen S. Hecht; *Univ. of Minnesota Cancer Center, Minneapolis, MN*
- TP 548 **devTOX quickPredict: A Rapid LC-MS-Based Metabolite Biomarker Assay to Predict Developmental Toxicity Using Human Cells; Paul R. West**; Egnash Laura; Alan Smith; Jessica Palmer; Kevin Conard; Mark Ross; Burr Fontaine; Preeti Bais; Elizabeth Donley; Robert Burrier; *Stemina Biomarker Discovery, Madison, WI*
- TP 549 **Aristolactam N-sulfate: A Highly Reactive Metabolite of Aristolochic Acid; Irina Zaitseva**; Viktoriya Siderenko; Sivaprasad Attaluri; Francis Johnson; Arthur P. Grollman; *Charles R. Iden*; *Stony Brook University, Stony Brook, NY*
- TP 550 **Analysis of All Citric Acid Cycle Metabolites by Liquid Chromatography – Tandem Mass Spectrometry; Andrew J. Worth**; Sankha Basu; Clementina Mesaros; Nathaniel W. Snyder; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*
- TP 551 **Rapid Determination of Tramadol and N-desmethyl Tramadol in Human Urine by HPLC-MS-MS Optimized Method; Mehdi Jalali**; *Pacific Toxicology Laboratory, Chatsworth, CA*
- TP 552 **Transformation of Aflatoxin B1 in Soil; Mustafa Selim<sup>1</sup>**; James Starr<sup>2</sup>; <sup>1</sup>East Carolina University, Greenville, NC; <sup>2</sup>U.S. Environmental Protection Agency, Research Triangle Park, NC
- TP 553 **DNA Adductomics Methodology Utilizing a High Resolution Accurate Mass MS<sup>n</sup> Approach for Analysis of Human DNA Samples; Peter Villalta**; Silvia Balbo; Pramod Upadhyaya; Stephen Hecht; *University of Minnesota, Minneapolis, MN*
- TP 554 **USP<467>: Benefits of Use Headspace GC-Mass Spectrometry System; Daniele Recenti<sup>1</sup>**; Roberta Lariccia<sup>1</sup>; Ilaria Ferrante<sup>1</sup>; Luigi Motti<sup>2</sup>; <sup>1</sup>DANI, Cologno Monzese, Italy; <sup>2</sup>Dani SA, Contone, Switzerland
- TP 555 **Automated Sample Preparation for Toxicology Screenings Workflows on Linear Ion Trap Instruments; Adrian Taylor<sup>1</sup>**; Michael Jarvis<sup>1</sup>; Jesse Seegmiller<sup>1</sup>; Oscar Cabrices<sup>2</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>GERSTEL, Inc., Linthicum, MD
- TP 556 **Evaluation of Mitochondrial Function Based on the Direct Single-Cell Molecular Analysis by Mass Spectrometry; Sachiko Date<sup>1</sup>**; Kiyoko Bando<sup>2</sup>; Jiro Deguchi<sup>2</sup>; Izuru Miyawaki<sup>2</sup>; Juki Kimura<sup>2</sup>; Hitoshi Funabashi<sup>2</sup>; Tsutomu Masujima<sup>1</sup>; <sup>1</sup>Quantitative Biology Center (QBiC), Riken, Osaka, Japan; <sup>2</sup>Dainippon Sumitomo Pharma Co., Ltd., Osaka, Japan

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- TP 557 **Measurement of Thiopurine Metabolites as a Companion Diagnostic Test to the Genotypic and Phenotypic Thiopurine Methyltransferase Assays; Stacy Dee**; Yvonne Wright; Russell Grant; *LabCorp, Burlington, NC*
- TP 558 **Improved UPLC Tandem Mass Spectrometry Assay for Uridine Diphosphate Galactose-4-epimerase Deficiency; Jie Chen<sup>1</sup>**; Gail A Ditewig Meyers<sup>1</sup>; Michael J Bennett<sup>1,2</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- TP 559 **Determination of 3-Epi-25-hydroxyvitamin D2 in Human Serum Using Liquid Chromatography-Tandem Mass Spectrometry; Susan Tai**; *NIST, Gaithersburg, MD*



- TP 560 **Development of an Improved Standard Reference Material for Vitamin D Metabolites in Serum;** Karen Phinney; Mary Bedner; Susan Tai; Lane Sander; Katherine Sharpless; Stephen Wise; *National Institute of Standards and Technology, Gaithersburg, MD*
- TP 561 **Results from the Initial Comparability Studies of the NIST/NIH Vitamin D Metabolites Quality Assurance Program;** Mary Bedner; Katrice Lippa; Susan Tai; *NIST, Gaithersburg, MD*
- TP 562 **Reducing Systematic Errors in the LC-MS/MS Determination of Vitamin D;** Dietrich Volmer; Julia Aspenleiter; *Saarland University, Saarbrücken, Germany*
- TP 563 **A Novel Method for the Extraction of 1 $\alpha$ , 25-dihydroxy-Vitamin D2/D3 and Analysis Using UHPLC-MS/MS;** Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Rhys Jones<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Gavin Jones<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; *<sup>1</sup>Biotage GB Limited, Cardiff, UK; <sup>2</sup>Biotage, Charlotte, NC*
- TP 564 **The Determination of Optimum Centrifugation Parameters when Designing a Robust and Sensitive 25OH-Vitamin D Assay using UPLC/MS;** Maria Cid; Stuart Coleman; *New York Presbyterian Hospital, New York, NY*
- TP 565 **The Search for 3-Epi-25 Hydroxy Vitamin D;** Jonathan Tang; William Fraser; *University of East Anglia, Norwich, UK*
- TP 566 **Simple, Accurate Quantitation of Nicotinic Acid and Nicotinamide in Human Plasma by Rapid Protein Precipitation Using HPLC-MS/MS;** Shuguang Li; Erica Pike; *Phenomenex, Torrance, CA*
- TP 567 **Evaluation of Acylcarnitines with Dicarboxylic Acid Residues as Candidate Markers for Neurodegenerative Syndromes;** Andrea Raffaelli<sup>1</sup>; Riccardo Donzelli<sup>2</sup>; Alessandro Saba<sup>3</sup>; Adriano Carpita<sup>2</sup>; Gabriele Siciliano<sup>3</sup>; *<sup>1</sup>CNR ICCOM - UOS Pisa, Pisa, Italy; <sup>2</sup>University of Pisa, Department of Chemistry, Pisa, Italy; <sup>3</sup>University of Pisa, Department of Medicine, Pisa, Italy*
- TP 568 **Challenges in the Conversion of a Multianalyte GC-MS Method to a High-Throughput LC-MS/MS Clinical Diagnostic Assay;** Lisa Ford; Qibo Zhang; Carolyn Sheffield; Jonathan McDunn; Robert Wolfert; *Metabolon, Research Triangle Park, NC*
- TP 569 **Simultaneous and Fast Analysis of Amino Acids, Acylcarnitines and Orotic Acid in Dried Blood Spots by Triple Quadrupole LC-MS/MS;** Scott Kuzdzal<sup>1</sup>; Hironori Kobayashi<sup>2</sup>; Toshikazu Minohata<sup>3</sup>; Yuki Hasegawa<sup>2</sup>; Ichiro Hirano<sup>3</sup>; Seiji Yamaguchi<sup>2</sup>; *<sup>1</sup>Shimadzu Scientific Instruments, Inc., Columbia, MD; <sup>2</sup>Shimane University Faculty of Medicine, Izumo, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan*
- TP 570 **Analysis of Dried Blood Spot Samples by High Resolution Mass Spectrometry – Validation of a Novel Method for Newborn Screening;** Julia Denes<sup>1</sup>; Steven L. Robinette<sup>1</sup>; Eszter Szabo<sup>2</sup>; Ildiko Szatmari<sup>2</sup>; Laszlo Szonyi<sup>2</sup>; Ernst W. Rauterberg<sup>3</sup>; Zoltan Takats<sup>1</sup>; *<sup>1</sup>Imperial College London, London, UK; <sup>2</sup>1st Dept. of Pediatrics, Semmelweis University, Budapest, Hungary; <sup>3</sup>Hesse Child Health Centre, Giessen, Germany*
- TP 571 **Determination of Desmosterol, Campesterol, Cholesterol, and  $\beta$ -sitosterol in Plasma Utilizing LC-MS/MS Technology in Clinical Diagnostics;** Jim Bruton; Joseph McConnell; Daniel Hoefner; Tara Dall; Thomas Dayspring; *Health Diagnostic Laboratory, Richmond, VA*
- TP 572 **Characterizing Blood Bile Alcohols in Cerebrotendinous Xanthomatosis (CTX); Promising Disease Markers Detectable in a Dried Bloodspot LC-ESI-MS/MS Test for CTX;** Andrea E DeBarber; Robert D Steiner; *Oregon Health & Science University, Portland, OR*
- TP 573 **Simplified Extraction of 3 Steroids from Biological Fluid for LC-MS/MS Analysis;** Silvia Bächer<sup>1</sup>; Michael Vogeser<sup>1</sup>; Christine Lehmann<sup>2</sup>; Robert Wohleb<sup>2</sup>; Roland Geyer<sup>2</sup>; *<sup>1</sup>Clinical Chemistry, University Hospital Munich, Munich, Germany; <sup>2</sup>Tecan Schweiz AG, Männedorf, Switzerland*
- TP 574 **Performance of the Absolute/DQ<sup>®</sup> Stero17 Kit on ABSciex, Waters and Thermo Scientific Triplequad Mass Spectrometers for Steroid Hormones Analysis;** Hai Pham Tuan; Doreen Kirchberg; Therese Koal; *BIOCRATES Life Sciences, Innsbruck, Austria*
- TP 575 **Quantification of Immunosuppressants by LC-MS/MS Ion Trap Analysis with a New Smart MRM Mode and Compound Verification by Library Search;** Andrea Kiehne; Birgit Schneider; Markus Peer; Markus Meyer; *Brüker Daltonik GmbH, Bremen, Germany*
- TP 576 **Cross Validation between LDTD-MS/MS and LC-MS/MS for the Determination of 4 Immunosuppressant Drugs in Whole Blood;** Gregory Blachon<sup>1</sup>; Kamisha Johnson-Davis<sup>2</sup>; Jean Lacoursiere<sup>1</sup>; Pierre Picard<sup>1</sup>; Serge Auger<sup>1</sup>; Annick Dion-Fortier<sup>1</sup>; *<sup>1</sup>Phytronix Technologies, Québec, Canada; <sup>2</sup>ARUP Laboratories, Salt Lake City, UT*
- TP 577 **High-Throughput Determination of 25-OH-Vitamin D2 and D3 in Plasma Using LDTD-MS/MS with Differential Mobility Spectrometry in 9 seconds Per Sample;** Alex Birsan<sup>1</sup>; Pierre Picard<sup>1</sup>; Gregory Blachon<sup>1</sup>; Michael Jarvis<sup>2</sup>; Serge Auger<sup>1</sup>; Adrian Taylor<sup>2</sup>; Jean Lacoursiere<sup>1</sup>; *<sup>1</sup>Phytronix Technologies Inc., Quebec, Canada; <sup>2</sup>AB SCIEX, Concord, Canada*
- Environmental Analysis:  
Pharmaceuticals and Pesticides, 578 – 607**
- TP 578 **A Strategy for an automated Unknown Screening Approach on Environmental Samples Using HRAM Mass Spectrometry;** Olaf Scheibner<sup>1,3</sup>; Maciej Bromirski<sup>1,3</sup>; Patricia van Baar<sup>2</sup>; Florian Wode<sup>2</sup>; Uwe Dünnebier<sup>2</sup>; Kristi Akervik<sup>1,3</sup>; Jamie Humphries<sup>1,3</sup>; *<sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Berliner Wasserbetriebe, Berlin, Germany; <sup>3</sup>Thermo Fisher Scientific, Austin, TX*
- TP 579 **Screening Environmental Samples for a Diverse Range of Compound Classes/Structures with Accurate Mass LC-MS and an Integrated Scientific Information System;** Gareth Cleland; Lauren Mullin; Claude Mallet; Jennifer Burgess; *Waters Corporation, Milford, MA*
- TP 580 **Ultra-sensitive Detection of Pharmaceutical and Personal Care Products (PPCP's) in Water with an Integrated On-Line Extraction (OLE)-UHPLC-MS/MS System;** Zicheng Yang; Helen Sun; Kefei Wang; *Bruker, Fremont, CA*
- TP 581 **Determination of Pharmaceuticals by Direct Aqueous Injection-HPLC/MS/MS in Source and Drinking Waters from 25 Municipal Treatment Plants;** Edward T. Furlong<sup>1</sup>; Mary C. Noriega<sup>1</sup>; Susan T. Glassmeyer<sup>2</sup>; Dana W. Kolpin<sup>3</sup>; *<sup>1</sup>National Water Quality Lab, U.S. Geological Survey, Denver, CO; <sup>2</sup>U.S. Environmental Protection Agency, Cincinnati, OH; <sup>3</sup>U.S. Geological Survey, Iowa City, IA*
- TP 582 **Determination of Pharmaceutical Compounds from Drinking and Surface Water at Low ng/L Levels Using Direct Aqueous Injection Triggered MRM LC-QQQ-MS;** László Toelgyesi<sup>1</sup>; Andreas Wanke<sup>2</sup>; Thomas Glauner<sup>1</sup>; Susanne Soelter<sup>1</sup>; *<sup>1</sup>Agilent Technologies, Waldbronn, Germany; <sup>2</sup>SMUL Sachsen, Nossen, Germany*
- TP 583 **Degradation Processes of Environmentally Relevant Pharmaceuticals;** Linyan Zhu<sup>1,2</sup>; Beatrix Santiago-Schuebel<sup>1</sup>; Agnieszka Kraj<sup>3</sup>; Zhiliang Zhu<sup>2</sup>; Yanling Qiu<sup>2</sup>; Stephan Kueppers<sup>1</sup>; *<sup>1</sup>Research Center Jülich, ZEA-3, Jülich, Germany; <sup>2</sup>Tongji University, Shanghai, China; <sup>3</sup>Antec, Zoeterwoude, The Netherlands*



- TP 584 **Natural Attenuation of Emerging Contaminants in the Critical Zone: Time of Flight Mass Spectrometry Measurement Approaches;** Rachel Maxwell<sup>1</sup>; Leif Abrell<sup>1</sup>; Andrea Conine<sup>2</sup>; Shane Snyder<sup>1</sup>; Jon Chorover<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Skidmore College, Saratoga Springs, NY
- TP 585 **LC-MS/MS for Screening and Quantifying Anti-Cancer Drugs and Metabolites in Waste Water Rejected in Mediterranean Sea;** Thérèse Schembri<sup>1</sup>; Mikael Levi<sup>2</sup>; François Gray<sup>1</sup>; Stéphane Moreau<sup>2</sup>; Claude Villard<sup>1</sup>; Pierre Boissery<sup>3</sup>; Daniel Lafitte<sup>1</sup>; <sup>1</sup>Aix Marseille Université, Inserm UMR 911 CRO2, Marseille, France; <sup>2</sup>Shimadzu France, Noisiel, France; <sup>3</sup>Agence de l'Eau Rhône Méditerranée & Corse, Marseille, France
- TP 586 **Determinaiton of Non-Steroidal Anti-Inflammatory Drugs in Environmental Water by Dispersive Liquid-Liquid Microextraction Coupled with Liquid Chromatography-Tandem Mass Spectrometry;** Shih-Shan Tai; Chung-Yu Chen; Maw-Rong Lee; National Chung-Hsing University, Taichung, Taiwan
- TP 587 **Removal of Matrix Effects Using Ion-Exchange SPE during Analysis of veterinary Antibiotics Present in Manure by LDTD-APCI-MS/MS;** Morgan Sollic<sup>1,2</sup>; Daniel Massé<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>Université de Montréal, Montréal, Canada; <sup>2</sup>Agriculture and Agri-Food Canada, Sherbrooke, Canada
- TP 588 **Identification and Structural Elucidation of Ozonation Transformation Products of Emerging Contaminants;** Pedro A. Segura; Angela Rodayan; Pearl Kaplan; Karim Saadi; Rachel Benoit; Viviane Yargeau; McGill University, Montréal, Canada
- TP 589 **Routine, Targeted and Non-Targeted Analysis of Environmental Contaminants of Emerging Concern – Development and Validation of a UHPLC-Orbitrap MS Method;** Paul Yang<sup>1</sup>; Tung Vi Nguyen<sup>2</sup>; Vince Pileggi<sup>1</sup>; Kristi Akervik<sup>3</sup>; Chunyan Hao<sup>1</sup>; Xiaoming Zhao<sup>1</sup>; Serei Thach<sup>1</sup>; Jennifer Newman<sup>1</sup>; Yafang Lu<sup>1</sup>; Sonya Kleywegt<sup>1</sup>; Shahram Tabe<sup>1</sup>; Ramin Farnood<sup>2</sup>; Charles Yang<sup>3</sup>; Jonathan Beck<sup>3</sup>; Maciej Bromirski<sup>3</sup>; Dipankar Ghosh<sup>3</sup>; <sup>1</sup>Ministry of the Environment, Etobicoke, Canada; <sup>2</sup>University of Toronto, Toronto, Canada; <sup>3</sup>Thermo Scientific, San Jose, CA
- TP 590 **Simultaneous Determination of Cationic and Anionic Pharmaceuticals Using an Online SPE LC and a High-Speed Polarity Switching ESI MS/MS;** Mitsuha Yoshikane<sup>1</sup>; Tairo Ogura<sup>2</sup>; Ichiro Hirano<sup>2</sup>; Yayoi Suzuki<sup>3</sup>; Shoji Nakayama<sup>3</sup>; <sup>1</sup>The University of Tokyo, Kashiwa, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>National Institute for Environmental Studies, Tsukuba, Japan
- TP 591 **Results of a National Scale Survey Investigating the Occurrence of Prescription Pharmaceuticals Present in Wastewater Discharges;** Angela Batt; Mitchell Kostich; Jim Lazorchak; U.S. Environmental Protection Agency, Cincinnati, OH
- TP 592 **Paper Spray Ionization of Herbicides from Dried Blood Spot Cards;** Steven L. Reeber; Sneha Gadi; Gary L. Glish; University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 593 **Determination of Glucocorticoid- And Mineralocorticoid-Active Compounds in Waste and River Waters by LC-MS/MS and in vitro Testing;** Adrian A Ammann<sup>1</sup>; Petra Macikova<sup>2</sup>; Ksenia J Groh<sup>1</sup>; Kristin Schirmer<sup>1</sup>; Marc J.-F. Suter<sup>1</sup>; <sup>1</sup>Eawag, Dübendorf, Switzerland; <sup>2</sup>Masaryk University, Brno, CZ
- TP 594 **Quantitative Determination of Antidepressants by Solvent Microextraction LC ESI-MS/MS in Biosolids Destined for Land Application;** Melissa M. Schultz; Lydia Niemi; Madigan Murphy; Katherine Stencel; The College of Wooster, Wooster, OH
- TP 595 **Analysis of Targeted and Non-Targeted Identified Contaminants in Storm Water Retention Ponds Using LC-HRMS with Online Solid Phase Extraction;** Jonathan Beck<sup>1</sup>; P. Lee Ferguson<sup>2</sup>; Gordon Getzinger<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Duke University, Durham, NC
- TP 596 **Trace Level Analysis of Herbicides in Drinking and Surface Water by Online-SPE LC/Triple Quadrupole MS to the Lower ppt Range;** Edgar Naegele; Agilent Technologies, Waldbronn, Germany
- TP 597 **Analysis of Diquat and Paraquat Using UHPLC-MS/MS and UHPLC-Orbitrap MS – Method Development, Matrix Effects and Performance;** Paul Yang<sup>1</sup>; Chunyan Hao<sup>1</sup>; Franca Morra<sup>1</sup>; Xiaoming Zhao<sup>1</sup>; Xiaodong Liu<sup>2</sup>; Charles Yang<sup>2</sup>; Jonathan Beck<sup>2</sup>; Maciej Bromirski<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; <sup>1</sup>Ministry of the Environment, Etobicoke, Canada; <sup>2</sup>Thermo Scientific, San Jose, CA
- TP 598 **Multi-Residue Method for the Target Analysis of Pesticides in Crops by Liquid Chromatography-Tandem Mass Spectrometry;** Nam-Sun Kim; SeongSoo Park; Hwa-Mi Lee; Mi-Jung Noh; Hyun-Sook Lee; Sungll Kim; SeungYoung Park; KeunHwa Choi; Dae Hyun Cho; Regional Food and Drug Administration, Incheon, Korea
- TP 599 **Rapid and Simultaneous Identification and Quantitation of Pesticides in different Matrices Using High Sensitive LC/MS/MS;** Karsten Ott<sup>1</sup>; Ugo Chiuminatto<sup>2</sup>; Sebastian Fabritz<sup>2</sup>; Jianru Stahl-Zeng<sup>2</sup>; <sup>1</sup>bilacon GmbH, Berlin, Germany; <sup>2</sup>AB Sciex, Darmstadt, Germany
- TP 600 **Sensitive Quantification of Pesticides at Low ppt Levels in Drinking Water Using High Performance Triple Quadrupole Mass Spectrometer;** Guifeng Jiang; Jia Wang; Marcus Miller; Terry Zhang; Jonathan Beck; Charles Yang; Dipankar Ghosh; Thermo Fisher Scientific, San Jose, CA
- TP 601 **High Throughput Analysis of Pesticide Residues in Raw Agricultural Commodities;** Leah Riter; Chad Wujcik; Monsanto, St. Louis, MO
- TP 602 **Improved Screening for 500 Pesticides in Matrix Using a LC-triple Quadrupole Mass Spectrometer;** Marcus Miller; Mary Blackburn; Dipankar Ghosh; Oleg Silva; ThermoFisher Scientific, San Jose, CA
- TP 603 **High-Throughput Simultaneous Analysis of Pesticides by Supercritical Fluid Chromatography/Orbitrap Mass Spectrometry;** Megumi Ishibashi<sup>1</sup>; Miho Sakai<sup>1,2</sup>; Takashi Ando<sup>2</sup>; Tomoko Hamasaka<sup>3</sup>; Shigeru Sakamoto<sup>3</sup>; Eiichiro Fukusaki<sup>1</sup>; Takeshi Bamba<sup>1</sup>; <sup>1</sup>Graduate School of Engineering, Osaka University, Suita, Japan; <sup>2</sup>Miyazaki Agricultural Research Institute, Miyazaki, Japan; <sup>3</sup>Thermo Fisher Scientific, Yokohama, Japan
- TP 604 **On-line SPE Coupled to UHPLC MS/MS for Analysis of Multiple TOCs in Water Using Simultaneous Positive and Negative Electrospray Ionization;** Tarun Anumol<sup>1</sup>; Sheher Mohsin<sup>2</sup>; Sylvain Merel<sup>1</sup>; Shane Snyder<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Agilent Technologies, Schaumburg, IL
- TP 605 **Simultaneous Screening Target and Non-Target Pesticides in Vegetable by GC/Q-TOF MS with Accurate Mass Ion Formula Database and Deconvolution Technique;** Fang Zhang<sup>1</sup>; Yinlong Guo<sup>1</sup>; Chongtian Yu<sup>2</sup>; zhe Cao<sup>2</sup>; Zhixu Zhang<sup>2</sup>; <sup>1</sup>Shanghai insititue of organic chemistry, Shanghai, China; <sup>2</sup>Agilent Technologies(China) Co., Ltd., Shanghai, China
- TP 606 **High Speed TOFMS for GC and GCxGC Endocrine Disrupting Compounds Characterization in Biological Samples for Environmental Risk Factors Assessment;** Daniela Cavagnino<sup>1</sup>; Antonella Siviero<sup>1</sup>; Alessandra Mantegazza<sup>1</sup>; Veronica Termopoli<sup>2</sup>; Pierangela Palma<sup>2</sup>; Giorgio Famiglini<sup>2</sup>; Anna Maria Lavezzi<sup>3</sup>; Luigi Matturri<sup>3</sup>; Achille Cappiello<sup>2</sup>; <sup>1</sup>DANI Instruments, Cologno Monzese,

Italy; <sup>2</sup>LC-MS Laboratory, DiSTeVA, University of Urbino, Urbino, Italy; <sup>3</sup>Research Center "Lino Rossi", University of Milan, Milan, Italy

- TP 607 **A Novel Screening Method for Anthropogenic Sewage Pollutants in Waste Water, Ground Water and Drinking Water Samples by LC-HRAM Analysis;** Sebastian Westrup; Nick Duczak; Michal Godula; *Thermo Fisher Scientific, San Jose, CA*

#### Elemental Analysis, 608 – 618

- TP 608 **Development of Capillary Electrophoresis Inductively Coupled Plasma Mass Spectrometry for Quantitative Analysis of Phosphorylated Peptide with Metrological Traceability;** Kyoung-Seok Lee<sup>1</sup>; Jinil Kim<sup>2</sup>; Yong-Hyeon Yim<sup>1</sup>; Su Kyeong Bang<sup>2</sup>; Tae Kyu Kim<sup>2</sup>; <sup>1</sup>KR/ISS, Yuseong-Gu, Korea; <sup>2</sup>Department of Chemistry, Pusan National University, Busan, Korea
- TP 609 **Optimizing Cold Cell LA-ICP-MS Conditions for the Analysis of Elemental Localization and Imaging of Biological Tissues;** Jason Hamilton; William Hoffman; Guido Verbeck; *University of North Texas, Denton, TX*
- TP 610 **Reducing Matrix Effect through Femtosecond Laser Ablation and Ionization;** Bochao Zhang; Wei Hang; *Xiamen University, Xiamen, China*
- TP 611 **Development of a Method Based on Tandem Inductively Coupled Plasma Mass Spectrometry for Determination of Calcium/Phosphorus Ratio in Teeth Samples;** Mohamed Amr<sup>1</sup>; Saeed Al-Meer<sup>1</sup>; Khalid Al-Saad<sup>1</sup>; Elham Fawzi<sup>2</sup>; <sup>1</sup>Qatar University, Doha, Qatar; <sup>2</sup>The Queen Dental Center, Doha, Qatar
- TP 612 **The State of the Matter: Providing Insight through Chemical Speciation;** Craig Westphal; *DuPont, Wilmington, DE*
- TP 613 **Analysis of Phosphorus in Some Environmental Samples by ESI - Mass Spectrometry and ICP - Mass Spectrometry;** Jerzy Mierzwa; *Tennessee State University, Nashville, TN*
- TP 614 **Determination of Iopromide in Environmental Waters by Ion Chromatography-ICP-MS;** Armando Durazo; Tarun Anumol; Shane A. Snyder; *University of Arizona, Tucson, AZ*
- TP 615 **Redox Speciation Analysis of Iron by Ion-Chromatography and ICP-MS Based on Speciated Isotope Dilution Mass Spectrometry (EPA Method 6800);** Mesay M. Wolle<sup>1</sup>; Timothy Fahrenholtz<sup>2</sup>; G. M. Mizanur Rahman<sup>2</sup>; Matt Pamuku<sup>2</sup>; H. M. "Skip" Kingston<sup>1</sup>; <sup>1</sup>Duquesne University, Pittsburgh, PA; <sup>2</sup>Applied Isotope Technologies, Pittsburgh, PA
- TP 616 **Rapid Detection of Metal Contaminants Using Ambient Mass Spectrometry;** Jamie Nizzia; Christopher Mulligan; *Illinois State University, Normal, IL*
- TP 617 **Ultra-fast LDTD-APCI-MS/MS Analysis of Steroid Hormones Oxidized in Surface Water Using Potassium Permanganate;** Paul Fayad<sup>1</sup>; Michele Prevost<sup>2</sup>; Sebastien Sauve<sup>1</sup>; <sup>1</sup>Universite de Montreal, Montreal, Canada; <sup>2</sup>Ecole Polytechnique de Montreal, Montreal, Canada
- TP 618 **Simultaneous Analysis of Heavy-Metals by ICP-MS: Efficiency of Clay, TiO<sub>2</sub> and SiO<sub>2</sub> Nanoparticles for the Removal of Toxic-Metals from Water;** Khalid A. Al-Saad<sup>1</sup>; Mohamed A. Amr<sup>1</sup>; Saeed H. Almeer<sup>1</sup>; Aisha N. Alsaygh<sup>1</sup>; Esraa Y. Abbas<sup>1</sup>; Mohammed A Abdul-Hakim<sup>1</sup>; Mohammed S. Muthana<sup>1</sup>; Siham S. Hersi<sup>1</sup>; Noor M. Bader<sup>1</sup>; Ahmed A. Ramadan<sup>1</sup>; Sakthivel Sundaresan<sup>2</sup>; Narendra Agnihotra<sup>2</sup>; <sup>1</sup>Qatar University, Doha, Qatar; <sup>2</sup>TCE QSTP-LLC, Doha, Qatar

#### Ion Mobility Applications, 619 – 661

- TP 619 **Using Ion Mobility Spectrometry to Screen Small Molecule Inhibitors for the Alzheimer's Disease Aβ42 Protein;** Xueyun Zheng; Michael Bowers; *University of California Santa Barbara, CA*
- TP 620 **Separation of Isomeric Cationized Diterpene Glycosides from *Stevia Rebaudiana* Bertoni Leaves by Traveling Wave Ion Mobility Mass Spectrometry (TWIM-MS);** Alessandra Tata<sup>1</sup>; Giovana Anceschi Bataglion<sup>1</sup>; Gustavo Henrique Martins Ferreira Souza<sup>2</sup>; Marcos Nogueira Eberlin<sup>1</sup>; <sup>1</sup>University of Campinas UNICAMP, Campinas (SP), Brazil; <sup>2</sup>MS Applications & Develop Lab, Waters Corporation, Sao Paulo, Brazil
- TP 621 **Separation and Characterization of Polymeric Architectures by Matrix Assisted Ionization Vacuum (MAIV)-Ion Mobility Spectrometry (IMS)-Mass Spectrometry (MS);** Lorelie Imperial<sup>1</sup>; Barbara Larsen<sup>2</sup>; Scott Grayson<sup>3</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>Department of Chemistry, Wayne State University, Detroit, MI; <sup>2</sup>The DuPont Company, Wilmington, DE; <sup>3</sup>Department of Chemistry, Tulane University, New Orleans, LA
- TP 622 **Ion Mobility-Mass Spectrometry Analysis of Globular Electrosprayed Polymer Ions Obtained via Charge Control;** Ernesto Criado Hidalgo<sup>1,2</sup>; Juan Fernández García<sup>1</sup>; Juan Fernández de la Mora<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>SEADM S.L., Boecillo, Spain
- TP 623 **Characterization of Amino Acid and Peptide Isomers Using Traveling Wave Ion Mobility Spectrometry-Mass Spectrometry;** Tawnya Flick; Chul Yoo; Iain Campuzano; Michael Bartberger; *Amgen, Inc., Thousand Oaks, CA*
- TP 624 **Spontaneous Cold Ionization and Characterization of Molecules from Surfaces by Matrix Assisted Ionization Vacuum Ion Mobility Spectrometry Mass Spectrometry;** Ellen D. Inutan; Sarah Trimpin; *Wayne State University, Detroit, MI*
- TP 625 **Hadamard Transform Atmospheric Pressure Ion Mobility Time-of-Flight Mass Spectrometry for Complex Sample Analysis;** Xing Zhang<sup>1</sup>; William Siems<sup>1</sup>; Stephan Graf<sup>2</sup>; Richard Knochenmuss<sup>2</sup>; Herbert Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Tofwerk AG, Thun, Switzerland
- TP 626 **Determination and Characterization of PFOS in Environmental Samples Using Travelling Wave Ion Mobility Mass Spectrometry;** Michael McCullagh<sup>1</sup>; Kendon Graham<sup>1</sup>; Dominic Roberts<sup>1</sup>; Kieran J. Neeson<sup>1</sup>; Jeff Goshawk<sup>1</sup>; Leonard Dillon<sup>1</sup>; Mike Hodgkinson<sup>1</sup>; Ingrid Ericson<sup>2</sup>; Bert van Bavel<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>MTM Research Centre, Örebro University, Örebro, Sweden
- TP 627 **A Novel Approach to the Reduction of False Positive and Negative Identifications in Screening of Pesticide Residues in Food Analysis;** Séverine Goscinnny<sup>1</sup>; Michael McCullagh<sup>2</sup>; Kieran Neeson<sup>2</sup>; Jeff Goshawk<sup>2</sup>; David Eatough<sup>2</sup>; Sara Stead<sup>2</sup>; Ramesh Rao<sup>2</sup>; Dominic Roberts<sup>2</sup>; <sup>1</sup>Scientific Institute of Public Health, Brussels, Belgium; <sup>2</sup>Waters, Manchester, UK
- TP 628 **Effective Analysis of Explosives with IMS-MS Using Corona Discharge Ionization;** Jihyeon Lee<sup>1</sup>; Soo Gyeong Cho<sup>2</sup>; Eun Mee Goh<sup>2</sup>; Sungman Lee<sup>3</sup>; Sung-Suk Koh<sup>3</sup>; Jeongkwon Kim<sup>1</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Agency for Defense Development, Daejeon, South Korea; <sup>3</sup>Sensor Tech Inc., Kyunggi-Do, South Korea
- TP 629 **Ion Evaporation from Amine-Nitrate Nanodrops Yields Singly-Charged "Magic" Octamer Cluster-Ion;** Juan Fernández García; Juan Fernández de la Mora; *Yale University, New Haven, CT*



- TP 630 **Characterization of Amyloid  $\beta$  / Neuropeptide interactions using Ion Mobility - Mass Spectrometry and Site-Direct Mutagenesis;** Molly T. Soper; Brandon T. Ruotolo; *Department of Chemistry, University of Michigan, Ann Arbor, MI*
- TP 631 **The Effects of Polar Side Chains and Multiple Charges on Conformational Preferences of Peptide Ions;** Chunying Xiao; David H. Russell; *Texas A&M University, College Station, Texas*
- TP 632 **Ion Cluster Effects on Differential Mobility as a Function of ESI Flow Rate;** Thomas Covey; Bradley Schneider; Jay Corr; *AB SCIEX, Concord, Canada*
- TP 633 **Ion Mobility Study of Isomeric Carbohydrates as their Group I Metal Cation Adducts: Evidence for Isomer-Specific Conformations;** Yuting Huang; Eric D. Dodds; *University of Nebraska-Lincoln, Lincoln, NE*
- TP 634 **Separation and Identification of Isomeric Glycans by Trapped Ion Mobility Spectrometry-Fourier Transform Mass Spectrometry;** Yi Pu<sup>1</sup>; Mark Ridgeway<sup>2</sup>; Melvin Park<sup>2</sup>; Cheng Lin<sup>3</sup>; Catherine E Costello<sup>1,3</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*; <sup>3</sup>*Boston University School of Medicine, Boston, MA*
- TP 635 **High Pressure Liquid Chromatography of Sugars and Pharmaceuticals using a single Ambient Pressure Ion Mobility LC Detector;** Stephen Davila; Cheng-Hui Yuan; Hermann Wollnik; Gary Eiceman; *New Mexico State University, Las Cruces, NM*
- TP 636 **Origin of Conformers Produced During Electrospray Ionization Revealed by Cryogenic Ion Mobility-Mass Spectrometry: A Benchmark Study Using Substance P;** Joshua A. Silveira<sup>1</sup>; Kyle L. Fort<sup>1</sup>; Nicholas A. Pierson<sup>2</sup>; David E. Clemmer<sup>2</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>*Texas A&M University, College Station, TX*; <sup>2</sup>*Indiana University, Bloomington, IN*
- TP 637 **Analyzing/Separating Isomers, Conformers, Isobaric Compounds and Other Closely Related Small Molecules: An IMS Case Study;** Filip Lemiere<sup>1,2</sup>; Frank Sobott<sup>1,2</sup>; Jasper Boschmans<sup>1</sup>; Eliane Goossens<sup>1</sup>; Debbie Dewaele<sup>1</sup>; <sup>1</sup>*Biomolecular Mass Spec., University of Antwerp, Antwerp, Belgium*; <sup>2</sup>*Centre for Proteomics, University of Antwerp, Antwerp, Belgium*
- TP 638 **Characterizing Conformation of Peptides in Low Dielectric Media Using Ion Mobility Mass Spectrometry;** Suk-Joon Hyung; Matthew Teague; Justin Stroh; Michael Shapiro; Xidong Feng; *Pfizer Worldwide Research, Groton, CT*
- TP 639 **Exploring nanoESI-DMS-MS/MS as a Rapid Quantitative Platform;** Amol Kifle<sup>1</sup>; Stephen Coy<sup>1</sup>; Adam Hall<sup>2</sup>; Sunita Yadav<sup>1</sup>; James Glick<sup>1</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Boston University, School of Medicine, Boston, MA*
- TP 640 **Improved Accuracy of Isobaric Tagging in Quantitative Proteomics Using High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS);** Eric Bonnell<sup>1</sup>; Dave Barnett<sup>2</sup>; Christelle Pomiès<sup>1</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montreal, Canada*; <sup>2</sup>*Atlantic Cancer Research Institute, Moncton, Canada*
- TP 641 **The Effects of Protein Glycation on Structural Dynamics of  $\alpha$ B-Crystallin;** Weston Struwe; Georg Hochberg; Justin Benesch; *University of Oxford, Oxford, UK*
- TP 642 **Separation and Relative Quantitation of Complex Lipid Regioisomers in Biological Extracts using Differential Mobility Spectrometry;** J. Larry Campbell<sup>1</sup>; Eva Duchoslav<sup>1</sup>; J. C. Yves Le Blanc<sup>1</sup>; Chris M. Lock<sup>1</sup>; Alan T. Maccarone<sup>2</sup>; Stephen J. Blanksby<sup>2</sup>; Todd W. Mitchell<sup>2</sup>; <sup>1</sup>*AB SCIEX, Concord, Canada*; <sup>2</sup>*University of Wollongong, Wollongong, NSW, Australia*
- TP 643 **Hofmeister Salts Recover a Misfolded Multiprotein Complex for Subsequent Structural Measurements in the Gas Phase;** Linjie Han; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- TP 644 **Combined Crosslinking and Ion Mobility-Mass Spectrometry for Structural Analysis of Protein Complexes;** Billy Clifford-Nunn; Linjie Han; Yueyang Zhong; Philip Andrews; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- TP 645 **Exploring the Potential of Ion Mobility-Mass Spectrometry in Protein Tyrosine Kinase Inhibitor Discovery;** Jessica N. Rabuck<sup>1</sup>; Matthew Soellner<sup>2</sup>; Brandon T. Ruotolo<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Michigan, Ann Arbor, MI*; <sup>2</sup>*College of Pharmacy, University of Michigan, Ann Arbor, MI*
- TP 646 **A Robotically-sampled Electrospray Ion Mobility-Mass Spectrometry Protocol for Structural Proteomics;** Yueyang Zhong; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- TP 647 **Structural Analysis of Transmembrane Spanning Peptides by Drift Tube Based Ion-Mobility Spectrometry;** Christian Klein; Christine Miller; Ruwan Kurulugama; Alexander Mordehai; Bill Barry; George Stafford; *Agilent Technologies, Santa Clara, CA*
- TP 648 **Probing Secondary Structure of Insulin B-chain by MS-CID-IM-MS;** Nathanael F Zinnel; David H. Russell; *Texas A&M University, College Station, TX*
- TP 649 **Insight into the Structure of Peptoids and Thioamide-Containing Peptoids by Ion-Mobility Mass Spectrometry (IMS);** Magdalena Zimnicka; *Institute of Organic Chemistry, PAS, Warsaw, Poland*
- TP 650 **Ion Mobility-Mass Spectrometry and Molecular Dynamics Simulations Reveal Structural Changes of Metallothionein: The Effects of Metal Binding on Conformation;** Shu-Hua Chen; Liuxi Chen; David Russell; *Texas A&M University, College Station, TX*
- TP 651 **Conformation and Binding Differences between Chemokine Analogs and Heparin as Determined by Ion Mobility Mass Spectrometry;** Youjin Seo; Christian Bleiholder<sup>2</sup>; Armann Andaya<sup>1</sup>; Julie Leary<sup>1</sup>; <sup>1</sup>*UC Davis, Davis, CA*; <sup>2</sup>*UC Santa Barbara, Santa Barbara, CA*
- TP 652 **Applying a High Throughput IMS-QTOF MS Platform to Complex Samples for Increased Molecular Coverage;** Erin Baker<sup>1</sup>; Kristin Burnum-Johnson<sup>1</sup>; Yehia Ibrahim<sup>1</sup>; Daniel Orton<sup>1</sup>; Elizabeth Torres<sup>1</sup>; William Danielson<sup>1</sup>; Kevin Crowell<sup>1</sup>; Matthew Monroe<sup>1</sup>; Gordon Slys<sup>2</sup>; Mary Lipton<sup>1</sup>; Thomas Metz<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Alex Mordehai<sup>2</sup>; Ed Darland<sup>2</sup>; George Stafford<sup>2</sup>; Gordon Anderson<sup>1</sup>; Richard Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- TP 653 **Structural Characterization of Disulfide-Bridged-Peptides;** Philippe Massonnet<sup>1</sup>; Loïc Quinton<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Nicolas Gilles<sup>2</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>*Laboratory of Mass Spectrometry, Ulg, Liège, Belgium*; <sup>2</sup>*CEA/DSV/iBiTec-S/SIMOPRO, Gif sur Yvette, France*
- TP 654 **Investigation of the Prebiotically Plausible Formation of Water-soluble Polyesters by Traveling Wave Ion Mobility-Mass Spectrometry;** Manshui Zhou<sup>1</sup>; Irena Mamajanov<sup>1</sup>; Francis Joseph Schork<sup>1</sup>; Ramanarayanan Krishnamurthy<sup>2</sup>; Martha A Grover<sup>1</sup>; Nicholas V. Hud<sup>1</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Scripps Research Institute, La Jolla, CA*
- TP 655 **Isomeric Separation and Structure Characterization of Polar Compounds in Petroleum by traveling Wave Ion Mobility Mass Spectrometry;** Priscila M. Lalli<sup>1,2</sup>; David C. Podgorski<sup>1,3</sup>; Yuri E. Corilo<sup>1,3</sup>; Marcos N. Eberlin<sup>2</sup>;



- Ryan P. Rodgers<sup>1,3</sup>; Alan G. Marshall<sup>1,4</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Thomson MS Laboratory, University of Campinas, Campinas, Brazil; <sup>3</sup>Florida State University Future Fuels Institute, Tallahassee, FL; <sup>4</sup>Florida State University, Department of Chemistry, Tallahassee, FL
- TP 656 **Global Peptide Collision Cross-section Profiling on a Travelling Wave Ion Mobility Mass Spectrometer;** Christopher B. Lietz; Chenxi Jia; Lingjun Li; *University of Wisconsin, Madison, WI*
- TP 657 **Collision Cross Sections and Reduced Mobilities of Endogenous Steroids in a Drift Tube IM-MS Using Nitrogen Bath Gas;** Christopher Crutchfield<sup>1</sup>; Stephanie Cologne<sup>1</sup>; Peter Backlund<sup>1</sup>; Christian Klein<sup>2</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Alex Mordehai<sup>2</sup>; Alfred L. Yergey<sup>1</sup>; <sup>1</sup>NIH, Columbia, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 658 **Influence of Drift Gas in the Separation of Hydroxybenzoic Acid Isomers (tautomers) via Traveling Wave Ion Mobility Mass Spectrometry (TWIM-MS);** Renan S. Galaverna; Giovana A. Bataglion; Gabriel Heerdt; Nelson H. Morgon; Marcos N. Eberlin; *State university of campinas, Campinas, Brasil*
- TP 659 **The Effect of Ion Temperature on the Conformation(s) of Gas-Phase Peptide Ions: An Ion Mobility-Mass Spectrometry Study;** Kyle L. Fort; Joshua A. Silveira; David H. Russell; *Texas A&M University, College Station, TX*
- TP 660 **Theoretical Investigation on the Ion Mobility Separation of Metal-Coordinated Oligosaccharide Isomers;** Yiqun Huang<sup>1</sup>; Erin Baker<sup>2</sup>; Catherine E. Costello<sup>1</sup>; Cheng Lin<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 661 **A Novel Approach to Improve Quantitation Accuracy and Proteome Coverage Upon Application of TWIMS (Travelling Wave Ion Mobility Mass Spectrometry);** Pavel Shliha; Laurent Gatto; Nick Bond; Michael Muelleder; Floriana Capuano; Markus Ralser; Kathryn Lilley; *University of Cambridge, Cambridge, UK*
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- TP 662 **In situ Analysis of Single Plant Cells by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation;** Linwen Zhang<sup>1</sup>; Bindesh Shrestha<sup>1</sup>; Éric Maréchal<sup>2</sup>; Denis Falconet<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, DC; <sup>2</sup>Université Joseph Fourier Grenoble, Grenoble, France
- TP 663 **Metabolic Analysis of Small Cell Populations by Plume Collimation in LAESI Mass Spectrometry with Ion Mobility Separation;** McKenzie Floyd; Akos Vertes; George Washington University, Washington, DC
- TP 664 **Metabolomic and Lipidomic Analysis of Live Microalgae by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation;** Sylwia Stopka<sup>1</sup>; Bindesh Shrestha<sup>1</sup>; Denis Falconet<sup>2</sup>; Éric Maréchal<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, District Of Columbia; <sup>2</sup>Université Joseph Fourier Grenoble, Grenoble, France
- TP 665 **Ex vivo Analysis of Lymnaea Organs by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation;** Laine Compton<sup>1</sup>; Zsolt Pirger<sup>2</sup>; Laszlo Mark<sup>3</sup>; Zita Laszlo<sup>2</sup>; Bindesh Shrestha<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, District of Columbia; <sup>2</sup>Hungarian Academy of Sciences, Tihany, Hungary; <sup>3</sup>University of Pecs, Pecs, Hungary
- TP 666 **LAESI Mass Spectrometry Imaging of Contact Lens Spoilage;** Holly Henderson; Brent Reschke; Matthew Powell; Callee Walsh; Trust Razunguzwa; *Protea Biosciences Group, Inc., Morgantown, WV*
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- TP 671 **Rapid Determination of Urinary Creatinine Levels Using Atmospheric Pressure Thermal Desorption Combined with Ion Mobility-Mass Spectrometry;** Neil Devenport<sup>1</sup>; James Reynolds<sup>1</sup>; Daniel Weston<sup>2</sup>; Colin Creaser<sup>1</sup>; <sup>1</sup>Loughborough University, Loughborough, UK; <sup>2</sup>AstraZeneca, Alderley Edge, UK
- TP 672 **Qualitative Analysis of 1-OHP with Extractive Electrospray Ionization Mass Spectrometry from a Wet Surface;** Jing Li; Eric Handberg; Huanwen Chen; *East China Institute of Tech., Nanchang, China*
- TP 673 **Detection of Exhaled Nitric Oxide by Extractive Electrospray Ionization Mass Spectrometry;** Susu Pan<sup>1</sup>; Yan Zhang<sup>1</sup>; Jianhua Ding<sup>1</sup>; Jiuyan Zhao<sup>2</sup>; Lanlan Zhu<sup>2</sup>; Qian Zeng<sup>1</sup>; Xinglei Zhang<sup>1</sup>; Eric Handberg<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Tech., Nanchang, China; <sup>2</sup>Nanchang University, Nanchang, China
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- TP 675 **Differentiation of Two Morphologically Similar Amazonian Aniba Species by Electron Spray Ionization Mass Spectrometry;** Carlos H.V. Fidelis<sup>1</sup>; Renan S. Galaverna<sup>1</sup>; Lauro E.S. Barata<sup>2</sup>; Paulo T. B. Sampaio<sup>3</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>State University of Campinas, Campinas, SP; <sup>2</sup>Federal University of Western Pará (UFOPA), Santarém, PA; <sup>3</sup>National Research Institute of Amazon, Manaus, AM
- TP 676 **Direct Analysis of Herbal Powders by Pipette-tip Electrospray Ionization Mass Spectrometry;** Haixing Wang; Zhong-Ping Yao; *The Hong Kong Polytechnic University, Hong Kong, China*
- TP 677 **Electrostatic-Spray Ionization Mass Spectrometry;** Liang Qiao<sup>1</sup>; Hubert Girault<sup>1</sup>; Romain Sartor<sup>1</sup>; Natalia Gasilova<sup>1</sup>; Elena Tobolkina<sup>1</sup>; Baohong Liu<sup>2</sup>; <sup>1</sup>École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Fudan University, Shanghai, China
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- TP 679 **Shvo's Catalyst in Chemoenzymatic Dynamic Kinetic Resolution of Amines - Inner or Outer Sphere Mechanism?** Cintia Milagre<sup>1</sup>; Boniek Vaz<sup>2</sup>; Marcos Eberlin<sup>3</sup>;

- Humberto Milagre<sup>1</sup>; <sup>1</sup>UNESP, Araraquara, Brazil; <sup>2</sup>Federal University of Goiás, Goiânia, Brazil; <sup>3</sup>UNICAMP, Campinas, Brazil
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- TP 682 **Quality Control Analysis of Cosmetic Compounds by Easy Ambient Sonic-Spray Ionization Mass Spectrometry;** Soraya Elkhatabi; Rosana Alberici; Marcos N. Eberlin; *Thomson Laboratory University of Campinas, UNICAMP, Campinas, SP, Brazil*
- TP 683 **Detection of Ginkgo Tablets Adulteration Using Easy Ambient Sonic Spray Ionization Mass Spectrometry;** Endler Borges<sup>1</sup>; Dietrich Volmer<sup>2</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>Unicamp, Campinas, Brazil; <sup>2</sup>Saarland University, Saarbrücken, Germany
- TP 684 **A Digital Microfluidic Surface Acoustic Wave Nebulization Chip for Direct Phosphoproteomic Analysis;** Yue Huang<sup>1</sup>; Michael Wilson<sup>1,2</sup>; Scott Heron<sup>1</sup>; John Chapman<sup>1</sup>; J. Scott Edgar<sup>3</sup>; Sung Hwan Yoon<sup>1,2</sup>; David R. Goodlett<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Maryland, Baltimore, MD; <sup>3</sup>Deurion LLC, Seattle, WA
- TP 685 **Preparative Scale Paper Spray for Small Scale Chemical Synthesis;** Xin Yan<sup>1</sup>; Xin Li<sup>1</sup>; Rodinei Augusti<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Federal University of Minas Gerais, Belo Horizonte, Brazil
- TP 686 **In-field Agrochemical Analysis Using Ambient Ionization and a Handheld Mass Spectrometer;** Pu Wei<sup>1</sup>; Joshua S. Wiley<sup>1</sup>; Jiangjiang Liu<sup>1</sup>; Chris Pulliam<sup>1</sup>; Ayanna U. Jackson<sup>2</sup>; Holger Tank<sup>2</sup>; Jeffrey R. Gilbert<sup>2</sup>; Jim Gifford<sup>2</sup>; Kerrn Yau<sup>2</sup>; John Whitteck<sup>2</sup>; Zheng Ouyang<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Dow AgroSciences, Indianapolis, IN
- TP 687 **In-situ Analysis of Corrosion Inhibitors Using Paper Spray Ionization Mass Spectrometry;** Fred Paul Mark Jjunju<sup>1</sup>; Anyin Li<sup>2</sup>; Abraham Badu-Tawiah<sup>2</sup>; Pu Wei<sup>2</sup>; Iman Roqan<sup>1</sup>; R. Graham Cooks<sup>2</sup>; <sup>1</sup>CEMSE KAUST, Thuwail, KSA; <sup>2</sup>Department of Chemistry Purdue University, West Lafayette, IN
- TP 688 **Improvement of Quantitative Performance of Paper Spray Mass Spectrometry by oxidative Treatment Of Paper Substrates;** Yuan Su; Jiangjiang Liu; R. Graham Cooks; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- TP 689 **Quantitative Analysis of Triglycerides and Fatty Acid Profiling in Oils and Oil Seeds Using Ambient Mass Spectrometry;** Jiangjiang Liu<sup>1</sup>; Pu Wei<sup>1</sup>; Joshua Wiley<sup>1</sup>; Ayanna Jackson<sup>2</sup>; Paresh Sanghani<sup>2</sup>; Jeffery Gilbert<sup>2</sup>; Brita McNew<sup>2</sup>; Zheng Ouyang<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Dow AgroSciences, Indianapolis, IN
- TP 690 **Direct Identification of Glycosyl Flavonoids in Bergamot Tissues by Leaf Spray Ambient Mass Spectrometry;** Fabio Mazzotti; Leonardo Di Donna; Domenico Taverna; Donatella Aiello; Anna Napoli; Giovanni Sindona; *Dipartimento di Chimica Università della Calabria, Arcavacata Di Rende, Italy*
- TP 691 **Method Development for Compositional Analysis of Free HS and HS in Proteoglycans from Human Serum and Saliva;** Wei Wei<sup>1</sup>; Rebecca Miller<sup>1</sup>; Susan Fisher<sup>2</sup>; Julie Leary<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>University of San Francisco Medical Center, San Francisco, CA
- TP 692 **High Temperature LC-MS Analysis of Native and Permethylated Glycans Derived from Glycoproteins;** Shiyue Zhou; Yunli Hu; James Blakmer; Yehia Mechref; *Texas Tech University, Lubbock, TX*
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- TP 694 **Isomeric Separation of Procainamide Labeled N-Glycans by Using Novel Superficially Porous Particle HILIC Column;** Shujuan Tao<sup>1</sup>; Yining Huang<sup>1</sup>; Barry Boyes<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center, UGA, Athens, GA; <sup>2</sup>Advanced Material Technology, Inc., Wilmington, DE
- TP 695 **Confident Identification of Isomeric N-glycan Structures by Combined Ion Mobility Mass Spectrometry and Hydrophilic Interaction Liquid Chromatography;** Yoshiki Yamaguchi<sup>1</sup>; Kenji Hirose<sup>2</sup>; Wataru Nishima<sup>1</sup>; Suyong Re<sup>1</sup>; Yuji Sugita<sup>1</sup>; <sup>1</sup>RIKEN, Wako-Shi, Japan; <sup>2</sup>Nihon Waters K.K., Osaka, Japan
- TP 696 **Nano-HILIC-Orbitrap-MS Combined with Linkage Specific Derivatization of Sialic Acid for Improved Characterization of Isomeric Sialylated N-Glycans in Cancer Biomarker Discovery;** Fateme Tousi<sup>1</sup>; William Hancock<sup>1</sup>; Marina Hincapie<sup>1</sup>; Jonathan Bones<sup>2</sup>; <sup>1</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>2</sup>NIBRT, Dublin, Ireland
- TP 697 **N-glycan Analysis of Immunoglobulin G by Enzymatic Release with Remove-iT Endo S and LC-MS;** Elizabeth McLeod; Paula Magnelli; Alicia Beliek; Xiaofeng Shi; Ellen Guthrie; *New England Biolabs, Ipswich, MA*
- TP 698 **A Fully Automated Workflow for LC-MS Analysis of Labeled and Native N-Linked Glycans Released From Proteins;** Udayanath Aich<sup>1</sup>; Julian Saba<sup>2</sup>; Xiaodong Liu<sup>1</sup>; Sergei Snovid<sup>3</sup>; Yury Agroskin<sup>1</sup>; Srinivasa Rao<sup>1</sup>; Chris Pohl<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, Sunnyvale, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Rockford, IL
- TP 699 **Data Analysis and Processing Strategy for Large Scale Mass Spectrometry N-linked Glycan Relative Quantification Studies;** Amber Taylor; S. Hunter Walker; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- TP 700 **Novel N-linked Glycan Relative Quantification Strategy via Stable-Isotope Labeled Hydrazone Formation and Application to Biomarker Discovery Efforts in Ovarian Cancer;** S. Hunter Walker<sup>1</sup>; Amber D. Taylor<sup>1</sup>; William A. Cliby<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Mayo Clinic College of Medicine, Rochester, MN
- TP 701 **Quantitative Analysis of Carbohydrates and Artificial Sweeteners in Food Samples Using LC/MS with Post-column Reagent Addition and APCI Interface;** Jie Xing<sup>1</sup>; Yin Ling Chew<sup>2</sup>; Zhe Sun<sup>1</sup>; Zhaoli Zhan<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; <sup>2</sup>Department of Chemistry, Faculty of Science, National University of Singapore, Singapore
- TP 702 **Profiling of Permethylated Glycans Released and Collected from Mouse Brain Sections Fixed to Microscopic Slides;** Yunli Hu; Shiyue Zhou; Sarah Khalil; Calvin Renteria; Yehia Mechref; *Texas Tech University, Lubbock, TX*

- TP 703 **Comparative N-glycomic Profiling Differentiates Primary Hepatocellular Carcinoma Tissue from Cirrhotic and Normal Liver Tissues**; Christa L. Feasley<sup>1</sup>; Matthew B. West<sup>1,3</sup>; Nikhil Mirjankar<sup>2</sup>; Barry K. Levine<sup>2</sup>; Christopher M. West<sup>1</sup>; Marie H. Hanigan<sup>1</sup>; <sup>1</sup>University of Oklahoma HSC, Oklahoma City, OK; <sup>2</sup>Oklahoma State University, Stillwater, OK; <sup>3</sup>Hough Ear Institute, Oklahoma City, OK
- TP 704 **Tissue O-glycans Change during Mouse Natural Aging**; Bum Jin Kim<sup>1</sup>; Hyoung Jin Jeong<sup>1</sup>; Serenus Hua<sup>1,2</sup>; Sureyya Ozcan<sup>1,2</sup>; Lauren Dimapasoc<sup>3</sup>; Ik-Soon Jang<sup>4</sup>; Jong-Soon Choi<sup>4</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>GRAST, Chungnam National University, Daejeon, South Korea; <sup>2</sup>Cancer Research Institute, Daejeon, South Korea; <sup>3</sup>University of California, Davis, CA; <sup>4</sup>Korea Basic Science Institute, Daejeon, South Korea
- TP 705 **N-glycan Profiling of the Urinary Exosome for Biomarker Discovery**; Nayoung Yun<sup>1</sup>; Seunghyup Jeong<sup>1</sup>; Serenus Hua<sup>1</sup>; Pyong-Gon Moon<sup>2</sup>; Moon Chang Baek<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>Chungnam National University, Daejeon, Korea; <sup>2</sup>Kyungpook National University, Daegu, Korea
- TP 706 **Mass Spectra Analysis of Bacteria-Resistant *bus-4* *Caenorhabditis elegans* Mutants Reveals Defects in O-glycosylation**; Lisa Parsons<sup>1</sup>; Rahman Mizanur<sup>2</sup>; Ewa Jankowska<sup>1</sup>; Jonathan Hodgkin<sup>3</sup>; Delia O'Rourke<sup>3</sup>; Dave Stroud<sup>3</sup>; John Cipollo<sup>1</sup>; <sup>1</sup>FDA, Bethesda, Md; <sup>2</sup>army, Bethesda, US; <sup>3</sup>Department of Biochemistry, University of Oxford, Oxford, UK
- TP 707 **Structural Determination of N-Glycans from Viral Glycoproteins by Ion Mobility Mass Spectrometry and Negative Ion Fragmentation**; David J. Harvey<sup>1</sup>; Christopher Scanlan<sup>1</sup>; Max Crispin<sup>1</sup>; Camille Bonomelli<sup>1</sup>; Thomas Bowden<sup>1</sup>; Bitto David<sup>1</sup>; Huiskenon Juha<sup>1</sup>; Matthew Edgeworth<sup>2</sup>; James Scrivens<sup>2</sup>; <sup>1</sup>University of Oxford, Oxford, UK; <sup>2</sup>University of Warwick, Coventry, UK
- TP 708 **Structural Elucidation of N-glycans Originating from Ovarian Cancer Cells Using High Vacuum MALDI Mass Spectrometry**; Matthew S. F. Choo<sup>1</sup>; Roberto Castangia<sup>2</sup>; Matthew E. Openshaw<sup>2</sup>; Omar Belgacem<sup>2</sup>; Stuart M. Haslam<sup>1</sup>; Anne Dell<sup>1</sup>; <sup>1</sup>Faculty of Natural Sciences, Imperial College, London, UK; <sup>2</sup>MALDI Applications Group, Shimadzu, Kratos, Manchester, UK
- TP 709 **MALDI and ESI MS-based Quantitative Analysis of N-linked Glycans Using Carbonyl-Reactive Tandem Mass Tags**; Yan Liu<sup>1,2</sup>; Xuefei Zhong<sup>1</sup>; Sergei Snovidia<sup>3</sup>; John C. Rogers<sup>3</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Xiamen University, Xiamen, China; <sup>3</sup>Thermo Fisher Scientific, Rockford, IL
- TP 710 **Detection and Quantification of Carbohydrates in the Murine Gastrointestinal Tract Following Antibiotic Treatment and During *Clostridium difficile* Infection**; Li Zhang<sup>1</sup>; Casey Theriot<sup>2</sup>; Thekkelnaycke Rajendiran<sup>1</sup>; Jaeman Byun<sup>1</sup>; Stephen Brown<sup>1</sup>; Vincent Young<sup>3</sup>; <sup>1</sup>University of Michigan, Metabolomics Core Facility, Ann Arbor, MI; <sup>2</sup>University of Michigan, Dept of Internal Medicine, Ann Arbor, MI; <sup>3</sup>The University of Michigan, Dept of Microbiology, Ann Arbor, MI
- TP 711 **Homeostasis of Plasma N-linked Glycome as Defined in the Domestic Hen Model of Spontaneous Ovarian Adenocarcinoma**; Amber Cook<sup>1</sup>; S. Hunter Walker<sup>1</sup>; Amber D. Taylor<sup>1</sup>; Adam M. Hawkrigge<sup>2</sup>; James N. Petitte<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Virginia Commonwealth University, Richmond, VA
- TP 712 **Method for the Analysis of 4-aminobenzoic Acid Ethyl Ester Derivatized N-linked Oligosaccharides from Cytopreservative Solutions**; Francis Murphy; Michael Finan<sup>1</sup>; Rodney Rocconi<sup>1</sup>; Lewis Pannell<sup>1</sup>; University of South Alabama, Mobile, AL
- TP 713 **Rapid Differentiation of Core- and Antennae-Fucosylation in N-glycans Using Procainamide Labeling and ESI-QTOF MS/MS**; Charles Nwosu; Hoi Kei (Natalie) Yau; Steven Becht; William Bakewell; *PPD, Middleton, WI*
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- TP 719 **Rapid N-linked Glycan Glycopeptide Analysis of the Biotherapeutic Erythropoietin (EPO) Using HILIC UPLC/FLR and Mass Spectrometry**; Mark Hilliard<sup>1</sup>; Pauline Rudd<sup>1</sup>; Jonathan Bones<sup>1</sup>; Ying Qing Yu<sup>2</sup>; <sup>1</sup>NIBRT, Dublin, Ireland; <sup>2</sup>Waters, Milford, Boston, MA
- TP 720 **Characterization of Glycopeptides in Tryptic Mixtures by 2D-UPLC (High/Low pH) – nanoESI-QToF**; Irina Perdivara; Kenneth B. Tomer; *NIEHS, Rtp, NC*
- TP 721 **Resolution of Sialylated Glycopeptides Using a Pentafluorophenylpropyl (F5) Stationary Phase**; Catherine A. Formolo; Karen W. Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
- TP 722 **Ion Mobility Mass Spectrometry of IgG Fc Glycopeptides from Different Subclasses**; Michiko Tajiri<sup>1</sup>; Feifei Zhu<sup>2</sup>; Maissa M. Gaya<sup>2</sup>; Yoshinao Wada<sup>1</sup>; David E. Clemmer<sup>2</sup>; <sup>1</sup>Osaka MCHRI, Izumi, Osaka, Japan; <sup>2</sup>Indiana University, Bloomington, IN
- TP 723 **Demonstration of Informational Power of Chip-Based Liquid Chromatography-Ion Mobility Spectrometry Mass Spectrometry for Glycopeptidomics**; Kshitij Khatri<sup>1</sup>; Qi Wang<sup>1</sup>; Crystal K. Cody<sup>2</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Catherine E. Costello<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 724 **A Robust LC-MS Based Workflow for Comparative Glycoproteomics with Online Glycopeptide Enrichment and Separation**; Kshitij Khatri<sup>1</sup>; Nancy Leymarie<sup>1</sup>; Gregory O. Staples<sup>2</sup>; Yu Huang<sup>1</sup>; Deborah R. Leon<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 725 **Highly Selective Enrichment of Sialylated Glycopeptides Using Titania Sol-Gels for MALDI-MS Applications**; H. Mehmet Kayili; Ömür Çelikbiçak; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- TP 726 **Magnetic Nanoparticle Technology for Sequestering Glycopeptides**; Edward Bodnar; Hélène Perreault; *University of Manitoba, Winnipeg, Canada*



- TP 727 **Comparison of Hydrazide Capture and Lectin Affinity Based Enrichment Methods for Glycoproteomics**; Yue Zhou; Peng Xue; Xiang Ding; Jun Wang; Fu quan Yang; *Institute of biophysics, CAS, Beijing, China*
- TP 728 **Sugar-azide Metabolic Labeling Combined with Alkyne-bead Capture for Efficient Isolation of Glycoproteins Involved in the Epithelial-Mesenchymal Transition**; Stephen Roper; Arch Martin; Benjamin Neely; E. Ellen Jones; Harry Drabkin; Robert Gemmill; Richard R Drake; *Medical University of South Carolina, Charleston, SC*
- TP 729 **Negative-Ion MALDI-QIT-TOF MS<sup>n</sup> of N-glycans Derivatized with Pyrene Butanoic Acid Hydrazide**; Kazuko Hirose-Hachisu; Junko Amano; *The Noguchi Institute, Tokyo, Japan*
- TP 730 **The GlycoFilter: A Simple and Comprehensive Sample Preparation Platform for Proteomics, N-Glycomics and Glycosylation Site Assignment**; Hui Zhou; John Froehlich; Andrew Briscoe; Richard Lee; *Boston Children's Hospital, Boston, MA*
- TP 731 **MALDI and ESI Evaluation of Glycopeptide Signal Strengths for Quantitative Label-Free Glycoproteomics: Demystifying Glycopeptide Ionisation Using Synthetically Produced Sialylated N-glycopeptides**; Kathrin Stavenhagen<sup>1,2</sup>; Hannes Hinneburg<sup>1</sup>; Morten Thaysen-Andersen<sup>3</sup>; Laura Hartmann<sup>1</sup>; Daniel Varón Silva<sup>1</sup>; Jens Fuchser<sup>4</sup>; Stephanie Kaspar<sup>4</sup>; Erdmann Rapp<sup>2</sup>; Peter H. Seeberger<sup>1,5</sup>; Daniel Kolarich<sup>1</sup>; <sup>1</sup>Max Planck Institute of Colloids and Interfaces, Berlin, Germany; <sup>2</sup>MPI for Dynamics of Complex Technical Systems, Magdeburg, Germany; <sup>3</sup>Macquarie University, Sydney, Australia; <sup>4</sup>Bruker Daltonics, Bremen, Germany; <sup>5</sup>Free University Berlin, Berlin, Germany
- TP 732 **Mass Spectrometry Analysis of NXS/T Glycosylation Sites in Recombinant Glycoproteins**; Izabela Sokolowska; Armand Ngounou Wetie; Urmi Roy; Christopher Talbot; Alisa Woods; Costel Darie; *Clarkson University, Potsdam, NY*
- TP 733 **Top-Down Analysis of Plasma-Derived and Recombinant Human Factor VII and Bovine Prothrombin Reveal Extensive, Cell-Line Related Heterogeneity of PTMs**; Stephen Harvey; Julie Kiriara; Lorraine Anderson; Matthew Wroblewski; Gary Nelsestuen; *University of Minnesota, Minneapolis, MN*
- TP 734 **Novel Strategy for Prediction of MS<sup>n</sup> Spectrum of Glycans from its Structure**; Hiromitsu Takaba<sup>1</sup>; Qi Xiaofeng<sup>1</sup>; Hiroshi Setogawa<sup>1</sup>; Atsushi Ogiwara<sup>2</sup>; Kazuko Hirose-Hachisu<sup>3</sup>; Mitsuhiro Kanazawa<sup>2</sup>; Junko Amano<sup>3</sup>; <sup>1</sup>Tohoku University, Sendai, Japan; <sup>2</sup>Reifycs Inc., Tokyo, Japan; <sup>3</sup>The Noguchi Institute, Tokyo, Japan
- TP 735 **Comparison of Trypsin and Nonspecific Digestions for Site Specific Characterization of Protein Glycans Utilizing New Software for Automated Matching and Scoring**; Evan Parker; Qiuting Hong; Andres Guerrero; Michael Xin Sun; Jincui Huang; Carlito Lebrilla; *UC, Davis, CA*
- TP 736 **GLIDE : GLycoprotein IDentification software**; Atsushi Ogiwara<sup>1</sup>; Hisae Anyoji<sup>1</sup>; Mitsuhiro Kanazawa<sup>1</sup>; Kazuko Hirose-Hachisu<sup>3</sup>; Hiromitsu Takaba<sup>2</sup>; Junko Amano<sup>3</sup>; <sup>1</sup>Reifycs Inc., Tokyo, Japan; <sup>2</sup>Tohoku University, Sendai, Japan; <sup>3</sup>The Noguchi Institute, Tokyo, Japan
- TP 737 **O-Glycomap-Sera: A Tool for Discovery of O-linked Glycopeptides in Human Serum Samples**; Jagadheshwar Balan<sup>1</sup>; Anoop Mayampurath<sup>1</sup>; Chuan-Yih Yu<sup>1</sup>; Yehia Mehcref<sup>2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN; <sup>2</sup>Texas Tech University, Lubbock, TX
- Food Safety, 738 – 772**
- TP 738 **Method Development for Trace Level Detection of N-Nitrosamines in Beer by GC-MS/MS**; Lai Chin Loo<sup>1</sup>; Cynthia Melanie Lahey<sup>1</sup>; Shao Hua Chia<sup>2</sup>; Fang Yan Li<sup>3</sup>; Yai Fong Chew<sup>3</sup>; Gee Siang Ling<sup>1</sup>; Sheot Harn Chan<sup>3</sup>; S. F. Y. Li<sup>2</sup>; <sup>1</sup>Shimadzu Asia Pacific Pte. Ltd., Singapore; <sup>2</sup>National University of Singapore, Singapore; <sup>3</sup>Food Safety Laboratory, Health Science Authority, Singapore
- TP 739 **Minimization of Carryover for High Throughput LC-MS/MS Analysis of 14 Mycotoxins in Beer**; Masayoshi Tamura<sup>1</sup>; Keiko Matsumoto<sup>2</sup>; Jun Watanabe<sup>2</sup>; Junko Iida<sup>2</sup>; Naoki Mochizuki<sup>1</sup>; <sup>1</sup>Asahi Group Holdings, Limited, Ibaraki, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- TP 740 **Determination of 20 Phthalic Acid Esters in Alcohol Drinks by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry**; Hengtao Dong; Jinting Yao; Hongyuan Hao; Luying Zhou; Qiang Li; Yuling Song; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu (China) Co., Ltd., Shanghai, China*
- TP 741 **Determination of Industrial Dyes in Foods by LCMS-IT-TOF**; Xiaozhen Chen<sup>1</sup>; Liying Huang<sup>1</sup>; Jin Wang<sup>1</sup>; Hui Cao<sup>1</sup>; Luying Zhou<sup>2</sup>; Jinting Yao<sup>2</sup>; Hengtao Dong<sup>2</sup>; Hongyuan Hao<sup>2</sup>; Taohong Huang<sup>2</sup>; Yuki Hashi<sup>2</sup>; <sup>1</sup>Zhejiang Institute of Quality Inspection Science, Hangzhou, China; <sup>2</sup>Shimadzu Global COE, Shimadzu (China) Co., Ltd, Shanghai, China
- TP 742 **Determination of the Derivatives of Nitrofurantol Metabolites in Marine Products by Ultra High Performance Liquid Chromatography/Triple Quadrupole Mass Spectrometry**; Xiongxiang Qiu; Jinting Yao; Song Zhan; Taohong Huang; *Shimadzu Global COE, Shimadzu (China) Co., Ltd. Guangzhou, China*
- TP 743 **Ultra High performance Liquid Chromatography Tandem Quadrupole-Time of Flight Mass Spectrometry for Simultaneous Screening Hazardous Compounds in Food Samples**; Chuanqi Zheng; *Agilent Technologies, Guangzhou, China*
- TP 744 **Determination of Six Major Ergot Alkaloids and Their Epimers in Wheat Using LC-MS/MS**; Mike Roscoe; Dainna Drul; Sheryl tittlemier; *Canadian Grain Commission, Winnipeg, Canada*
- TP 745 **Direct Analysis of 4-Methylimidazole in Foods using Paper Spray Mass Spectrometry**; Anyin Li<sup>1</sup>; Pu Wei<sup>1</sup>; Hsu-Chen Hsu<sup>1</sup>; Linfan Li<sup>2</sup>; Zheng Ouyang<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Biomedical Engineering, Purdue University, West Lafayette, IN
- TP 746 **Rapid Simultaneous Assay of 25 Mycotoxins in a Variety of Food Samples by UHPLC-MS/MS Using Fast Polarity Switching**; Eric Capodanno<sup>1</sup>; Stéphane Moreau<sup>2</sup>; Mikael Levi<sup>2</sup>; <sup>1</sup>Phytocontrol, Nîmes, France; <sup>2</sup>Shimadzu France, Noisiel, France
- TP 747 **Development and Application of an Exact Mass LC-MS/MS Library for Screening of Mycotoxins and Fungal Metabolites in Food and Feed**; Elisabeth Varga<sup>1</sup>; Thomas Glauner<sup>2</sup>; Bernhard Wuest<sup>2</sup>; Michael Sul yok<sup>1</sup>; Rainer Schuhmacher<sup>1</sup>; Rudolf Krska<sup>1</sup>; Franz Berthiller<sup>1</sup>; <sup>1</sup>University of Natural Resources and Life Sciences, Tulln, Austria; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- TP 748 **Identification and Quantification of 19 Phthalic Acid Esters in Chinese Liquors Using GC-MS/MS**; Xing Jiangtao; Gao Peng; Wang Furong; Fan Jun; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Beijing, China*

- TP 749 **Identification and Quantitation of Beta-Agonists in Beef and Pork Extracts Using Ultra-High Performance Liquid Chromatography Tandem Mass Spectrometry with Triggered Multiple Reaction Monitoring**; Shan-An Chan; Agilent, Taipei, Taiwan
- TP 750 **Using Ion Mobility Mass Spectrometry to Identify Multiple Protonation Sites and Different Fragmentation Patterns Within the Fluoroquinolone Class of Antibiotics**; Michael McCullagh<sup>1</sup>; Sara Stead<sup>1</sup>; David Eatough<sup>1</sup>; Kieran Neeson<sup>1</sup>; Jeff Goshawk<sup>1</sup>; Wouter de Keizer<sup>2</sup>; Aldert Bergwerff<sup>2</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>RnAssays BV, Utrecht, The Netherlands
- TP 751 **Rapid Screening of Sorbic and Benzoic Acids in Soy Sauce by Direct Analysis in Real Time Time-of-Flight Mass Spectrometry**; Xiaojing Ding<sup>1</sup>; Junwei Huang<sup>2</sup>; Shan Zhao<sup>1</sup>; Jing Zhang<sup>1</sup>; Echo W. Jia<sup>2</sup>; Bing Shao<sup>1</sup>; Charles C. Liu<sup>2</sup>; <sup>1</sup>Beijing Centre for Disease Control and Prevention, Beijing, China; <sup>2</sup>ASPEC Technologies Limited, Beijing, China
- TP 752 **Multi Antibiotic Residue Detection - Status quo and Challenges for Confirmatory and Screening approaches**; Nelli Jochim<sup>1</sup>; Lutz Hartig<sup>1</sup>; Scarlett Biselli<sup>1</sup>; Sebastian Westrup<sup>2</sup>; <sup>1</sup>Eurofins WEJ Contaminants, Hamburg, Germany; <sup>2</sup>Thermo Scientific, Dreieich, Germany
- TP 753 **HighResolution Mass Spectrometric Characterization of Toxic Jatropha Factors from Jatropha curcas: Possible Contaminants in Animal Feed and Non-Food Grade Glycerin**; Hiranthi Jayasuriya; Upul Nishshanka; Renate Reimschuessel; Chaitali Chattopadhyay; FDA, CVM, Laurel, MD
- TP 754 **Rapid, High Throughput Quantitation of Thujone in Absinthe by UHPLC-MS-MS**; Jared Russell; Jeffrey Dahl; Shimadzu Scientific Instruments, Columbia, MD
- TP 755 **Analysis of Non-steroidal Anti-inflammatory Drugs in Food Matrices by Means of HPLC-MS/MS**; Pavel Metalnikov; Alexandre Komarov; Alexandre Panin; VGNI, Moscow, Russian Federation
- TP 756 **Overcoming Challenges of Protein Sample Preparation for Food Allergen Analysis**; Rachel Lieberman<sup>1</sup>; Brian Feild<sup>1</sup>; Scott Kuzdzal<sup>1</sup>; Kevin Meyer<sup>2</sup>; Nick Herold<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Perfinity Biosciences, Inc., West Lafayette, IN
- TP 757 **Development and Evaluation of a Standardized Method for Food Contaminant Analysis Based on Liquid-Liquid-Extraction or QuEChERS, UHPLC and HRAM Platform**; Jinyuan Wang; Jonathan Beck; Charles Yang; Guifeng Jiang; Jennifer Massi; Thermo Fisher Scientific, San Jose, CA
- TP 758 **High-Throughput Screening of Illegal Drugs in Functional Foods by Ultra Performance Liquid Chromatography Coupled with Quadrupole-Time Of Flight Mass Spectrometry**; Qiaozhen Guo; Jie Yin; Jing Zhang; Bing Shao; Beijing Center for Disease Control and Prevention, Beijing, China
- TP 759 **Determination of 62 Non-Dioxin-Like PCBs and 7 indicatorPCBs in Food**; Jungju Seo; Jijeong Ryu; Seunghye Ahn; Korea Basic Science Institute, Seoul, South Korea
- TP 760 **Determination of Antibiotics in Honey by LC-MSMS – The Replacement Three Methods with One Single Method**; Leena Saari; Finnish Food Safety Authority, Helsinki, Finland
- TP 761 **Determination of Arsenic Speciation in Rice Grain by IC-ICP-MS**; Cheong-Tae Kim<sup>1</sup>; Youn-Jee Kim<sup>1</sup>; Dae-Hyun Kim<sup>1</sup>; Seung-Il Yang<sup>2</sup>; Jung-Kun Lee<sup>1</sup>; <sup>1</sup>NONGSHIM CO., LTD, Seoul, South Korea; <sup>2</sup>ThermoFisher Scientific-Korea, Seoul, South Korea
- TP 762 **Comparison of Low-Resolution MS<sup>n</sup> Data and High- Resolution Mass Spectrometric Data for Non-Targeted Analysis Using Spectral Data Interpretation Software**; Carrie Sisk<sup>1</sup>; Ann Knolhoff<sup>2</sup>; Timothy Croley<sup>2</sup>; <sup>1</sup>Commonwealth of Virginia DCLS, Richmond, VA; <sup>2</sup>FDA, CFSAN, College Park, MD
- TP 763 **Analysis of Antibiotics in Food Matrix Using LC High Resolution Accurate Mass Spectrometry**; Jia Wang; Charles Yang; Dipankar Ghosh; Thermo Fisher Scientific, San Jose, CA
- TP 764 **Improving a Regulatory Method to Quantify Triarylmethane Dyes in Fish Tissue**; Sarah Pierce; Darin Files; Haejung An; Eugene Chang; Han Paek; US Food & Drug Administration, Irvine, CA
- TP 765 **Extraction of Jatropha Factors from Glycerin for Analysis using LC/MS**; Bethany Subel; Jonathan Litzau; FDA, Cincinnati, OH
- TP 766 **Proteomic Analysis of Poor and Robust Colonizing Campylobacter jejuni Isolates from Chick Cecum**; Yuan Gao<sup>1</sup>; Kidon Sung<sup>1</sup>; Saeed Khan<sup>1</sup>; Kelli Hiatt<sup>2</sup>; Eric Line<sup>2</sup>; Oh-Gew Kweon<sup>1</sup>; Carl Cerniglia<sup>1</sup>; Li-Rong Yu<sup>1</sup>; <sup>1</sup>National Center for Toxicological Research, US FDA, Jefferson, AR; <sup>2</sup>Agricultural Research Service, USDA, Athens, GA
- TP 767 **Comparison Quantitation Ability of Quadrupole-Orbitrap HR/AM MS and Triple Quadrupole MS in Food Additives within Candies**; Shu-Hui Lee; Hsin-Hung Huang; Wei-Shun Lai; Mass Solutions Technology, New Taipei City, Taiwan
- TP 768 **A Study of the Presence of Arecoline and Guvacoline in Saliva of 'Betel-Quid' Chewer Using Ion Trap LC/MS**; A. F. M. Motiur Rahman; Mohamed W. Attwa; Adnan, A. Kadi; King Saud University, Riyadh, SAUDI ARABIA
- TP 769 **Direct Detection of Illegal Additives in Red Wine Using MALDI-FTMS**; Hai Pu; Nan Hu; Ow Saw Yen; Bruker, Beijing, China
- TP 770 **Identification of True and Fake Wines Using Single Photon Ionization Mass Spectrometry**; Cao Li<sup>1</sup>; Ya-Fei Zhou<sup>1</sup>; Ya-Li Liu<sup>1,3</sup>; Wei Gao<sup>2</sup>; Zhen Zhou<sup>2</sup>; Eric Handberg<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Tech., Nanchang, China; <sup>2</sup>Shanghai University, Shanghai, China; <sup>3</sup>Hebei University of Technology, Tianjin, China
- TP 771 **Nanotile based UPLC - Mass Spectrometry for Anabolic Steroids Analysis in Food Safety**; Arjen Gerssen<sup>1</sup>; Eric O. van Bennekom<sup>1</sup>; Marco H. Blokland<sup>1</sup>; Saskia S. Sterk<sup>1</sup>; Michel W.F. Nielsen<sup>1,2</sup>; <sup>1</sup>RIKILT - Institute of Food Safety, Wageningen UR, Wageningen, The Netherlands; <sup>2</sup>Laboratory of Organic Chemistry, Wageningen UR, Wageningen, The Netherlands
- TP 772 **Determination of Urethane in Chinese Rice Wine by Supported Liquid Extraction Coupled and Gas Chromatography-Mass Spectrometry**; Suzi Qin; Jack Liu; Wan Wang; Guotao Lu; Bonna-Agela Technologies, Tianjin, China





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

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### Mass Spectrometry - History & Education, 001 – 002

- WP 001 **Origin, Growth, and Development of the Mass Spectrometry Societies;** P. Jane Gale<sup>1</sup>; Michael A. Grayson<sup>2</sup>; <sup>1</sup>Gale-Bentz Consulting, Southborough, MA; <sup>2</sup>Retired, St. Charles, MO
- WP 002 **Chem./Bio. 429 - Experimental Genomics and Proteomics. An Interdisciplinary Upper-Division Laboratory Course for Undergraduates;** Charlotte Platner; Jacquelyn Blake-Hedges; Samuel Clamons; Ruth Dana; Adam Drici; Sophia Dudte; Gregory Ginsburg; Veronica Gray; Alexandra Mellis; Allison Roberts; Charles Thompson; Stephanie Wraith; Mark Forsyth; Margaret Saha; Kurt Williamson; John Poutsma; *College of William & Mary, Williamsburg, VA*

### Nanomaterials, 003 – 012

- WP 003 **Functionalized Gold Nanoparticle Coated Surfaces for the Detection of Biomolecules by Laser Desorption/Ionization Mass Spectrometry;** Alyssa L. M. Marsico; Brian Creran; Bradley Duncan; Vikas Nandwana; Vincent M. Rotello; Richard W. Vachet; *University of Massachusetts, Amherst, MA*
- WP 004 **Improving MS Sensitivity for Underivatized Carbohydrates with Diamond Nanoparticles in MALDI;** Hsun Lee; Chia-Chen Wang; Chieh-Lin Wu; Yin-Hung Lai; Jia-Der Lin; Yi-Sheng Wang\*; *Genomics Research Center, Academia Sinica, Taipei 115, Taiwan, ROC*
- WP 005 **Investigating the Impact of Nanoparticle Surface Ligand Structures on Protein Adsorption by Mass Spectrometry;** Shang Zeng; Wenwan Zhong; *University of California, Riverside, CA*
- WP 006 **Graphene/Polyaniline Nanocomposite Along with MALDI-MS for Sensitive Detection of Small Biomolecules;** Nadnudda Rodthongkum<sup>1</sup>; Nipapan Ruecha<sup>1</sup>; Voravee Hoven<sup>1</sup>; Richard Vachet<sup>2</sup>; Orawon Chailapakul<sup>1</sup>; <sup>1</sup>Chulalongkorn University, Bangkok, Thailand; <sup>2</sup>University of Massachusetts, Amherst, MA
- WP 007 **A Sol-Gel Derived Silver Nanoparticle Embedded Thin Film for Mass Spectrometry-Based Biosensing;** Roberto Gamez; David Russell; *Texas A&M University, College Station, TX*

- WP 008 **Mass Spectrometric Analysis of Impurities in Crystalline Organic Semiconductors;** Anna Voloshenko<sup>1</sup>; Ke Jie Tan<sup>2</sup>; Christian Kloc<sup>2</sup>; Rimma Shelkov<sup>1</sup>; Sergey Sladkevich<sup>1</sup>; Peter Prikhodchenko<sup>1</sup>; Jenny Gun<sup>1</sup>; Ovadia Lev<sup>1</sup>; <sup>1</sup>The Hebrew University of Jerusalem, Jerusalem, Israel; <sup>2</sup>Nanyang Technological University, Singapore

- WP 009 **Mass Spectrometric Analysis of Species Evolution in Mesoporous Silica Synthesis;** Ivy Hwee Lim; Ferdi Schüth; Wolfgang Schrader; *Max-Planck-Institut für Kohlenforschung, Mülheim An Der Ruhr, Germany*

- WP 010 **Phenylboronic Acid-Decorated Lectins for Specific Enrichment of Glycoproteins and Their Glycoproteomic Application;** Ying-Wei Lu<sup>1</sup>; Chih-Wei Chien<sup>1</sup>; Po-Chiao Lin<sup>2</sup>; Sz-Wei Wu<sup>3</sup>; Chang-Yang Chen<sup>4</sup>; Chia-Li Han<sup>3</sup>; Kay-Hooi Khoo<sup>3</sup>; Chun-Cheng Lin<sup>1</sup>; Yu-Ju Chen<sup>3</sup>; <sup>1</sup>National Tsing Hua University, Hsinchu, Taiwan; <sup>2</sup>National Sun Yat-sen University, Kaohsiung, Taiwan; <sup>3</sup>Academia Sinica, Taipei, Taiwan; <sup>4</sup>National Taiwan Normal University, Taipei, Taiwan

- WP 011 **Photocatalytic Nanoweb for Matrix-Free MALDI-TOF Mass Spectrometry;** Jo-Il Kim<sup>1</sup>; Su-Yeol Ryu<sup>2</sup>; Seung-Yeop Kwak<sup>2</sup>; Min-Jung Kang<sup>3</sup>; Jae-Chul Pyun<sup>1</sup>; <sup>1</sup>Yonsei University, Seoul, Republic of Korea; <sup>2</sup>Seoul National University, Seoul, Republic of Korea; <sup>3</sup>Korea Institute of Science and Technology, Seoul, Republic of Korea

- WP 012 **TiO<sub>2</sub> Nanowire Array for Matrix-Free MALDI-TOF Mass Spectrometry;** Jo-Il Kim<sup>1</sup>; Min-Jung Kang<sup>2</sup>; Jae-Chul Pyun<sup>1</sup>; <sup>1</sup>Yonsei University, Seoul, Republic of Korea; <sup>2</sup>Korea Institute of Science and Technology, Seoul, Republic of Korea

### Environmental Analysis: General II, 013 – 035

- WP 013 **LC/QTOF Confirmation of Previously Unreported Microcystins in Alberta Lake Waters;** Ralph Hindle<sup>1</sup>; Xu Zhang<sup>2</sup>; <sup>1</sup>Vogon Laboratory Services Ltd., Cochrane, Canada; <sup>2</sup>Alberta Centre for Toxicology, Calgary, Canada

- WP 014 **Using LDTD-APCI-MS/MS for the Ultrafast Analysis of Emerging Contaminants;** Sébastien Sauv  ; *Universit   de Montr  al, Montr  al, Canada*

- WP 015 **The Comprehensive Analysis of CID MS/MS Spectra Of Bisphenol A Derivatives;** Wei Zou; Anupama Aditham; Qi Gavin; Jianwen She; *California Department of Public Health, Richmond, CA*



- WP 016 **Analysis of Naphthenic Acids in Tissue by Liquid Chromatography Tandem Mass Spectrometry;** Million Woudneh; Coreen Hamilton; Guanghui Wang; Jonathan Benskin; John Cosgrove; *AXYS Analytical Services Ltd., Sidney, Canada*
- WP 017 **High-Throughput LC-MS/MS assay of Phthalates;** Hui Qiao; Sha Joshua Ye; Changtong Hao; *IONICS Mass Spectrometry Group Inc, Bolton, Canada*
- WP 018 **QuEChERS Extraction for the Determination of Free Microcystins in Fish Muscle Using Liquid Chromatography/Tandem Mass Spectrometry;** Xu Zhang; David Kinniburgh; *ACFT, University of Calgary, Calgary, Canada*
- WP 019 **Analysis of Fish Tissue for Perfluorinated Compounds by Reversed Phase High Performance Liquid Chromatography Multiple Reaction Monitoring Tandem Mass Spectrometry;** Michael Stagliano; Joseph Colombo; Paul Gulyas; Matthew Geiger; Bonnie Taffe; *Mi. Dept. of Community Health, Lansing, MI*
- WP 020 **Cyanobacterial Toxins Analysis by Direct Aqueous Injection High Performance Liquid Chromatography – Quadrupole Linear Ion Trap Tandem Mass Spectrometry;** Curtis Hedman<sup>1</sup>; Stacy Tremintin<sup>2</sup>; William Krick<sup>1</sup>; <sup>1</sup>*WI State Lab of Hygiene, Madison, WI*; <sup>2</sup>*AB SCIEX, Foster City, CA*
- WP 021 **Full Scan Tandem Quadrupole Mass Spectrometry for the Determination of Novel Chlorinated Environmental Pollutants;** Qian Wang; Gergana Georgieva; M. Paul Chiarelli; *Loyola University, Chicago, IL*
- WP 022 **Drinking Water Disinfection by Peracetic Acid and Disinfection Byproducts Studied by UFLC-MS/MS and GC-MS;** Honglan Shi<sup>1</sup>; Ruipu Mu<sup>1</sup>; Yongbo Dan<sup>1</sup>; Qihua Wu<sup>1</sup>; Danielle West<sup>1</sup>; Yinfu Ma<sup>1</sup>; John Yang<sup>2</sup>; Bin Hua<sup>2</sup>; Enos Inniss<sup>3</sup>; <sup>1</sup>*Missouri University of Science and Technology, Rolla, MO*; <sup>2</sup>*Lincoln University, Jefferson City, MO*; <sup>3</sup>*University of Missouri, Columbia, MO*
- WP 023 **Tandem Quadrupole Mass Spectrometry for the Determination of Glucuronides Found in Surface and Waste Water;** Matthew Reichert; Deepika Panawennage; Gergana Georgieva; M. Paul Chiarelli; *Loyola University, Chicago, IL*
- WP 024 **Fast Analysis of Cyanobacterial Toxins in Water by Online Preconcentration-Orbitrap MS and Flow Injection-LC-MS/MS and Removal Properties of Chlorination;** Jaewon Choi<sup>1</sup>; Jeheon Jang<sup>1</sup>; Yuns Kim<sup>1</sup>; Charles Yang<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; <sup>1</sup>*Kwater, Daejeon, South Korea*; <sup>2</sup>*ThermoFisher, San Jose, CA*
- WP 025 **The Effects of Acid Pretreatment on the Measurement of 28 VOC Metabolites in Urine by UPLC-ESI-MS/MS;** Liqun Wang; K. Udeni Alwis; Yu Qiu; Benjamin Blount; *Center for Disease Control and Prevention, Chamblee, GA*
- WP 026 **Simultaneous Analysis of Alkylphenol Ethoxylates Using Ultra-High Speed LC-MS/MS;** Daisuke Kasai<sup>1</sup>; Jun Watanabe<sup>2</sup>; Keiko Matsumoto<sup>2</sup>; Koji Takinami<sup>1</sup>; <sup>1</sup>*Nissenken Quality Evaluation Center, Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- WP 027 **Determination of Ten Nitrosamines in Drinking Water by Gas Chromatography/Electron Ionization Tandem Mass Spectrometry;** Peng Gao<sup>1</sup>; Jun Fan<sup>1</sup>; Changqing Lin<sup>2</sup>; <sup>1</sup>*Shimadzu (China) Co., Ltd, Shanghai, China*; <sup>2</sup>*Putuo Environmental Monitoring Station, Shanghai, China*
- WP 028 **Analysis of Linear Alkylbenzene Sulfonate in Environmental Water Using Online SPE LC System Coupled with LC-MS/MS;** Benjamin Figard<sup>1</sup>; Keiko Matsumoto<sup>2</sup>; Jun Watanabe<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, INC., Columbia, MD*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- WP 029 **From Source Water to Tap Water to Swimming Pool and Spa Water: Effects of Disinfectants and Implications for Exposure/Toxicity;** Eric Daiber<sup>1</sup>; Susan Richardson<sup>1</sup>; Sridevi Anduri<sup>1</sup>; David DeMarini<sup>2</sup>; Ernest Blatchley<sup>3</sup>; Mehrnaz Afifi<sup>3</sup>; <sup>1</sup>*US EPA, NERL, Athens, GA*; <sup>2</sup>*U.S. EPA, NHEERL, RTP, NC*; <sup>3</sup>*Purdue University, West Lafayette, IN*
- WP 030 **A Comparison of the Use of Online SPE and Large Volume Injection Using LC-MS/MS for the Detection of Environmental Contaminants;** Stephen J. Lock; Pamela Stoddart; *ABSCIEX, Warrington, UK*
- WP 031 **Reliable Analysis of Priority Pollutants in Water by GC/HRMS with Faster, Cheaper, and Safer Sample Preparation;** Olga Polyakova<sup>1</sup>; Dmitry Mazur<sup>1</sup>; Slava Artaev<sup>2</sup>; Albert T. Lebedev<sup>1</sup>; <sup>1</sup>*Moscow State University, Moscow, Russian Federation*; <sup>2</sup>*Leco Corporation, St. Joseph, MI*
- WP 032 **Solid Phase Micro-extraction (SPME) with Gas Chromatography/Mass Spectrometry (GC/MS) to Quantify Polar Haloamides in Drinking Water;** Brandon Jessie; Christine N. Dalton; *Carson-Newman College, Jefferson City, TN*
- WP 033 **Determination of Microcystins in Drinking Water by Ultra High Performance Liquid Chromatography/Triple Quadrupole Mass Spectrometry;** Jinting Yao; Hongyuan Hao; Yin Huo; Hengtao Dong; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Shanghai, China*
- WP 034 **Quantitative Determination of Disinfection Byproduct Haloacetic Acids in Drinking Water Using Liquid Chromatography Tandem Mass Spectrometry;** Jinyuan Wang<sup>1,2</sup>; Xiaodong Liu<sup>1,2</sup>; Jonathan Beck<sup>1,2</sup>; Charles Yang<sup>1,2</sup>; Guifeng Jiang<sup>1,2</sup>; Richard Jack<sup>1,2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Sunnyvale, CA*
- WP 035 **N-nitrosodimethylamine (NDMA) Analysis in Water Using GC Triple Quadrupole Mass Spectrometry in Positive Chemical Ionization Mode;** Anthony Macherone<sup>2</sup>; Alandra Kahl<sup>1</sup>; Darryl Jones<sup>1</sup>; Lisa Lowe<sup>1</sup>; Shane Snyder<sup>1</sup>; <sup>1</sup>*University of Arizona, Tucson, AZ*; <sup>2</sup>*Agilent Technologies, Wilmington, DE*

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- WP 036 **Sulfur Rich Crude Oil and Bitumen Analysis on the Molecular Level by APPI and LDI FT-ICR Mass Spectrometry;** Matthias Witt; Jochen Friedrich; *Bruker Daltonik GmbH, Bremen, Germany*
- WP 037 **Dissolved Organic Matter in Lake Superior: A Study Combining Characterization by ESI FT-ICR MS, UV-Visible Spectroscopy and Isotopic Analysis;** Hongyu Li; Elizabeth Minor; *Large Lakes Observatory, University of Minnesota, Duluth, MN*
- WP 038 **Integrated Alkane, PAH, and Petroleum Biomarker Analysis by Tandem GC/MS;** Stephan Baumann; *Agilent Technologies, Inc., Santa Clara, CA*
- WP 039 **Applying Differential Mobility Spectrometry with Unique Gas-Phase Separations to the Analysis of Naphthenic Acids;** J. Larry Campbell<sup>1</sup>; Takeo Sakuma<sup>1</sup>; Andre Schreiber<sup>1</sup>; Paul Winkler<sup>1</sup>; John V. Headley<sup>2</sup>; Kerry M. Peru<sup>2</sup>; <sup>1</sup>*AB SCIEX, Concord, Canada*; <sup>2</sup>*Water Sci. Tech. Directorate, Environment Canada, Saskatoon, SK, Canada*
- WP 040 **GCxGC Profiling of Naphthenic Acid Esters in Oil Sands Composite Tailings;** David Bowman<sup>1</sup>; David Alonso<sup>2</sup>; Lorne Fell<sup>2</sup>; Joe Binkley<sup>2</sup>; Brian McCarty<sup>1</sup>; <sup>1</sup>*McMaster University, Hamilton, Canada*; <sup>2</sup>*Leco Corporation, St Joseph, MI*

- WP 041 **Characterization of Carbonaceous Particulate Matter Using Thermal Extraction Followed by Pyrolysis with Gas Chromatography Mass Spectrometry; Alena Kubatova;** Josef Beranek; Richard Cochran; Haewoo Jeong; Evgenii Kozliak; *University of North Dakota, Grand Forks, ND*
- WP 042 **Characterization of 2.5 Micron Particulate Borne Semivolatile Organic Compounds by GCxGC-TOFMS and UHPLC-Orbitrap MS – Method Development, Performance and Applications; Paul Yang<sup>1</sup>;** Nicholas Karellas<sup>1</sup>; Adrienne Boden<sup>1</sup>; Xiaoming Zhao<sup>1</sup>; Mike Spencer<sup>1</sup>; Chunyan Hao<sup>1</sup>; Stephanie Lemanik<sup>1</sup>; Gerald Ladwig<sup>1</sup>; Charles Yang<sup>2</sup>; Kristi Akervik<sup>2</sup>; Maciej Bromirski<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; *Ministry of the Environment, Etobicoke, Canada; <sup>2</sup>Thermo Scientific, San Jose, CA*
- WP 043 **Calibration of a Membrane Inlet Mass Spectrometer for Environmental Monitoring; Simon Maher;** Boris Brkic; Stephen Taylor; *University of Liverpool, Liverpool, UK*
- WP 044 **Detection of Nitrated and Oxygenated Polycyclic Aromatic Hydrocarbons Using Atmospheric Pressure Chemical Ionization High Resolution Mass Spectrometry; Richard Cochran;** Alena Kubatova; *University of North Dakota, Grand Forks, ND*
- Energy: Hydrocarbons and Petrochemical, 045 – 069**
- WP 045 **Oil Spill Source Identification by Principal Component Analysis of Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectra; Yuri E. Corilo<sup>1,2</sup>;** David C. Podgorski<sup>1,2</sup>; Amy M. McKenna<sup>1,3</sup>; Ryan P. Rodgers<sup>1,2</sup>; Karin L. Lemkau<sup>4</sup>; Christopher M. Reddy<sup>4</sup>; Alan G. Marshall<sup>1,3</sup>; *National High Magnetic Field Laboratory - FSU, Tallahassee, FL; <sup>2</sup>Future Fuels Institute - FSU, Tallahassee, FL; <sup>3</sup>Department of Chemistry and Biochemistry - FSU, Tallahassee, FL; <sup>4</sup>Woods Hole Oceanographic Institute, Woods Hole, MA*
- WP 046 **Improved Relative Abundance and Overall Sensitivity by Optimized Modifier/Analyte Concentration in Positive Ion Electrospray Crude Oil FT-ICR-MS; Brian M. Ruddy<sup>1</sup>;** Christopher L. Hendrickson<sup>2</sup>; Alan G. Marshall<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2</sup>; *Florida State University, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL*
- WP 047 **Development of High-Field Orbitrap FTMS-based Platform for Petroleum Analysis; Konstantin O. Zhurov;** Anton N. Kozhinov; Yury O. Tsybin; *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
- WP 048 **Characterization of Petroleum Fractions Using Mass Spectrometry Tools; Hung Pham<sup>1</sup>;** Haiyan Wang<sup>1</sup>; Howard Greenberg<sup>1</sup>; Matthew Unterfenger<sup>1</sup>; Wayne Rathbun<sup>1</sup>; Jonathan Pierson<sup>1</sup>; Paul Adams<sup>1</sup>; Gil Jones<sup>1</sup>; Kendall Guyer<sup>1</sup>; Dave Hindenlang<sup>2</sup>; *UOP LLC, A Honeywell Company, Des Plaines, IL; <sup>2</sup>Honeywell International Inc., Morristown, NJ*
- WP 049 **FT-ICR-MS – Studying the Effects of Ion Suppression on Crude Oil Mass Spectral Response Using Standard Compounds and Systems; Melissa Brown;** Ning Sanguantrakun; Ken Chanthamontri; Thomas Oldenburg; Steve Larter; *PRG, University of Calgary, Calgary, Canada*
- WP 050 **Petroleomics at Moderate Mass Resolution; Fan Huang;** Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- WP 051 **Ionization of Hydrocarbons by Atmospheric Solid Analysis Probe (ASAP) and Atmospheric Pressure Gas Chromatography (APGC); Chunping Wu;** Kuangnan Qian; Kathleen Edwards; Clifford Walters; Anthony Mennito; Christopher Jurtschenko; *ExxonMobil Research & Engineering Co., Annandale, NJ*
- WP 052 **Comparisons and Characterization of Different Asphaltenes Using Novel Ion Mobility-Mass Spectrometry Comparison Software ; Eleanor Riches<sup>1</sup>;** Jeremie Ponthus<sup>2</sup>; *Waters Corporation, Manchester, UK; <sup>2</sup>IFP Energies Nouvelles, Lyon, France*
- WP 053 **Isolation and Characterization of Interfacial Material from Athabasca Bitumen by Ultrahigh Resolution FT-ICR Mass Spectrometry; Amy Clingenpeel<sup>1</sup>;** Jacqueline Jarvis<sup>1</sup>; Winston Robbins<sup>2</sup>; Alan Marshall<sup>1,3</sup>; Ryan Rodgers<sup>1,3</sup>; *Florida State University Department of Chemistry, Tallahassee, FL; <sup>2</sup>Consultant, Brunswick, ME; <sup>3</sup>Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*
- WP 054 **Comparing LDI-FT-ICR and LDI-TOF/TOF Mass Spectrometry to Characterize Vacuum Residue of Colombian Crude Oils; Enrique Mejía-Ospino<sup>1</sup>;** Rafael Cabanzo<sup>1</sup>; Jorge Armando Orrego-Ruiz<sup>2</sup>; Andrea Gómez<sup>2</sup>; Yustina Rodriguez<sup>2</sup>; *Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Instituto Colombiano de Petróleos (ICP-Ecopetrol), Piedecuesta, Colombia*
- WP 055 **Asphaltene Analysis by TLC MALDI-TOF-MS; Martha L. Chacón<sup>1</sup>;** Andrea Gómez-Escudero<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; *Escuela de Química, Univ Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Instituto Colombiano del Petróleo, Ecopetrol, Piedecuesta, Colombia*
- WP 056 **A CAD Study on Ionized Model Compounds of Asphaltenes Containing Varying Alkyl Side Chains and Different Aromatic Core Sizes; Mohammad Sabir Aqueel;** James Riedeman; Hilkka Kenttamaa; *Purdue University, West Lafayette, IN*
- WP 057 **Examination of Solvent/Reagent Effects on Collisionally Activated Dissociation of Ionized Asphaltenes Using Atmospheric Pressure Chemical Ionization; Matthew Hurt;** Priya Murria; Hilkka Kenttamaa; *Purdue University, West Lafayette, IN*
- WP 058 **Structural Comparison of Asphaltenes of Different Origins by Using Tandem Mass Spectrometry; Weijuan Tang;** *Purdue University, West Lafayette, IN*
- WP 059 **Characterization of Nitrogen Containing Compounds in Vacuum Gas Oils Resins by ESI FT-ICR MS and HT-GCxGC/MS; Laure Boursier<sup>1</sup>;** Jérémie Ponthus<sup>1</sup>; Vincent Souchon<sup>1</sup>; Cyril Dartiguelongue<sup>1</sup>; Didier Thiébaud<sup>2</sup>; *IFP New Energy, Solaize, France; <sup>2</sup>UMR 7195 PESCA - ESPCI Paris Tech, Paris, France*
- WP 060 **Quantitative Analysis of Long Chain Fatty Acids Present in a Type I Kerogen Using ESI-FT-ICR-MS and Compared With GC-FID; Albert W. Kamga<sup>1</sup>;** Francoise Behar<sup>2</sup>; Patrick G. Hatcher<sup>1</sup>; *Department of Chemistry and Biochemistry, ODU, Norfolk, VA; <sup>2</sup>TOTAL, Paris, France*
- WP 061 **Quantitation of Asphaltene Inhibitors in Crude Oil by LC-TOF MS; Steven Rowland<sup>1</sup>;** Winston Robbins<sup>3</sup>; Ryan Rodgers<sup>1,2</sup>; *Florida State University, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Future Fuels Institute, Tallahassee, FL*
- WP 062 **High-Throughput Analysis Method for Straight Chain Alkanes Using LDTD-MS/MS; Pascal Belisle;** Gregory Blachon; Annick Dion; Serge Auger; Pierre Picard; *Phytronix Technologies, Quebec City, Canada*
- WP 063 **Targeted Petroleomics: Using High-Resolution TOF-MS to Evaluate the Efficiency of Acid and Sulfur Compound Removal from Crude Oil; Kevin Siek<sup>1</sup>;** Julie Hernández<sup>2</sup>; Clécio Klitzke<sup>3</sup>; Joe Binkley<sup>1</sup>; Jeffrey S. Patrick<sup>1</sup>; Rubens Maciel-Filho<sup>2</sup>; Marcos Eberlin<sup>3</sup>; *LECO Corporation, Saint Joseph, MI; <sup>2</sup>UNICAMP Separation Process Development Laboratory, Campinas SP, Brazil; <sup>3</sup>Thomson Mass Spectrometry Laboratory UNICAMP, Campinas SP, Brazil*



- WP 064 **Characterization of Heteroatom-Containing Aromatics in Crude Oil on a Research-Type High-Field Orbitrap MS by Utilization of a Deuterated Derivatization Reaction;** XuXiao Wang; Wolfgang Schrader; *Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany*
- WP 065 **Identification of Sulfur Compounds in Petroleum Samples Using Derivatization with Mass Deficient Reagents;** Ting Wang<sup>1</sup>; Daniel Jupiter<sup>2</sup>; Laxman Devkota<sup>1</sup>; Kevin Chambliss<sup>1</sup>; Kevin Pinney<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Baylor Univerisy, Waco, TX*; <sup>2</sup>*Texas A&M Health and Science Center, Temple, TX*
- WP 066 **Geotracers by FT-ICR MS;** Hendrik Muller<sup>1</sup>; Khaled Arouri<sup>2</sup>; Saroj Panda<sup>1</sup>; Adnan Al-Hajji<sup>1</sup>; <sup>1</sup>*Research and Development Center, Saudi Aramco, Dhahran, Saudi Arabia*; <sup>2</sup>*EXPEC Advanced Research Center, Saudi Aramco, Dhahran, Saudi Arabia*
- WP 067 **Petroleum Biomarkers Analyzed by Atmospheric Pressure Gas Chromatography Tandem Mass Spectrometry (APGC/MS/MS);** Douglas Stevens<sup>1</sup>; Quan Shi<sup>2</sup>; Chang Samuel Hsu<sup>3,4</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*China University of Petroleum, Beijing, China*; <sup>3</sup>*Florida State University, Tallahassee, FL*; <sup>4</sup>*Petro Bio Oil Consulting, Tallahassee, FL*
- WP 068 **Investigating Polyaromatic Sulfur Heterocycles in Model Systems and Crude Oil Using Atmospheric Pressure Chemical Ionization Orbitrap Mass Spectrometry;** Nadim Hourani<sup>1</sup>; Ma'an Amad<sup>1</sup>; Jan Andersson<sup>2</sup>; Mani Sarathy<sup>1</sup>; <sup>1</sup>*King Abdullah University Of Science and Technology, Thuwal, Saudi Arabia*; <sup>2</sup>*University of Muenster, Muenster, Germany*
- WP 069 **An Approach to Analysis and Visualization of Crude Oil Samples;** Manhoi Hur<sup>1</sup>; Yunju Cho<sup>2</sup>; Sungwhan Kim<sup>2</sup>; Eve Syrkin Wurtele<sup>1</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Kyungpook National University, Daegu, South Korea*
- Small Molecules: Quantitative Analysis III, 070 – 097**
- WP 070 **Method Development and Validation of an Assay for the Quantitation of Balsalazide in Human Plasma by Basic Reversed-Phase LC-MS/MS;** Melissa Meyer; Sara Clemens; Nancy Zheng; Zong-Ping Zhang; *PPD, Middleton, WI*
- WP 071 **High Sensitivity and Low Sample Volume Method Development for Quantitation of Fluticasone Propionate and Salmeterol in Human Plasma by LC-MS/MS;** Nancy Zheng; Jun Wang; Zong-Ping Zhang; *PPD Inc, Middleton, WI*
- WP 072 **Simultaneous Determination of Pioglitazone and Celecoxib in Mouse Plasma by nanoLC-MS;** Hong Wang<sup>1</sup>; Hiroyuki Katayama<sup>1</sup>; Mark Schliekelman<sup>2</sup>; Sam Hanash<sup>1</sup>; <sup>1</sup>*MD Anderson Cancer Center, Houston, TX*; <sup>2</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*
- WP 073 **Development of a Mass Spectrometric Method for Quantitating Sex Steroids in Human Serum;** Kerry M. Wooding; Chris A. Johnson; Joseph A. Hankin; Robert M. Barkley; Andrew P. Bradford; Nanette Santoro; Robert C. Murphy; *University of Colorado Denver AMC, Aurora, CO*
- WP 074 **Determination of Abiraterone in Human Plasma by LC-MS/MS;** Lan Li; Yuan-Shek Chen; Kumar Ramu; QPS, LLC, Newark, DE
- WP 075 **Quantitative Determination of Irsogladine in Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry;** Haejong Jang; Yuchang Choi; Kyunghwan Kim; Seungwoo Kang; *International Scitntific Standard, Chuncheon, South Korea*
- WP 076 **A Validated Method for the Determination of Adefovir in Human Plasma by Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry;** Won Seok Nam; Seo Hyun Yoon; Kyung-Sang Yu; In-Jin Jang; Joo-Youn Cho; *Seoul National University College of Medicine, Seoul, South Korea*
- WP 077 **A Sub-Picogram LC-MS/MS Method for the Analysis of Mometasone Furoate in Human Plasma;** Veniamin Lapko; Alan Dzerk; Karl Linderholm; Roger Coe; Brandon Retke; Mike Merrill; Curtis Sheldon; *Celerion, Inc, Lincoln, NE*
- WP 078 **Simultaneous Quantification of 15 Drugs of Abuse in Oral Fluid and Plasma by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry;** Yuling Song; Jinting Yao; Xiongxiang Qiu; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu (China) Co., LTD, Shanghai, China*
- WP 079 **Sensitive LC-MS/MS Quantitation of Thyroid Hormones in Serum;** Changtong Hao; Hui Qiao; Chuck Jolliffe; Sha Joshua Ye; *IONICS Mass Spectrometry, Bolton, ON, Canada*
- WP 080 **Highly Sensitive LC-MS/MS Quantification of Underivatized 1a,25-dihydroxyvitamin D3 Comparing Various Sample Extraction Methods;** Sha Joshua Ye; Changtong Hao; Hui Qiao; *IONICS Mass Spectrometry, Bolton, ON Canada*
- WP 081 **Developing High Throughput 2D-LC-MS/MS Method for Quantification of Vitamin D which Overcomes Challenges of Chemiluminescent Immunoassay;** Sreekala Narayanan<sup>1</sup>; Anura .V Kurpad<sup>1</sup>; Siji Joseph<sup>2</sup>; Sudha Rajagopalan<sup>2</sup>; Amit Kumar Mandal<sup>1</sup>; Suresh Babu C.V<sup>2</sup>; <sup>1</sup>*St. John's Research Institute, Bangalore, India*; <sup>2</sup>*Agilent Technologies, Bangalore, India*
- WP 082 **Development and Validation for the Determination of (E)-/(Z)-vitamin K1 Isomers in Human Plasma by LC-MS/MS;** Jingguo Hou; Melvin Tan; Ravi Orugunty; Xiaodong Zhu; Thomas Horvath; Jing Zhou; Gregory Poch; Michael Sullivan; Edward Wells; Steve Unger; *WWCT, Austin, TX*
- WP 083 **UHPLC-MS-MS Quantitation of Flavonoids, Terpene Lactones, and Detection of Unwanted Pesticides and Pharmaceuticals in Ginkgo Biloba Natural Dietary Products;** Frederic L Ciner<sup>1</sup>; Thomas Hayes<sup>1</sup>; Rachel Lieberman<sup>2</sup>; Jeffrey Dahl<sup>2</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, SOE, Raleigh, NC*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*
- WP 084 **An Alternative USP Method for the Analysis of Impurities in Riboflavin (Vitamin B2) Using LC-MS-MS;** Nicolas J. Hauser<sup>1</sup>; Jenna E. Milliken<sup>2</sup>; Carmen T. Santasania<sup>3</sup>; <sup>1</sup>*RTC/Sigma-Aldrich, Laramie, WY*; <sup>2</sup>*Department of Chemistry, University of Wyoming, Laramie, WY*; <sup>3</sup>*Supelco/Sigma-Aldrich, Bellefonte, PA*
- WP 085 **Application of DBS for the Quantitative Determination of Midazolam and Hydroxymidazolam Using an AB Sciex 6500 QTrap LC-MS/MS System;** Alexandre Pimenov; Jeffry Plomley; Mohamed Makhoulfi; *Charles River Laboratories, Senneville, Canada*
- WP 086 **Automatic LC/MS/MS Method to Quantitate Eicosapentaenoic acid (EPA) in Rat Plasma;** Rachel Sun; Jordan Nally; Tim Shoaf; *BASi, West Lafayette, IN*
- WP 087 **Quantification of Midazolam and 1-Hydroxymidazolam in Human Plasma Using API-4000 LC-MS/MS Systems with Higher Specificity and Lower Background Noise;** Guangchun Zhou; Nicole Roenker; Yong-Xi Li; *Medpace, Cincinnati, OH*
- WP 088 **A Simple, Direct Quantification of Carboplatin in Human Plasma Using Liquid Chromatography-Tandem Mass Spectrometry;** Tian-Sheng Lu; Elise Malinowski; Nicole Roenker; Yong-Xi Li; *Medpace, Cincinnati, OH*



- WP 089 **A Robust LC-MS/MS Analytical Method for Quantification of  $\beta$ -Lapachone: A Novel Chemotherapeutic Agent for the Treatment of Solid Tumors;** Claudia Meek<sup>1</sup>; Erling Beck<sup>1</sup>; David Boothman<sup>2</sup>; David Gerber<sup>2</sup>; Richard Leff<sup>1</sup>; <sup>1</sup>*School of Pharmacy, Texas Tech University HSC, Dallas, TX*; <sup>2</sup>*Harold C. Simmons Cancer Center, UT Southwestern, Dallas, TX*
- WP 090 **Two-Dimensional Liquid Chromatography/In-Source Fragmentation and Tandem Mass Spectrometry for Quantification of 2-Hydroxypropyl- $\beta$ -Cyclodextrin in Human Plasma;** Xuntian Jiang; Hui Jiang; Rohini Sidhu; Jean E Schaffer; Daniel S Ory; *Washington University, St. Louis, MO*
- WP 091 **Determination of Leelamine in Mouse Plasma by Liquid Chromatography/Electrospray Tandem Mass Spectrometry;** Min Song; Miri Hong; Oh Kwang Kwon; Doohyun Lee; Suyoun Lee; Taeho Lee; Sangkyu Lee; *Kyungpook National University, Daegu, Korea*
- WP 092 **Development of a HPLC-MS/MS Assay to Measure Irinotecan and Its Main Metabolites in Plasma. Preliminary Pharmacokinetic Evaluation in Cancer Patients;** Elena Marangon; Elisa Mazzega; Giuseppe Toffoli; *National Cancer Institute of Aviano, Aviano, Italy*
- WP 093 **Determination of Ceftiofur Metabolite Desfuroylceftiofur Cysteine Disulfide in Bovine Ileum by LC-MS/MS;** Gajendiran Mahadevan; Shixia Feng; Oscar A. Chiesa; *Center for Veterinary Medicine, FDA, Laurel, MD*
- WP 094 **Development and Validation of a Sensitive LC-MS/MS Method for Analysis of Midazolam and Their Metabolites in Human Plasma and Urine;** Ganesh Moorthy; Praveen Srivastava; Vu Nguyen; Jeffrey Barrett; Athena Zuppa; *The Children's Hospital of Philadelphia, Philadelphia, PA*
- WP 095 **Rapid and Robust Analysis Method for Quantifying Antidepressants and Major Metabolites in Human Serum by UHPLC-MS/MS;** Vincent Goudriaan<sup>1</sup>; Christ Pijnenburg<sup>2</sup>; Jacob Diepenbroek<sup>2</sup>; Jan Giesbertsen<sup>2</sup>; Annemieke Vermeulen Windsant-v.d. Tweel<sup>2</sup>; <sup>1</sup>*Shimadzu Benelux BV, 's-Hertogenbosch, Netherlands*; <sup>2</sup>*ZANOB BV, 's-Hertogenbosch, Netherlands*
- WP 096 **Quantitative Determination of Ultralow Level of Azelastine and Its Metabolite, Desmethylazelastine in Human Plasma via Two-Dimensional HPLC with MS/MS Detection;** Jingduan Chi; Zong-Ping Zhang; *PPD Inc, Madison, WI*
- WP 097 **Development a UHPLC-MS/MS Method for Determination of Clopidogrel, Clopidogrel Acid, and Clopidogrel Active Metabolite H4 in Human Plasma;** Wenyi Hua; Michael Lesslie; Brian T. Hoffman; Daniel Mulvana; *Advion Bioanalytical Labs, a Quintiles Company, Ithaca, NY*
- Diagnostic Clinical Chemistry: Small Molecules II, 098 – 116**
- WP 098 **Sensitive Assay of Free Thyroid Hormones by Online SPE-UHPLC-MS/MS in Human Plasma;** Maureen Ramero; Stéphane Moreau; Mikael Levi; *Shimadzu France, Noisiel, France*
- WP 099 **Quantification of Testosterone from Dried Blood Spots Using Liquid Chromatography Tandem Mass Spectrometry;** Richard E. Mathieu<sup>1</sup>; Catherine P. Riley<sup>1</sup>; Carmen L. Wiley<sup>1,2</sup>; <sup>1</sup>*Pathology Associates Medical Laboratories, Spokane, WA*; <sup>2</sup>*Providence Sacred Heart Medical Center, Spokane, WA*
- WP 100 **LC-ESI-MS/MS Multi-Target Quantification Method of Derivatized Catecholamines and Serotonin Applied to Clinical Analysis;** Elias Tessaro<sup>1,2</sup>; Giovana Bataglion<sup>1</sup>; Phellipe Amaral<sup>1,2</sup>; Gianfranco Zampieri<sup>3</sup>; Diogo Baldim<sup>3</sup>; <sup>1</sup>*UNICAMP, Campinas, Brazil*; <sup>2</sup>*LABMASS Laboratory, Campinas, Brazil*; <sup>3</sup>*Salomão & Zoppi Diagnósticos, São Paulo, Brazil*
- WP 101 **Simultaneous Analysis of Urinary Metanephines, Catecholamines and Serotonin by ESI-LC-MS/MS with Solid Phase Extraction Sample Preparation;** Murat Celik; Hasan Ozgen; Avni Cavdar; *Zivak Technologies, Kocaeli, Turkey*
- WP 102 **Sensitive Liquid Chromatography Mass Spectrometry Method for measuring Plasma Metanephines;** Catherine Riley<sup>1</sup>; Richard E. Mathieu<sup>1</sup>; Carmen L. Wiley<sup>1,2</sup>; <sup>1</sup>*Pathology Associates Medical Laboratories, Spokane, WA*; <sup>2</sup>*Providence Sacred Heart Medical Center, Spokane, WA*
- WP 103 **Use of a 2  $\mu$ m Ultra High Performance Liquid Chromatography Column and High Resolution MS in the Clinical Laboratory;** Ling Bei<sup>1</sup>; Michael Schulz<sup>1</sup>; Petra Lewits<sup>1</sup>; Patrik Appelblad<sup>1</sup>; Hans-Ake Lakso<sup>2</sup>; Joern Schneede<sup>2</sup>; <sup>1</sup>*EMD Millipore, Billerica, MA*; <sup>2</sup>*Dep Clinical Pharmacology Umeå University Hospital, Umeå, Sweden*
- WP 104 **Diagnosis of Breast Cancer Based on Lipid Profiles Obtained by MALDI-TOF Mass Spectrometry;** Hung Su<sup>1</sup>; Ya-Fei Bao<sup>1</sup>; Yi-Tzu Cho<sup>2</sup>; Jentaie Shiea<sup>1</sup>; Pei-Yung Nien<sup>3</sup>; Ya-Hui Chang<sup>3</sup>; Ming-Feng Hou<sup>3</sup>; <sup>1</sup>*National Sun Yat-Sen Univ., Kaohsiung, Taiwan*; <sup>2</sup>*Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan*; <sup>3</sup>*Kaohsiung Medical University Hospital, Kaohsiung, Taiwan*
- WP 105 **Development of a Method for the Diagnosis of Adrenoleukodystrophy Using Liquid Chromatography-Mass Spectrometry;** Kazuhiro Kida<sup>1</sup>; Hideki Nakajima<sup>1</sup>; Teruhiko Miwa<sup>1</sup>; Jun Watanabe<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; Torayuki Okuyama<sup>1</sup>; Masafumi Onodera<sup>1</sup>; Junichiro Fujimoto<sup>1</sup>; <sup>1</sup>*National Center for Child Health and Development, Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*
- WP 106 **Determination of Polyols (polyols) in Urine by Gas Chromatography-Chemical Ionization Mass Spectrometry;** Charles Kroll; Mark Magera; Perry Loken; Brenda Holmen; Dietrich Matern; Dimitar Gavrilov; Silvia Tortorelli; Devin Oglesbee; Piero Rinaldo; Kimiyo Raymond; *Mayo Clinic, Rochester, MN*
- WP 107 **Mucopolysaccharide Quantitation in Urine by LC-MS/MS;** Jean M Lacey; Mark J Magera; Dimitar K Gavrilov; Silvia Tortorelli; Devin Oglesbee; Piero Rinaldo; Kimiyo M Raymond; Dietrich Matern; *Mayo Clinic, Rochester, MN*
- WP 108 **Clinical Diagnostics Approaches of Lysosomal Storage Diseases on DBSs by Fluorimetry and MRM-MS Using Identical  $\alpha$ -hydroxy-coumarin based substrates;** Claudia Cozma<sup>1</sup>; Marius-Ionut Iurascu<sup>1</sup>; Gabriela Paraschiv<sup>1</sup>; Laura Ion<sup>2</sup>; Alina Brandusa Petre<sup>2</sup>; Adolf Muhl<sup>3</sup>; Stefan Maeser<sup>3</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*University of Konstanz, Konstanz, Germany*; <sup>2</sup>*Al.I. Cuza University, Iasi, Romania*; <sup>3</sup>*Centogene AG, Freiburg & Rostock, Germany*
- WP 109 **Nicotine and Metabolites: Evaluation of Supported Liquid Extraction Approaches prior to UPLC-MS/MS Analysis;** Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Adam Senior<sup>1</sup>; Rhys Jones<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Gavin Jones<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage US, Charlotte, NC*
- WP 110 **Fast On-Line SPE-UHPLC-MS/MS Quantitative Analysis of Multiclass Antibiotics in Human Plasma for Emergency Diagnostic;** Mikael LEVI; Maureen Ramero; Stephane Moreau; *Shimadzu France, Marne La Vallée Cedex 2, France*
- WP 111 **Quantification of Serum Voriconazole by Liquid Chromatography and Tandem Mass Spectrometry;** Karina Helena Morais Cardozo; Jessica Silva Salgueiro; Valdemir Melechco Carvalho; *Fleury Group, São Paulo, Brazil*

- WP 112 **Concentrations of Arsenic in Human Urine: A Correlation between Total Arsenic by ICP-MS and Speciated Arsenic by HPLC-ICP-MS;** Indranil Sen; Wei Zou; *CA Dept of Public Health, Richmond, CA*
- WP 113 **Comparison of Two Sample Preparation Methods for Analyzing Pain Management Drugs in Urine;** Xuejun Zang; Igor Gavin; Krishna Mallia; Asha Oroskar; Anil Oroskar; *Orochem Technologies Inc., Lombard, IL*
- WP 114 **An Enzyme Assay Mass Screening System for Adenosine Deaminase Deficiency from Dried Blood Spots Using a DART MS/MS;** Hideki Nakajima<sup>1</sup>; Teruhiko Miwa<sup>1</sup>; Kazuhiro Kida<sup>1</sup>; Jun Watanabe<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; Torayuki Okuyama<sup>1</sup>; Masafumi Onodera<sup>1</sup>; Junichiro Fujimoto<sup>1</sup>; <sup>1</sup>*National Center for Child Health and Development, Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*
- WP 115 **Positive and Negative Mode PESI-MS for Cancer Diagnostics;** Mridul Kanti Mandal<sup>1</sup>; Kentaro Yoshimura<sup>2</sup>; Subhrakanti Saha<sup>1</sup>; Md. Obaidur Rahman<sup>1</sup>; Yasuo Shida<sup>1</sup>; Sen Takeda<sup>2</sup>; Hiroshi Nonami<sup>3</sup>; Kenzo Hiraoka<sup>1</sup>; <sup>1</sup>*CERC, University of Yamannashi, Kofu, Japan*; <sup>2</sup>*Faculty of Medicine, University of Yamannashi, Chuo, Japan*; <sup>3</sup>*Faculty of Agriculture, Ehime University, Matsuyama, Japan*
- WP 116 **Catalytic Pyrolysis Metal Oxide Laser Ionization (CP-MOLI MS) Fatty Acid Profiling for Bacterial Identification;** Kirk Jensen<sup>1</sup>; Casey McAlpin<sup>1</sup>; Christopher Cox<sup>1</sup>; Robert Cody<sup>2</sup>; Jon Rees<sup>3</sup>; Kent Voorhees<sup>1</sup>; <sup>1</sup>*Colorado School of Mines, Golden, CO*; <sup>2</sup>*JEOL USA, Peabody, MA*; <sup>3</sup>*Centers for Disease Control, Atlanta, GA*
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- WP 117 **Method Scalability for Drugs of Abuse Extraction from Urine using Supported Liquid Extraction prior to UPLC-MS/MS Analysis;** Lee Williams<sup>1</sup>; Rhys Jones<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Kerry Stephens<sup>1</sup>; Steve Jordan<sup>1</sup>; Gavin Jones<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage, Charlotte, NC*
- WP 118 **High Performance Cost Efficient LC-MS/MS Solution for NIDA-5 Panel Using New Dual Channel Prelude SPLC System and Quantum-Ultra Mass Spectrometer;** Haiqiang Yu; Kristine Van Natta; Marta Kozak; *ThermoFisher Scientific, San Jose, CA*
- WP 119 **Direct Mass Imaging of Ketamine Distribution in Single Scalp Hair by MALDI-CASI-FTMS;** Ping Xiang<sup>1</sup>; Hai Pu<sup>2</sup>; Min Shen<sup>1</sup>; <sup>1</sup>*Institute of Forensic Sciences, Shanghai, China*; <sup>2</sup>*Bruker, Beijing, China*
- WP 120 **A Reversed-Phase LC-MS/MS Method for the Quantitation of Ethyl Glucuronide and Ethyl Sulfate in Human Urine;** Frances Carroll; Sharon Lupo; Chris Denicola; Ty Kahler; Paul Connolly; *Restek Corporation, Bellefonte, PA*
- WP 121 **Rapid Screening and Semi-Quantitative Analysis for Forensic Drugs in Blood Using Liquid Chromatography Triple Quadrupole Mass Spectrometry;** Thomas Hayes<sup>1</sup>; Keiko Kudo<sup>2</sup>; Toshikazu Minohata<sup>3</sup>; Kiyotaka Usui<sup>4</sup>; Noriaki Shima<sup>5</sup>; Munehiro Katagi<sup>6</sup>; Hitoshi Tsuchihashi<sup>6</sup>; Koichi Suzuki<sup>6</sup>; Ichiro Hirano<sup>3</sup>; Noriaki Ikeda<sup>2</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Inc., Columbia, MD*; <sup>2</sup>*Kyushu University, Fukuoka, Japan*; <sup>3</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>4</sup>*Tohoku University Graduate School of Medicine, Sendai, Japan*; <sup>5</sup>*Osaka Prefectural Police, Osaka, Japan*; <sup>6</sup>*Osaka Medical College, Takatsuki, Japan*
- WP 122 **Direct Analysis Using Paper-Spray Mass Spectrometry: Method Development for the Rapid Screening of Drugs of Abuse for Forensic Toxicology;** Maria C. Prieto Conaway<sup>1</sup>; Nicholas E. Manicke<sup>2</sup>; Marta Kozak<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Purdue University, West Lafayette, IN*
- WP 123 **Characterization and Classification of Heroin from Illicit Heroin Seizures by GC/Q-TOF;** Dmitry Koluntaev<sup>1</sup>; Sergei Syromyatnikov<sup>2</sup>; Igor Sarychev<sup>2</sup>; Sofia Aronova<sup>3</sup>; <sup>1</sup>*InterLab, Inc., Moscow, Russia*; <sup>2</sup>*Federal Drug Control Service of Russian Federation, Moscow, Russia*; <sup>3</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- WP 124 **Cocaine and Metabolites: Method Development Strategies Using Supported Liquid Extraction from Urine Prior to UPLC-MS/MS Analysis;** Rhys Jones<sup>1</sup>; Lee Williams<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Kerry Stephens<sup>1</sup>; Steve Jordan<sup>1</sup>; Gavin Jones<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage, Charlotte, NC*
- WP 125 **Rapid and Sensitive Quantitation of THC and Metabolites in Urine by Microflow LC-MS/MS;** Daniel Blake<sup>1</sup>; Julie Moriceau<sup>1</sup>; Sylvain Dulaurent<sup>2</sup>; Jean-Michel Gaulier<sup>2</sup>; Aymeric Morla<sup>1</sup>; <sup>1</sup>*AB SCIEX, Warrington, UK*; <sup>2</sup>*CHU Dupuytren Limoges, Limoges, France*
- WP 126 **Direct Quantification of 11-nor- $\Delta^8$ -tetrahydrocannabinol-9-carboxylic Acid and Its Glucuronide in Urine Using Liquid Chromatography-Tandem Mass Spectrometry;** Jin-Young Kim; Woonyong Kwon; Sungill Suh; Moon Kyo In; *Supreme Prosecutors' Office, Seoul, Korea*
- WP 127 **Ultrafast, Ultra-selective High-Throughput Forensic Drug Screening in Urine Using SPE/MS/MS;** Vaughn Miller; Michelle Romm; Kari Schlicht; Nikunj Parikh; Mohamed Youssef; Maxcy Stroman; William LaMarr; Can Ozbai; *Agilent Technologies, Wakefield, MA*
- WP 128 **Rapid LC-MS/MS Screening Method for Fourteen JWH-type Synthetic and Natural Cannabinoids in Counterfeit Samples;** Philippe Lebel; Karen C. Waldron; Alexandra Furtos; *Université de Montréal, Montréal, Canada*
- WP 129 **Rapid Generation of Synthetic Cannabinoids' "Metabolite Fingerprints" following Human Hepatocyte Metabolism and High Resolution Mass Spectrometry Analysis;** Ariane Wohlfarth<sup>1</sup>; Adarsh Gandhi<sup>1</sup>; Shaokun Pang<sup>2</sup>; Hua-fen Liu<sup>2</sup>; Mingshe Zhu<sup>3</sup>; Marilyn Huestis<sup>1</sup>; <sup>1</sup>*NIDA, NIH, Baltimore, MD*; <sup>2</sup>*AB Sciex, Foster City, CA*; <sup>3</sup>*Bristol-Myers Squibb, Princeton, NJ*
- WP 130 **Rapid Analysis of Synthetic Cathinones (bath salts) by LC/Triple Quadrupole Mass Spectrometry;** Flaubert Mbeunkui; Joseph Wiegel; Brent Dixon; *Physicians Choice Laboratory Services, Charlotte, NC*
- WP 131 **Analysis of Cathinones in Bath Salts by Direct Sample Analysis TOF MS;** Noelle Elliott<sup>1</sup>; Amanda Leffler<sup>2</sup>; Avinash Dalmia<sup>1</sup>; Frank Dorman<sup>2</sup>; Carl Schwarz<sup>1</sup>; <sup>1</sup>*PerkinElmer, Shelton, CT*; <sup>2</sup>*Penn State University, University Park, PA*
- WP 132 **Implementation of Bench-Top Quadrupole Orbitrap Ultra High Resolution Mass Spectrometer in Quantitative Analysis of Synthetic Cathinones in Urine Samples;** Marta Kozak; Kristine Van Natta; Shijun Sheng; *Thermo Fisher Scientific, San Jose, CA*
- WP 133 **Trapping 'Spice': A Comprehensive Automated LC-Ion Trap-MS Screening Approach for the Detection of 38 Synthetic Cannabinoids in Serum;** Laura M. Huppertz; Stefan Kneisel; Volker Auwärter; Jürgen Kempf; *Institute of Legal Medicine, University Freiburg, Freiburg, Germany*
- WP 134 **Confirmation and Quantification of Synthetic Cannabinoids in a Sample of "Spice" by GC/TOF-MS;** Chiara Abate<sup>1</sup>; Ilaria Ferrante<sup>1</sup>; Luigi Motti<sup>2</sup>; <sup>1</sup>*DANI, Cologno Monzese, Italy*; <sup>2</sup>*Dani SA, Contone, Switzerland*

- WP 135 **Development of a LC-MS/MS Analytical Strategy Based on Class-Characteristic Fragmentation Pathways to Detect Synthetic Cannabinoids in Different Matrices;** Monica Mazzarino; Xavier de la Torre; Ilaria Fiocco; Francesco Botrè; *Antidoping laboratory, Rome, Italy*
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- WP 136 **Recombinant “IMS TAG” Proteins - A Method for Validating MALDI - Ion Mobility Separation - Mass Spectrometry Imaging (MALDI-IMS-MSI);** Laura Cole<sup>1</sup>; Khaled Mahmoud<sup>2</sup>; Gillian Tozer<sup>3</sup>; Simona Francese<sup>1</sup>; David Smith<sup>1</sup>; Malcolm Clench<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>Al-Jouf University, Sakaka, Kingdom of Saudi Arabia; <sup>3</sup>Sheffield University, Sheffield, UK
- WP 137 **Optimization of A New Method for Spatial Profiling of N-linked Glycan Expression in Tissues by MALDI Mass Spectrometry Imaging;** Thomas Powers<sup>1</sup>; E. Ellen Jones<sup>1</sup>; Anand Mehta<sup>2</sup>; Richard R Drake<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Drexel Institute for Biotechnology and Virology, Doylestown, PA
- WP 138 **MALDI Imaging Mass Spectrometry (MALDI-IMS) of Colon Adenocarcinoma Formalin-Fixed Paraffin-Embedded Tissues;** Irene (Eirini) Panderi (Panteri)<sup>1,2</sup>; Lulu Cao<sup>2</sup>; Lelia Noble<sup>2</sup>; Kimberly Perez<sup>3</sup>; Dionysios Pantazatos<sup>2</sup>; <sup>1</sup>University of Athens, Pharmacy, Pharm.Chemistry, Athens, Greece; <sup>2</sup>COBRE Center for Cancer Research, Brown Medical, Providence, RI; <sup>3</sup>Rhode Island Hospital, Brown Medical, Providence, RI
- WP 139 **Identification of Accumulated Ceramide Species in a Farber Disease Mouse Model by MALDI-MS Imaging;** Shaaalee Dworski<sup>1</sup>; Ellen Jones<sup>2</sup>; Abdulfatah Alayoubi<sup>1</sup>; Jeffrey A. Medin<sup>1</sup>; Richard Drake<sup>2</sup>; <sup>1</sup>University of Toronto, Toronto Ontario, Canada; <sup>2</sup>Medical University of South Carolina, Charleston, SC
- WP 140 **Microwave-Assisted Enzymatic Digestion On-Tissue for Membrane Protein Analysis with MALDI Imaging Mass Spectrometry;** Jamie L Wenke; Kevin L Schey; *Department of Biochemistry, Vanderbilt University, Nashville, TN*
- WP 141 **The Effect of Heat-Induced Tissue Stabilization on the MS- and Histo-Architecture of Mouse Brain;** Ricardo J. Carreira<sup>1</sup>; Cecilia Eriksson<sup>2</sup>; Walid M. Abdelmoula<sup>1</sup>; Reinald Shyti<sup>1</sup>; René J.M. van Zeijl<sup>1</sup>; Sandra H. van Heiningen<sup>1</sup>; Else A. Tolner<sup>1</sup>; Arn M.J.M. van den Maagdenberg<sup>1</sup>; Jouke Dijkstra<sup>1</sup>; Per E. Andrén<sup>2</sup>; Liam A. McDonnell<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>2</sup>Uppsala University, Uppsala, Sweden
- WP 142 **Detection of Individual Cells in Tissue Using MALDI-TOF Imaging at 10 µm Pixel Size;** Eckhard Belau<sup>1</sup>; Jane-Marie Kowalski<sup>2</sup>; Janine Rattke<sup>1</sup>; Alice Ly<sup>3</sup>; Soeren-Oliver Deininger<sup>1</sup>; Detlev Suckau<sup>1</sup>; Axel Walch<sup>3</sup>; Marius Ueffing<sup>3</sup>; Michael Becker<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Helmholtz-Zentrum München, Munich, Germany
- WP 143 **Identifying and Imaging Lipid Oxidation Products by MALDI-MS<sup>n</sup>: A Multivariate Approach;** Whitney L. Stutts<sup>1</sup>; Gert B. Eijkel<sup>2</sup>; Ron M.A. Heeren<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>Chemistry Department, University of Florida, Gainesville, FL; <sup>2</sup>FOM Institute AMOLF, Amsterdam, NL
- WP 144 **Peptide Bead Arrays Measured by Mass Spectrometry Imaging;** Vladislav Bergo; *Adeptrix Corp, Boston, MA*
- WP 145 **MALDI Imaging of Rat Testis at 10µm Pixel Size and 200k Mass Resolution;** Jens Fuchser; Eckhard Belau; Soeren-Oliver Deininger; Michael Becker; *Bruker Daltonik GmbH, Bremen, Germany*
- WP 146 **Novel Workflow Combining MALDI Imaging and LC-MALDI for Obtaining Identification and Spatial Localization of Proteins from Eye Lens Tissue;** Sergei Dikler; Jane-Marie Kowalski; D. Shannon Cornett; *Bruker Daltonics Inc., Billerica, MA*
- WP 147 **Improved Sensitivity in the Detection of Low Abundance Proteins in Virtual 2D Gels;** Karen Lohnes; Fred Kobzeff; Andrea Rivera; Robert Gunsalus; Joseph Loo; Rachel Ogorzalek Loo; *University of California, Los Angeles, CA*
- WP 148 **Imaging of Lipids in Rat Heart by MALDI-MS;** Shelley N Jackson; Ludovic M Muller; Kathrine Baldwin; Amina S Woods; *NIDA-IRP, NIH, Baltimore, MD*
- WP 149 **Profiling of a Cell Population Using MALDI Mass Spectrometry Imaging;** Ta-Hsuan Ong; David Kissick; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois, Urbana, IL*
- WP 150 **Separation Effects Caused by the Dried-Droplet Sample Preparation for MALDI Mass Spectrometry of Synthetic Polymers;** Stefan Johannes Gabriel<sup>1</sup>; Steffen Weidner<sup>1</sup>; Ulrich Panne<sup>1</sup>; Clemens Schwarzwinger<sup>2</sup>; <sup>1</sup>Federal Institute for Material Research BAM, Berlin, Germany; <sup>2</sup>Johannes Kepler University JKU, Linz, Austria
- WP 151 **Matrix Application Method Optimization for MALDI-MS Imaging (MSI) of Metabolites during Nitrogen Fixation in the Medicago truncatula-Sinorhizobium meliloti Symbiosis;** Erin Gemperline<sup>1</sup>; Vivian Hui Ye<sup>2</sup>; Muthusubramanian Venkateshwaran<sup>3</sup>; Jean-Michel Ané<sup>3</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>UW-Madison Department of Chemistry, Madison, WI; <sup>2</sup>UW-Madison School of Pharmacy, Madison, WI; <sup>3</sup>UW-Madison Department of Agronomy, Madison, WI
- WP 152 **Towards 3-Dimensional MALDI MS Molecular Imaging of the Optic Chiasm;** David M. G. Anderson<sup>1</sup>; Raf Van de Plas<sup>1</sup>; Kevin L. Schey<sup>1</sup>; Anne Solga<sup>2</sup>; David H. Gutmann<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>2</sup>Washington University School of Medicine, St. Louis, MO
- WP 153 **Fixation of Single Sections and Whole Organs in Formal Lithium Improves *in-situ* Characterisation and Imaging of Lipids by Mass Spectrometry;** Rian L. Griffiths; Joscelyn Sarsby; Emily J. Guggenheim; Alan M. Race; Rory T. Steven; Andrew D. Palmer; Patricia Lalor; Josephine Bunch; *University of Birmingham, Birmingham, UK*
- WP 154 **High Spatial Resolution Imaging of Lipids in Formalin-fixed Cardiac Tissue by MALDI Imaging MS;** Peggy Angel<sup>1</sup>; Andrey Zavalin<sup>1</sup>; H. Scott Baldwin<sup>2</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>Dept Biochem, Vanderbilt University, Nashville, TN; <sup>2</sup>Dept Cell & Dev Biol, Peds, Vanderbilt University, Nashville, TN
- WP 155 **Imaging and Accurate Mass Identifications of Intact Proteins above 10 kDa Using Multiply Charged Ions and High Resolution MS;** David G. Rizzo; Jeffrey M. Spraggins; Kristie L. Rose; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- WP 156 **1,5-Diaminonaphthelene Pre-Coated Targets for MALDI Imaging of Lipids;** Junhai Yang<sup>1</sup>; Richard Caprioli<sup>1,2</sup>; <sup>1</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>2</sup>Pharmacology and Medicine, Vanderbilt University, Nashville, TN
- WP 157 **Monitoring Time-Dependent Lipid Degradation on Tissue Sections by MALDI Imaging Mass Spectrometry;** Heath Patterson; Aurélien Thomas; Pierre Chaurand; *University of Montreal, Montreal, Canada*



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- WP 158 **MSiReader: A Free Open Source Vendor-Neutral Matlab Interface to View and Analyze High Resolving Power MS Imaging Data;** Kenneth P. Garrard; Guillaume Robichaud; Jeremy A. Barry; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- WP 159 **Exploration of Tensor Decomposition for Imaging Mass Spectrometry;** Yousef El Aalamat<sup>1,4</sup>; Raf Van de Plas<sup>2</sup>; Nico Verbeeck<sup>1,4</sup>; Bart De Moor<sup>1,4</sup>; Etienne Waelkens<sup>3,4</sup>; <sup>1</sup>*KU Leuven, ESAT-SCD/ iMinds Future Health Dept., Leuven, BE*; <sup>2</sup>*Vanderbilt University, Nashville, TN*; <sup>3</sup>*KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, BE*; <sup>4</sup>*KU Leuven, Sybioma, Leuven, BE*
- WP 160 **Customizable Open-Source Mass Spectrometry Imaging (MSI) Data Processing Tool for Use with the .mzxml Data File Format;** Cynthia Kaeser; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- WP 161 **Mass Spectrometry Imaging Software Assisting Labeled Normalization and Quantitation with Standardized Open Access Format;** Patrik Källback; Anna Nilsson; Mohammadreza Shariatgorji; Per E. Andrén; *Uppsala University, Uppsala, Sweden*
- WP 162 **Pathology Interface for Mass Spectrometry (PIMS): A Web-Based Collaborative Tool for Histology-Directed Mass Spectrometry Experiments;** Jeremy L. Norris<sup>1</sup>; Erin H. Seeley<sup>1</sup>; Tina Tsui<sup>1</sup>; Alireza Sepehr<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University School of Medicine, Nashville, TN*; <sup>2</sup>*Harvard Beth Israel Deaconess Medical Center, Boston, MA*
- WP 163 **Going Beyond Imaging Mass Spectrometry: Fusing Information Across Different Imaging Technologies;** Raf Van de Plas; Junhai Yang; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- WP 164 **Extensible Software for the Processing of Spectrometry Imaging Data Sped Up Using GPGPU;** Alan M. Race; Andrew D. Palmer; Rory T. Steven; Joscelyn Sarsby; Rian L. Griffiths; Iain B. Styles; Josephine Bunch; *University of Birmingham, Birmingham, UK*
- WP 165 **An Intelligent Data Compression Workflow for the Analysis of Biomedical Mass Spectrometry Images;** Andrew Palmer; Rory Steven; Rian Griffiths; Alan Race; Joscelyn Sarsby; Emily Guggenheim; Patricia Lalor; Iain Styles; Josephine Bunch; *University of Birmingham, Birmingham, UK*
- WP 166 **Deeper Insights through Integration: Linking Imaging Mass Spectrometry Data with Anatomical Data;** Nico Verbeeck<sup>1,3</sup>; Junhai Yang<sup>2</sup>; Bart De Moor<sup>1,3</sup>; Richard Caprioli<sup>2</sup>; Etienne Waelkens<sup>3,4</sup>; Raf Van de Plas<sup>2</sup>; <sup>1</sup>*ESAT-SISTA / iMinds Future Health Dept., KU Leuven, Leuven, Belgium*; <sup>2</sup>*Vanderbilt University, Nashville, TN*; <sup>3</sup>*Sybioma, KU Leuven, Leuven, Belgium*; <sup>4</sup>*Dept. of Cellular & Molecular Medicine, KU Leuven, Leuven, Belgium*
- WP 167 **Targeted Ion Imaging MS: Evaluation of New Algorithms to Reduce Acquisition and Processing Time;** Paul Murray; Keith Richardson; Emmy Hoyes; Chris Jones; Richard Chapman; Jeff Brown; *Waters Corporation, Manchester, UK*
- WP 168 **Investigation of Different Hierarchical Clustering Approaches for Protein Identification Directly from Tissue Section in a MALDI Imaging Experiment;** Mark Towers<sup>1</sup>; Laura M. Cole<sup>2</sup>; Malcolm R. Clench<sup>2</sup>; Emmanuelle Claude<sup>1</sup>; <sup>1</sup>*Waters corporation, Manchester, UK*; <sup>2</sup>*Biomedical Research Centre, Sheffield Hallam Uni, Sheffield, UK*
- WP 169 **A New 64-Bit Software Application for MS Image Processing;** Damon Barbacci; Thomas Egan; J. Albert Schultz; *Ionwerks, Inc., Houston, TX*

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- WP 170 **Imaging Mass Spectrometry in Three-Dimensional Cell Culture Systems for Evaluation of Therapeutics;** Xin Liu; Amanda Hummon; *University of Notre Dame, Notre Dame, IN*
- WP 171 **Imaging Analysis of the Brain Distribution of Verapamil by Liquid Extraction Surface Analysis (LESA) Mass Spectrometry;** Kenichi Watanabe; Jun Tadano; Toichiro Yamada; Chihiro Ishikawa; Takao Watanabe; Tetsuya Nakagawa; Naruaki Nomura; Masashi Yabuki; *Dainippon Sumitomo Pharma Co., Ltd., Suita, Osaka, Japan*
- WP 172 **Potential Markers of Tumour Viability and Necrosis in CA-4-P Treated Fibrosarcomas Employing a Multimodal Proteomic Approach;** Laura Cole<sup>1</sup>; Jo Bluff<sup>2</sup>; Vikki Carolan<sup>1</sup>; Martyn Paley<sup>2</sup>; Gillian Tozer<sup>2</sup>; Malcolm Clench<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, BMRC, Sheffield, UK*; <sup>2</sup>*University of Sheffield, Sheffield, UK*
- WP 173 **Semi-Quantitative Analysis for Distribution of CNS Drugs and Metabolites in Rat Brain by Liquid Extraction Surface Analysis Mass Spectrometry;** Jun Tadano; Toichiro Yamada; Kenichi Watanabe; Tetsuya Nakagawa; Naruaki Nomura; Masashi Yabuki; *Dainippon Sumitomo Pharma Co., Ltd., Suita, Japan*
- WP 174 **Imaging LA-ICP-MS as a Powerful Tool for the Investigation of Pd-tagged Photosensitizers in Tumor Spheroids;** Ann-Christin Bülter; Christoph A. Wehe; Franziska Blaske; Olga Reifschneider; Uwe Karst; *Westfälische Wilhelms-Universität Münster, Münster, Germany*
- WP 175 **Extracting More from QWBA's with Liquid Extraction Surface Analysis (LESA): Identifying Drug and Metabolites Directly from Whole Rat Sections;** William Hardesty; Jill Pirhalla; Stephen Castillino; *GlaxoSmithKline, King of Prussia, PA*
- WP 176 **Investigating the Correlation between Plasma PK Analysis with Tissue Abundance and Distribution by using MS Imaging and Profiling;** John G. Swales<sup>1,2</sup>; Peter Webb<sup>1</sup>; Malcolm Clench<sup>2</sup>; Richard Goodwin<sup>1</sup>; <sup>1</sup>*Astrazeneca, Macclesfield, UK*; <sup>2</sup>*Sheffield Hallam University, Sheffield, UK*
- WP 177 **Validation of Observed Metabolite to Parent Drug Abundance Ratios from IR-MALDESI MSI by Performing LC-MS on Adjacent Tissue Sections;** Kristin M. Klinc<sup>1</sup>; Jeremy A. Barry<sup>1</sup>; Guillaume Robichaud<sup>1</sup>; Reid Groseclose<sup>2</sup>; David Wagner<sup>2</sup>; Stephen Castellino<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*GlaxoSmithKline, Research Triangle Park, NC*
- WP 178 **Mapping the Distribution of Intranasally Administered Oxytocin (OXT) in Rat Brain Using MALDI Imaging Mass Spectrometry;** Bingming Chen; Hui Ye; Mohan Gautam; Jingxin Wang; Robert Thorne; Lingjun Li; *School of Pharmacy, University of Wisconsin, Madison, WI*
- WP 179 **High Spatial and Mass Resolution Imaging to Assess Ocular Drug Delivery;** Cristine Quiaison<sup>1</sup>; Sheerin K. Shahidi-Latham<sup>1</sup>; Katherine A. Kellersberger<sup>2</sup>; Brian J. Dean<sup>1</sup>; <sup>1</sup>*Genentech Inc., South San Francisco, CA*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*
- WP 180 **Imaging Mass Spectrometry of Pharmaceutical Drugs Using a High Mass Resolution MALDI-SpiralTOF-TOF;** Ayumi Kubo<sup>1</sup>; Takaya Satoh<sup>1</sup>; Robert A. DiPasquale<sup>2</sup>; Naoki Moriguchi<sup>3</sup>; Hisanao Hazama<sup>3</sup>; Kunio Awazu<sup>3</sup>; Michisato Toyoda<sup>4</sup>; <sup>1</sup>*JEOL Ltd., Tokyo, Japan*; <sup>2</sup>*JEOL USA, Inc., Peabody, MA*; <sup>3</sup>*Graduate School of Engineering, Osaka University, Osaka, Japan*; <sup>4</sup>*Graduate School of Science, Osaka University, Osaka, Japan*

- WP 181 **Mass Spectrometry Imaging of Raclopride and Fexofenadine in Whole Body Mouse Tissue Using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS);** Callee Walsh; Pamela Williams; Gregory Boyce; Brent Reschke; Holly Henderson; Matthew Powell; Trust Razunguzwa; *Protea Biosciences, Morgantown, WV*
- WP 182 **Mass Spectrometric Imaging of Potential Lipid Biomarkers in Shiverer Mice by Desorption Electrospray Ionization for Neurologic Diseases;** Daniel Waldon; Liyu Yang; *Biogen idec, Cambridge, MA*
- WP 183 **MALDI Mass Spectrometry Imaging (MALDI-MSI) of Pyrazinamide, Pyrazinoic Acid and Moxifloxacin in Clinical TB Lung Biopsies;** Brendan Prideaux<sup>1</sup>; Markus Stoeckli<sup>2</sup>; Dieter Staab<sup>2</sup>; Gregory Morandi<sup>2</sup>; Clifton E Barry<sup>3</sup>; Laura E Via<sup>3</sup>; Danielle Weiner<sup>3</sup>; Veronique Dartois<sup>1</sup>; <sup>1</sup>*Public Health Research Institute, UMDNJ, Newark, NJ*; <sup>2</sup>*Novartis Institutes for BioMedical Research, Basel, Switzerland*; <sup>3</sup>*Tuberculosis Research Section, NIAID, Bethesda, MD*
- WP 184 **Blood-Brain Barrier Drug Targeting by Mass Spectrometry Imaging in Early ADME Profiling;** Anna Nilsson; Richard Goodwin; Henrik Loden; Charlotta Wallinder; Sergio Estrada; Niklas Marklund; Mats Larhed; Per E. Andrén; *Uppsala University, Uppsala, Sweden*
- WP 185 **Development of Combined PK/PD Studies of RAF/MEK/mTOR Inhibitors for the Treatment of Pediatric Low-Grade Astrocytomas by MALDI Mass Spectrometry Imaging;** David Calligaris<sup>1,2</sup>; Xiaohui Liu<sup>1,2</sup>; Daniel Feldman<sup>1,2</sup>; Christopher J. Thompson<sup>3</sup>; Jennifer L. Ide<sup>1,2</sup>; Mark Marchionni<sup>4</sup>; Sara Buhrlage<sup>4</sup>; Michael L. Easterling<sup>3</sup>; Nathanael Gray<sup>4</sup>; Charles D. Stiles<sup>4</sup>; Nathalie Y. Agar<sup>1,2</sup>; <sup>1</sup>*Brigham & Women's Hospital, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*Bruker Daltonics, Inc., Billerica, MA*; <sup>4</sup>*Dana Farber Cancer Institute, Boston, MA*
- WP 186 **MALDI-Imaging Mass Spectrometry (MALDI-IMS) Analysis of Mouse Liver Injected with Gold and Copper Nanoparticles;** Dionysios Pantazatos<sup>1,2</sup>; Irene (Eirini) Panderi (Panteri)<sup>1,4</sup>; Liangran Guo<sup>3</sup>; Wei Lu<sup>3</sup>; <sup>1</sup>*COBRE Center for Cancer Research and Development, Providence, RI*; <sup>2</sup>*Warren Alpert Medical School, Brown University, Providence, RI*; <sup>3</sup>*University of Rhode Island, College of Pharmacy, Kingston, RI*; <sup>4</sup>*University of Athens, Pharmacy, Pharm.Chemistry, Athens, Greece*
- WP 187 **Developing Imaging Mass Spectrometry in 3D Cell Cultures;** Amanda B. Hummon; Eric Weaver; Xin Liu; Haohang Li; Dorothy Ahlf; *University of Notre Dame, Notre Dame, IN*
- WP 188 **MALDI-MS Imaging of LCL124 (SPG103) Tissue Distribution and Molecular Effects on Lipids and Glycans in a Prostate Tumor Xenograft Model;** Ellen Jones; Xiang Liu; James Norris; Richard Drake; *Medical University of South Carolina, Charleston, SC*
- WP 189 **Pharmaco-Imaging Analysis of Anti-cancer Agents in Tumor Tissues Using Mass Microscope;** Shuichi Shimma; Yuki Takashima; Akinobu Hamada; *National Cancer Center Research Institute, Tokyo, Japan*
- WP 190 **Cosmetic Analysis Using MALDI-MSI – "Cosmetomics";** Diogo De Oliveira; Sabrina de Bona Sartor; Mônica Ferreira Siqueira; Rodrigo Ramos Catharino; *INNOVARE Biomarkers Lab, University of Campinas, Campinas, Brasil*
- WP 191 **A nano-PALDI Protocol for Anticancer Drugs Tumor Uptake and Distribution Studies;** Enrico Davoli; Lavinia Morosi; Pietro Spinelli; Maria G. Carrera; Raffaella Giavazzi; Massimo Zucchetti; Maurizio D'Incalci; *Mario Negri Institute, Milano, Italy*
- WP 192 **MALDI-MS Imaging of the Molecular Profile Changes Resulting from Sphingosine Kinase Inhibition in an Orthotopic Pancreatic Cancer Model;** Peng Gao; E. Ellen Jones; Thomas Powers; Stephen Roper; Benjamin Neely; Drew Schoenling; Charles Smith; Richard R Drake; *Medical University of South Carolina, Charleston, SC*
- WP 193 **Use of High Resolution MSI Combined with Metabolomics Study to Evaluate Drug Efficacy and Impact onto Biological Environment;** David Bonnel<sup>1</sup>; Gregory Hamm<sup>1</sup>; Guillaume Hochart<sup>1</sup>; Fred Fack<sup>2</sup>; Olivier Keunen<sup>2</sup>; Fabien Pamelard<sup>1</sup>; Raphael Legouffe<sup>1</sup>; Simone Niclou<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>*ImaBiotech, MS Imaging Department, Lille, France*; <sup>2</sup>*CRP Santé, Luxembourg*
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- WP 194 **Imaging of Molecular Distribution in Areca Nut by Desorption Electrospray Ionization Mass Spectrometry (DESI-MS);** Amitava Srimany; R. G. Hemalatha; Danica Glenda Pinto; Hemanta R. Naik; T. Pradeep; *IIT Madras, Chennai, India*
- WP 195 **Small Molecules Detection with an Ultrashort Pulsed Laser Ablation VUV Postionization TOF-MS;** Yang Cui; Chhavi Bhardwaj; Slobodan Milasinovic; Robert Gordon; Luke Hanley; *Univ. of Illinois at Chicago, Chicago, IL*
- WP 196 **Laser Ablation Atmospheric Pressure Photoionization Mass Spectrometry Imaging of Sage Leafs;** Anu Vaikkinen<sup>1</sup>; Bindesh Shrestha<sup>2</sup>; Risto Kostainen<sup>1</sup>; Akos Vertes<sup>2</sup>; Tiina J. Kauppila<sup>1</sup>; <sup>1</sup>*University of Helsinki, Helsinki, Finland*; <sup>2</sup>*George Washington University, Washington, DC*
- WP 197 **Whole-Body DESI Imaging of Clozapine and Its Metabolite;** Jingzhou Liu; Zhiyang Zhao; Yohannes Teffera; *Amgen, Cambridge, MA*
- WP 198 **Direct Coupling of TLC with MALDI-TOF Mass Spectrometry for Analysis of Extracted Phospholipids from DMXAA Treated Xenograft Tumor;** Afnan Batubara<sup>1</sup>; Malcolm Clench<sup>1</sup>; Paul Loadman<sup>2</sup>; Chris Sutton<sup>2</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*University of Bradford, Bradford, UK*
- WP 199 **MALDI Tissue Imaging: Identification of Amino Acid and Neurotransmitter Metabolites;** M. Lisa Manier; Jeffrey M. Spraggins; Michelle L. Reyzer; Jeremy L. Norris; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- WP 200 **MALDI Imaging of Metabolites During the Germination of a Corn Seed;** Adam Feenstra<sup>1,2</sup>; Andrew Korte<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames Laboratory/USDOE, Ames, IA*
- WP 201 **MALDI Imaging of Forensic Samples by Using a Spiral-Trajectory Ion Optics Time-of-Flight Mass Spectrometer;** Masaaki Ubukata; John Dane; Robert B. Cody; Donna Guarrera; Masateru Shibata; *JEOL USA, Inc., Peabody, MA*
- WP 202 **Localization of Endogenous Metabolites in Diabetic Mouse Brain Tissue Using MALDI Imaging Mass Spectrometry;** Michelle L. Reyzer<sup>1</sup>; Andre Kleinridders<sup>2</sup>; Heather Ferris<sup>2</sup>; Jeffrey M. Spraggins<sup>1</sup>; C. Ronald Kahn<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Joslin Diabetes Center, Harvard University, Boston, MA*
- WP 203 **MALDI-IMS-MSI Examination of Emollient Treated Living Skin Equivalent for Lipidomic and Small Molecule Analysis;** Christopher Mitchell; *BMRC, Sheffield, UK*
- WP 204 **Rat Skeletal Muscle Fiber Differentiation Using Mass Spectrometric Imaging (MSI) and Tandem MS (MS<sup>n</sup>);** Yu-Hsuan Tsai<sup>1</sup>; Timothy Garrett<sup>2</sup>; Christy Carter<sup>3</sup>; Richard Yost<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Florida, Gainesville, FL*; <sup>2</sup>*Department of Pathology, University of Florida, Gainesville, FL*; <sup>3</sup>*Dept. Aging & Geriatric Research, Univ of Florida, Gainesville, FL*

- WP 205 **Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry for Chemical Imaging of Plant Metabolites**; Gargey Yagnik<sup>1,2</sup>; Andrew Korte<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames lab US DOE, Ames, IA
- WP 206 **Promethazine as a PET Probe for Amyloid Beta in Alzheimer's Disease Using MALDI Imaging Mass Spectrometry**; Chad Chumbley; Richard McClure; Michelle Reyzer; Wellington Pham; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- WP 207 **Mass Spectrometry Imaging of Leaf Surface Using Platinum Vapor Deposition Assisted Laser Desorption/Ionization**; Tomoyuki Ozawa; Hideya Kawasaki; Ryuichi Arakawa; *Kansai University, Osaka, Japan*
- WP 208 **Spatial Correlation Combined with Hierarchical Clustering Analysis for Reducing Complex Multi-Dimensional MALDI Imaging Dataset**; Hernando Olivos<sup>1,2</sup>; Kieran Neeson<sup>1,2</sup>; Emmanuelle Claude<sup>1,2</sup>; Mark Towers<sup>1,2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Waters Corporation, Beverly, MA
- WP 209 **Investigations into Adjuvant Efficacy upon the Surface Distribution and Penetration of a Herbicide into Plant Leaves by LAESI-MS Imaging**; Stephen Rumbelow<sup>1</sup>; Gregory Lindner<sup>1</sup>; Holly Henderson<sup>2</sup>; Alicia Morgan<sup>2</sup>; Haddon Goodman<sup>2</sup>; <sup>1</sup>Croda Inc, New Castle, DE; <sup>2</sup>Protea Biosciences Group Inc., Morgantown, WV
- WP 210 **MALDI-MS Imaging and Quantitation of Acetylcholine in Mouse Brain after Administration of Cholinesterase Inhibitor Using Deuterated CHCA as Matrix**; Mohammadreza Shariatgorji<sup>1</sup>; Nicoletta Schintu<sup>2</sup>; Per Svenningsson<sup>2</sup>; Per. E Andrén<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institute, Stockholm, Sweden
- WP 211 **Imprinting and MALDI-MS Imaging of Metabolites from Soybean Leaves**; Adam Klein<sup>1,2</sup>; Gargey Yagnik<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames Laboratory US-DOE, Ames, IA
- WP 212 **In situ Quantitative Protein-Metal Co-Localization Using Imaging by Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry**; Dominic Hare<sup>1,2</sup>; Peng Lei<sup>2</sup>; Scott Ayton<sup>2</sup>; Rudolf Grimm<sup>3</sup>; Jessica George<sup>2</sup>; Robert Cherny<sup>2</sup>; Paul Adlard<sup>2</sup>; Ashley Bush<sup>2</sup>; David Finkelstein<sup>2</sup>; Philip Doble<sup>1</sup>; <sup>1</sup>University of Technology, Sydney, Broadway, Australia; <sup>2</sup>Florey Institute of Neuroscience and Mental Health, Melbourne, Australia; <sup>3</sup>Agilent Technologies, Santa Clara, CA
- WP 213 **Carbon Nanodots as a Novel Matrix for the Analysis of Small Molecules by MALDI-TOF MS**; Chen Suming; Nie Zongxiu; *Institute of Chemistry Chinese Academy of Sciences, Beijing, China*
- WP 214 **Visualizing Metabolites in Plants and Insects with High Resolution AP-SMALDI MS Imaging**; Dhaka Bhandari; Andreas Roempp; Bernhard Spengler; *Justus Leibig University Giessen, Giessen, Germany*
- WP 215 **Distribution and Identification of Molecular Interactions between Tomato Roots and Bacterial Biofilms**; Delphine Debois<sup>1</sup>; Emmanuel Jourdan<sup>2</sup>; Nicolas Smargiasso<sup>1</sup>; Marc Ongena<sup>3</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>University of Liege, Liège, Belgium; <sup>2</sup>University of Liege - CWBI, Liege, Belgium; <sup>3</sup>University of Liege Gembloux Agro-Bio Tech, Gembloux, Belgium
- WP 216 **Imaging of Lipids in Rat Sciatic Nerve**; Roberto Fernandez<sup>1</sup>; Javier Diez-Garcia<sup>2</sup>; Miguel Alaminos<sup>3</sup>; Begoña Castro Feo<sup>2</sup>; Alejandro Garcia-Garcia<sup>2</sup>; Jose A. Fernandez<sup>1</sup>; <sup>1</sup>Universidad del Pais Vasco, Leioa, Spain; <sup>2</sup>Histocell S. L., Derio, Sp; <sup>3</sup>University of Granada, Granada, Spain
- WP 217 **Imaging Mass Spectrometry: Insights into the Interactive Metabolome of Pseudomonas aeruginosa**; Vanessa Phelan<sup>1</sup>; Wilna Moree<sup>1</sup>; Alexandra Koumoutsis<sup>2</sup>; Suzanne Noble<sup>2</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>UC, San Diego, La Jolla, CA; <sup>2</sup>University of California, San Francisco, CA
- WP 218 **MALDI Imaging MS of Metabolites in Human Cancer Tissues**; Tim Dekker; Emrys Jones; René van Zeijl; Willem Corver; Rob Tollenaar; André Deelder; Hans Morreau; Wilma Mesker; Liam McDonnell; *Leiden University Medical Center, Leiden, Netherlands*
- WP 219 **Identifying the Neuroanatomical Substrate Involved in ICVNPY Inhibition of Reinstatement of Cocaine-Induced Behavior in Rats by MALDI Imaging**; Leila Hosseinzadehshahri; *Buffalo, NY*
- WP 220 **Complimentary Use of MALDI FTICR-MS and TOF-SIMS Imaging Approaches in an Invertebrate**; Manuel Liebeke<sup>1</sup>; Jens Fuchser<sup>2</sup>; Katherine A. Kellersberger<sup>3</sup>; Sarah Fearn<sup>4</sup>; David McPhail<sup>4</sup>; Jacob G. Bundy<sup>1</sup>; <sup>1</sup>Department of Surgery and Cancer, Imperial College, London, UK; <sup>2</sup>Bruker Daltonik, GmbH, Bremen, DE; <sup>3</sup>Bruker Daltonics, Inc., Billerica, MA; <sup>4</sup>Department of Materials, Imperial College, London, UK
- WP 221 **Structural Properties of Metabolites that Dominate the Ionization Efficiency in MALDI with 9-Aminoacridine as the Matrix**; Daichi Yukihiro; Daisuke Miura; Yoshinori Fujimura; Mitsuru Shindo; Hiroyuki Wariishi; *Kyushu University, Fukuoka, Japan*
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- WP 223 **Scoring Methods for Interpreting Mass Spectra of Unknown Structures Using the MASSPEC Algorithm**; Marshall M. Siegel<sup>1</sup>; Gary Walker<sup>1</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>MS Mass Spec Consultants, Fair Lawn, NJ; <sup>2</sup>Cerno Bioscience, Norwalk, CT
- WP 224 **Fragmentation Outcome Modelling: Prototype Software for Prediction of CID Fragment Ions for Small Molecule Structures**; Kirsten Hobby<sup>1</sup>; Richard Gallagher<sup>2</sup>; Neil Loftus<sup>1</sup>; <sup>1</sup>Shimadzu MS/BU, Manchester, UK; <sup>2</sup>AstraZeneca, Macclesfield, UK
- WP 225 **Automated Tool for Substructure Annotation of Accurate Mass MS/MS Spectra**; Yan Ma; Tobias Kind; Oliver Fiehn; *University of California, Davis, CA*
- WP 226 **Method for Assessing the Statistical Significance of Mass Spectral Similarities by Using BLAST Statistics**; Fumio Matsuda; Hiroshi Tsugawa; Eiichiro Fukusaki; *Osaka University, Suita, Japan*
- WP 227 **Accurate Mass Report Generation with Spectral Accuracy Isotope Scoring within a High Throughput Laboratory**; Christopher Williams<sup>1</sup>; Yongdong Wang<sup>2</sup>; Leo Xu<sup>2</sup>; Ming Gu<sup>2</sup>; <sup>1</sup>Swansea University, Swansea, UK; <sup>2</sup>Cerno Bioscience, Norwalk, CT
- WP 228 **Increasing LC/MS Workflow Capacity with Data Analysis by Exception Strategies**; Timothy Dunne; Chan C. K; Travis Mathewson; Holly McKeith; Rosalia Gonzales; *Pfizer, Groton, CT*
- WP 229 **Critical Assessment of Small Molecule Identification: Results of the Inaugural CASMI Contest 2012**; Emma Schymanski; Steffen Neumann<sup>2</sup>; <sup>1</sup>Eawag: Swiss Federal Institute of Aquatic Science, Dübendorf, Switzerland; <sup>2</sup>Leibniz Institute of Plant Biochemistry, Halle (Saale), Germany



- WP 230 **Towards a Workflow for the Automated Structural Elucidation of Unknowns from MS/MS Spectra;** Gerard Hopfgartner<sup>1</sup>; Abhinandan KR<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Lyle Burton<sup>2</sup>; Ron Bonner<sup>2</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>AB Sciex, Concord, ON, Canada
- WP 231 **Identification of Unknown Metabolites Using Tandem MS: Improving the Quality of Fragmentation Trees;** Kai Dührkop; Kerstin Scheubert; Sebastian Böcker; *Friedrich-Schiller University Jena, Jena, Germany*
- WP 232 **Integrating Datasets from Drug Metabolism and Bioanalytical Studies and Fixing the Missing Link for Quan/Qual;** Mark D. Wrona; Craig Dorschel; Yun W. Alelyunas; Kevin Cook; Stephen McDonald; Paul D. Rainville; *Waters Corporation, Milford, MA*
- WP 233 **Characterization of Oxidative Forced Degradation Products Using Fragment Ion Search;** Chunang (Christine) Gu<sup>1</sup>; Jane Li<sup>1</sup>; Kate Comstock<sup>2</sup>; Alan Deese<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
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- WP 234 **Characteristic Retro-Diels-Alder Fragmentation of Four Cephalosporins and Their Δ-3 Isomers in Positive and Negative Mode: An Experimental and Theoretical Study;** Jian-Qin Qian<sup>1,2</sup>; Chang-Qin Hu<sup>1</sup>; <sup>1</sup>National Institutes for Food and Drug Control, Beijing, China; <sup>2</sup>Peking Union Medical College, Beijing, China
- WP 235 **Fundamental Study of Mechanisms of Collision-Activated Dissociation of Ionized Asphaltenes' Model Compounds Using a Linear Quadrupole Ion Trap Mass Spectrometer;** James Riedeman; Nadine Njoya; David Borton; Matt Hurt; Hilikka Kenttämää; *Purdue University, West Lafayette, IN*
- WP 236 **Structural Elucidation of Small Drug Molecules Using Q-TOF, LTQ-Orbitrap and GC-ESI-MS with Supersonic Molecular Beams (SMB);** Lena von Sydow<sup>1</sup>; Anja Ekdahl<sup>1</sup>; Carina Leandersson<sup>1</sup>; Marie Tysk-Rönnqvist<sup>2</sup>; Aviv Amirav<sup>3</sup>; <sup>1</sup>AstraZeneca R&D, Mölndal, Sweden; <sup>2</sup>AstraZeneca Operations, Södertälje, Sweden; <sup>3</sup>Tel Aviv University, Tel Aviv, Israel
- WP 237 **Novel Glutathione Conjugates of Phenyl Isocyanate Studied by Ultra-Performance Liquid Chromatography/ Electrospray Ionization Mass Spectrometry;** Tove Johansson Mali'n; Crister Åstot; *Swedish Defense Research Agency, Umeå, Sweden*
- WP 238 **Mass Spectrometric Detection of Local Anesthetics Masking Prohibited Practice of Inducing Limb Soring in Walking Horses to Enhance Appeal;** Szabolcs Szarka; Laszlo Prokai; *UNT Health Science Center, Fort Worth, TX*
- WP 239 **Investigation of an Impurity in Carboplatin through a Forced Degradation Study;** Jeffrey Selenka<sup>1</sup>; Cynthia Sanderson<sup>2</sup>; <sup>1</sup>PPD Inc., Madison, WI; <sup>2</sup>AB SCIEX, Framingham, MA
- WP 240 **Unusual Degradation Products of Selective β-Amyloid Aggregation Inhibitor BTB01473;** Ludmila Alexandrova<sup>1</sup>; Paul A. Novick<sup>2</sup>; Vijay S. Pande<sup>2</sup>; Allis Chien<sup>1</sup>; <sup>1</sup>Stanford University Mass Spectrometry, Stanford, CA; <sup>2</sup>Stanford University, Chemistry Department, Stanford, CA
- WP 241 **On-line Nanopore Optical Interferometry-Mass Spectrometry for Screening and Quantifying Small Molecule-Protein Interactions;** Iain D. G. Campuzano; Paul D. Schnier; Klaus Michelsen; *Amgen Inc., Thousand Oaks, CA*
- WP 242 **Fast Analysis of Stereo and Structural Related Isomers using Supercritical Fluid Chromatography-Mass Spectrometry;** Yugin Dai; Lisa Zang; *Agilent Technologies, Santa Clara, CA*
- WP 243 **Principal Component Analysis of Laser Desorption Postionization Mass Spectrometry Data for Mixed/ Coculture Biofilms;** Chhavi Bhardwaj<sup>1</sup>; Yang Cui<sup>1</sup>; Theresa Hofstetter<sup>2</sup>; Suet Liu<sup>2</sup>; Hans C. Bernstein<sup>3</sup>; Ross P. Carlson<sup>3</sup>; Musahid Ahmed<sup>2</sup>; Luke Hanley<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL; <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>3</sup>Montana State University, Bozeman, MT
- WP 244 **New Methodology for the Analysis of Highly Hydrophobic Calixarenes by MALDI-TOF Mass Spectrometry;** Vincent Guérineau<sup>1</sup>; Vincent Huc<sup>2</sup>; David Touboul<sup>1</sup>; Baptiste Boutonnet<sup>2</sup>; Cyril Martini<sup>2</sup>; Alain Brunelle<sup>1</sup>; <sup>1</sup>CNRS, Institut de Chimie des Substances Naturelles, Gif-sur-Yvette, France; <sup>2</sup>Université Paris-Sud, ICMO, Orsay, France
- WP 245 **Creation of Uniquely Deep and Rich Datasets for the Structural Elucidation of Metabolites in Quan/Qual Analyses;** Jonathan L. Josephs<sup>1</sup>; Timothy Stratton<sup>2</sup>; William Humphreys<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Pennington, NJ; <sup>2</sup>Thermo Scientific, San Jose, CA
- WP 246 **Application of Mass Spectrometry to Support Authentication and Characterization of Counterfeit Pharmaceuticals;** Michael Peddicord; Charles Pathirana; Holly Shackman; Mark Bolgar; Scott Miller; *Bristol-Myers Squibb, New Brunswick, NJ*
- WP 247 **Application of MALDI-Mass Spectrometry to Investigation of Active Layer Degradation in Organic Solar Cells;** Evgenia Akhmetova; Matthew McMahon; Santhosh Narasimhachary; Charles L. Wilkins; *University of Arkansas, Fayetteville, AR*
- WP 248 **LCMSMS Technique Reveals the Structure of New Impurity in Valproic Acid, an Anticonvulsant Drug – Unseen in GC Analysis!;** Arugavur Ponnusamy Kannan<sup>1</sup>; D. Easwaramoorthy<sup>1</sup>; Raman Palvannanathan<sup>2</sup>; Mohan Kasi<sup>2</sup>; Saravanan Subramanian<sup>2</sup>; Janani Thyagarajan<sup>2</sup>; Venkat Manohar<sup>2</sup>; <sup>1</sup>Dept. of Chemistry B.S.Abdur Rahman University, Chennai, India; <sup>2</sup>IICMS, Chennai, India
- WP 249 **Understanding the role of Solvent Media towards Peroxide Degradation Products of Lenalidomide, an Anticancer Compound Using LCMSMS Technique;** Janani Thyagarajan<sup>1</sup>; Raman Palvannanathan<sup>1</sup>; Mohan Kasi<sup>1</sup>; Govindarajan Chandramohan<sup>1</sup>; Saravanan Subramanian<sup>1</sup>; Thaminum Ansari Abubacker<sup>2</sup>; Venkat Manohar<sup>1</sup>; <sup>1</sup>IICMS, Chennai, India; <sup>2</sup>Muthuramgam Govt. Arts College, Vellore, Tamil Nadu, India
- WP 250 **Characterization of Hitherto Unknown Process Related Impurities of Crizotinib through Multiple Collision LCMSMS Analysis;** Saravanan Subramanian<sup>1</sup>; Thaminum Ansari Abubacker<sup>2</sup>; Mohan Kasi<sup>1</sup>; Govindarajan Chandramohan<sup>1</sup>; Rampriya Uthayakumar<sup>1</sup>; Raman Palvannanathan<sup>1</sup>; Arvind Thyagarajan<sup>1</sup>; Venkat Manohar<sup>1</sup>; <sup>1</sup>IICMS, Chennai, India; <sup>2</sup>Muthuramgam Govt. Arts College, Vellore, Tamil Nadu, India
- WP 251 **Identification of an Unknown Photo-degradant in Active Pharmaceutical Ingredient;** Meng Xu; Hongfei Yue; John Castoro; *Bristol-Myers Squibb, New Brunswick, NJ*
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- WP 252 **Identification of Tamoxifen Metabolites in Human Serum using the iHumite Workflow: Metabolite Prediction, LC-HRMS and MS Vendor Independent Data Processing;** Peter L. Jacobs<sup>1,2</sup>; Lars Ridder<sup>3</sup>; Marco Ruijken<sup>4</sup>; Hilde Rosing<sup>5</sup>; Nynke G.L. Jager<sup>6</sup>; Jos H. Beijnen<sup>5</sup>; Richard R. Bas<sup>1</sup>; William D. van Dongen<sup>1</sup>; <sup>1</sup>TNO Triskelion, Zeist, The Netherlands; <sup>2</sup>MSam, Oss, The Netherlands; <sup>3</sup>Wageningen University, Wageningen, The Netherlands; <sup>4</sup>MsMetrix, Maarssen, The Netherlands; <sup>5</sup>Slotervaart Hospital, Netherlands Cancer Institute, Amsterdam, The Netherlands

- WP 253 **iPeaks: Isotope Pattern Matching for Fast and Sensitive Drug Metabolite Detection using High Resolution Mass Spectrometry**; Marco Ruijken; *MsMetrix, Maarssen, Netherlands*
- WP 254 **Evaluation of Xevo G2-S Q-ToF and UNIFI Software for the Identification and Relative Quantitation of Metabolites**; Richard Clayton<sup>1</sup>; Richard Lock<sup>2</sup>; Lucy Fernandes<sup>2</sup>; <sup>1</sup>Covance, Harrogate, UK; <sup>2</sup>Waters Ltd, Manchester, UK
- WP 255 **Comparison of MS/MS<sup>all</sup> with SWATH<sup>™</sup> and Information Dependent Acquisition Methods for Increased Throughput in Metabolic Soft-Spot Identification Using HRMS**; Veronica Zelesky<sup>1</sup>; Richard Schneider<sup>1</sup>; John Janiszewski<sup>1</sup>; Yves LeBlanc<sup>2</sup>; Eva Duchoslav<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>AB SCIEX, Concord, Canada
- WP 256 **Automated Metabolite Identification and Profiling in Non-Specific Fragmentation High Resolution Accurate Mass Spectrometry Data**; Eva Duchoslav; Gordana Ivosev; Ignat Shilov; Hesham Ghobarah; Lyle Burton; *AB SCIEX, Concord, Canada*
- WP 257 **Increasing the Number of Identified Metabolites from in-vitro and in-vivo Samples with All Ion Fragmentation on an Orbitrap Mass Spectrometer**; Joseph T. Marini; Jie Ding; Donald L. McKenzie; *Covance, Madison, WI*
- WP 258 **Multiple Fragmentation Techniques for Comprehensive Metabolite Identification**; Jack Cunliff<sup>1</sup>; Kelly Wang<sup>2</sup>; Gene Eiserberg<sup>2</sup>; Tim Stratton<sup>1</sup>; Kate Comstock<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Gilead Sciences, Inc., Foster City, CA
- WP 259 **Using HRAM Survey Analysis Combined with Rapid MS2 Data to Develop a Fragmentation Based Detection Workflow for Structure ID Acquisition**; Tim Stratton; *Thermo Fisher Scientific, San Jose, CA*
- WP 260 **Electrochemically Initiated Reactions Upfront MS - EC/MS an Unknown Panacea?** Martin Eysberg; Agnieszka Kraj; Hendrik-Jan Brouwer; Nico Reinhoud; Jean-Pierre Chervet; *Antec, Zoeterwoude, The Netherlands*
- WP 261 **In vitro Mimicry of Metabolism of Xanthohumol by Electrochemistry Combined with LC-DAD-MS/MS**; Andries P. Bruins<sup>1</sup>; Jan F. Stevens<sup>2</sup>; Ulrik Jurva<sup>3</sup>; <sup>1</sup>University of Groningen, Groningen, Netherlands; <sup>2</sup>Oregon State University, Corvallis, OR; <sup>3</sup>AstraZeneca, Mölndal, Sweden
- WP 262 **Use of On-Line Electrochemistry/High-Resolution Mass Spectrometry for the Estimation of the Site of Glucuronidation**; Kazuyoshi Nozaki<sup>1</sup>; Kenji Tabata<sup>1</sup>; Toshio Teramura<sup>1</sup>; Mitsuo Takayama<sup>2</sup>; <sup>1</sup>Astellas Pharma Inc., Tsukuba, Japan; <sup>2</sup>Yokohama City University, Yokohama, Japan
- WP 263 **Automation Strategies for an Electrochemistry/MS Method for Metabolism Studies**; Hannah Simon; Michael Kießhauer; Uwe Karst; *University of Münster, Münster, Germany*
- WP 264 **Utility of Data-Independent LC/MS<sup>E</sup> with Ion Mobility to Increase Coverage of Nefazodone Metabolites from in-vivo Matrices**; Joseph T. Marini<sup>1</sup>; Andrew G. Baker<sup>2</sup>; Jie Ding<sup>1</sup>; Donald L. McKenzie<sup>1</sup>; <sup>1</sup>Covance, Madison, WI; <sup>2</sup>Waters Corporation, Pleasanton, CA
- WP 265 **Evaluation of Differential Mobility Techniques for Quantitative and Qualitative Identification Workflows in Pharmaceutical Environments**; Keith Goodman; Paul Clemens; James Ferguson; Loren Olson; *AB SCIEX, San Jose, CA*
- WP 266 **Analysis of Urine Samples using Microflow LC Coupled to Differential Ion Mobility Spectrometry**; Carmel Seto; Pauline Vollmerhaus; Alina Dindyal-Popescu; Deolinda Fernandes; Takeo Sakuma; *AB SCIEX, Concord, Canada*
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- WP 268 **Identification of Human Drug Metabolites with Poor Mass Spectrometric Response Using LC-MS Assisted by TopCount Radioactive Detection**; Manfred Zell; Christophe Husser; *F. Hoffmann-La Roche Ltd, Basel, Switzerland*
- WP 269 **Investigation of Metabolism of Peptide Drug by <sup>127</sup>I-tagging Follow by Analyses Using Capillary UPLC Coupled to ICP-MS and ESI-LTQ/Orbitrap**; Heng-Keang Lim; *Janssen Pharmaceuticals R&D, Raritan, NJ*
- WP 270 **Molecular Level Probing of the Mechanism and Biological Activity of Metal-based Anticancer Drug Candidates by ESI FT-ICR Mass Spectrometry**; Zhihua Yang; Dajena Tomco; Claudio N. Verani; Mary T. Rodgers; *Wayne State University, Detroit, MI*
- WP 271 **Characterization of Bromopride and Metoclopramide N-O-glucuronides in Human Hepatocytes by HPLC/ESI/FTMS/MS and Hydrogen Deuterium Exchange**; Jennifer L. Bushee<sup>1</sup>; Christine E. Dunne<sup>2</sup>; Kevin Colizza<sup>1</sup>; Amanda Cirello<sup>1</sup>; Upendra A. Argikar<sup>1</sup>; <sup>1</sup>Novartis, Cambridge, MA; <sup>2</sup>Northeastern University, Boston, MA
- WP 272 **Mass Spectrometric Study of the Nitration and Halogenation of the  $\beta_2$ -Agonist Albuterol**; Larry Sallans<sup>1</sup>; Stephen Macha<sup>1</sup>; Kari Brown<sup>1</sup>; Dennis McGraw<sup>1,2</sup>; Melinda Butsch Kovacic<sup>1,3</sup>; Sara Stigler<sup>1,3</sup>; Bradley Britigan<sup>4,5</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>Veterans Affairs Medical Center, Cincinnati, OH; <sup>3</sup>Cincinnati Children's Hospital, Cincinnati, OH; <sup>4</sup>University of Nebraska Medical Center, Omaha, NE; <sup>5</sup>Veterans Affairs Medical Center - NE/Western IA, Omaha, NE
- WP 273 **Investigations of Sulfation Phenotyping and Kinetics of Raloxifene and the Active Metabolites of Tamoxifen**; Lori Coward<sup>1</sup>; Greg Gorman<sup>1</sup>; Teresa Wilborn<sup>2</sup>; Gwen Nance<sup>2</sup>; <sup>1</sup>Pharmaceutical Sciences Research Institute, Samford University, Birmingham, AL; <sup>2</sup>McWhorter School of Pharmacy, Samford University, Birmingham, AL
- WP 274 **Turning Drug Glucosides into Glucuronides – Making Fungal Incubations Work Together with Chemical Derivatization**; Axel Rydevik<sup>1</sup>; Ulf Bondesson<sup>1,2</sup>; Mario Thevis<sup>3</sup>; Mikael Hedeland<sup>1,2</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>National Veterinary Institute (SVA), Uppsala, Sweden; <sup>3</sup>German Sport University, Cologne, Germany
- WP 275 **Unusual Phase I and Phase II Metabolites Prepared by Biotransformation and Their Unexpected MS/MS Fragmentation**; Andreas Fredenhagen; Juergen Kuehnoel; Matthias Kittelmann; Kirsten Schroer; Stephan Luetz; Reiner Aichholz; Lukas Oberer; *Novartis Institutes for BioMedical Research, Basel, Switzerland*
- WP 276 **Evaluation of the Fungus *Cunninghamella elegans* as a Model for the Formation of Reactive Metabolites Using Glutathione Trapping and UHPLC/HRMS**; Axel Rydevik<sup>2</sup>; Anna Hellqvist<sup>2</sup>; Ulf Bondesson<sup>1</sup>; Mikael Hedeland<sup>1</sup>; <sup>1</sup>Nat'l Veterinary Institute, Uppsala, Sweden; <sup>2</sup>Uppsala University, Uppsala, Sweden
- WP 277 **UHPLC-MS-MS with Fast Precursor Ion and Neutral Loss Scanning and Glutathione Trapping for Detecting Reactive Metabolites of Licorice**; Ke Huang; Richard B. van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- WP 278 **A Reactive Metabolite Investigation of Fenclozic Acid by LC-UV-MSMS**; Scott Martin<sup>1</sup>; Malcolm clench<sup>2</sup>; <sup>1</sup>Astrazeneca, Macclesfield, UK; <sup>2</sup>Sheffield Hallam university, Sheffield, UK



- WP 279 **Proteomic Characterization of Ocular S9 Fractions for Biotransformation Studies in Ophthalmic Drug Discovery**; Joshua L. Johnson; Jennifer L. Bushee; Upendra A. Argikar; Amin Kamel; Shawn Harriman; *NIBR, Cambridge, MA*
- WP 280 **A Comparison of LC-MS and a Prototype Microfluidics-MS Device in the Metabolite Identification of *in-vitro* and *in-vivo* Samples**; Philip Tiller<sup>1</sup>; Mark D. Wrona<sup>2</sup>; Yun W. Alelyunas<sup>2</sup>; Catalin Doneanu<sup>2</sup>; Paul D. Rainville<sup>2</sup>; <sup>1</sup>*RMI Laboratories, North Wales, PA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- WP 281 **Characterization of Long Lasting Plasma Radioactivity in Monkey following Single Oral Dose of C-14 labeled Merck Compound A**; Yuxia Liang; Sheri Smith; Kelem Kassahun; Thomayant Prueksaritanont; Dan Cui; *PPDM, Merck, West Point, PA*
- WP 282 **LC-MS<sup>n</sup> Analysis of Metabolites of ST-255, a Novel Anti-Lassa Virus Compound**; X. Steven Yan; Brian Furmansk; Daniela Kropf; Dongcheng Dai; Jim Burgeson; Candace Lovejoy; Sean Amberg; Shanthakumar Tyavanagimatt; Janet Leeds; *SIGA Technologies, Inc., Corvallis, OR*
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- WP 283 **Determination of Opiates and Opioids in Dried Blood Spots Using Novel Flow-Through Technology Coupled to LC/MS/MS**; Dennis Nagtalon<sup>1</sup>; Kevin McCann<sup>1</sup>; Na Pi Parra<sup>1</sup>; Ken Lewis<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*OpAns, Durham, NC*
- WP 284 **Rapid Online LC-TOF-MS Analysis of Glycated Hemoglobin from dried Blood Spots Using Automated Direct Flow-Through Elution**; Robert J. Seward<sup>1</sup>; Dhvani Shah<sup>1</sup>; Jonathan Wilson<sup>1</sup>; Catherine Stacey<sup>1</sup>; Christel Hempen<sup>2</sup>; <sup>1</sup>*PerkinElmer, Waltham, MA*; <sup>2</sup>*Spark Holland, Emmen, The Netherlands*
- WP 285 **Advancing Quantitative Dried Blood Spot Analysis Using Temperature-Enhanced Flow-Through Desorption Coupled Online to Solid-Phase Extraction and Mass Spectrometry**; Christel Hempen; Lena Knecht; Bert Ooms; *Spark Holland B.V., Emmen, Netherlands*
- WP 286 **Application of Micro Fluidic LC/MS/MS for the Quantification Rosuvastatin from Dried Blood Spots: A Clinical Study Example**; Robert Plumb<sup>2</sup>; Nicola Gray<sup>1</sup>; Ian Wilson<sup>2</sup>; Paul Rainville<sup>1</sup>; <sup>1</sup>*Waters, Milford, MA*; <sup>2</sup>*Imperial College, London, UK*
- WP 287 **Direct Automated Analysis of Dried Blood Spots (DBS) by 2D LC-HRMS: Effects of Hematocrit on DBS Results**; Regina Oliveira<sup>1</sup>; Jack Henion<sup>1</sup>; Enaksha Wickremsinhe<sup>2</sup>; <sup>1</sup>*Advion Bioanalytical Labs, a Quintiles Company, Ithaca, NY*; <sup>2</sup>*Drug Disposition, Eli Lilly and Company, Indianapolis, IN*
- WP 288 **Development of a Molecular Filtration Membrane Substrate as an Alternative for DBS LC/MS Bioanalyses**; Robert Sturm<sup>1</sup>; Jack Henion<sup>1</sup>; Richard Abbott<sup>2</sup>; Phillip Wang<sup>3</sup>; <sup>1</sup>*Advion Bioanalytical Labs, a Quintiles company, Ithaca, NY*; <sup>2</sup>*Shire Pharmaceuticals, Basingstoke, UK*; <sup>3</sup>*Shire Development, Wayne, PA*
- WP 289 **Comparison of Proteins in Liquid and Dried Blood Spot Samples by HPLC/ESI-MS/MS**; Andrew Chambers<sup>1</sup>; Andrew Percy<sup>1</sup>; Darryl Hardie<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*
- WP 290 **Heat Stabilized Blood Spots as Alternative to Standard DBS Sampling – Analyte Stability and Coextraction of Matrix Proteins**; Karl Skold<sup>1</sup>; David Zeeberg<sup>1</sup>; Daniel Blessborn<sup>2</sup>; Karnrawee Kaewkhao<sup>2</sup>; Olof Skold<sup>1</sup>; Martin Ahnoff<sup>3</sup>; <sup>1</sup>*Denator AB, Uppsala, Sweden*; <sup>2</sup>*Mahidol University, Bangkok, Thailand*; <sup>3</sup>*University of Gothenburg, Gothenburg, Sweden*
- WP 291 **Determination of Eight Metabolically Unstable Drugs in Blood by Heat-Stabilized DBS and LC-MS/MS**; Olof Skold<sup>1</sup>; Karl Skold<sup>1</sup>; David Zeeberg<sup>1</sup>; Gunnar Häggglund<sup>4</sup>; Eskil Hermansson<sup>4</sup>; Peter Abrahamsson<sup>2</sup>; Martin Ahnoff<sup>3</sup>; <sup>1</sup>*Denator AB, Gothenburg, Sweden*; <sup>2</sup>*Agilent Technologies, Gothenburg, Sweden*; <sup>3</sup>*University of Gothenburg, Gothenburg, Sweden*; <sup>4</sup>*Q&Q labs AB, Gothenburg, Sweden*
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- WP 292 **Targeted Ion Mobility and Liquid Chromatography-Mass Spectrometry Metabolomic Strategies for Glucose Quantitation in Exhaled Breath Condensate for Cystic Fibrosis Studies**; Maria Monge<sup>1</sup>; Jose Perez<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Manshui Zhou<sup>1</sup>; Arlene Stecenko<sup>2</sup>; Facundo Fernández<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Emory University School of Medicine, Atlanta, GA*
- WP 293 **Quantitative Analysis of Small Molecule Neurotransmitters Secreted by hESCs Derived Serotonergic Neurons via Capillary Electrophoresis-Electrospray Ionization-Multiple Reaction Monitoring**; Xuefei Zhong; Hui Ye; Jianfeng Lu; Su-chun Zhang; Lingjun Li; *University of Wisconsin, Madison, WI*
- WP 294 **Quantification of AQC Derivatized Polyamines in Bovine Intraluminal Fluids by UPLC-MS/MS after Solid Phase Extraction**; Maxim Maheux; Claude-Paul Lafrance; *TransBIOTech, Levis, Canada*
- WP 295 **The Potential of Two Dimensional Liquid Chromatography in Mass Spectrometric Assays of the Primary Metabolome**; Kristaps Klavins<sup>1,2</sup>; Dinh Binh Chu<sup>1</sup>; Stefan Neubauer<sup>1</sup>; Stephan Hann<sup>1,2</sup>; Gunda Koellensperger<sup>1,2</sup>; <sup>1</sup>*BOKU - Vienna, Vienna, Austria*; <sup>2</sup>*Austrian Centre of Industrial Biotechnology (ACIB), Vienna, Austria*
- WP 296 **Simultaneous Analysis of Hydrophilic Metabolites on Central Carbon Metabolic Pathway, Amino Acids and Nucleotides by Triple Quadrupole LC/MS/MS**; Tsuyoshi Nakanishi<sup>1</sup>; Takako Hishiki<sup>2,3</sup>; Makoto Suematsu<sup>2,3</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*School of Medicine, Keio University, Tokyo, Japan*; <sup>3</sup>*JST ERATO Suematsu Gas Biology Project, Tokyo, Japan*
- WP 297 **Differential Analysis for Quantitative Metabolomics Using Isotope-Labeling and LC-HRMS: Data Processing Strategies**; Michel Wagner<sup>1</sup>; Yasmin Boukhedimi<sup>1</sup>; Leanne Ohlund<sup>1</sup>; Tze Chieh Shiao<sup>1</sup>; Amelie Vezina<sup>1</sup>; Borhane Annabi<sup>1</sup>; Alex P. Parker<sup>2</sup>; Sarah Jenna<sup>1</sup>; Rene Roy<sup>1</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>*UQAM, Montreal, Canada*; <sup>2</sup>*University of Montreal, Montreal, CA*
- WP 298 **Mild Base Catalyzed Deuteration of Polyphenolics for Improving their Quantification in Cold Hardy Wines by Multiple Reaction Monitoring Mass Spectrometry**; Cecilia Gentle<sup>1,2</sup>; Mikel Roe<sup>1</sup>; Adrian Hegeman<sup>1</sup>; Jerry Cohen<sup>1</sup>; <sup>1</sup>*University of Minnesota, St. Paul, MN*; <sup>2</sup>*Anoka-Ramsey Community College, Coon Rapids, MN*
- WP 299 **An Isotope Label Free Quantification Method for Plant Secondary Metabolites by New Developed Make-Up Liquid Chromatography System**; Che-I Liao; Ya-an Lin; Min-Jane Chen; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan*
- WP 300 **Separation and Complementary ESI-MS/MS and ICP-DRC-MS Detection of Coenzyme A Compounds**; Stefan Neubauer; Dinh Binh Chu; Kristaps Klavins; Stephan Hann; Gunda Koellensperger; *BOKU - Vienna, Vienna, Austria*



- WP 301 **Addressing the Bottlenecks in Metabolomics: Making an Expedient Transition from Global Profiling to Targeted Quantitation;** Mark Sanders<sup>1</sup>; Kevin McHale<sup>1</sup>; Adam Takvam<sup>2</sup>; Michael Athanas<sup>3</sup>; Mark Szewc<sup>1</sup>; Jamie Humphries<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific NJ, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific TX, Austin, TX; <sup>3</sup>Thermo Fisher Scientific CA, San Jose, CA
- WP 302 **Development, Validation and Application of a Novel UPLC-ESI/MS/MS Method for Simultaneous Quantitative Profiling of 14 Endocannabinoids in Biological Matrices;** Sandra Gouveia; Malin Nording; *Department Chemistry, Umea University, Umea, Sweden*
- WP 303 **Quantitative and Qualitative Metabolomics of Neuronal Cell Culture Challenged with Illicit Drugs: A Unified GC/MS/MS and LC/MS/MS approach;** Maria Wenner; Catherine Rawlinson; Joel Gummer; Ian Mullaney; Garth Maker; Robert Trengove; *Murdoch University, Murdoch, Australia*
- WP 304 **Use of CI and EI for Enhanced Selectivity and Sensitivity for the Analysis of Phytohormones;** Catherine Rawlinson<sup>1</sup>; Lars Kamphuis<sup>2</sup>; Paul Wynne<sup>4,5</sup>; Karam Singh<sup>2</sup>; Riki Kitano<sup>3</sup>; Bruce Fraser<sup>4,5</sup>; Robert Trengove<sup>1</sup>; <sup>1</sup>Murdoch University, Murdoch, Australia; <sup>2</sup>CSIRO Plant Industry, Perth, Australia; <sup>3</sup>Shimadzu Corporation, Tokyo, Japan; <sup>4</sup>Shimadzu Scientific Instruments (Oceania), Palmerston North, New Zealand; <sup>5</sup>Shimadzu Scientific Instruments (Oceania), Melbourne, Australia
- WP 305 **Screening of Nandrolone Misuse in Horses by GC-MS/MS Steroid Profiling and Confirmation by UPLC-MS/MS Steroid Esters Detection in Blood;** Zied Kaabia<sup>1,2</sup>; Gaud Dervilly-Pinel<sup>1</sup>; Marie-Agnès Popot<sup>2</sup>; Ludovic Bailly-Chouriberry<sup>2</sup>; Philippe Plou<sup>2</sup>; Yves Bonnaire<sup>2</sup>; Bruno Le Bizet<sup>1</sup>; <sup>1</sup>LABERCA, Nantes, France; <sup>2</sup>LCH, Paris, France
- WP 306 **Highly Sensitive Method for Quantification of Estradiol, Estrone, and Keto-Androgen Metabolites from Human Serum;** Lisa Bottalico<sup>1,2</sup>; Kannan Rangiah<sup>3</sup>; Jasbir Arora<sup>4</sup>; Clementina Mesaros<sup>1,2</sup>; Ian A. Blair<sup>1,2</sup>; <sup>1</sup>Center for Cancer Pharmacology, Philadelphia, PA; <sup>2</sup>University of Pennsylvania School of Medicine, Philadelphia, PA; <sup>3</sup>NCBS, Center for Cellular and Molecular Platforms, Bangalore, India; <sup>4</sup>HFL Sport Science, LGC Health Sciences, KY
- WP 307 **Comprehensive Analysis of Neurotransmitters from Planarian Extract Using UHPLC-MS/SRM Method;** Kannan Rangiah<sup>1</sup>; Dasaradhi Palakodeti<sup>2</sup>; <sup>1</sup>Scientist, C-CAMP, Bangalore, India; <sup>2</sup>Scientist, inSTEM, Bangalore, India
- WP 308 **Metabolomics Investigation of Ovalbumin-Induced Murine Asthmatic Model;** Jun Yang; Jennifer Bratt; Lisa Franzi; Nicholas Kenyon; Bruce Hammock; *University of California, Davis, CA*
- WP 309 **Investigation of Gender Differences in the Hepatic Metabolome of Genotyped Sockeye Salmon (*Oncorhynchus nerka*) Using a Targeted Metabolomics Approach;** Jonathan Benskin<sup>1,2</sup>; Michael Ikonomou<sup>2</sup>; Ralf Bogumil<sup>3</sup>; John Cosgrove<sup>1</sup>; <sup>1</sup>AXYS Analytical Services Ltd., Sidney, Canada; <sup>2</sup>Institute of Ocean Sciences, Sidney, Canada; <sup>3</sup>BIOCRATES Life Sciences AG, Innsbruck, Austria
- WP 310 **Dynamics of Acylsugar Biosynthesis and Metabolism in *Solanum* Glandular Trichome Development;** Zhenzhen Wang; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- WP 311 **Targeted Metabolomic Analysis of Nucleosides in Biological Fluids by Isotope Dilution Liquid Chromatography Electrospray Ionization Tandem Mass Spectrometry;** Jaeman Byun; Anna Mathew; Subramaniam Pennathur; *University of Michigan, Ann Arbor, MI*
- WP 312 **Metabolomic Profiling Reveals Biochemical Pathways Associated with Ethnic Disparity in Breast Cancer;** Nagireddy Putluri<sup>1</sup>; Atsushi Terunuma<sup>2,3</sup>; Tim D. Veenstra<sup>4</sup>; Prachi Mishra<sup>2,3</sup>; Ewy A. Mathe<sup>2,3</sup>; Tiffany H. Dorsey<sup>4</sup>; Ming Yi<sup>4</sup>; Tiffany A. Wallace<sup>4</sup>; Haleem J. Issaq<sup>4</sup>; J. Keith Killian<sup>4</sup>; Holly S. Stevenson<sup>4</sup>; Edward D. Karoly<sup>5</sup>; King Chan<sup>4</sup>; Susmita Samanta<sup>1</sup>; Daniel C. Edelman<sup>4</sup>; Jacob Wulff<sup>4</sup>; Adrienne M. Starks<sup>2,3</sup>; Yinneng Yang<sup>2,3</sup>; Rick A. Kittles<sup>6</sup>; Harry G. Yfantis<sup>7</sup>; Dong H. Lee<sup>7</sup>; Rachel Schiff<sup>1</sup>; Robert M. Stephens<sup>4</sup>; Paul S. Meltzer<sup>4</sup>; Arun Sreekumar<sup>1</sup>; Stefan Ambs<sup>4</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX; <sup>2</sup>National Institutes of Health, Bethesda, MD; <sup>3</sup>National Institutes of Health, Bethesda, MD; <sup>4</sup>National Cancer Institute, Bethesda, MD; <sup>5</sup>Metabolon Inc, Durham, NC; <sup>6</sup>University of Illinois, Chicago, IL; <sup>7</sup>Pathology and Laboratory Medicine, Baltimore, MD
- WP 313 **Application of Metabolomics to Characterize Differences between Plasma and Nipple Aspirate Fluid, a Potential Source of Novel Breast Cancer Biomarkers;** Jessica Miller<sup>1</sup>; Patricia Thompson<sup>1</sup>; Andrew Baker<sup>2,3</sup>; Steven Lai<sup>2,3</sup>; H-H Sherry Chow<sup>1</sup>; <sup>1</sup>University of Arizona Cancer Center, Tucson, AZ; <sup>2</sup>Waters Corporation, Pleasanton, CA; <sup>3</sup>Waters Corporation, Milford, MA
- WP 314 **Metabolomic Comparison of Serum Changes in Focal Segmental Glomerulosclerosis (FSGS) – Preliminary Study;** Chih-Chuan Yu<sup>1</sup>; Chen-Chin Chang<sup>1</sup>; Lai-Chuan Chang<sup>1</sup>; Hung-Chun Chen<sup>2</sup>; <sup>1</sup>Biotech Total Solutions Co., Ltd., Taipei, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 315 **MALDI-TOF MS Quantitation of Targeted Metabolite Disease Markers from Human Plasma;** Nivedita Bhattacharya<sup>1</sup>; Ajeet Singh<sup>1</sup>; Avinash Ghanate<sup>1</sup>; Gaurav Bharadwaj<sup>2</sup>; Trayambak Basak<sup>2</sup>; Shantanu Sengupta<sup>2</sup>; Venkateswarlu Panchagnula<sup>1</sup>; <sup>1</sup>CSIR-National Chemical Laboratory, Pune, India; <sup>2</sup>CSIR-Institute of Genomics and Integrative Biology, New Delhi, India
- WP 316 **Metabolomic Study of Malaria-Borrelia Co-Infection in Murine Model;** Izabella Surowiec<sup>1</sup>; Maria Nelson<sup>2</sup>; Sven Bergström<sup>2</sup>; Johan Trygg<sup>1</sup>; Johan Normark<sup>2</sup>; <sup>1</sup>Department of Chemistry, Umeå University, Umeå, Sweden; <sup>2</sup>Department of Molecular Biology, Umeå University, Umeå, Sweden
- WP 317 **A Global LC-MS Metabolomics Approach for Biomarker Identification in Patients with Nonalcoholic Fatty Liver Disease;** Rainey Patterson<sup>1</sup>; Romina Lomonaco<sup>2</sup>; Nishanth Sunny<sup>2</sup>; Kenneth Cusi<sup>2</sup>; Timothy Garrett<sup>3</sup>; David Powell<sup>1</sup>; Richard Yost<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>2</sup>Division of Endocrinology, University of Florida, Gainesville, FL; <sup>3</sup>Department of Pathology, University of Florida, Gainesville, FL
- WP 318 **Evaluation of Home Sampling DBS and Micro Fluidic LC/MS for Monitoring the Effects of Rosuvastatin on Cholesterol and Triglyceride Levels;** Robert Plumb<sup>1</sup>; Ian Wilson<sup>1</sup>; Nicola Gray<sup>1</sup>; Paul Rainville<sup>2</sup>; <sup>1</sup>Imperial College, London, UK; <sup>2</sup>Waters, Milford, MA
- WP 319 **Determination of Hydroxyeicosatetraenoic Acids in Prostate Cancer Serum Samples Using UHPLC-MS/MS;** Giovanny Rodríguez-Blanco<sup>1</sup>; Peter Burgers<sup>1</sup>; Lennard Dekker<sup>1</sup>; Jan Ijzerman<sup>2</sup>; Mirella Vredenburg-van den Berg<sup>3</sup>; Ellen Schenk<sup>3</sup>; Guido Jenster<sup>3</sup>; Theo Luider<sup>1</sup>; <sup>1</sup>Neurology Department, Erasmus Medical Center, Rotterdam, Netherlands; <sup>2</sup>Department of Surgery, Erasmus Medical Center, Rotterdam, Netherlands; <sup>3</sup>Urology Department, Erasmus Medical Center, Rotterdam, Netherlands
- WP 320 **Plasma Metabolites Associated with Acute Exacerbations of Chronic Obstructive Pulmonary Disease;** Makedonka Gulcevi<sup>1</sup>; Cavan Reilly<sup>1</sup>; Steven

Harvey<sup>1</sup>; Joseph Dalluge<sup>1</sup>; Prescott Woodruff<sup>2</sup>; Christine Wendt<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of California, San Francisco, CA

WP 321 **Assessment of Gut Microbiome Using Metabolomics Analysis of Body Fluids**; Shucha Zhang; Karen Corbin; Xueqing Zhao; Steven Zeisel; *UNC Chapel Hill, Kannapolis, NC*

WP 322 **Identification of Metabolites Cleared by the Kidney with High Efficiency Using Orbitrap Metabolomics Platform**; Pavel Aronov<sup>1</sup>; Tammy Sirich<sup>2</sup>; Natalie Plummer<sup>2</sup>; Allis Chien<sup>3</sup>; Timothy Meyer<sup>2</sup>; <sup>1</sup>Thermo Scientific, San Jose, CA; <sup>2</sup>Department of Medicine, Stanford University, Stanford, CA; <sup>3</sup>Mass Spectrometry Laboratory, Stanford University, Stanford, CA

WP 323 **Metabolomics Input in a Search for Chronic Kidney Disease Targets Utilizing Clinical Cross-Platform Omics Data Integration**; Vladimir Tolstikov; Alexander Nikolayev; Dennis Laska; Ming-Shan Kuo; Kevin Duffin; *Eli Lilly and Company, Indianapolis, IN*

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WP 324 **An Advanced CE-QTOF Technique for the Rapid Characterization of Amino Acids in Herbal Medicines**; Tao Bo; Zhengxiang Zhang; Xiaorong Ran; Jianzhong Li; *Agilent Technologies, Beijing, China*

WP 325 **Sake-omics: Development and Application of Advanced GC-MS Methods for Speciation of Quality Components in Sake Varietals**; Doug D. Carlton Jr.; Kevin A. Schug; *The University of Texas at Arlington, Arlington, TX*

WP 326 **Rapid Analysis of Triglycerides and Fatty Acids in Food Oils Using DART-MS with High-Speed Polarity Switching**; Shun Wada<sup>1</sup>; Jun Watanabe<sup>2</sup>; Keiko Matsumoto<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; Shingo Toda<sup>3</sup>; <sup>1</sup>Japan Inst. of Oil & Fats, Other Foods Inspection, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>AMR, Inc., Tokyo, Japan

WP 327 **Quantitative Analysis of  $\alpha$ - and  $\beta$ - acids in Hops by Paper Spray Ionization**; Gregg Hasman; Andre Venter; *Western Michigan University, Kalamazoo, MI*

WP 328 **Rapid Amino Acid Content Analysis in Soybeans and Other Foodstuffs Utilizing Microwave Hydrolysis Coupled with Desorption Electrospray Ionization Mass Spectrometry**; Jonathan R. Person; Christopher C. Mulligan; *Department of Chemistry, Illinois State University, Normal, IL*

WP 329 **New Method for the Analysis of Antioxidants in Vegetable Oils Using an Hybrid SFC/UHPLC System with MS Detection**; Patric Hoerth<sup>1</sup>; Maria Rambla-Alegre<sup>2</sup>; Martin Vollmer<sup>1</sup>; Gerd Vanhoenacker<sup>2</sup>; <sup>1</sup>Agilent Technologies, Waldbronn, Germany; <sup>2</sup>Research Institute for Chromatography, Kortrijk, Belgium

WP 330 **Use of Supercritical Fluid Chromatography /Mass Spectrometry for Rapid Separation of Fat Soluble Vitamins, A, D, E and K**; Jennifer Van Anda<sup>1</sup>; Terry Berger<sup>2</sup>; <sup>1</sup>Agilent Technologies, Little Falls, DE; <sup>2</sup>SFC Solutions, Englewood, FL

WP 331 **Analysis of Water-Soluble B Vitamins in Infant Formula Using Automated Online Sample Preparation with LC/MS**; Yang Shi; *Thermo Fisher Scientific, Franklin, MA*

WP 332 **Queued and Ready to Run? Testing the Stability of Vitamin Extracts While in Queue Using Triple Quadrupole LC/MS/MS Analysis**; Jeremy Post<sup>1</sup>; Susan Leonard<sup>2</sup>; Christopher Gilles<sup>1</sup>; Scott Kuzdzal<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Shimadzu Scientific Instruments, Marlborough, MA

WP 333 **Characterization of Flavored Tobacco with GCxGC-TOFMS and GC-HR-TOFMS**; Elizabeth Humston-Fulmer; Jeff Patrick; Joe Binkley; *LECO, St. Joseph, MI*

WP 334 **High Throughput Profiling of Phytic Acid, Inositol Phosphates and Inorganic Phosphate in Seed Extracts with Flow Injection Electrospray Mass Spectrometry**; David Mccaskill; Josh Flook; Scott Greenwalt; Beth Blakeslee; *Dow AgroSciences, Indianapolis, IN*

WP 335 **LC-MS Analysis of Food and Food Additives with Monolithic Silica Columns**; David Lentz<sup>1</sup>; Stephan Altmaier<sup>2</sup>; Egidijus Machtejevas<sup>2</sup>; Karin Cabrera<sup>2</sup>; <sup>1</sup>EMD Millipore, Billerica, MA; <sup>2</sup>Merck Millipore Merck KGaA, Darmstadt, Germany

WP 336 **Characterization and Quantitation of Capsaicin and Related Pungent Agents in Chili Peppers and Hot Sauces by LC/MS/MS**; Seyed Sadjadi; J Preston; Sky Countryman; Zeshan Aqeel; *Phenomenex, Inc, Torrance, CA*

WP 337 **Comprehensive Analysis of Caecal Contents of the Human Flora-associated (HFA) Mice by High Resolution LC-QTOF Mass Spectrometry**; Masahiko Takino<sup>1</sup>; Motoi Tamura<sup>2</sup>; <sup>1</sup>Agilent Technologies Japan, Tokyo, Japan; <sup>2</sup>the National Food Research Institute, Tsukuba, Japan

WP 338 **Elemental Non-Targeted Profiling of 66 Whiskies Using ICP-MS**; Helene Hopfer<sup>1,2</sup>; Thomas S. Collins<sup>1,3</sup>; Jenny Nelson<sup>2,4</sup>; Susan Ebeler<sup>1,2</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Food Safety and Measurement Facility, Davis, CA; <sup>3</sup>Treasury Wine Estates, Napa, CA; <sup>4</sup>Agilent Technologies, Santa Clara, CA

WP 339 **Metabolic Profiling of Wines from Various Geographic Regions and Chateaux Using UHPLC-ESI/QTOF-MS Technique Combined with Principle Components Analysis**; Shen Han<sup>1</sup>; Jinhua Wang<sup>1</sup>; Ying Liu<sup>1</sup>; Qi Zhou<sup>1</sup>; Meiling Lu<sup>2</sup>; <sup>1</sup>Beijing Entry-Exit Bureau of Inspect. and Quarant., Beijing, CN; <sup>2</sup>Agilent Technologies, Beijing, CN

WP 340 **Application of Non-Targeted High Resolution Mass Spectrometry to Monitoring Tea Fermentation Level and Origin**; Karl Fraser<sup>2</sup>; Don Otter<sup>2</sup>; Geoff Lane<sup>2</sup>; Siew-Young Quek<sup>1</sup>; Yacine Hemar<sup>1</sup>; <sup>1</sup>University of Auckland, Auckland, New Zealand; <sup>2</sup>AgResearch, Palmerston North, New Zealand

WP 341 **A Novel Strategy for *in situ* Label-Free Imaging of a Bioactive Polyphenol**; Yoshinori Fujimura<sup>1</sup>; Yoon Hee Kim<sup>2</sup>; Takatoki Hagihara<sup>2</sup>; Masako Sasaki<sup>2</sup>; Daichi Yukihiro<sup>2</sup>; Tatsuhiko Nagao<sup>2</sup>; Daisuke Miura<sup>1</sup>; Shinichi Yamaguchi<sup>3</sup>; Kazunori Saito<sup>4</sup>; Hiroyuki Wariishi<sup>2</sup>; Koji Yamada<sup>2</sup>; Hirofumi Tachibana<sup>2</sup>; <sup>1</sup>ICMRN, Kyushu University, Fukuoka, Japan; <sup>2</sup>Faculty of Agriculture, Kyushu University, Fukuoka, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan; <sup>4</sup>Bruker Daltonics K.K., Yokohama, Japan

WP 342 **Identification of Structural Isomers of Methylated Flavonols by UHPLC Coupled High Resolution QTOF Mass Spectrometry**; ChengYing Ma<sup>1</sup>; Haipeng Lv<sup>1</sup>; Xingzhong Zhang<sup>1</sup>; Zongmao Chen<sup>1</sup>; Jiang Shi<sup>1</sup>; Zhi Lin<sup>1</sup>; Meiling Lu<sup>2</sup>; Shan Zhou<sup>2</sup>; <sup>1</sup>Tea Research Institute, CAAS, Hangzhou, CN; <sup>2</sup>Agilent Technologies, Beijing, CN

WP 343 **A Global Proteomics Approach for the Detection and Characterization of Gluten in Food**; Katherine L. Fiedler; Sara C. McGrath; John H. Callahan; Mark M. Ross; *CFSAN, U.S. FDA, College Park, MD*

WP 344 **Characterization and Quantification of Peanut Allergens Using Ion Mobility Data Independent Label Free Strategies**; Philip Johnson<sup>2</sup>; Lee A Gethings<sup>1</sup>; Justin Marsh<sup>2</sup>; James Langridge<sup>1</sup>; Clare Mills<sup>2</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>University of Manchester, Manchester, UK



- WP 345 **Site-Specific Detection of Radicals on  $\alpha$ -lactalbumin after riboflavin-Sensitized Reaction, Detected by Immuno-Spin Trapping, ESR and MS;** Trine Dalsgaard<sup>1</sup>; Mathilde Triquigneaux<sup>2</sup>; Leesa Deterding<sup>2</sup>; Fiona Summers<sup>2</sup>; Kalina Rangelova<sup>2</sup>; Grith Mortensen<sup>1</sup>; Ronald Mason<sup>2</sup>; <sup>1</sup>Aarhus University, Tjele, Denmark; <sup>2</sup>NIEHS/NIH, Research Triangle Park, NC
- WP 346 **Identification of AGE Modifications to Peanut Allergens Using LC-ESI Based Mass Spectrometry;** Katina L. Johnson<sup>1</sup>; Geoffrey A. Mueller<sup>1</sup>; Soheila Maleki<sup>2</sup>; Allison Schrozman<sup>3</sup>; Anna Pomes<sup>4</sup>; Lori Edwards<sup>1</sup>; Hajeung Park<sup>5</sup>; Leesa Deterding<sup>1</sup>; Kenneth B. Tomer<sup>1</sup>; Robert London<sup>1</sup>; Jason G. Williams<sup>1</sup>; <sup>1</sup>National Institute of Environmental Health Science, Research Triangle Park, NC; <sup>2</sup>USDA, New Orleans, LA; <sup>3</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>4</sup>INDOOR Biotechnologies, Charlottesville, VA; <sup>5</sup>The Scripps Research Institute, Jupiter, FL
- WP 347 **Rapid Throughput Extraction of Human Milk Oligosaccharides to Allow Studies on Larger Cohorts;** Lauren M. Dimapasoc; Sarah Totten; Carol Stroble; L. Renee Ruhaak; Carlito B. Lebrilla; *University of California, Davis, CA*
- WP 348 **Milk Protein Identification and Relative Quantification by Capillary LC Coupled with Novel Hybrid High Resolution Mass Spectrometer;** Terry Zhang; David Horn; Guifeng Jiang; Charles Yang; Dipankar Ghosh; *ThermoFisher, San Jose, CA*
- WP 349 **Mass Spectrometry Based Glycan Arrays for Determining Specificity of Glycosidases in Bacteria;** Sarah Totten; Santiago Ruiz-Moyano; David Mills; Carlito Lebrilla; *University of California, Davis, CA*
- WP 350 **Digestomics of Human Milk Proteins in Term and Premature Infants;** David Dallas<sup>1</sup>; Andres Guerrero<sup>1</sup>; Nora Khaldi<sup>2</sup>; Bruce German<sup>1</sup>; Daniela Barile<sup>1</sup>; Mark Underwood<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>UC Dublin, Dublin, Ireland
- WP 351 **Metabolite Fingerprinting Using High Resolution Mass Spectrometry of Feces from Rats Fed Resistant Starch;** Tim Anderson; R. Sam Houk; Roger Jones; Diane Birt; Yinsheng Zhao; John McClelland; *Iowa State University, Ames, IA*
- WP 352 **Determination of fortified and endogenous folates in food-based Standard Reference Materials by isotope-dilution liquid chromatography-tandem mass spectrometry;** Johanna Camara; Mark Lowenthal; Karen Phinney; *NIST, Gaithersburg, MD*
- WP 353 **Analysis of Triglycerides in Plant Oils by Direct Analysis in Real Time;** Igor Gavin; Anil Oroskar; Asha Oroskar; *Orochem Technologies Inc., Lombard, IL*
- WP 354 **A New, Sensitive Method for Lignan Metabolite Detection of Flaxseed-Fed Mice Using LC-MS/MS;** Rong Tsao<sup>1</sup>; Honghui Zhu<sup>1</sup>; Sha Joshua Ye<sup>2</sup>; Lisa M. Cousins<sup>2</sup>; <sup>1</sup>Guelph Food Research Centre, Agriculture & Agri-F, Guelph, ON, Canada; <sup>2</sup>IONICS Mass Spectrometry, Bolton, ON, Canada
- WP 355 **Identification of Wax Esters by LCMS in Cloudy Canola Oil;** Susan Seegers; Tiffanie West; *Bunge North America, Bradley, IL*
- WP 356 **Determination of 3-chloro-1,2-propanediol in Soy Sauce Samples with Supported Liquid Extraction and GC-MS;** Suzi Qin; Jack Liu; Wan Wang; Guotao Lu; *Bonna-Agela Technologies, Tianjin, China*
- WP 357 **Direct Detection of Chloramphenicol in Honey by Neutral Desorption-Extractive Electrospray Ionization Mass Spectrometry;** Xi Zhang<sup>1,2</sup>; Li-Ping Luo<sup>2</sup>; Xi-Mo Dai<sup>1</sup>; <sup>2</sup>Xiao-Wei Fang<sup>1</sup>; Eric Handberg<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Technology, Nanchang, China; <sup>2</sup>Nanchang University, Nanchang, China
- WP 358 **Rapid Screening of Sulfur fumigated Chinese Star Anise by Surface Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry;** Xi-Mo Dai<sup>1,2</sup>; Li-Ping Luo<sup>1</sup>; Xi Zhang<sup>1,2</sup>; Ya-Li Liu<sup>2,3</sup>; Xiao-Wei Fang<sup>2</sup>; Eric Handberg<sup>2</sup>; Huanwen Chen<sup>2</sup>; <sup>1</sup>Nanchang University, Nanchang, China; <sup>2</sup>East China Institute of Technology, Nanchang, China; <sup>3</sup>Hebei University of Technology, Tianjin, China
- WP 359 **Cadmium-Lead Chemical Signatures Characteristic to the Harvest Areas of the American Oyster, by ICP-MS: A Regulatory and Environmental Monitoring Tool;** Marc E. Engel; *FDACS, Tallahassee, FL*
- WP 360 **Liquid Chromatography – Mass Spectrometry Method for the Quantitative Determination of Residues of Selected Veterinary Hormones in Powdered Milk-Based Commodities;** Stefan Ehling; Murali Reddy; *Abbott Nutrition, Columbus, OH*
- WP 361 **Direct-EL/LC-MS in Food Safety Applications. Multicomponent Analysis of Environmental Contaminant Residues in Milk Based Raw Materials;** Achille Cappiello<sup>1</sup>; Fabiana Capriotti<sup>1</sup>; Giorgio Famigliini<sup>1</sup>; Pierangela Palma<sup>1</sup>; Veronica Termopoli<sup>1</sup>; Nicholas Cellar<sup>2</sup>; <sup>1</sup>University of Urbino, Urbino, Italy; <sup>2</sup>Abbott Nutrition, Columbus, OH
- WP 362 **Rapid Quantitative Detection of Residual Malachite Green in Drinking and Aquaculture Water Samples by Extractive Electrospray Ionization Mass Spectrometry (EESI-MS);** Xiaowei Fang; Susu Pan; Liang Zhu; Xinglei Zhang; Eric Handberg; Huanwen Chen; *East China Institute of Tech., Nanchang, China*
- WP 363 **Coupling Neutral Desorption to Dielectric Barrier Discharge Ionization Mass Spectrometry for Direct Analysis of Oil Samples;** Yafei Zhou<sup>1</sup>; Zhongchen Wu<sup>2</sup>; Cao Li<sup>1</sup>; Nannan Wang<sup>1</sup>; Saijin Xiao<sup>1</sup>; Xinglei Zhang<sup>1</sup>; Eric Handberg<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Tech., Nanchang, China; <sup>2</sup>Shandong University, Weihai, China
- WP 364 **Desorption Atmospheric Pressure Chemical Ionization Mass Spectrometry and Pattern Classification to Identify the Molecular Cause of Aging in Lotus Seeds;** Ximo Dai<sup>1,3</sup>; Liping Luo<sup>1,1</sup>; Xi Zhang<sup>1,3</sup>; Yongzhong Ouyang<sup>2</sup>; Eric Handberg<sup>3</sup>; Huanwen Chen<sup>3</sup>; <sup>1</sup>Nanchang University, Nanchang, China; <sup>2</sup>Hebei University of Technology, Tianjin, China; <sup>3</sup>East China Institute of Tech., Nanchang, China
- WP 365 **Analysis of  $\alpha$ -dicarbonyl Process Contaminants in High Fructose Corn Syrup and Carbonated Soft Drinks by UHPLC-DAD-ESI-MS/MS;** Sabrina Gensberger; Monika Pischetsrieder; *University of Erlangen-Nuremberg, Erlangen, Germany*
- WP 366 **Multi-Target Screening for 138 Veterinary Drugs in Meat Using Liquid Chromatography High Resolution Mass Spectrometry;** Feng Qin<sup>1</sup>; Xiaoyan Li<sup>1</sup>; Ke Wang<sup>1</sup>; Chengyuan Cai<sup>2</sup>; Yongming Xie<sup>2</sup>; Huaien Zhu<sup>2</sup>; <sup>1</sup>Shanghai Institute of Food and Drug Control, Shanghai, China; <sup>2</sup>ABSCIEX, Shanghai, China
- WP 367 **Rapid Identification of Veterinary Drugs from Different Matrices Using High Resolution LC/MS/MS and Library Search;** Franziska Spitzbarth<sup>1</sup>; Günther Kempe<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; Alexander Eilfeld<sup>2</sup>; <sup>1</sup>LUA Sachsen, Chemnitz; <sup>2</sup>AB Sciex, Leipzig, Germany
- WP 368 **Determination of 68 Veterinary Drugs in Marine Products by Ultra High Performance Liquid Chromatography/Triple Quadrupole Mass Spectrometry;** Lingling Shen; Jinting Yao; Caiyong Lin; Xiongxiang Qiu; Qisheng Zhong; Song Zhan; Taohong

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- Huang; Shimadzu Global COE, Shimadzu (China) Co., Ltd., Guangzhou, China
- WP 369 **Analysis of Multiclass Veterinary Drug Residues in Baby Food by Ultra Fast Chromatography with High Performance Triple Quadrupole Mass Spectrometry;** Charles T. Yang; Mary Blackburn; Dipankar Ghosh; *Thermo Fisher Scientific, San Jose, CA*
- WP 370 **Multi-residue Screening and Confirmation of Veterinary Drugs in Tissue Samples by LC-MS/MS with New Triggered MRM Acquisition;** Guenther Kempe<sup>2</sup>; Thomas Glauner<sup>1</sup>; Franzika Spitzbarth<sup>2</sup>; *<sup>1</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>2</sup>LUA Saxony, Chemnitz, Germany*
- WP 371 **Automated Solid Phase Extraction (SPE)-LC/MS/MS Method for the Determination of Acrylamide in Brewed Coffee Samples;** Fred Foster; John Stuff; Edward Pfannkoch; *Gerstel, Inc., Linthicum, MD*
- WP 372 **Organizing the Masses;** Daniel L. Sweeney; *MathSpec, Inc., Arlington Heights, IL*
- H/D Exchange, Software and Hardware, 373 – 385**
- WP 373 **Peptide-Dependent Amide Back Exchange Rates Limit the Utility of Subtractive Analysis as a Method for Increased HDX-MS Resolution;** Joey Sheff; *University of Calgary, Calgary, Canada*
- WP 374 **Assessing Lab-to-lab Reproducibility of Deuterium Measurement in Hydrogen Deuterium Exchange Mass Spectrometry Analysis;** Barbara Sullivan; *Waters, Beverly, MA*
- WP 375 **Online SCX and RP extraction method for H/D Exchange Mass Spectrometry of Samples Containing Macromolecular Crowding Agents;** Farai Rusinga; David Weis; *University of Kansas, Lawrence, KS*
- WP 376 **An Improved HDX Platform Workflow for Enhanced Separation, Digestion, and Data Analysis;** Joomi Ahn<sup>1</sup>; Michael Eggertson<sup>1</sup>; Keith Faden<sup>1</sup>; Han Joo Lee<sup>1</sup>; John Engen<sup>2</sup>; *<sup>1</sup>Waters Corp, Milford, MA; <sup>2</sup>Northeastern University, Boston, MA*
- WP 377 **Applications of an Automated Hydrogen Deuterium Exchange Platform to Epitope Mapping of Antibody-Antigen Complexes;** Jon Fitchett; Kai Zhang; Bryan E Jones; *Lilly Biotech Center-San Diego, San Diego, CA*
- WP 378 **Overcoming Peak Capacity Limitations Imposed by Hydrogen Exchange Quench Conditions;** Bradley B. Stocks<sup>1</sup>; Thomas E. Wales<sup>1</sup>; Martha Stapels<sup>2</sup>; Keith Faden<sup>2</sup>; Michael Eggertson<sup>2</sup>; Geoff Gerhardt<sup>2</sup>; John R. Engen<sup>1</sup>; *<sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Waters Corporation, Milford, MA*
- WP 379 **A Single-Droplet Digital Microfluidics System for Hydrogen-Deuterium Exchange Mass Spectrometry;** Huijiang Ding; Puneet Souda; Christopher M. Ryan; Kym Faull; Julian Whitelegge; *University of California, Los Angeles, CA*
- WP 380 **Fully Automated HDX-MS on a Microfluidic Platform – Solving Problems Related to Small Volume Sample Preparation, Protein Adsorption, and Carryover;** Yunan Miao<sup>1</sup>; Gregory Staples<sup>2</sup>; Reid A. Brennen<sup>2</sup>; Hongfeng Yin<sup>2</sup>; Kevin Killeen<sup>2</sup>; Terry Lee<sup>1</sup>; *<sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Agilent Laboratories, Santa Clara, CA*
- WP 381 **Software for Automated HDX-MS Data Analysis and Visualization;** Seungjin Na<sup>1</sup>; Jae-Jin Lee<sup>2</sup>; Kong-Joo Lee<sup>2</sup>; Eunok Paek<sup>1</sup>; *<sup>1</sup>Hanyang University, Seoul, Korea; <sup>2</sup>Ewha Womans University, Seoul, Korea*
- WP 382 **How to Obtain Conformational Structures of Protein in Solution from Higher Charge States in HDX and Top-Down ECD ESI MS?** Teerapat Rojsajakul; Fred King; *Department of Chemistry, West Virginia University, Morgantown, WV*
- WP 383 **H/D Exchange Mass Spectrometry in Atmospheric Pressure ESI-MS Interface for Enumeration of Labile Hydrogens in Complex Mixtures;** Yury Kostyukevich<sup>1, 4</sup>; Alexey Kononikhin<sup>1, 2</sup>; Igor Popov<sup>2, 4</sup>; Oleg Kharybin<sup>1, 3</sup>; Eugene Nikolaev<sup>1, 3</sup>; *<sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>3</sup>Orehovich Institute of Biomedical Chemistry, Moscow, Russia; <sup>4</sup>Moscow Institute of Physics and Technology, Moscow, Russia*
- WP 384 **Improvements to the HDX Workbench Software for High Throughput Analysis of HDX MS Data;** Bruce D. Pascal; Michael J. Chalmers; Graham M. West; Scott Novick; Devrishi Goswami; David Marciano; Patrick R. Griffin; *The Scripps Research Institute, Scripps Florida, Jupiter, FL*
- WP 385 **Binomial Fitting Provides a Powerful Method for the Analysis of H/D Exchange Data;** Miklos Guttman; Kelly Lee; *University of Washington, Seattle, WA*
- H/D Exchange: Protein Structure/Function II, 386 – 400**
- WP 386 **Structural Confirmation of Potential Cancer Therapeutic: Pyruvate Kinase Activator Restores Active Conformation to M2 Isoform;** Graham M West<sup>1</sup>; Dimitrios Anastasiou<sup>2</sup>; Bruce Pascal<sup>1</sup>; Michael Chalmers<sup>1</sup>; Lewis Cantley<sup>3</sup>; Patrick Griffin<sup>1</sup>; *<sup>1</sup>Scripps Research Institute, FL, Jupiter, FL; <sup>2</sup>Division of Physiology and Metabolism, MRC-NIMR, London, UK; <sup>3</sup>Dpt of Systems Biology, Harvard Medical School, Boston, MA*
- WP 387 **Using Hydrogen-Deuterium Exchange to Probe the Structure of Phosphorylase Kinase, a Complex with 325 kDa of Unique Sequence;** Mary Ashley Rimmer; Antonio Artigues; Maria T. Villar; Gerald M. Carlson; *University of Kansas Medical Center, Kansas City, KS*
- WP 388 **Substrate Channeling in Phosphodiesterase-Protein Kinase A Interactions Mediates cAMP Signal Termination: Monitoring Transient Ternary Complexes by HDXMS;** Srinath Krishnamurthy; *NUS, Singapore*
- WP 389 **Structural Dynamics and Ligand Dependent Activation of IDH1 R132H Probed by HDX-MS;** Devrishi Goswami<sup>1</sup>; Michael Chalmers<sup>1</sup>; Carlos Perez<sup>2</sup>; Stephen Antonyamsy<sup>2</sup>; Bruce Pascal<sup>1</sup>; Jeffrey Dodge<sup>2</sup>; Patrick Griffin<sup>1</sup>; *<sup>1</sup>The Scripps Research Institute, Jupiter, FL; <sup>2</sup>Lilly Research Laboratories, Eli Lilly and company, Indianapolis, IN*
- WP 390 **H/DX Mass Spectrometry Reveals Features of SecA Dimeric Interface and a Conformational Change from Open to Closed Forms upon Dimerization;** Yuetian Yan<sup>1</sup>; Andy Wowor<sup>2</sup>; Jun Zhang<sup>3</sup>; James Cole<sup>4</sup>; Debra Kendall<sup>5</sup>; Michael Gross<sup>1</sup>; *<sup>1</sup>Dept of Chemistry, Washington University, Saint Louis, MO; <sup>2</sup>Dept of Chem and Biochem, Colorado College, Colorado Springs, CO; <sup>3</sup>Department of Drug Product Development, Amgen Inc, Seattle, WA; <sup>4</sup>Department of Chemistry, University of Connecticut, Storrs, CT; <sup>5</sup>Dept of Pharmaceutical Sciences, U. of Connecticut, Storrs, CT*
- WP 391 **Thermodynamic Stability of Protective Antigen Measured by His-HDX-MS;** Vennela Mullangi<sup>1, 3</sup>; James Bann<sup>2</sup>; David Anderson<sup>1</sup>; Masaru Miyagi<sup>3</sup>; *<sup>1</sup>Cleveland State University, Cleveland, OH; <sup>2</sup>Wichita State University, Wichita, KS; <sup>3</sup>Case Western Reserve University, Cleveland, OH*
- WP 392 **Characterizing Protein Dynamics and Higher Order Structure in a Conformer-Specific Fashion with Top-Down HDX MS/MS: A Case of Ubiquitin;** Guanbo Wang; Rinat R. Abzalimov; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- WP 393 **Effect of Ligand binding on Conformational Dynamics of DAHP Synthase Using Microfluidics Enabled Hydrogen/ Deuterium Exchange;** Tamanna Rob<sup>1</sup>; Naresh Balachandran<sup>2</sup>; Paul Berti<sup>2</sup>; Derek Wilson<sup>1</sup>; *<sup>1</sup>York University, Toronto, Canada; <sup>2</sup>McMaster University, Hamilton, ON, Canada*

- WP 394 **HDX-MS in Pharmaceutical Analysis: Defining the Epitopes of Drug-Bound Proteins;** Rebecca Rose; Hannah Maple; John Porter; Richard Taylor; Rachel Garlish; *UCB, Slough, UK*
- WP 395 **Pinpointing Conformational Differences between Protein Variants by HDX-MS and ETD (HDX-ETD);** Signe T. Seger<sup>1,2</sup>; Mette D. Andersen<sup>2</sup>; Jens Breinholt<sup>2</sup>; Christine B. Schjødt<sup>2</sup>; Johan Faber<sup>2</sup>; Kasper D. Rand<sup>1</sup>; <sup>1</sup>*University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Novo Nordisk A/S, Biopharmaceuticals Research Unit, Måløv, Denmark*
- WP 396 **Solution-Phase H/D Exchange for Charge State +12 and +13 Ions of Bovine Ubiquitin Revealed by Top-down ECD ESI FTICR MS;** Xiaqing Xu; Teerapat Rojsajakul; Fred King; *Department of Chemistry, West Virginia University, Morgantown, WV*
- WP 397 **Analysis of cGMP/cAMP Binding to the PKGI Beta Regulatory Domain by HDX Using High Resolution Orbitrap Mass Spectrometer;** Sheng Li; Bryant Kou; Virgil Woods, Jr; Darren E. Casteel; *UCSD, La Jolla, CA*
- WP 398 **Probing Inhibition of Insulin Fibrillation by 1, 2-Bis[4-(3-sulfonatopropoxyl)phenyl]-1,2-Diphenylethane with Hydrogen/Deuterium Exchange – Mass Spectrometry;** Matthew Cummings; Teerapat Rojsajakul; Fred King; *Department of Chemistry, West Virginia University, Morgantown, WV*
- WP 399 **A HDX/MS Analysis of the Interaction between Human Tumor Necrosis Factor-Alpha (TNF-alpha) and anti-TNF-alpha Agents;** Shiori Nakazawa<sup>1,2</sup>; Noritaka Hashii<sup>2</sup>; Nana Kawasaki<sup>1,2</sup>; <sup>1</sup>*Hokkaido Univ., Sapporo, Japan*; <sup>2</sup>*Natl. Inst. Health Sci., Tokyo, Japan*
- WP 400 **Suicide Inhibition of Oncogenic K-Ras G12C Proceeds via Shift to the Inactive Conformation;** Rane Harrison<sup>1</sup>; Sang Min Lim<sup>2,3</sup>; Kenneth Westover<sup>4</sup>; Nathanael Gray<sup>2,3</sup>; John Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*Dana-Farber Cancer Institute, Boston, MA*; <sup>4</sup>*University of Texas Southwestern Medical Center, Dallas, TX*
- Proteins: Non-Covalent Interactions, 401 – 421**
- WP 401 **Assembly of the Bacteriophage T7 Replisome Probed by Native Electrospray Ionization Top-Down Mass Spectrometry;** Hao Zhang; Jamie R. Wallen; Weidong Cui; Robert E. Blankenship; Thomas E. Ellenberger; Michael L. Gross; *Washington University, St. Louis, MO*
- WP 402 **Probing the Molecular Mechanism of Photoprotective Quenching in Cyanobacteria by Native Mass Spectrometry and Protein Cross-linking;** Hao Zhang; Haijun Liu; Mindy Prado; Michael L. Gross; Robert E. Blankenship; *Washington University, Saint Louis, MO*
- WP 403 **Nanodiscs Can Fly: Investigating the Ionization and Dissociation Mechanisms of Lipoprotein Macromolecules;** Michael Marty<sup>1</sup>; Hao Zhang<sup>2</sup>; Weidong Cui<sup>2</sup>; Robert Blankenship<sup>2</sup>; Michael Gross<sup>2</sup>; Stephen Sligar<sup>1</sup>; <sup>1</sup>*University of Illinois Urbana-Champaign, Urbana, IL*; <sup>2</sup>*Washington University St. Louis, St. Louis, MO*
- WP 404 **Binding Affinities Determination of the Norovirus P Particle with HBGA Oligosaccharides;** Ling Han<sup>1</sup>; Elena Kitova<sup>1</sup>; Ming Tan<sup>2</sup>; Xi Jiang<sup>2</sup>; John Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*; <sup>2</sup>*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*
- WP 405 **Quantification of Protein Binding to Cell Receptors by Electrospray Ionization Mass Spectrometry;** Hong Lin; Yixuan Zhang; Elena N. Kitova; John S. Klassen; *Department of Chemistry, University of Alberta, Edmonton, Canada*
- WP 406 **Dissociation Pathways Observed for Multisubunit Protein-Ligand Complexes in the Gas Phase;** Yixuan Zhang; Lu Deng; Elena Kitova; John Klassen; *U of Alberta, Edmonton, Canada*
- WP 407 **A Novel Method for Determining the Binding Site Location of FGFR1 Kinase Inhibitors;** Helen Beeston<sup>1</sup>; Jan Griesbach<sup>2</sup>; Jason Breed<sup>2</sup>; Richard Norman<sup>2</sup>; Julie Tucker<sup>2</sup>; Geoff Holdgate<sup>2</sup>; Alison E. Ashcroft<sup>1</sup>; <sup>1</sup>*Faculty of Biological Sciences, University of Leeds, Leeds, UK*; <sup>2</sup>*Astrazeneca UK Ltd, Macclesfield, UK*
- WP 408 **Probing Interactions of Different Glycoforms of Antithrombin-III with Heparin Octasaccharides Using Native Electrospray Ionization Mass Spectrometry ;** Rinat Abzalimov; Burcu Baykal; Stephen Eyles; Paul Dubin; *UMASS, Amherst, MA*
- WP 409 **Investigation of the Interaction between Gadolinium and Transferrin by Mass Spectrometric Analysis;** Kristina Wentker; Christine Brauckmann; Olga Reifschneider; Helene Faber; Christoph A. Wehe; Uwe Karst; *University of Münster, Münster, Germany*
- WP 410 **Determination of Non-Covalent Bound Ligands and Metals to Transferrin in Clinically Relevant Samples;** Jake W. Pawlowski; Cedric E. Bobst; Igor A. Kaltashov; *UMASS, Amherst, MA*
- WP 411 **Mass Spectrometry Reveals Synergistic Binding of Nucleotides, Lipids and Drugs to a Multidrug Resistance Efflux Pump;** Julien Marcoux<sup>1</sup>; Sheila Wang<sup>1</sup>; Argyris Politis<sup>1</sup>; Jerome Ma<sup>1</sup>; Philip Biggin<sup>1</sup>; Geoffrey Chang<sup>2</sup>; Nina Morgner<sup>1</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*Scripps Research Institute, La Jolla, CA*
- WP 412 **Pulsed and Continuous Infrared Laser Photodissociation of Soluble and Membrane Protein Complexes in a Modified QToF Mass Spectrometer;** Victor A. Mikhailov<sup>1</sup>; Todd Mize<sup>1</sup>; Matt Bush<sup>2</sup>; Carol Robinson<sup>1</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*University of Washington, Seattle, US*
- WP 413 **Improved Structural Characterization of Stable Non-Covalent Protein Complexes by Surface Induced Dissociation (SID);** Xin Ma; *The Ohio State University, Columbus, OH*
- WP 414 **Probing Protein-Ligand Interactions Involved in Neurodegenerative Disease Using Native Electrospray Ionization Top-Down Mass Spectrometry;** Priya Wongkongkathep; Sheng Yin; Becky Chan; Madhuri Chattopadhyay; Joan Valentine; Gal Bitan; Joseph Loo; *UCLA, Los Angeles, CA*
- WP 415 **Structural Characterization of Protein Complexes by Electron Capture Dissociation and Top-Down Native Mass Spectrometry;** Jiang Zhang; G. Reza Malmirchegini; Robert Clubb; Joseph Loo; *Univ. California, Los Angeles, CA*
- WP 416 **Fourier Transform Ion Cyclotron Resonance Mass Spectrometry of Protein Complexes;** Paul Spier<sup>1</sup>; Lindsay Morrison<sup>2</sup>; Jeremy Wolff<sup>1</sup>; Christopher Thompson<sup>1</sup>; Vicki Wysocki<sup>2</sup>; <sup>1</sup>*Bruker Daltonics, Billerica, MA*; <sup>2</sup>*Ohio State University, Columbus, OH*
- WP 417 **Native Salt-Bridge Structure of Proteins by ETD followed by CID;** Zhe Zhang; Shaynah Browne; Vachet Richard; *University of Massachusetts, Amherst, MA*
- WP 418 **Direct Coupling of Ion Exchange Chromatography and Native Electrospray Mass Spectrometry for Routine Analysis of Biological Complexes at Endogenous Levels;** Zachary Quinkert; Paul D. B. Olinares; Júlio C. Padovan; Brian T. Chait; *The Rockefeller University, New York, NY*



- WP 419 **Molecular Weight Analysis of Macromolecular Complexes by LiquiScan-ES**; [Elisbeth Loecken](#); Sherrie Elzey; *TSI, Inc., Shoreview, MN*
- WP 420 **Native Mass Spectrometry and Global H/D Exchange of Whole Proteins and Noncovalent Protein Complexes by Surface Acoustic Wave Nebulization**; [Lucas Monkkonen](#); J. Scott Edgar; Scott Heron; Eri Nakatani; Carlos E. Catalano; David R. Goodlett; *University of Washington, Seattle, WA*
- WP 421 **Role of Histidine Rich Epitopes in the Formation of Non-Covalent Complexes**; [Aurelie Roux](#); Ludovic M. Muller; Luciana Tovo Rodrigues; Amina S. Woods; *NIH/NIDA IRP, Baltimore, MD*
- Antibody & Antibody Drug Conjugates, 422 – 446**
- WP 422 **Native Orbitrap Mass Spectrometry Yields Higher Resolution and Potential for Relative Quantitation of Complex Antibody Mixtures**; [Natalie Thompson](#)<sup>1</sup>; Sara Rosati<sup>1</sup>; Linda J.A. Hendriks<sup>2</sup>; John de Kruijff<sup>2</sup>; Mark Throsby<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*Merus, Utrecht, Netherlands*
- WP 423 **Using MALDI-TOF MS to Screen for Monoclonal Gammopathies in Serum and Urine**; David Barnidge<sup>1</sup>; Tim Griffin<sup>2</sup>; Tom Krick<sup>2</sup>; [David Murray](#)<sup>1</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*; <sup>2</sup>*University of Minnesota, St. Paul, MN*
- WP 424 **Investigating Structure/ Function Relationships of Immunoglobulin Molecules Using Shape Selective Mass Spectrometry**; [Matthew Edgeworth](#); James Scrivens; *University of Warwick, Coventry, UK*
- WP 425 **Rapid Disulfide Bond Analysis of a Recombinant Monoclonal IgG Using Electron Transfer Dissociation**; [Daniel Clark](#); Eden Go; Heather Desaire; *University of Kansas, Lawrence, KS*
- WP 426 **Development of a Peptide Affinity Column for anti-TNF- $\alpha$  Monoclonal Antibodies**; [Noritaka Hashii](#); Ryosuke Kuribayashi; Akira Harazono; Shiori Nakazawa; Nana Kawasaki; *National Institute of Health Sciences, Tokyo, Japan*
- WP 427 **Improved Characterization of the Serum Antibody Response through Selective Enrichment and 193 nm Photodissociation of IgG Heavy Chain CDR3 Peptides**; [Victoria Cotham](#); Yariv Wine; George Georgiou; Jennifer Brodbelt; *University of Texas, Austin, TX*
- WP 428 **Simultaneous Peptide Mapping, Posttranslational Modifications and Major N-glycosylation Characterization of Trastuzumab by Sheathless CE-ESI-MS/MS - Comparison to nanoLC-MS/MS**; Rabah Gahoual<sup>1</sup>; Alicia Burr<sup>1</sup>; Jean-Marc Busnel<sup>2</sup>; Lauriane Kuhn<sup>3</sup>; Philippe Hamman<sup>3</sup>; Alain Beck<sup>4</sup>; [Yannis Francois](#)<sup>1</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>*LSMIS, University of Strasbourg, Strasbourg, France*; <sup>2</sup>*Beckman Coulter Inc., Brea, CA*; <sup>3</sup>*BMC, University of Strasbourg, Strasbourg, France*; <sup>4</sup>*Centre d'immunologie Pierre Fabre, Saint-Julien-en-Genevois, France*
- WP 429 **CE-UV/MALDI-MS: A New Platform for Proteomic and Intact Protein Characterization**; Michael Biacchi<sup>1</sup>; Anja Resemann<sup>2</sup>; Pierre-Olivier Schmit<sup>3</sup>; Alain Beck<sup>4</sup>; Yannis Francois<sup>1</sup>; [Emmanuelle Leize](#)<sup>1</sup>; <sup>1</sup>*LSMIS, University of Strasbourg, Strasbourg, France*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Bruker Daltonique S.A, Wissembourg, France*; <sup>4</sup>*Centre d'immunologie Pierre Fabre, Saint-Julien-en-Genevois, France*
- WP 430 **Complementary Glycan Quantitation Strategies Based on High Sensitivity NanoLC/MS**; [Mellisa Ly](#); Gregory Staples; Hongfeng Yin; Kevin Killeen; *Agilent Labs, Agilent Technologies, Santa Clara, CA*
- WP 431 **Identification of Pyroglutamate and O-linked Glycosylation on Anti-IL17A Peptide Anti-IL22 Antibody Bispecific Genetic Fusion**; [Eric Sousa](#)<sup>1</sup>; Xiaotian Zhong<sup>1</sup>; Elizabeth Kieras<sup>1</sup>; Aaron D'Antona<sup>1</sup>; J. Christian Baber<sup>1</sup>; Joel Desharnais<sup>2</sup>; Lauren Wood<sup>2</sup>; Deborah Luxenberg<sup>1</sup>; Mark Stahl<sup>1</sup>; Ronald Kriz<sup>1</sup>; Laura Lin<sup>1</sup>; Will Somers<sup>1</sup>; Lori Fitz<sup>1</sup>; Jill Wright<sup>1</sup>; Tao He<sup>1</sup>; <sup>1</sup>*Pfizer, Cambridge, MA*; <sup>2</sup>*CovX, San Diego, CA*
- WP 432 **Characterization of Hydrophobic Interaction Chromatography (HIC) Fractionated Antibody Bioconjugates**; [Michael Bacica](#); Ryan Preston; Robert Murphy; *Pfizer/CovX, San Diego, CA*
- WP 433 **Quantitative Profiling of NHS Drug Conjugation Sites on IgG1 Based Antibody Drug Conjugates using Data Independent Analysis**; [Dan Rock](#)<sup>1</sup>; Kelli Jonakin<sup>2</sup>; Eric Johansen<sup>2</sup>; <sup>1</sup>*Amgen Inc, Seattle, WA*; <sup>2</sup>*ABSCIEX, Foster City, CA*
- WP 434 **Optimizing the Enzymatic Subunit Generation with IdeS for High Throughput Structure Verification of Therapeutic Antibodies by Middle-Down Mass Spectrometry**; Fredrik Olsson<sup>1</sup>; Linda Andersson<sup>1</sup>; [Matthew Willetts](#)<sup>2</sup>; Wolfgang Jabs<sup>3</sup>; Anja Resemann<sup>3</sup>; Waltraud Evers<sup>3</sup>; Carsten Baessmann<sup>3</sup>; Detlev Suckau<sup>3</sup>; <sup>1</sup>*Genovis AB, Lund, Sweden*; <sup>2</sup>*Bruker Daltonics Inc, Billerica, MA*; <sup>3</sup>*Bruker Daltonik GmbH, Bremen, Germany*
- WP 435 **Combination of Online Fractionation and ETD-UHR QTOF to Enhance Middle-Down Monoclonal Antibodies Characterization**; [Guillaume Tremintin](#)<sup>1</sup>; Wolfgang Jabs<sup>2</sup>; <sup>1</sup>*Bruker Daltonics, Fremont, CA*; <sup>2</sup>*Bruker Daltonik, Bremen, Germany*
- WP 436 **Rapid Analysis of Intact Antibody-drug Conjugates(ADCs) by UPLC Q-TOF MS**; [Wei Jia](#)<sup>1</sup>; ChuanFei Yu<sup>2</sup>; Kai Gao<sup>2</sup>; <sup>1</sup>*Waters Shanghai, Beijing, China*; <sup>2</sup>*China National institutes for food and drug control, Beijing, China*
- WP 437 **Paired Acquisition of Spectra for Monoclonal Antibody Sequencing**; Natalie Castellana; *Digital Proteomics, LLC., San Diego, CA*
- WP 438 **Analytical Solutions for Pharmacokinetic Analysis of Antibody Drug Conjugates**; [Kan Zhu](#); Roxana Garcia Caro; Karen Wang; *Novartis, Cambridge, MA*
- WP 439 **Advanced LC-MS Methods for Characterization and Heterodimer Purity Assessment of Bispecific Antibodies**; [Jeremy Woods](#)<sup>1</sup>; Thomas Spreter von Kreudenstein<sup>2</sup>; Gordon Ng<sup>2</sup>; Surjit B. Dixit<sup>2</sup>; Hongwei Xie<sup>1</sup>; <sup>1</sup>*KBI Biopharm, Durham, North Carolina*; <sup>2</sup>*Zymeworks, Inc., Vancouver, BC, Canada*
- WP 440 **FC antibody Fragments Analysis Using MALDI ISD**; [Sega Ndiaye](#)<sup>1,2</sup>; Angélique Boedec<sup>1</sup>; François Gray<sup>2</sup>; Florence Lhospice<sup>1</sup>; Claude Villard<sup>2</sup>; Rima Ait-Belkacem<sup>2</sup>; Christian Belmont<sup>1</sup>; Daniel Lafitte<sup>2</sup>; <sup>1</sup>*Innate Pharma, Marseille, Fr*; <sup>2</sup>*Aix-Marseille Université, Marseille, France*
- WP 441 **Direct Coupling of Protein-A HPLC with Mass Spectrometry: A Useful Approach to Analyze Monoclonal IgG Antibody-Maytansinoid Conjugates from Complex Matrices**; [Megan Ellis](#); Lintao Wang; Alexandru C. Lazar; *ImmunoGen, Inc., Waltham, MA*
- WP 442 **Intact Mass Analysis of Monoclonal Antibody (MAb) Charge Variants Separated Using Linear pH Gradient**; [Shanhua Lin](#); Zhiqi Hao; Wim Decrop; Julia Baek; Udayanath Aich; Patrick Bennett; Srinivasa Rao; Yury Agroskin; Chris Pohl; *Thermo Fisher Scientific, Sunnyvale, CA*
- WP 443 **Rapid Peptide Mapping via Automated Integration of On-line Digestion, Separation and Mass Spectrometry for the Analysis of Therapeutic Proteins**; [Esther Lewis](#); Zhiqi Hao; Patrick Bennett; *Thermo Fisher Scientific, San Jose, CA*



- WP 444 **Characterization of Monoclonal Antibody Glycoforms Using a Novel Glycan Column Technology and Bench-Top Orbitrap LC-MS/MS;** Zhiqi Hao<sup>1</sup>; Udayanath Aich<sup>2</sup>; Julian Saba<sup>1</sup>; Rosa Viner<sup>1</sup>; Xiaodong Liu<sup>2</sup>; Srinivasa Rao<sup>2</sup>; Chris Pohl<sup>2</sup>; Andreas Hühmer<sup>1</sup>; Patrick Bennett<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>ThermoFisher Scientific, Sunnyvale, CA
- WP 445 **Characterization of Disulfide-linked and Glycosylated Intact Monoclonal Antibodies by Ultrahigh Resolution ETD with LC-MS Topdown Approach;** Shiaw-Lin Wu<sup>1</sup>; Zhiqi Hao<sup>2</sup>; David Horn<sup>2</sup>; Andreas FR Hühmer<sup>2</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 446 **IgG1 Thioether Bond Formation *in vivo*;** Qingchun Zhang; Matthew R. Schenauer; John D. McCarter; Amgen, Thousand Oaks, CA
- Analysis of Biosimilars, 447 – 452**
- WP 447 **Applying Multiple Orthogonal Analytical Methodologies for Comprehensive Biosimilar Comparability Assessment;** Henry Shion; Vera Ivleva; Ying Qing Yu; Tom Wheat; Weibin Chen; Waters Corp., Milford, MA
- WP 448 **N-linked Glycan Profile Comparison between the Innovator and a Biosimilar Etanercept;** Ying-Qing Yu; Waters Corporation, Milford, MA
- WP 449 **Determination of O-Glycosylation Site and O-glycan Profile at the Site on Etanercept Using UPLC-MS/MS;** Jung-Keun Suh<sup>1</sup>; Hyong-Ha Kim<sup>2</sup>; <sup>1</sup>Korean German Institute of Technology, Seoul, South Korea; <sup>2</sup>Korea Research Institute of Standards and Science, Seoul, Korea
- WP 450 **Qualitative and Quantitative Characterization of Therapeutic Antibody Using High Speed and High Resolution Mass Spectrometry;** Byung-Hee Shin<sup>1</sup>; Eric Johansen<sup>2</sup>; Justin Lim<sup>3</sup>; Jason Neo<sup>3</sup>; <sup>1</sup>AB Sciex Korea Ltd, Seoul, South Korea; <sup>2</sup>AB Sciex, Foster City, CA; <sup>3</sup>AB Sciex Ltd., Singapore
- WP 451 **Utilizing a Novel Compact Mass Spectrometer (CMS) in the Real-Time Monitoring of a Continuous Solution Phase Peptide Synthesis;** Daniel Eikel<sup>1</sup>; Shahnaz Ghassemi<sup>2</sup>; Simon Prosser<sup>1</sup>; <sup>1</sup>Advion Inc., Ithaca, NY; <sup>2</sup>Synpure LLC, Charlottesville, VA
- WP 452 **Optimization of Qualitative and Quantitative Follicle Stimulating Hormone Analyses by High Performance Mass Spectrometry;** Dipankar Malakar; Annu Uppal; Faraz Rashid; Manoj Pillai; AB Sciex, India, Gurgaon, India
- Biomarkers: Discovery, 453 – 475**
- WP 453 **Utilizing Mass Spectrometry-Based Profiling System to Identify Cellular Response Proteins Induced by Silk Fibroin Surface-Modified Biomaterials;** Ming-Hui Yang<sup>1</sup>; Tze-Wen Chung<sup>1</sup>; Yu-Chang Tyan<sup>2</sup>; <sup>1</sup>National Yunlin University of Science & Technology, Yunlin, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 454 **Aptamer-Based Tool for Lung Cancer Biomarker Discovery;** Yury Glazyrin<sup>1</sup>; Olga Kolovskaya<sup>1</sup>; Galina Zamay<sup>1</sup>; Anna Zamay<sup>1</sup>; Evgeny Erkaev<sup>1</sup>; Alexey Krat<sup>2</sup>; Maxim Berezovskiy<sup>3</sup>; Yaroslav Lyutvinskiy<sup>4</sup>; Roman Zubarev<sup>4</sup>; Tatyana Zamay<sup>1</sup>; <sup>1</sup>Krasnoyarsk State Medical University, Krasnoyarsk, Russia; <sup>2</sup>Krasnoyarsk Regional Clinical Oncological Center, Krasnoyarsk, Russia; <sup>3</sup>University of Ottawa, Ottawa, Canada; <sup>4</sup>Karolinska Institutet, Stockholm, Sweden
- WP 455 **Comparison of Pancreas-Specific Proteins Using an Accurate Mass and Time Tag Approach in Hu-14 Depleted and Un-Depleted Pancreatic Juice;** Jana Rocker<sup>1</sup>; Lee Thompson<sup>2</sup>; Dean Billheimer<sup>3</sup>; Lewis Pannell<sup>1</sup>; <sup>1</sup>Mitchell Cancer Institute, Mobile, AL; <sup>2</sup>Mobile Infirmary Medical Center, Mobile, AL; <sup>3</sup>University of Arizona, Tucson, AZ
- WP 456 **Development of Methods for Information-Driven MS/MS (ID-MS/MS) for Increased Identification Rates in Bottom-Up Proteomics of Human Blood Serum;** Peter Brechlin<sup>1</sup>; Stuart Pengelley<sup>1</sup>; Pierre-Olivier Schmit<sup>2</sup>; Ow Sawyen<sup>3</sup>; Dirk Wunderlich<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonique S.A., Wissembourg, France; <sup>3</sup>Bruker Daltonics Inc, Beijing, China
- WP 457 **Detection of Cellular Response to an *in vitro* Challenge with Bacterial Gram-Negative Lipopolysaccharides (LPS) in Peripheral Blood Mononuclear Cells (PBMCs);** David A Sarracino<sup>1</sup>; Jennifer Sutton<sup>1</sup>; Maryann Vogelsang<sup>1</sup>; Bryan Krastins<sup>1</sup>; Gregory Byram<sup>1</sup>; Amol Prakash<sup>1</sup>; Gouri Vadali<sup>1</sup>; Vineet Gupta<sup>2</sup>; Mary F Lopez<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Cambridge, MA; <sup>2</sup>Rush University Medical Center, Chicago, IL
- WP 458 **Proteomics Analysis of Leishmania exosomes;** Brajesh Singh; Jason Weirather; Patrick Kelly; Yalan Li; R. Marshall Pope; Mary Wilson; University of Iowa, Iowa City, IA
- WP 459 **Quantitative and Facile Analysis of the ATP-binding Proteome of *Mycobacterium tuberculosis*: Disease State Biomarkers and Novel Therapeutic Targets;** Lisa Wolfe<sup>1,2</sup>; Jessica Prenni<sup>2</sup>; Karen Dobos<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Proteomics and Metabolomics Facility, Fort Collins, CO
- WP 460 **LC-MS Based Detection and Quantification of N-glycans in Human Serum Samples;** Tsung-Heng Tsai<sup>1</sup>; Minkun Wang<sup>1</sup>; Cristina Di Poto<sup>1</sup>; Yi Zhao<sup>1</sup>; Yunli Hu<sup>2</sup>; Shiyue Zhou<sup>2</sup>; Yehia Mechref<sup>2</sup>; Habtom Ressom<sup>1</sup>; <sup>1</sup>Georgetown University, Washington, DC; <sup>2</sup>Texas Tech University, Lubbock, TX
- WP 461 **Quantification of the Airway Mucin-Interactome in the Beta ENaC-transgenic Mouse Using Mass Spectrometry;** Rui Cao; Alessandra Livraghi-Butrico; Tiffany Wang; Wanda O'Neal; Mehmet Kesimer; University of North Carolina, Chapel Hill, NC
- WP 462 **Comparative Analysis of the Proteomic Changes of Amniotic Fluid in Different Gestational Age for Lung Development;** Jingxin Wang<sup>1</sup>; Shigetoshi Yokoyama<sup>2</sup>; Robert Cunningham<sup>3</sup>; Xin Sun<sup>2</sup>; Lingjun Li<sup>3</sup>; <sup>1</sup>Neuroscience Training Program, UW, Madison, WI; <sup>2</sup>Laboratory of Genetics, UW, Madison, WI; <sup>3</sup>School of Pharmacy, UW, Madison, WI
- WP 463 **Probing Phosphatidylcholine Metabolites and Diagnostic Biomarkers for Early Stage Lung Cancer Using nanoMate-FTICR MS;** Yumei Guo; Zhili Li; IBMS, CAMS&PUMC, Beijing, China
- WP 464 **Quantitative Proteomics in Non-Case versus Control Studies;** Lauren Devine<sup>1</sup>; Ingo Ruczinski<sup>2</sup>; Keith West<sup>2</sup>; Kerry Schulze<sup>2</sup>; Robert Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins Mass Spec and Proteomics Facility, Baltimore, MD; <sup>2</sup>Johns Hopkins School of Public Health, Baltimore, MD
- WP 465 **An Adductomic Approach to Measure and identify Hemoglobin Adducts of Possible Genotoxic Compounds Using LC-MS;** Henrik Carlsson; Hans von Stedingk; Ulrika Nilsson; Margareta Törnqvist; Stockholm University, Stockholm, Sweden
- WP 466 **Altered Expression of Sialylated Glycoproteins in Ovarian Cancer Using a Lectin Array and LC-MS/MS;** Jing Wu<sup>1</sup>; Xiaolei Xie<sup>2</sup>; Song Nie<sup>1</sup>; Ronald Buckanovich<sup>1</sup>; David Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Caprion Proteomics US LLC, Menlo Park, CA
- WP 467 **Potential Lipid Biomarker Identification in Hepatocellular Carcinoma;** Guangxiang Wu<sup>1</sup>; Yiyun (Sherry) Wang<sup>2</sup>; Nicholas J. Skill<sup>3</sup>; Mary A. Maluccio<sup>3</sup>; Patrick L. Love<sup>2</sup>; <sup>1</sup>Biomarker Center of Excellence, Covance, Greenfield, IN; <sup>2</sup>In Vivo Pharmacology-Receptor Occupancy, Covance, Greenfield, IN; <sup>3</sup>Indiana University School of Medicine, Indianapolis, IN

- WP 468 **Discovery of Glyco-Biomarkers of Complications in Diabetes;** Di Wu<sup>1</sup>; Helen Colhoun<sup>2</sup>; Michael Ferguson<sup>1</sup>; <sup>1</sup>College of Life Sciences, University of Dundee, Dundee, UK; <sup>2</sup>Medical Research Institute, University of Dundee, Dundee, UK
- WP 469 **Mass-Spectrometry Based Analysis of Human Blood Sera Peptidome for a Search of Socially Significant Disease Biomarkers;** Georgy Arapidi<sup>1,2</sup>; Rustam Ziganshin<sup>1</sup>; Sergey Kovalchuk<sup>1</sup>; Igor Azarkin<sup>1</sup>; Olga Ivanova<sup>1</sup>; Nikolay Anikanov<sup>1</sup>; Dmitry Kamaev<sup>1</sup>; Vadim Govorun<sup>1</sup>; Vadim Ivanov<sup>1</sup>; <sup>1</sup>Institute of Bioorganic Chemistry, RAS, Moscow, Russian Federation; <sup>2</sup>Moscow Institute of Physics and Technology, Moscow, Russian Federation
- WP 470 **A Novel Quantification Model for Discovering Glycopeptide Biomarkers;** Anoop Mayampurath<sup>1</sup>; Ehwang Song<sup>2</sup>; Chuan-yih Yu<sup>1</sup>; Yehia Mechref<sup>2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Texas Tech University, Lubbock, TX
- WP 471 **Biomarker Discovery for Radiation Induced Tissue Damage Via Un-Targeted Mass Spectrometry Based Metabolomics;** Jace W. Jones; Alexander Bennett; Ann M. Farese; Thomas J. MacVittie; Maureen A. Kane; *University of Maryland, Baltimore, MD*
- WP 472 **Metformin Decreases Glyco-Oxidation Markers: A Study Utilizing Multiple Reaction Monitoring;** Owen Kinsky<sup>1,6</sup>; Michael Kimzey<sup>1,6</sup>; Serena Allred<sup>2,6</sup>; Tarun Anumol<sup>3,6</sup>; Hussein Yassine<sup>4,6</sup>; Craig Stump<sup>4,6</sup>; George Tsapralis<sup>1,6</sup>; Shane Snyder<sup>3,6</sup>; Dean Billheimer<sup>5,6</sup>; Terrence Monks<sup>1,6</sup>; Serrine Lau<sup>1,6</sup>; <sup>1</sup>SEWHSC, Dept. of Pharm/Tox, College of Pharmacy, Tucson, AZ; <sup>2</sup>Division of Epidemiology and Biostatistics, Tucson, AZ; <sup>3</sup>Dept. of Chemical & Environmental Engineering, Tucson, AZ; <sup>4</sup>College of Medicine, Tucson, AZ; <sup>5</sup>AZ Stat. Cons. Lab, Dept. of Ag. and Biosys. Eng., Tucson, AZ; <sup>6</sup>University of Arizona, Tucson, AZ
- WP 473 **MALDI TOF/TOF Determination of Serum Plasminogen Sialylation Profile from Patients with Gastric Precancerous Lesions;** Catarina Gomes<sup>1</sup>; Andreia Almeida<sup>2</sup>; Alexandre Ferreira<sup>2</sup>; Celso Reis<sup>1,3</sup>; Hugo Osorio<sup>1,3</sup>; <sup>1</sup>IPATIMUP, Porto, Portugal; <sup>2</sup>Department of Chemistry, University of Aveiro, Aveiro, Portugal; <sup>3</sup>Faculty of Medicine, University of Porto, Porto, Portugal
- WP 474 **Integrating Targeted Strategies for Characterization and Quantification Using Orbitrap Technology and Novel Software for Targeted Glycoprotein/Peptide Studies;** Sucharita Dutta<sup>1</sup>; Julian Saba<sup>2</sup>; Scott Peterman<sup>2</sup>; Sergei Snovidia<sup>2</sup>; Lifang Yang<sup>1</sup>; Julius Nyalwidhe<sup>1</sup>; Oliver Semmes<sup>1</sup>; <sup>1</sup>Leroy T. Canoles Cancer Center - EVMS, Norfolk, VA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific -Rockford, Rockford, IL
- WP 475 **Biomarker Screening for Drug-Induced Nephrotoxicity in Rats Using UPLC-MS<sup>E</sup>;** Liuxi Chen<sup>1</sup>; Brad Williams<sup>2</sup>; Jonathan Phillips<sup>1</sup>; Scott Geromanos<sup>2</sup>; Vladimir Papov<sup>1</sup>; <sup>1</sup>Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT; <sup>2</sup>Waters Corporation, Milford, MA
- Biomarker Quantitation: New Methods, 476 – 489**
- WP 476 **Application of DiLeu Isobaric Tandem-Mass Tags to Quantitative Proteomic Analyses of Cerebrospinal Fluid from Alzheimer's Disease Patients;** Dustin Frost; Jingxin Wang; Robert Cunningham; Cynthia Carlsson; Lingjun Li; *University of Wisconsin, Madison, WI*
- WP 477 **Extraction and Quantitation of Biomarkers from Human Plasma in the Low Nanogram Range with a Rapid and Economical Method;** Jun Wang<sup>1</sup>; Lingjun Li<sup>2</sup>; Zong-Ping Zhang<sup>1</sup>; <sup>1</sup>PPD, Middleton, U.S.; <sup>2</sup>University of Wisconsin, Madison, WI
- WP 478 **Utilizing MFLC/MS/MS for Large Molecule Quantitative Bioanalysis;** Casey Johnson; Jennifer Zimmer; Chad Christianson; Shane Needham; *Alturas Analytics, Moscow, ID*
- WP 479 **Improved Throughput and Reproducibility for Targeted Protein Quantification Using a New High Performance Triple Quadrupole Mass Spectrometer;** Reiko Kiyonami; Mary Blackburn; Andreas Hühner; *ThermoFisher Scientific, San Jose, CA*
- WP 480 **Ultrathroughput Multiple Reaction Monitoring Mass Spectrometry for Protein Biomarker Validation in Nondepleted Serum;** Mary Joan Castillo; Adam Jay McShane; Xudong Yao; *University of Connecticut, Storrs, CT*
- WP 481 **Defining Expectations for iTRAQ Analysis of Urinary Proteins by a Common, Cost-Conscious Approach;** Yun Jiang<sup>1</sup>; Matthew Wroblewski<sup>1</sup>; Yan Zhang<sup>2</sup>; Gary Nelsestuen<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of Rochester, Rochester, NY
- WP 482 **TMTcalibrator – A Novel Method Delivering Low ng/ml Sensitivity for Targeted MS Assays in Biological Fluids;** Ian Pike<sup>1</sup>; Emma Lahert<sup>1</sup>; Claire Russell<sup>1</sup>; Christopher Löfner<sup>2</sup>; Stephan Jung<sup>2</sup>; Sasa Koncarevic<sup>2</sup>; Malcolm Ward<sup>1</sup>; <sup>1</sup>Proteome Sciences plc, London, UK; <sup>2</sup>Proteome Sciences R&D GmbH & Co. KG, Frankfurt, Germany
- WP 483 **Effective Coupling of CITP/CZE with nanoESI-MS Using Advanced Interface Technologies for High Sensitivity Sample Quantification;** Keqi Tang<sup>1</sup>; Chengcheng Wang<sup>2</sup>; Cheng S. Lee<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific NW National Laboratory, Richland, WA; <sup>2</sup>University of Maryland, College Park, MD
- WP 484 **Targeted Mass Spectrometric Approach Coupled with Long Gradient Separation Enables Highly Sensitive, Large Scale Protein Quantification in a Single Analysis;** Tujin Shi<sup>1</sup>; Thomas L. Fillmore<sup>2</sup>; Rui Zhao<sup>2</sup>; Athena A. Schepmoes<sup>1</sup>; Carrie D. Nicora<sup>1</sup>; Yuqian Gao<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Tao Liu<sup>1</sup>; Karin D. Rodland<sup>1</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; David G. Camp<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>PNNL, Richland, WA; <sup>2</sup>Environmental Molecular Sciences Laboratory, PNNL, Richland, WA
- WP 485 **Metal-tag Labeling Coupled with Multiple Reaction Monitoring-Mass Spectrometry for Absolute Quantitation of Proteins;** Yangjun Zhang; Xueying Wang; Xin Wang; Hongjun Lin; Xiaohong Qian; *Beijing Proteome Research Ctr, Beijing, China*
- WP 486 **Evaluating the Ruggedness of Nanospray on a Curtain Gas-Triple Quadrupole MS Equipped with Emitter Rinsing;** Amanda Berg; Helena Svobodova; Ben Ngo; Gary Valaskovic; *New Objective, Inc., Woburn, MA*
- WP 487 **Automation of Immunoprecipitation via Magnetic Beads on the Perkin Elmer Janus Platform for Biomarker Analyses;** Richard Wong; Baomin Xin; Timothy Olah; *Bristol-Myers Squibb, Pennington, NJ*
- WP 488 **Targeted Protein Quantification for Human Plasma Samples by MRM and MRM-HR;** Xiaomin Song<sup>1</sup>; Thiri Zaw<sup>1</sup>; Ardeshir Amirkhani<sup>1</sup>; Chris Hodgkins<sup>2</sup>; Mark Molloy<sup>1</sup>; <sup>1</sup>APAF, Macquarie University, Sydney, Australia; <sup>2</sup>ABSCIEX, Sydney, Australia
- WP 489 **A High-Throughput and Reproducible Workflow for MRM Analysis of Biological Samples;** Qin Fu<sup>1</sup> (equal contribution); Michael Kowalski<sup>2</sup> (equal contribution); Weihua Ji<sup>1</sup>; Jie Zhu<sup>1</sup>; Graham Threadgill<sup>3</sup>; Christie Hunter<sup>4</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Beckman Coulter Life Sciences, Indianapolis, IN; <sup>3</sup>Beckman Coulter, Inc., Fullerton, CA; <sup>4</sup>AB Sciex, Foster City, CA



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- WP 490 **Development of an Online Size Exclusion Chromatography-Mass Spectrometry Method for Characterization of Highly Heterogeneous Protein Samples;** Khaja Muneeruddin; Rinat Abzalimov; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- WP 491 **Online- Bioaffinity- Mass Spectrometry for “Top-Down” Structure and Affinity Determination of  $\alpha$ -Synuclein Aggregation;** Michael Przybylski<sup>1</sup>; Stefan Slamnoi<sup>1</sup>; Mihaela Stumbaum<sup>1,2</sup>; Camelia Vlad<sup>1,2</sup>; Kathrin Lindner<sup>1</sup>; Christiaan Karreman<sup>1</sup>; Marcel Leist<sup>1</sup>; Bastian Henger<sup>3</sup>; <sup>1</sup>*Universitat Konstanz, Konstanz, Germany*; <sup>2</sup>*SAW-Instruments GmbH, Bonn, Germany*; <sup>3</sup>*Boehringer Ingelheim GmbH & Co KG, ZNS Research, Biberach, Germany*
- WP 492 **Phosphorylation of the Sae2 Endonuclease Regulates Its Solubility and Activity in DNA Repair;** Qiong Fu; Chia-fang Lee; Julia Chow; Maria D. Person; Tanya T. Paull; *The University of Texas, Austin, TX*
- WP 493 **Mapping synphilin-1 Binary Interactions Using Isotopically Tagged Cross-Linking and Mass Spectrometry;** Xiaobin Xu<sup>1</sup>; Han Hu<sup>2</sup>; Anatoli B. Meriin<sup>2</sup>; Nava Zaarur<sup>2</sup>; Nancy Leymarie<sup>2</sup>; Yi Pu<sup>1</sup>; Mark E. McComb<sup>2</sup>; Michael Y. Sherman<sup>2</sup>; Catherine E. Costello<sup>1,2</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*
- WP 494 **Mapping Protein-DNA Interactions Using UV Cross-linking and Mass Spectrometry;** Fiona Flett<sup>1</sup>; David Clarke<sup>2</sup>; Pat Langridge Smith<sup>2</sup>; Logan Mackay<sup>2</sup>; Heidrun Interthal<sup>1</sup>; <sup>1</sup>*School of Biology, University of Edinburgh, Edinburgh, UK*; <sup>2</sup>*School of Chemistry, University of Edinburgh, Edinburgh, UK*
- WP 495 **Protein Structures and Protein-Protein Interactions: Identifying Links;** James Bruce; Juan Chavez; Chunxiang Zheng; Chad Weisbrod; Arti Navare; Xia Wu; Jimmy Eng; Sayaka Shibata; Shaday Michan; Richard Harkewicz; *University of Washington, Seattle, WA*
- WP 496 **A Combination of ChIP Seq and Mass Spectrometry Methods Provides Complementary Proteomic and Genomic Data;** Clive S. D'Santos<sup>1</sup>; Hisham Mohammed<sup>2</sup>; Christopher Taylor<sup>1</sup>; Aurelian Serandour<sup>2</sup>; Gordon D. Brown<sup>2</sup>; H. Raza Ali<sup>2</sup>; Kelly Holmes<sup>2</sup>; Jessica Robinson<sup>2</sup>; Amel Saadi<sup>2</sup>; John Stingl<sup>2,3</sup>; Carlos Caldas<sup>2,3</sup>; Jason S. Carroll<sup>2,3</sup>; <sup>1</sup>*Proteomic Core Facility, CRUK Cambridge Institute, Cambridge, CB20RE*; <sup>2</sup>*CRUK Cambridge Institute, Cambridge, UK*; <sup>3</sup>*Department of Oncology, University of Cambridge, Cambridge, UK*
- WP 497 **Protein Cross-Linking of Multi-Protein Complex of S100A8 and S100A9 with TLR4/MD2: Considerations Regarding Chemistry and Efficiency;** Alena Dreiling; Thomas Vogl; Johannes Roth; Simone Koenig; *University of Muenster, Muenster, Germany*
- WP 498 **Identification of Stress-Dependent Interactors of the MAP Kinase Sty1 in *Schizosaccharomyces pombe*;** Guadalupe Espadas<sup>1</sup>; Esther Paulo<sup>2</sup>; Francesco M. Mancuso<sup>1</sup>; Elena Hidalgo<sup>2</sup>; Eduard Sabidó<sup>1</sup>; <sup>1</sup>*Proteomics Unit CRG/UPF, Barcelona, Spain*; <sup>2</sup>*Universitat Pompeu Fabra, Barcelona, Spain*
- WP 499 **Topology of the Anaphase Promoting Complex/Cyclosome Studied by CBDPS (cyanurbiotindipropionylsuccinimide) Crosslinking;** Nicole Sessler<sup>1</sup>; Taka-Aki Ichu<sup>2</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*University of Victoria, Victoria, Canada*; <sup>3</sup>*Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada*
- WP 500 **Determination of Outer Dynein Arm Protein Complex Topology using Chemical Crosslinking and LC/MS/MS Analysis;** Kevin Blackburn<sup>1</sup>; Andrew Argo<sup>1</sup>; Lawrence Ostrowski<sup>2</sup>; Michael B. Goshe<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*
- WP 501 **Chaperones Identified from Affinity Purification-MS/MS Facilitate Epilepsy-Associated Mutant GABA<sub>A</sub> Receptor Folding in the Endoplasmic Reticulum;** Yajuan (Megan) Wang; Xiao-Jing Di; Mark R. Chance; Ting-Wei Mu; *Case Western Reserve University, Cleveland, OH*
- WP 502 **Fluorescence Complementation Affinity Proteomics to Study Kinase Substrate Interactions;** Lingfei Zeng; Chih-Chao Hsu; Chang-Deng Hu; Andy Tao; *Purdue University, West Lafayette, IN*
- WP 503 **Applications of the Fc-III Tagged Protein Expression System for Studying Protein Complexes;** Shan Feng; Gulishana Adeljiang; Yiyi Gong; Lixiao Gu; Haiteng Deng; *Tsinghua University, Beijing, China*
- WP 504 **Magic Lysis Buffer Improves the Efficiency of Immunoprecipitation-LC/MS/MS (IP-MS) with Less Non-Specific Interactions and Stronger Retention of Binding Protein Partners;** Susanne Breitkopf<sup>1</sup>; Min Yuan<sup>1</sup>; John Neveu<sup>3</sup>; John M Asara<sup>1,2</sup>; <sup>1</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*ESI Source Solutions, Woburn, MA*
- WP 505 **iTRAQ Stable Isotope Labeling and Multiple Immunoaffinity Matrices for Enhanced Mass Spectrometric Identification of Protein Complex Constituents;** Sricharan Bandhakavi<sup>1</sup>; Michael Early<sup>1</sup>; Jonathan Kohn<sup>1</sup>; Ebbing de Jong<sup>2</sup>; Timothy Griffin<sup>2</sup>; <sup>1</sup>*Bio-Rad Laboratories, Hercules, CA*; <sup>2</sup>*University of Minnesota, MN*
- WP 506 **ARL13B, PDE6D, and CEP164 Form a Functional Network for INPP5E Ciliary Targeting;** R. Marshall Pope; Yalan Li; Val C. Sheffield; Seongjin Seo; *University of Iowa, Iowa City, IA*
- WP 507 **Single-step Affinity Isolation and Rapid Non-Denaturing Elution of Endogenous Protein Complexes with Subsequent LC-MS Characterization;** Paul Dominic B. Olinares; Zachary T. Quinkert; Amelia D. Dunn; Julio C. Padovan; Brian T. Chait; *The Rockefeller University, New York, NY*
- WP 508 **An Improved MS Strategy for Probing Protein-Protein Interaction and Its Application in the Study of Tumor Cell Chemotaxis;** Ruibing Chen; Yanping Wang; Ning Zhang; *Tianjin Medical University, Tianjin, China*
- WP 509 **A High-Throughput, Mass-Spectrometry-Based Platform for Rapid Profiling of Human Protein Interaction Networks;** Edward L. Huttlin<sup>1</sup>; Lily Ting<sup>1</sup>; Raphael Bruckner<sup>1</sup>; Melanie Gygi<sup>1</sup>; Robert Obar<sup>1</sup>; Virginia Guarani-Pereira<sup>1</sup>; Ramin Rad<sup>1</sup>; Deepak Kolippakkam<sup>1</sup>; Bo Zhai<sup>1</sup>; Stanley Tam<sup>1</sup>; Fana Gebreab<sup>1</sup>; Myriam Boukhali<sup>1</sup>; Joao Paulo<sup>1</sup>; Timothy Harris<sup>2</sup>; Spyros Artavanis-Tsakonas<sup>1</sup>; Mathew Sowa<sup>1</sup>; J. Wade Harper<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Biogen, Cambridge, MA*
- WP 510 **Defining DNA Sensing Mechanisms during Host Innate Immunity and Viral Immunosuppression;** Benjamin Diner; Tuo Li; John Fuesler; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- WP 511 **Quantitation of Proteins in Ribosomes and Ribosome Assembly Complexes by LC-MS<sup>E</sup>;** Romel Dator; Kirk Gaston; Patrick Limbach; *University of Cincinnati, Cincinnati, OH*
- WP 512 **Evolution of the Protein Stoichiometry in the L12 Stalk of Bacterial and Organellar Ribosomes;** Ingo Wohlgemuth<sup>1</sup>; Iakov Davydov I.<sup>2</sup>; Irena I. Artamonova<sup>3</sup>;



Alexander G. Tonevitsky<sup>4</sup>; Marina V. Rodnina<sup>1</sup>; Henning Urlaub<sup>1,5</sup>; <sup>1</sup>MPI for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>SRC Bioclinicum, Moscow, Russia; <sup>3</sup>Russian Academy of Science, Moscow, Russia; <sup>4</sup>Lomonosov Moscow State University, Moscow, Russia; <sup>5</sup>University Medical Center Göttingen, Göttingen, Germany

- WP 513 **Mass Spectrometric Binding Study on Novel Anticancer Agents as Tubulin Depolymerizer;** Sool Yeon Cho<sup>1</sup>; Benjamin S. Hoffman<sup>2</sup>; Amol Padgaonkar<sup>1</sup>; Stephen C. Cosenza<sup>1</sup>; Venkat Palella<sup>3</sup>; Muralidhar R. Mallireddigari<sup>3</sup>; D.R.C. Venkata Subbaiah<sup>1</sup>; Revathi Patti<sup>3</sup>; M. V. Ramana Reddy<sup>1</sup>; E. Premkumar Reddy<sup>1</sup>; John Roboz<sup>1</sup>; <sup>1</sup>Chan School of Medicine at Mount Sinai, New York, NY; <sup>2</sup>The Fels Cancer Institute, Temple University, Philadelphia, PA; <sup>3</sup>Onconova Therapeutics, Inc., Newtown, PA
- WP 514 **Role of Lysine Residues in the Interaction of Blood Coagulation Factor VIII with Its Clearance Receptor Low-Density Lipoprotein Receptor-Related Protein;** Maartje Van Den Biggelaar<sup>1</sup>; Johan H Faber<sup>2</sup>; Marleen Zuurveld<sup>1</sup>; Carmen van der Zwaan<sup>1</sup>; Jesper J Madsen<sup>2</sup>; Ole H Olsen<sup>2</sup>; Henning R Stennicke<sup>2</sup>; Koen Mertens<sup>1</sup>; Alexander B. Meijer<sup>1</sup>; <sup>1</sup>Sanquin Research, Amsterdam, Netherlands; <sup>2</sup>Novo Nordisk, Copenhagen, Denmark

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- WP 515 **A Suitability Study of Commonly-Used Isolation Techniques for Microtubule Associated Protein Tau by LC-MS;** Robert Pelot<sup>1,2</sup>; Jon Reed<sup>1</sup>; Gogce Crynen<sup>1</sup>; Corbin Bachmeier<sup>1</sup>; James Evans<sup>1</sup>; Laila Abdullah<sup>1</sup>; Fiona Crawford<sup>1</sup>; <sup>1</sup>Roskamp Institute, Bradenton, FL; <sup>2</sup>The Open University, Milton Keynes, UK
- WP 516 **Oxidative Post-Translational Modifications of Amyloidogenic Light Chain Proteins from a Patient with Amyloid Light Chain Amyloidosis;** Yanyan Lu; Yan Jiang; Tatiana Prokaeva; Yang Mao; Lawreen Connors; Catherine Costello; Boston University, Boston, MA
- WP 517 **Analysis of PTM Crosstalk in Photosynthetic Model Organisms Using a 2D Gel-Based Approach;** Silas Rodrigues; Leslie Hicks; Donald Danforth Plant Science Center, Saint Louis, MO
- WP 518 **Analysis of Protein Isoform in HEK293T Using New N-terminome Strategy;** Jeonghun Yeom<sup>1,2</sup>; Cheolju Lee<sup>1,2</sup>; <sup>1</sup>Korea institute science and technology, Seoul, Korea; <sup>2</sup>University of Science and Technology, Daejeon, Korea
- WP 519 **a-N-methylation of DDB2 and Its Function in Nucleotide Excision Repair;** Qian Cai; Yinsheng Wang; University of California, Riverside, CA
- WP 520 **Identification of indole-3-acetic Acid Modified Proteins of Arabidopsis;** Peng Yu<sup>1</sup>; Jutta Ludwig-Müller<sup>2</sup>; Adrian Hegeman<sup>1</sup>; Jerry Cohen<sup>1</sup>; <sup>1</sup>University of Minnesota, Falcon Heights, MN; <sup>2</sup>TU-Dresden, Dresden, Germany
- WP 521 **Characterization of Triose Phosphate Isomerase in Drosophila Presenilin Mutant;** Jong Bok Seo<sup>1</sup>; Soo Young Kim<sup>1</sup>; Young Ho Koh<sup>2</sup>; <sup>1</sup>Korea Basic Science Institute, Seoul, South Korea; <sup>2</sup>Hallym University, Anyang, Republic of Korea
- WP 522 **Probing the Transmural Molecular Heterogeneity of the Heart Using High-Resolution Top-Down Mass Spectrometry;** Zachery Gregorich; Wei Guo; Timothy Hacker; Ying Ge; UW, Madison, WI
- WP 523 **Qualitative Examination of the Diversity of Protein Post-Translational Modifications Present in Model Prokaryotic and Eukaryotic Organisms;** Ritin Sharma<sup>2</sup>; Rachel Adams<sup>2</sup>; Paul Abraham<sup>2</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN
- WP 524 **Characterization of Extensive Post-translational Modification of Endogenous Human p53;** Caroline DeHart<sup>1</sup>; Jasdave S. Chahal<sup>2</sup>; S. J. Flint<sup>1</sup>; David H. Perlman<sup>3</sup>; <sup>1</sup>Dept. of Molecular Biology, Princeton University, Princeton, NJ; <sup>2</sup>Whitehead Institute for Biomedical Research, MIT, Cambridge, MA; <sup>3</sup>Proteomics and Mass Spec. Core, Princeton Univ., Princeton, NJ
- WP 525 **Discovering the Role of Post-translational Modifications in Regulation of Protein Activities in Diabetes using an in vivo SILAC approach;** Soraya Hoelper; Hendrik Nolte; Thomas Braun; Marcus Krüger; Max-Planck-Institute for Heart and Lung Research, Bad Nauheim, Germany
- WP 526 **Comparative Analysis of RNA Polymerase II Reveals Potential Evolutionary Conserved Posttranslational Modified Sites Amongst Schizosaccharomyces pombe and Saccharomyces cerevisiae;** Selene Swanson<sup>1</sup>; Charles Banks<sup>1</sup>; Zhihui Wen<sup>1</sup>; Brad Groppe<sup>1</sup>; Laurence Florens<sup>1</sup>; Michael Washburn<sup>1,2</sup>; <sup>1</sup>Stowers Institute for medical research, Kansas City, mo; <sup>2</sup>University of Kansas Medical Center, Kansas City, KS
- WP 527 **Deep Characterization of Combinatorial Post-Translational Modifications in a Natural Microbial Community;** Zhou Li<sup>1,2</sup>; Yingfeng Wang<sup>2</sup>; Nicholas Justice<sup>3</sup>; Tae-Hyuk Ahn<sup>2</sup>; Robert Hettich<sup>1,2</sup>; Jillian Banfield<sup>3</sup>; Chongle Pan<sup>1,2</sup>; <sup>1</sup>University of Tennessee, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>University of California, Berkeley, CA
- WP 528 **Calorie Restriction and SIRT3 Trigger Global Reprogramming of the Mitochondrial Protein Acetylome;** Kristin Dittenhafer-Reed<sup>1</sup>; Alex Hebert<sup>1</sup>; Wei Yu<sup>1</sup>; Derek Bailey<sup>2</sup>; Ebru Selin Selen<sup>3</sup>; Joshua Carson<sup>3</sup>; Melissa Boersma<sup>1</sup>; Michael Westphall<sup>5</sup>; David Pagliarini<sup>3</sup>; Tomas Prolla<sup>7</sup>; Fariba Assadi-Porter<sup>3,6</sup>; Sushmita Roy<sup>4</sup>; Joshua Coon<sup>1,5</sup>; John Denu<sup>1</sup>; <sup>1</sup>Department of Biomolecular Chemistry, Madison, WI; <sup>2</sup>Department of Chemistry, Madison, WI; <sup>3</sup>Department of Biochemistry, Madison, WI; <sup>4</sup>Dept of Biostatistics and Medical Informatics, Madison, WI; <sup>5</sup>Genome Center of Wisconsin, Madison, WI; <sup>6</sup>National Magnetic Resonance Facility at Madison, Madison, WI; <sup>7</sup>Department of Genetics and Medical Genetics, Madison, WI
- WP 529 **Radical Acetylation: Possible Routes of Epigenetic Modifications of Proteins;** Atecla Nunciata Lopes Alves<sup>1</sup>; Sheila Barreto Guterres<sup>1</sup>; Emanuel Carrilho<sup>2</sup>; Maria Aparecida Juliano<sup>1</sup>; Etelvino Jose Henriques Bechara<sup>1</sup>; Nilson Antonio Assunção<sup>1</sup>; <sup>1</sup>Unifesp, Sao Paulo, Br; <sup>2</sup>Universidade de Sao Paulo, Sao Paulo, Br
- WP 530 **Comprehensive Profiling of Protein Lysine Acetylation in Escherichia coli;** Kai Zhang<sup>1</sup>; Shuzhen Zheng<sup>1</sup>; Jeong Soo Yang<sup>2</sup>; Yingming Zhao<sup>2</sup>; Yue Chen<sup>2</sup>; Zhongyi Cheng<sup>2</sup>; <sup>1</sup>Nankai University, Tianjin, China; <sup>2</sup>The University of Chicago, Chicago, IL
- WP 531 **Quantitative Profiling of Lysine Acetylation in Mouse Tissues by AcetylScan;** Hongbo Gu<sup>1</sup>; Matthew Stokes<sup>1</sup>; Ailan Guo<sup>1</sup>; Kimberly Lee<sup>1</sup>; Jianmin Ren<sup>1</sup>; Xiaoying Jia<sup>1</sup>; Meghan Duncan<sup>2</sup>; Vipin Suri<sup>2</sup>; Jeffrey Silva<sup>1</sup>; <sup>1</sup>Cell Signaling Technology, Danvers, MA; <sup>2</sup>Sirtris, A GSK Company, Cambridge, MA
- WP 532 **Enhanced Ionization Efficiency in ESI by Dimethylation of Amines Compared to Acetylation of Amines;** Kyungcho Cho; Jeongwon Kang; JiHye Hong; KwangPyo Kim; Konkuk university, Seoul, Korea
- WP 533 **Distinct Lysine Methylation Profiles of Outer Membrane Protein B in Virulent and Avirulent Rickettsiae Revealed by LCMS;** Guanghui Wang<sup>1</sup>; Amila Abeykoon<sup>2</sup>; Chien-Chung Chao<sup>3</sup>; Wei-Mei Ching<sup>3</sup>; David Yang<sup>2</sup>; Marjan Gucak<sup>1</sup>; <sup>1</sup>NHLBI, NIH, Bethesda, MD; <sup>2</sup>Georgetown University, Washington, DC; <sup>3</sup>Naval Medical Research Center, Silver Spring, MD

- WP 534 **A Dual-Enzyme and Dual-Activation Strategy for Comprehensive and Accurate Characterization of Protein Arginine-Methylation in Trypanosoma brucei Mitochondrion**; Jun Li; Chengjian Tu; Bo An; Jun Qu; *University at Buffalo, Buffalo, NY*
- WP 535 **Proteome-Wide Screening of Lysine Succinylation in Escherichia coli Reveals Its Broad Roles in Cellular Metabolism**; Minjia Tan<sup>1,2</sup>; Yue Chen<sup>1</sup>; Zhongyu Xie<sup>1</sup>; Zhike Lu<sup>1</sup>; Yingming Zhao<sup>1</sup>; <sup>1</sup>*University of Chicago, Chicago, IL*; <sup>2</sup>*Shanghai Institute of Materia Medica, Shanghai, China*
- WP 536 **The First Mammalian Succinylome Analysis Reveals SIRT5-mediated Lysine Desuccinylation and Its Roles in Diverse Cellular Pathways**; Yue Chen<sup>1</sup>; Chao Peng<sup>1</sup>; Minjia Tan<sup>1,2</sup>; Lunzhi Dai<sup>1</sup>; Zhongyu Xie<sup>1</sup>; Yingming Zhao<sup>1</sup>; <sup>1</sup>*University of Chicago, Chicago, IL*; <sup>2</sup>*Shanghai Institute of Materia Medica, Shanghai, China*
- WP 537 **Statistical Approaches to Infer Kinase Pathway Activation from Mass Spectrometry-Based Phosphoproteomics Data**; Pedro R. Cutillas; *Imperial College London, London, UK*
- WP 538 **In-gel Visualization and Identification of Phosphoproteomes**; Linna Wang; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
- WP 539 **Low pH Differential Thiol Labeling Agents for Studying Cellular Redox-based Regulation Using MS**; Christopher A Bonham; Aaron J Steevensz; Qiudi Geng; Panayiotis O Vacratsis; *Dept. of Chem. and Biochem., University of Windsor, Windsor, ON, Canada*
- Peptides: PTM Identifications, 540 – 574**
- WP 540 **Highly Efficient Ionization of Phosphopeptides at Low pH by Desorption Electrospray Ionization Mass Spectrometry**; Ning Pan<sup>1</sup>; Pengyuan Liu<sup>1</sup>; Weidong Cui<sup>2</sup>; Bo Tang<sup>3</sup>; Jingmin Shi<sup>3</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>*Ohio University, Athens, OH*; <sup>2</sup>*Washington University, St. Louis, MO*; <sup>3</sup>*Shandong Normal University, Jinan, China*
- WP 541 **Electron-Transfer and Higher-Energy Collision Dissociation, ETHcD, Provides for Full Peptide Sequence Coverage and Unambiguous Phosphosite Localization**; Christian Frese<sup>1</sup>; Dirk Nolting Nolting<sup>2</sup>; Jens Griep-Raming<sup>2</sup>; Henk van den Toorn<sup>1</sup>; Houjiang Zhou<sup>1</sup>; Thomas Taus<sup>3</sup>; Karl Mechtler<sup>3</sup>; Maarten Altelaar<sup>1</sup>; Albert J. R. Heck<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>3</sup>*IMP - Research Institute of Molecular Pathology, Vienna, Austria*
- WP 542 **Extending the Phosphoproteomics Toolkit**; Amanda Patrick; Nicolas Polfer; *University of Florida, Gainesville, FL*
- WP 543 **Data Independent Analysis – A New Strategy for Discovery of Phosphopeptides in Complex Proteome Samples**; Joerg Dojahn; Christian Baumann; *AB SCIEX, Darmstadt, Germany*
- WP 544 **Investigation and Characterization of Potential Dimetallic Tags for the Selective Recognition and Protection of Phosphate Ester Groups in CAD Activation**; Simon Svane; Christine J. McKenzie; Frank Kjeldsen; *University of Southern Denmark, Odense M, Denmark*
- WP 545 **Coupling Immobilized Alkaline Phosphatase-based Automated Diagonal Capillary Electrophoresis to Tandem Mass Spectrometry for Phosphopeptide Analysis**; Si Mou; Liangliang Sun; Norman Dovichi; *University of Notre Dame, Notre Dame, IN*
- WP 546 **Nucleus Phosphoproteome Reveals that EGF Regulates Alternative Splicing through mTORC1 Pathway in MDA-MB-468 Cells**; Xianwei Chen<sup>1</sup>; Dan Guo<sup>1</sup>; Xiaomin Lou<sup>1</sup>; Ju Zhang<sup>1</sup>; Jin Zi<sup>2</sup>; Jun Zhang<sup>1</sup>; Quanhui Wang<sup>1,2</sup>; Haidan Sun<sup>1</sup>; Zhaohui Wang<sup>1</sup>; Yuan Wang<sup>1</sup>; Weixin Guo<sup>1</sup>; Jiao Guo<sup>1</sup>; Feng Xian<sup>1</sup>; Jia Zhang<sup>3</sup>; Yang Li<sup>3</sup>; Yusheng Dong<sup>3</sup>; Liang Lin<sup>2</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>*Beijing Institute of Genomics, CAS, Beijing, China*; <sup>2</sup>*BGI-Shenzhen, Shenzhen, China*; <sup>3</sup>*Beijing Protein Innovation, Beijing, China*
- WP 547 **Optimization of Lectin Enrichment of Glycopeptides for Identification of Site-Specific Core-Fucosylation in Human Serum**; Zhijiang Tan; *University of Michigan, Ann Arbor, MI*
- WP 548 **Quantitative Site-Specific Glycosylation on HIV-1 Envelope Glycoprotein**; Tsung-Ping Lin; Chein-Hung Chen; Jennifer M. Lo; Che Alex Ma; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taipei, Taiwan*
- WP 549 **Automatic Glycopeptide Sequencing by Y1 Ion (AGSY)**; Chein-Hung Chen<sup>1</sup>; Hsin-Yu Hsieh<sup>1</sup>; Pang-Hung Hsu<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>*Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*National Taiwan Ocean University, Keelung, Taiwan*
- WP 550 **Identification of Prostate Specific Antigen Glycosylation in Clinical Urine Samples by Mass Spectrometry**; Chun-Jen Hsiao<sup>1,2</sup>; Chein-Hung Chen<sup>1</sup>; Hsin-Yu Hsieh<sup>1</sup>; Wen Horng Yang<sup>3</sup>; Tzong-Shin Tzai<sup>3</sup>; Chung Hsuan (Winston) Chen<sup>1,2</sup>; <sup>1</sup>*Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*National Yang-Ming University, Taipei, Taiwan*; <sup>3</sup>*National Cheng Kung University Hospital, Tainan, Taiwan*
- WP 551 **Characterization of Sialylated Glycopeptides in Caseinoglycomacropeptide by Tandem Mass Spectrometry with Electron Transfer Dissociation and High Energy Collision Dissociation**; Haiying Li; Finn Kirpekar; *University of Southern Denmark, Odense, Denmark*
- WP 552 **Modifications of Cysteine and MS Data Complexity**; Jens T Vanselow; Andreas Schlosser; *Rudolf-Virchow-Zentrum, University Wuerzburg, Wuerzburg, Germany*
- WP 553 **Improvements in the Mass Spectrometric Detection of S-Glutathionylated Peptides Using Multiple Fragmentation Approaches**; Susana Comte-Walters; Jennifer Rutherford Bethard; Lauren Ball; Joachim Uys; *Medical Univ of S Carolina, Charleston, SC*
- WP 554 **Capturing Reversibly Oxidized Cysteines in the Myocardium Using Thiol-Disulfide Exchange**; Jana Paulech; Nestor Solis; Max Puckeridge; Kiersten Liddy; Melanie White; Stuart Cordwell; *The University of Sydney, Sydney, Australia*
- WP 555 **Defining Novel Redox-Regulated Targets of Growth Factor Signaling Using Differential Alkylation, Thiopropyl Sepharose Enrichment, and Label-Free Quantitative Proteomics**; Jason Held; Tara Srinivasan; Alexandria D'Souza; Birgit Schilling; Gary Scott; Christopher Benz; Bradford Gibson; *Buck Institute for Age Research, Novato, CA*
- WP 556 **Characterization of a Post-translational Oxidative Modification in a Fetal Hemoglobin (γ-V68M→D) Associated with the Blue Baby Syndrome**; Michael Strader<sup>1</sup>; Wayne Hicks<sup>1</sup>; Ah-Lim Tsai<sup>2</sup>; Gang Wu<sup>2</sup>; John Olson<sup>3</sup>; Mitchell Weiss<sup>4</sup>; Todd Mollan<sup>1</sup>; Abdu Alayash<sup>1</sup>; <sup>1</sup>*FDA/CBER, Rockville, Md, MD*; <sup>2</sup>*University of Texas-Houston Medical School, Houston, TX*; <sup>3</sup>*Rice University, Houston, TX*; <sup>4</sup>*The Children's Hospital of Philadelphia, Philadelphia, PA*
- WP 557 **Stable Isotope Labeling with <sup>18</sup>O to Examine Oxidative Processes in Fetal Hemoglobin with a Met to Asp Conversion**; Wayne Hicks; Michael Strader; Todd Mollan; Abdu Alayash; *Food and Drug Administration, Gaithersburg, MD*

- WP 558 **Mass Spectrometry Characterization of Acrolein Protein Targets in the Liver: Focus On Site-Specific Analysis;** Yiyiing Zhu; Carthene Bazemore-Walker; *Brown University, Providence, RI*
- WP 559 **A Simple Work Flow for Identification of Acylated Proteins by LC MS/MS Using Sequentially Connected C4 and C18 Columns;** Wei Chen; Colin Gottlieb; Maurine Linder; Robert Sherwood; Hong Jiang; Hening Lin; Sheng Zhang; *Cornell University, Ithaca, NY*
- WP 560 **Mass Spectral Enhanced Detection of UbIs Using SWATH Acquisition: MEDUSA™ -Utilizing the Chemical Derivatization Dependent Generation of Isopeptide Diagnostic Ions;** Navin Chicooree<sup>1,2</sup>; John Griffiths<sup>1</sup>; Yvonne Connolly<sup>1</sup>; Thomas Knapman<sup>3</sup>; Christie Hunter<sup>4</sup>; Duncan Smith<sup>1</sup>; <sup>1</sup>*Paterson Institute for Cancer Research, Manchester, UK*; <sup>2</sup>*School of Chemistry, University of Manchester, Manchester, UK*; <sup>3</sup>*AB SCIEX, Phoenix House, Warrington, UK*; <sup>4</sup>*AB SCIEX, Foster City, CA*
- WP 561 **Identification of Ubiquitinated Synaptic Proteins and Discovery of Lys29 Poly-Ubiquitin Function Using Ubiquitin K29R Mutant Cells;** Chan-Hyun Na; Drew Jones; Yanling Yang; Xusheng Wang; Yanji Xu; Junmin Peng; *St Jude Children's Research Hospital, Memphis, TN*
- WP 562 **Large-scale Global Identification of Protein Lysine Methylation *in vivo*;** Xing-Jun Cao<sup>1</sup>; Anna M. Arnaudo<sup>1,2</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Princeton University, Princeton, NJ*
- WP 563 **Pitfalls in Identification of Lysine/Arginine Methylation by MS - Influence of Sample Preparation;** Bettina Sarg<sup>1</sup>; Shadab Allipour Birgani<sup>2</sup>; Gerald Brosch<sup>2</sup>; Klaus Faserl<sup>1</sup>; Leopold Kremser<sup>1</sup>; Herbert Lindner<sup>1</sup>; <sup>1</sup>*Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria*; <sup>2</sup>*Division of Molecular Biology, Biocenter, Innsbruck, Austria*
- WP 564 **Differentiation of Symmetric/Asymmetric Dimethylated Arginine-containing Peptides Using MALDI Tandem Mass Spectrometry;** Matthew Openshaw<sup>1</sup>; Yuzo Yamazaki<sup>2</sup>; Omar Belgacem<sup>1</sup>; Takeshi Kawamura<sup>3</sup>; <sup>1</sup>*Kratos Analytical, Manchester, UK*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*University of Tokyo, Tokyo, Japan*
- WP 565 **Identifying Citrullinated Peptides in Complex Mixtures: Comparison of Label-Free and Chemical Modification Methods;** Manolo D. Plasencia<sup>1</sup>; Henry W. Rohrs<sup>2</sup>; Michael L. Gross<sup>2</sup>; Emil R. Unanue<sup>1</sup>; <sup>1</sup>*Washington University School of Medicine, St. Louis, MO*; <sup>2</sup>*Washington University, St. Louis, MO*
- WP 566 **Direct Identification of Tyrosine Sulfation in Peptide Anions using 193 nm Ultraviolet Photodissociation;** Michelle Robinson; Jennifer Brodbelt; *University of Texas at Austin, Austin, TX*
- WP 567 **Side-Chain Losses in Electron Capture Dissociation Improves the Identification of Pt(II)-modification Sites on Peptides and Proteins;** Huilin Li; Jonathon Snelling; Mark Barrow; James Scrivens; Peter Sadler; Peter O'Connor; *University of Warwick, Coventry, UK*
- WP 568 **S- to N-palmitoyl Migration during Proteomic Sample Preparation;** Yuhuan Ji; Catherine E. Costello; Cheng Lin; *Biochem Dept, Boston University School of Medicine, Boston, MA*
- WP 569 **Sensitive Peptide Identification with Multiple Unexpected Modifications;** June Snedecor; Nuno Bandeira; *UCSD, La Jolla, CA*
- WP 570 **Posttranslational Modifications in Human Synaptic Microdomains of Human Brain Tissue Discovered Utilizing ABSciex Protein Pilot;** Guy Uechi; Matthew MacDonald; Mani Balasubramani; Robert Sweet; Nathan Yates; *University of Pittsburgh, Pittsburgh, PA*
- WP 571 **Identification of Phosphorylation Sites in Chk2 Kinase;** Henry W. Rohrs<sup>1</sup>; Ilan Geerloff-Vidavskiy<sup>2</sup>; Manolo Plasencia<sup>1</sup>; Hao Zhang<sup>1</sup>; Alan Davis<sup>1</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Anurag Agarwal<sup>1</sup>; Reid Townsend<sup>1</sup>; Helen Piwnicka-Worms<sup>1</sup>; <sup>1</sup>*Washington University, St Louis, MO*; <sup>2</sup>*FDA, St. Louis, MO*
- WP 572 **A large Synthetic Phosphopeptide Library for Mass Spectrometry Based Proteomics;** Harald Marx<sup>1</sup>; Simone Lemeer<sup>1</sup>; Jan Schliep<sup>1</sup>; Lucrece Matheron<sup>2</sup>; Shabaz Mohammed<sup>2</sup>; Juergen Cox<sup>3</sup>; Matthias Mann<sup>3</sup>; Albert Heck<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technical University Munich, Freising, Germany*; <sup>2</sup>*Utrecht University, Utrecht, NL*; <sup>3</sup>*Max-Planck Institute for Biochemistry, Munich, DE*
- WP 573 **Elucidation of Direct Substrates of Abelson Tyrosine Kinase in Cancer Cells Through Multiple Drug Treatments and Sensitive Kinase Assay Linked-Phosphoproteomics;** Justine Arrington; Liang Xue; W. Andy Tao; *Purdue University, West Lafayette, IN*
- WP 574 **Titanium Dioxide Photocatalytic Oxidation of Phosphopeptides for Simulation of *in vivo* Oxidation Reactions;** Miina Ruokolainen; Elisa Ollikainen; Tiina Sikanen; Risto Kostiaainen; Tapio Kotiaho; *University of Helsinki, Helsinki, Finland*
- Informatics: Peptide Identification/Characterization I, 575 – 596**
- WP 575 **Improved Recovery of Information from Mass Spectrometric Data When the Amount of Sample is Severely Limited;** Himanshu Grover<sup>1</sup>; Sarah Keegan<sup>1</sup>; Jonathan Giuffrida<sup>1</sup>; Siyang Li<sup>2</sup>; Vladimir Brusic<sup>3</sup>; Shashi Murthy<sup>2</sup>; Barry L. Karger<sup>2</sup>; Alexander R. Ivanov<sup>2</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>*New York University, New York, NY*; <sup>2</sup>*Northeastern University, Boston, MA*; <sup>3</sup>*Dana-Farber Cancer Institute, Boston, MA*
- WP 576 **Untargeted Peptide Identification in SWATH™-MS Using Spectral Library Search;** Jian Wang<sup>1</sup>; Monika Tuchosilka<sup>2</sup>; Brett Larsen<sup>2</sup>; Stephen Tate<sup>3</sup>; Anne-Claude Gingras<sup>2</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>*UCSD, La Jolla, CA*; <sup>2</sup>*Samuel Lunenfeld Research Institute at Mount Sinai, Toronto, Canada*; <sup>3</sup>*AB-SCIEX, Concord, Canada*
- WP 577 ***De novo* Sequencing of Toxins from Predatory Sea Snails;** Yong Kil<sup>1</sup>; Wilfred Tang<sup>1</sup>; Chris Becker<sup>1</sup>; Marshall Bern<sup>1</sup>; Julita Imperial<sup>2</sup>; Baldomera Olivera<sup>2</sup>; David Fenyo<sup>3</sup>; Beatrix Ueberheide<sup>3</sup>; <sup>1</sup>*Protein Metrics Inc., San Carlos, CA*; <sup>2</sup>*University of Utah, Salt Lake City, UT*; <sup>3</sup>*New York University, New York, NY*
- WP 578 **Comprehensive Characterization of Porcine and Bovine Trypsin Digestion;** Scott Walmsley<sup>1</sup>; Paul Rudnick<sup>2</sup>; Yuxue Liang<sup>2</sup>; Qian Dong<sup>2</sup>; Stephen Stein<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 579 **Peptide *de novo* Sequencing Result Validation;** Lian Yang<sup>1</sup>; Baozhen Shan<sup>1</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>*Bioinformatics Solutions Inc., Waterloo, Ontario*; <sup>2</sup>*University of Waterloo, Waterloo, Canada*
- WP 580 **Whole Protein *de novo* Sequencing with LC-MS/MS;** Lian Yang<sup>1</sup>; Baozhen Shan<sup>1</sup>; Mingjie Xie<sup>1</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>*Bioinformatics Solutions Inc., Waterloo, ON*; <sup>2</sup>*University of Waterloo, Waterloo, Canada*
- WP 581 **Computational Methods for Untargeted Protein Identification Using Data Independent SWATH Acquisition;** Chih-Chiang Tsou<sup>1</sup>; Monika Tucholska<sup>2</sup>; Brett Larsen<sup>2</sup>; Anne-Claude Gingras<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Samuel Lunenfeld Research Institute, Toronto, Canada*



- WP 582 **Hypothesis-driven Analysis: An Alternative Approach to Handle Data-Independent Acquisition Data of Peptides from a Novel Hybrid Orbitrap (Q-OT-qIT) Mass Spectrometer;** Ying Sonia Ting<sup>1</sup>; Jarrett D. Egerton<sup>1</sup>; Gennifer E. Merrihew<sup>1</sup>; Richard S. Johnson<sup>1</sup>; Lukas Käll<sup>2</sup>; Jesse D. Canterbury<sup>3</sup>; Reiko Kiyonami<sup>3</sup>; Michael Senko<sup>3</sup>; Vlad Zabrouskov<sup>3</sup>; Brendan MacLean<sup>1</sup>; William Stafford Noble<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Royal Institute of Technology, Solna, Sweden; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- WP 583 **Fragmentation Patterns of EThcD Spectra of Phosphopeptides and Glycopeptides;** Marshall Bern<sup>1</sup>; Yong J. Kil<sup>1</sup>; Wilfred Tang<sup>1</sup>; Chris Becker<sup>1</sup>; Christian Frese<sup>2</sup>; Maarten Altelaar<sup>2</sup>; Shabaz Mohammed<sup>2</sup>; Albert Heck<sup>2</sup>; John Syka<sup>3</sup>; Ryan Bomgardner<sup>3</sup>; Rosa Viner<sup>3</sup>; <sup>1</sup>Protein Metrics Inc., San Carlos, CA; <sup>2</sup>Utrecht University, Utrecht, Netherlands; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- WP 584 **Annotating the R. norvegicus Genome Using Mass Spectrometry;** Jennifer Teubl<sup>1</sup>; Manor Askenazi<sup>3</sup>; Meera Prasad<sup>1</sup>; Peter Lobel<sup>2</sup>; David Fenyó<sup>1</sup>; <sup>1</sup>NYU Langone Medical Ctr, NY, NY; <sup>2</sup>Rutgers University, Piscataway, NJ; <sup>3</sup>The Ionomix Initiative, Arlington, MA
- WP 585 **Identifying Proteins in Zebrafish Embryos Using Spectral Libraries Generated from Dissected Adult Organs and Tissues;** Suzanne J. van der Plas-Duivestijn<sup>1</sup>; Yassene Mohammed<sup>1</sup>; Hans Dalebout<sup>1</sup>; Annemarie H. Meijer<sup>2</sup>; Alex A. Henneman<sup>1</sup>; André M. Deelder<sup>1</sup>; Herman P. Spaik<sup>2</sup>; Magnus Palmblad<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, The Netherlands; <sup>2</sup>Leiden University, Leiden, The Netherlands
- WP 586 **Integrative Genome, Transcriptome and Proteome Analysis of Rat Livers from Two Different Genetic Backgrounds;** Teck Yew Low<sup>1</sup>; Sebastian van Heesch<sup>2</sup>; Henk van den Toorn<sup>1</sup>; Piero Giansanti<sup>1</sup>; Alba Cristobal<sup>1</sup>; Bas van Breukelen<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; Victor Guryev<sup>3</sup>; Edwin Cuppen<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>University of Utrecht, Utrecht, Netherlands; <sup>2</sup>Hubrecht Institute, Utrecht, Netherlands; <sup>3</sup>University of Groningen, Groningen, Netherlands
- WP 587 **iPRG-2013: Proteome Informatics Research Group Study: Using RNA-Seq Data to Refine Proteomic Data Analysis;** Robert Chalkley<sup>1</sup>; Nuno Bandeira<sup>2</sup>; Matthew Chambers<sup>3</sup>; John Cottrell<sup>4</sup>; Eric Deutsch<sup>5</sup>; Eugene Kapp<sup>6</sup>; Henry Lam<sup>7</sup>; Thomas Neubert<sup>8</sup>; Rui-Xiang Sun<sup>9</sup>; Olga Vitek<sup>10</sup>; Susan Weintraub<sup>11</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>University of California, San Diego, CA; <sup>3</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>4</sup>Matrix Science Ltd, London, UK; <sup>5</sup>Institute for Systems Biology, Seattle, WA; <sup>6</sup>Walter & Eliza Hall Institute of Medical Research, Melbourne, Australia; <sup>7</sup>University of Science and Technology, Hong Kong, China; <sup>8</sup>New York University School of Medicine, New York, NY; <sup>9</sup>Chinese Academy of Sciences, Beijing, China; <sup>10</sup>Purdue University, West Lafayette, IN; <sup>11</sup>University of Texas Health Science Center, San Antonio, TX
- WP 588 **Impact of Amino Acid Substitutions on Peptide Fragmentation Pattern in Tandem Mass Spectrometry;** Chao Ji; Randy Arnold; Haixu Tang; Predrag Radivojac; Indiana University, Bloomington, IN
- WP 589 **A Proteogenomic Workflow to Enhance the Annotation of Novel Microbial Genomes: Case Study of T. thermohydrosulfuricus WC1;** Tobin J. Verbeke; Vic Spicer; Richard Sparling; David Levin; Oleg V. Krokhnin; University of Manitoba, Winnipeg, Canada
- WP 590 **Using Orthogonal Techniques for Protein-Peptide Separation to Generate Comprehensive HDMSe Mass Spectral Libraries from an E. coli Model System;** Justin D. Topp<sup>3</sup>; Michael Nold<sup>5</sup>; Ezra S. Abrams<sup>2</sup>; Charles L. Farnsworth<sup>1</sup>; Scott Geromanos<sup>5</sup>; Manor Askenazi<sup>4</sup>; Jeffrey C. Silva<sup>1</sup>; <sup>1</sup>Cell Signaling Technology, Danvers, MA; <sup>2</sup>Sage Science Inc., Beverly, MA; <sup>3</sup>Gordon College, Wenham, MA; <sup>4</sup>The Ionomix Initiative, Arlington, MA; <sup>5</sup>Waters Corporation, Milford, MA
- WP 591 **Importing Data into Protein Prospector's MS-Viewer;** Peter R Baker; Alma Burlingame; Robert Chalkley; UCSF, San Francisco, CA
- WP 592 **Development of High Resolution MS/MS Library of Peptides from Protein Digestion;** Xiaoyu Yang; Pedaturs Neta; Lisa Kilpatrick; Yuri Mirokhin; Yuxue Liang; Dmitri Tchekhovskoi; Jeri Roth; Stephen Stein; NIST, Gaithersburg, MD
- WP 593 **Combining Demultiplexing and Label-free Quantification for High-resolution Data-independent Acquisition LC-MS/MS Analyses;** Aivett Bilbao<sup>1,2</sup>; Ying Zhang<sup>1</sup>; Dario Bottinelli<sup>1</sup>; Bandar Alghanem<sup>1</sup>; Frédéric Nikitin<sup>2</sup>; Jeremy Luban<sup>3</sup>; Caterina Strambio De Castillia<sup>3</sup>; Markus Mueller<sup>2</sup>; Frédérique Lisacek<sup>2</sup>; Emmanuel Varesio<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland; <sup>3</sup>University of Massachusetts, Worcester, MA
- WP 594 **Optimization of MS/MS Spectral Library Searching for High Mass Accuracy Spectra of Peptides;** Kan Zhu; Wenguang Shao; Yingwei Hu; Henry Lam; The Hong Kong University of Science and Technology, Hong Kong, China
- WP 595 **OpenSWATH: Automated, Targeted Analysis of Mass Spectrometric Data Generated by Data-Independent Acquisition;** Hannes Roest<sup>1</sup>; George Rosenberger<sup>1</sup>; Pedro Navarro<sup>1</sup>; Ludovic Gillet<sup>1</sup>; Sasa Miladinovic<sup>1,2</sup>; Olga Schubert<sup>1</sup>; Witold Wolski<sup>4</sup>; Johan Malmstroem<sup>3</sup>; Lars Malmstroem<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>Biognosys AG, Schlieren, Switzerland; <sup>3</sup>Department of Immunotechnology, Lund University, Lund, Sweden; <sup>4</sup>SyBIT project of SystemsX.ch, Zurich, Switzerland
- WP 596 **Software for Integrated and Interactive Visualization of LC-MS Data and Peptide Identification Results;** Zefeng Zhang; Bioinformatics Solutions Inc., Waterloo, Canada
- Informatics: Post-Translational Modifications, 597 – 607**
- WP 597 **Identification of Putative PTM Cross-Talk Motifs from Large-Scale Experimental Datasets;** Mao Peng; Arjen Scholten; Albert J.R. Heck; Bas van Breukelen; Utrecht University, Utrecht, Netherlands
- WP 598 **GlycoMap\_Align: An Application for Annotation of Glycoproteins through Alignment of Glycomaps;** Abhinav Mathur<sup>1</sup>; Anoop Mayampurath<sup>1</sup>; Chuan-Yih Yu<sup>1</sup>; Ehwang Song<sup>2</sup>; Yehia Mechref<sup>2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Texas Technical University, Lubbock, TX
- WP 599 **Characterization of a-N-methylation of Centromere Protein CENP-B;** Xiaoxia Dai<sup>1</sup>; Zi Wang<sup>1</sup>; Koichiro Otake<sup>2</sup>; Changjun You<sup>1</sup>; Qian Cai<sup>1</sup>; Hiroshi Masumoto<sup>2</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, CA; <sup>2</sup>Kazusa DNA Research Institute, Kisarazu, Japan
- WP 600 **Synthesis, Fragmentation and RPLC Separation of S-Palmitoyl Peptides;** Zhiyu Li; Vikas Pejaver; Randy Arnold; Suchetana Mukhopadhyay; David Clemmer; Predrag Radivojac; Indiana University - Bloomington, Bloomington, IN
- WP 601 **An Informatics Workflow for the Analysis of the Heavily N-glycosylated gp120;** Audra Hargett<sup>1</sup>; Milan Raska<sup>1,2</sup>; Stacy Hall<sup>1</sup>; Qing Wei<sup>1</sup>; Katerina Zachova<sup>2</sup>; Zhi-Qiang Huang<sup>2</sup>; Lydie Czernekova<sup>2</sup>; Zina Moldoveanu<sup>1</sup>; Jan Novak<sup>1</sup>; Amol Prakash<sup>3</sup>; Chris Becker<sup>4</sup>; Marshall Bern<sup>4</sup>; Scott Peterman<sup>3</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>Palacky University in Olomouc, Olomouc, Czech Republic; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>Protein Metrics, San Carlos, CA

- WP 602 **A Phospho-peptide Spectrum Library for Improved Targeted Assays;** Barbara Frewen<sup>1</sup>; Scott Peterman<sup>1</sup>; Bryan Krastins<sup>1</sup>; Gregory Byram<sup>1</sup>; David Sarracino<sup>1</sup>; John Sinclair<sup>2</sup>; Claus Jorgensen<sup>2</sup>; Amol Prakash<sup>1</sup>; Mary Lopez<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, BRIMS, Cambridge, MA; <sup>2</sup>The Institute of Cancer Research, London, UK
- WP 603 **Sipros/ProRata: A Software Package for Identification and Quantification of Proteins, Modifications and Stable Isotope Incorporation in Microbial Communities;** Yingfeng Wang; Tae-Hyuk Ahn; Zhou Li; Chongle Pan; Oak Ridge National Lab, Oak Ridge, TN
- WP 604 **Detecting Drug Induced Protein Adducts with Tandem Mass Spectrometry;** Markus Muller<sup>1</sup>; Paola Antinori Malaspina<sup>2,3</sup>; Adelina Acosta Martin<sup>2,3</sup>; Youssef Daali<sup>4</sup>; Denis Hochstrasser<sup>4</sup>; Pierre Lescuyer<sup>2,4</sup>; Alexandre Scherl<sup>2,3</sup>; <sup>1</sup>SIB, Geneva, Switzerland; <sup>2</sup>Biomedical Proteomics Research Group, Geneva, Switzerland; <sup>3</sup>Swiss Center of Applied Human Toxicology, Geneva, Switzerland; <sup>4</sup>Geneva University Hospitals, Geneva, Switzerland
- WP 605 **STRAP PTM: Differential Characterization by PTM Counting and Much More;** Jean L. Spencer; Vivek N. Bhatia; Stephen A. Whelan; Christian F. Heckendorf; Catherine E. Costello; Mark E. McComb; Boston University School of Medicine, Boston, MA
- WP 606 **A Robust Mechanism to Capture Protein Evidences and PTMs in UniprotKB;** Pierre-Alain Binz<sup>1</sup>; Edouard de Castro<sup>1</sup>; Nicole Redaschi<sup>1</sup>; Delphine Baratin<sup>1</sup>; Severine Duvaud<sup>1</sup>; Lydie Bougueleret<sup>1</sup>; Ioannis Xenarios<sup>1</sup>; Alan Bridge<sup>1</sup>; The UniProt Consortium<sup>1,2</sup>; <sup>1</sup>Swiss Institute of Bioinformatics, Geneva 4, Switzerland; <sup>2</sup>EBI and PIR, Hinxton and Washington, UK and DC
- WP 607 **Unbiased Phosphopeptide Analysis Using the Distributions of All Theoretically Possible Peptides;** Rovshan Sadygov; University of Texas, Galveston, TX
- Peptides: Quantitative Analysis II, 608 – 643**
- WP 608 **NeuQuant: An Open-Access Software Toolbox for Neutron Encoded (NeuCode) Quantification Technologies;** Anna E. Merrill; Alexander S. Hebert; Derek J. Bailey; Michael S. Westphall; Joshua J. Coon; University of Wisconsin, Madison, WI
- WP 609 **Direct Comparison of Metabolic Labeling by SILAC and Chemical Labeling by Stable Isotope Dimethyl Labeling in Single Runs;** Ho-Tak Lau; Hyongwon Danny Suh; Shao-En Ong; Univ of Washington, Seattle, WA
- WP 610 **Absolute Quantification of Cellular Ras Isoform Abundance Using PSAQ and Dynamic SILAC Coupled with SRM;** Craig Mageean<sup>1</sup>; John Griffiths<sup>2</sup>; Yvonne Connolly<sup>2</sup>; Michael Clague<sup>1</sup>; Duncan Smith<sup>2</sup>; Ian Prior<sup>1</sup>; <sup>1</sup>University of Liverpool, Crown Street, UK; <sup>2</sup>Paterson Institute for Cancer Research, Manchester, UK
- WP 611 **SILAC Labeling and Mass Spectral Analysis Reveals Temporal Changes in Nbn Protein Interactions and PTMs in Response to DNA Damage;** Andrea Matlock<sup>1</sup>; Philip Compton<sup>2</sup>; Dina Bai<sup>3</sup>; Jeffrey Shabanowitz<sup>3</sup>; Patrick Concannon<sup>4</sup>; Donald Hunt<sup>3</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>Northwestern, Evanston, IL; <sup>3</sup>University of Virginia, Charlottesville, VA; <sup>4</sup>University of Florida, Gainesville, FL
- WP 612 **Study on the Mechanism of Palmitate-Induced Insulin Resistance in C2C12 Myoblasts Using SILAC Based Quantitative Proteomic Analysis;** Xiulan Chen; Shasha Wei; Fuquan Yang; Institute of Biophysics, CAS, Beijing, China
- WP 613 **Incorporation Rate of Heavy Isotope-labeled Lysine in Non-Generational Metabolic Labeling in Mice;** Tasha Agreste<sup>1</sup>; Michael Ford<sup>2</sup>; Richard Jones<sup>2</sup>; Kevin Millis<sup>1</sup>; John C. Rogers<sup>3</sup>; <sup>1</sup>Cambridge Isotope Laboratories, Andover, MA; <sup>2</sup>MS Bioworks, Ann Arbor, MI; <sup>3</sup>Thermo Fisher Scientific, Rockford, IL
- WP 614 **Quantitative Dimethyl Labeling Strategy for the Investigation of the Global Effects of Aneuploidy on the Proteome;** Leigh Weston<sup>1</sup>; Kerry Bauer<sup>1</sup>; Darawalee Wangsa<sup>2</sup>; Thomas Ried<sup>2</sup>; Amanda Hummon<sup>1</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, IN; <sup>2</sup>National Institutes of Health, Bethesda, MD
- WP 615 **Cross Validation of MALDI-TOF MS Label Free Profiling and LC/MS Based Stable Isotopic Labeling Strategies for Peptide Quantitation;** Sarah Dowd; Elena Romanova; Jonathan Sweedler; University of Illinois at Urbana-Champaign, Urbana, IL
- WP 616 **Development of Novel 8-plex N,N-dimethylated Leucine (DiLeu) Isobaric Labels for Quantitative Proteomics and Peptidomics;** Tyler Greer; Dustin Frost; Feng Xiang; Zhidan Liang; Lingjun Li; University of Wisconsin, Madison, WI
- WP 617 **Improving High Throughput in Relative Protein Quantitation from 6 to 10 Plex;** Rosa Viner<sup>1</sup>; Ryan Bomgarden<sup>2</sup>; Michael Blank<sup>1</sup>; John Rogers<sup>2</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Rockford, IL
- WP 618 **Assessing Non-Mitotic Pathways of an Aurora Kinase Inhibitor Using Chemical Labelling and Label-Free MS Approaches;** Matthew McKay; Judith Nicholson; Mark Molloy; APAF, Macquarie University, Sydney, Australia
- WP 619 **Application of Microbore Hollow Fiber Enzymatic Reactor (mHFER)-based <sup>18</sup>O-labeling Approach to Quantitative Proteomics;** Sun Young Lee; So-Young Kim; Dukjin Kang; Korea Research Institute of Standards and Science, Daejeon, South Korea
- WP 620 **ABRF-sPRG 2013 Study: Development and Characterization of a Stable Isotope Labeled Peptide Standard for Quantitative Proteomics Applications;** Christopher Colangelo<sup>1</sup>; Craig Dufresne<sup>2</sup>; Alexander Ivanov<sup>3</sup>; Antonius Koller<sup>4</sup>; Brett Phinney<sup>5</sup>; Kristie Rose<sup>6</sup>; Paul Rudnick<sup>7</sup>; Brian Searle<sup>8</sup>; Scott Shaffer<sup>9</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Thermo Fisher Scientific, West Palm Beach, FL; <sup>3</sup>Northeastern University, Boston, MA; <sup>4</sup>Stony Brook University, Stony Brook, NY; <sup>5</sup>University of California, Davis, CA; <sup>6</sup>Vanderbilt University, Nashville, TN; <sup>7</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>8</sup>Proteome Software, Portland, OR; <sup>9</sup>University of Massachusetts Medical School, Worcester, MA
- WP 621 **Trimethylation Enhancement using Diazomethane (TrEnDi): Rapid On-Column Methylation of Peptides and Proteins to Permit Quantitative Analysis Using Tandem Mass Spectrometry;** Karl Wasslen; Stephen Wood; Jeffrey Manthorpe; Jeffrey C. Smith; Carleton University, Department of Chemistry, Ottawa, Canada
- WP 622 **Intestinal Proteome Study in Insulin-Resistant Patients by a Combination of iTRAQ, MRM and SWATH;** Sylvie Bourassa<sup>1</sup>; Isabelle Kelly<sup>1</sup>; Benjamin Nehmé<sup>1</sup>; Frédéric Fournier<sup>1</sup>; André J. Tremblay<sup>2</sup>; Benoit Lamarche<sup>2</sup>; Patrick Couture<sup>2</sup>; Arnaud Droit<sup>1,3</sup>; <sup>1</sup>CHU de Quebec Research Center, Laval University, Quebec, Canada; <sup>2</sup>INAF, Laval University, Quebec, Canada; <sup>3</sup>Department of Molecular Medicine, Laval University, Quebec, Canada
- WP 623 **Quantitative Assessment of Differential Protein Expression in the Hemicellulolytic Bacterium *Clostridium stercoarium* Using iTRAQ and SWATH approaches;** Peter D. McQueen<sup>1,2</sup>; John Schellenberg<sup>1</sup>; Vic Spicer<sup>1</sup>; Richard Sparling<sup>1</sup>; David Levin<sup>1</sup>; John Wilkins<sup>1,2</sup>; Oleg Krokhin<sup>1,2</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, Canada



- WP 624 **Highly Sensitive Determination of Therapeutic Peptides in Human Plasma Using Orthogonal HILIC-RP Column Switching and Tandem Mass Spectrometric Detection;** Eric W. Ma; Moucun Yuan; Michael Tingler; William Mylott Jr; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- WP 625 **Improved Identification and Relative Quantification of Sites of Oxidation in Model Peptides and Protein Systems by Electron-Transfer Dissociation (ETD);** Xiaoyan Li; Joshua S. Sharp; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- WP 626 **Comparison of Peptide Fragmentation and Bioanalysis among Different LC/MS Approaches for the Quantification of Glucagon and Its Analogs in Plasma;** Hang Zeng<sup>1</sup>; Zhenmin Liang<sup>1</sup>; Catherine Bentzley<sup>2</sup>; David Moore<sup>1</sup>; <sup>1</sup>*HL Roche, Inc., Nutley, NJ*; <sup>2</sup>*University of the Sciences, Philadelphia, PA*
- WP 627 **An Augmented Label-Free Differential Analysis Workflow Enhances Peptide Identifications and Understanding of Alcohol Preference;** Scott Goulding<sup>1</sup>; Nicholas Bateman<sup>2</sup>; Nicholas Shulman<sup>3</sup>; Michael MacCoss<sup>3</sup>; Karen Szumlanski<sup>4</sup>; Christine Wu<sup>2</sup>; <sup>1</sup>*University of Colorado Anschutz Medical Campus, Aurora, CO*; <sup>2</sup>*University of Pittsburgh, Pittsburgh, PA*; <sup>3</sup>*University of Washington, Seattle, WA*; <sup>4</sup>*University of California, Santa Barbara, CA*
- WP 628 **Proteomics Profiling of Cancer Cell Lines Using High Flow Chromatography and Electrospray Ionization Technique;** Vadira B. Bhat<sup>1</sup>; Dawn Stickle<sup>1</sup>; Anne E. Blackwell<sup>1</sup>; Umesh T. Sankpal<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE*; <sup>2</sup>*MD Anderson Cancer Center Orlando, Orlando, FL*
- WP 629 **Liver Mitochondria Proteomics Employing High Resolution MS Technology;** Jenny T.C. Ho<sup>1</sup>; Loïc Dayon<sup>2</sup>; John Corthésy<sup>2</sup>; Umberto De Marchi<sup>2</sup>; Antonio Núñez<sup>2</sup>; Andreas Wiederkehr<sup>2</sup>; Rosa Viner<sup>3</sup>; Michael Blank<sup>3</sup>; Steven Danielson<sup>3</sup>; Madalina Oppermann<sup>1</sup>; Martin Hornshaw<sup>1</sup>; Martin Kussmann<sup>2,4</sup>; <sup>1</sup>*Thermo Fisher Scientific, Hemel Hempstead, UK*; <sup>2</sup>*Nestlé Institute of Health Sciences, Lausanne, Switzerland*; <sup>3</sup>*ThermoFisher Scientific, San Jose, CA*; <sup>4</sup>*Ecole Polytechnique Fédérale Lausanne (EPFL), Lausanne, Switzerland*
- WP 630 **Method Optimization for Cardiovascular Proteomic Mass Spectrometry Analysis of Reversible Cysteine Oxidation in CatTG Mice;** Chunxiang Yao<sup>1,2</sup>; Jessica Behring<sup>2</sup>; Deborah A. Siwik<sup>3</sup>; Catherine E. Costeool<sup>1</sup>; Wilson Colucci<sup>3</sup>; Richard A. Cohen<sup>2</sup>; Mark E. McComb<sup>1,2</sup>; Markus M. Bachschmid<sup>1,2</sup>; <sup>1</sup>*CPC and CBMS, BUSM, Boston, MA*; <sup>2</sup>*Vascular Biology Section, BUSM, Boston, MA*; <sup>3</sup>*Myocardial Biology Unit, BUSM, Boston, MA*
- WP 631 **Large Molecule Quantification by HRMS: "Sensitive Calcitonin Bioanalysis Using Targeted Selected Ion Monitoring and High Resolving Power";** Jean-Nicholas Mess<sup>1</sup>; Louis-Philippe Morin<sup>1</sup>; Gene Ciccimaro<sup>2</sup>; Maroun El Khoury<sup>3</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>*Algorithme Pharma Inc., Laval, Quebec, Canada*; <sup>2</sup>*Thermo Scientific, Sommerset, NJ*; <sup>3</sup>*Thermo Scientific, Montreal, Quebec, Canada*
- WP 632 **Comprehensive Cancer Cell Proteomics: Providing a Global Counterpoint to Genomic Approaches;** Corey Bakalarski<sup>1</sup>; Richard Neve<sup>1</sup>; Mamie Yu<sup>1</sup>; Suresh Selvaraj<sup>1</sup>; Anthony Possemato<sup>2</sup>; Sean Beausoleil<sup>2</sup>; Peng Yue<sup>1</sup>; David Dornan<sup>1</sup>; Richard Bourgon<sup>1</sup>; William Forrest<sup>1</sup>; Donald Kirkpatrick<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*; <sup>2</sup>*Cell Signaling Technology, Danvers, MA*
- WP 633 **Reduced Abundance of Protein Phosphatase 1 Regulatory Subunit 12B in Diabetes Revealed by Targeted Proteomics;** Monique Lewis; Danjun Ma; Michael A. Caruso; Xiangmin Zhang; Zhengping Yi; *Wayne State University, Detroit, MI*
- WP 634 **The Analysis of Human Parathyroid Hormone 1-34 (Teriparatide) by LC-MS/MS: Challenges and Lessons Learned;** Erin E. Chambers<sup>1</sup>; Mary Lame<sup>1</sup>; Jon Bardsley<sup>2</sup>; Eileen Collins<sup>2</sup>; Sally Hannam<sup>2</sup>; Elizabeth Thomas<sup>2</sup>; Kenneth J. Fountain<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*ICON PLC, Manchester, UK*
- WP 635 **Identification and Quantification of Peptide Hormones in Sea Lamprey Brain Tissues by Electrospray Ionization Tandem Mass Spectrometry;** Huiyong Wang; Yu-Wen Chung-Davidson; Ke Li; Weiming Li; *Michigan State University, East Lansing, MI*
- WP 636 **Casein Kinase I  $\delta$  Substrates Associated with Migraine;** Huan Kang; Emily Bates; John Prince; *Brigham Young University, Provo, Utah*
- WP 637 **A Detergent Free, Label Free Quantification Method with High Sensitivity and Throughput for CYP Enzymes via LC/MS/MS;** Ji Zhang; Jimmy Li; Bingli Ma; Cindy Xia; Jing-Tao Wu; Matt Jones; *Millennium :The Takeda Oncology Company, Cambridge, MA*
- WP 638 **Proteomic Analysis of Rhizome Specificity across Plant Kingdom;** Fernanda Salvato; *University of Missouri, Columbia, MO*
- WP 639 **Quantitation of Low Levels of Heat Shock Protein 90 in Serum of Cervical Cancer Patients by Selected Reaction Monitoring;** Coskun Guzel<sup>1</sup>; Natalia I. Govorukhina<sup>2</sup>; Klaske A. ten Hoor<sup>3</sup>; Lennard J.M. Dekker<sup>1</sup>; Harry Hollema<sup>3</sup>; Harry G. Klip<sup>3</sup>; Ate G.J. van der Zee<sup>3</sup>; Alexander Boichenko<sup>1</sup>; Boichenko<sup>2</sup>; Rainer Bischoff<sup>2</sup>; Theo M. Luider<sup>1</sup>; <sup>1</sup>*Erasmus Medical Center, Rotterdam, the Netherlands*; <sup>2</sup>*University of Groningen, Groningen, the Netherlands*; <sup>3</sup>*University Medical Centre Groningen, Groningen, the Netherlands*
- WP 640 **Challenge in Trying to Reach Femtogram per Milliliter (fg/mL) Sensitivity in Plasma for the Quantification of a Cyclic Peptide: Desmopressin;** Louis-Philippe Morin<sup>1</sup>; France Landry<sup>1</sup>; Jean-Nicholas Mess<sup>1</sup>; Kelli Jonakin<sup>2</sup>; Mauro Aiello<sup>2</sup>; Xavier Misonne<sup>2</sup>; Gary Impey<sup>2</sup>; Johnny Cardenas<sup>2</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>*Algorithme Pharma Inc., Laval, Quebec, Canada*; <sup>2</sup>*AB Sciex, Concord, Ontario, Canada*
- WP 641 **Absolute Quantitation of Yeast Kinases by Means of LC-MS/MS Using QconCat and SRM Technologies;** Philip J Brownridge<sup>1</sup>; Victoria Harman<sup>1</sup>; Simon Cubbon<sup>2</sup>; Johannes PC Vissers<sup>2</sup>; Craig Lawless<sup>3</sup>; Simon J Hubbard<sup>3</sup>; Robert J Beynon<sup>1</sup>; <sup>1</sup>*Protein Function Group, University of Liverpool, Liverpool, UK*; <sup>2</sup>*Waters Corporation, Manchester, UK*; <sup>3</sup>*Faculty of Life Sciences, University of Manchester, Manchester, UK*
- WP 642 **Detection of HIV Peptides Using Selective Reaction Monitoring Mass Spectrometry: An *in vitro* Study;** Xiaolin Li; John C Tilton; Daniela M Schlatzer; *Case Western Reserve University, Cleveland, OH*
- WP 643 **Glucagon Bioanalysis by LC-MS: "Unprecedented Level of Sensitivity (10pg/mL) for a Novel Formulation";** Jean-Nicholas Mess<sup>1</sup>; Louis-Philippe Morin<sup>1</sup>; Mauro Aiello<sup>2</sup>; Xavier Misonne<sup>2</sup>; Gary Impey<sup>2</sup>; Johnny Cardenas<sup>2</sup>; Josee Michon<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>*Algorithme Pharma Inc., Laval - Quebec, Canada*; <sup>2</sup>*AB SCIEX, Concord - Ontario, Canada*

#### Phosphopeptides: Enrichment Methods, 644 – 668

- WP 644 **Application of Immobilized Metal Ion Affinity Chromatography (IMAC) Enrichment for Bacterial Phosphopeptide Analysis;** Yi Qu; Si Wu; Rui Zhao; Erika Zink; Daniel Orton; Ronald Moore; Da Meng; Therese Clauss; Joshua Aldrich; Mary Lipton; Ljiljana Paša-Tolić; *PNNL, Richland, WA*



- WP 645 **Differentiation of Ion Exchange Materials for Phosphopeptide Fractionation;** Qing-Run Li; Qing-Qing Wu; Rong Zeng; *Shanghai Institutes for Biological Sciences, Shanghai, China*
- WP 646 **The Phosphopeptide Shootout: A Study of Reproducibility in IMAC Phosphopeptide Enrichment;** Nicholas M. Riley; Gregory K. Potts; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- WP 647 **An Enzyme Assisted RP-RPLC Approach for In-Depth Human Liver Phosphoproteome Analysis;** Yangyang Bian<sup>1</sup>; Chunxiao Song<sup>1</sup>; Mingming Dong<sup>1</sup>; Wenhai Jin<sup>2</sup>; Lihai Guo<sup>2</sup>; Yongming Xie<sup>2</sup>; Mingliang Ye<sup>1</sup>; Hanfa Zou<sup>1</sup>; <sup>1</sup>*Dalian Institute of Chemical Physics, Dalian, Liaoning Province, China*; <sup>2</sup>*Asia Pacific Application Support Center, AB SCIEX, Shanghai, China*
- WP 648 **Reducing Sample Size and Improving Numbers of Identified Proteins: Phosphoproteomic Studies with SCX-IMAC and IMAC-RP Methods;** Xiaoshan Yue; Amanda Hummon; *Notre Dame, Notre Dame, IN*
- WP 649 **Comparison of Resins for Metal Oxide Affinity Chromatography with Mass Spectrometry Detection for the Determination of Phosphopeptides;** Ales Tichy<sup>1</sup>; Barbora Salovska<sup>2</sup>; Ivo Fabrik<sup>1</sup>; Jirina Vavrova<sup>1</sup>; <sup>1</sup>*University of Defence, Hradec Kralove, Czech Republic*; <sup>2</sup>*Faculty of Medicine, Hradec Kralove, Czech Republic*
- WP 650 **Dimetal Phosphate Ester Stabilization and Strong-Cation Exchange Chromatography (DIMPES-SCX): A Novel Approach for Phosphopeptide Enrichment;** Thiago Verano-Braga; Simon Svane; Christine McKenzie; Frank Kjeldsen; *University of Southern Denmark, Odense, Denmark*
- WP 651 **A Streamlined Protocol for High Content Phosphoproteomics;** Francesca Zappacosta; Gilbert Scott; Michael Huddleston; Dean McNulty; Timothy Sikorski; Roland Annan; *GlaxoSmithKline, Collegeville, PA*
- WP 652 **Enhanced Phosphopeptide Identification in Bacteria by Stepwise Hydroxy Acid-Modified Metal Oxide Chromatography with Elevated Sample Loading Capacity;** Miao-Hsia Lin; Yasushi Ishihama; *Kyoto university, Kyoto, Japan*
- WP 653 **Highly Specific Phosphopeptide Enrichment Using a Novel Tantalum-based Sol-gel for MALDI-MS Applications;** Ömür Çelikbıçak; Mehmet Atakay; Ülkü Güler; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- WP 654 **A Mild Phosphopeptide Desorption Strategy in Anion Exchange Based Enrichment Applications for Mass Spectrometry Analysis;** Mehmet Atakay; Ömür Çelikbıçak; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- WP 655 **Close Examination of Tyrosine Phosphopeptide Enrichment and Its Application to Syk and Lyn Signaling Pathways;** Keerthi Jayasundera; Anton Iliuk; Shenrui Mahorney; Liang Xue; Andrew Nguyen; Robert Geahlen; W. Andy Tao; *Purdue University, West Lafayette, IN*
- WP 656 **Improved Identification of Akt Substrate Motif Phosphorylation in LC-MS/MS with a Tandem Affinity Enrichment Approach;** Taylur Ma; Victoria Pham; Jennie Lill; Kebing Yu; *Genentech, Inc., South San Francisco, CA*
- WP 657 **Targeted Phosphoproteomics Analysis of Immunoaffinity Enriched Tyrosine Phosphorylation in Mouse tissue;** Ravi Kumar Krovvidi<sup>1</sup>; Leo Bonilla<sup>1</sup>; Charles L Farnsworth<sup>2</sup>; Jeffrey C Silva<sup>2</sup>; <sup>1</sup>*Agilent Technologies India Pvt. Ltd, Bangalore, India*; <sup>2</sup>*Cell Signaling Technology, Inc, Danvers, CT*
- WP 658 **Complementation of Ti, Zr and Fe-based PolyMAC for In-Depth Phosphoproteome Analysis of B cell Signaling;** Anton Iliuk<sup>1</sup>; Keerthi Jayasundera<sup>2</sup>; Wen-hong Wang<sup>2</sup>; Robert Geahlen<sup>2</sup>; Weiguo Andy Tao<sup>2</sup>; <sup>1</sup>*Tymora Analytical Operations, West Lafayette, IN*; <sup>2</sup>*Purdue University, West Lafayette, IN*
- WP 659 **Quantitative Profiling of Signaling Pathways Using Immunoaffinity Purification and LC-MS/MS;** Matthew P. Stokes; Jian Min Ren; Kimberly A. Lee; Xiaoying Jia; Jeffrey C. Silva; *Cell Signaling Technology, Danvers, MA*
- WP 660 **A Novel Strategy Employing a Phosphatase Trapping Mutant for the Enrichment of Phosphoarginine, an Unconventional Type of Protein Phosphorylation;** Débora Broch Trentini; Tim Clausen; Karl Mechtler; *Institute of Molecular Pathology (IMP), Vienna, AUSTRIA*
- WP 661 **Sunny-side Up: First UV MALDI-ToF-MS Phosphopeptide Analysis Using a Solidified Ionic Liquid Matrix (SILM);** Gargee Mukherjee<sup>1</sup>; Claudia Röwer<sup>1</sup>; Manuela Russ<sup>1</sup>; Chris Protzel<sup>2</sup>; Oliver Hakenberg<sup>2</sup>; Cornelia Koy<sup>1</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, Rostock, Germany*; <sup>2</sup>*Urology Clinic and Polyclinic, University Medicine, Rostock, Germany*
- WP 662 **Old Tools in a New Jacket: Phosphopeptide Enrichment by TiO<sub>2</sub> and IMAC Columns;** Simone Lemeer; Benjamin Ruprecht; Heiner Koch; Max Mundt; Bernhard Kuster; *Technische Universität München, Freising, Germany*
- WP 663 **The Phosphoproteome of *Chlamydomonas reinhardtii* Determined by TiO<sub>2</sub>-HILIC and HILIC-PolyMAC Workflows Coupled to nanoLC-MS/MS;** Brian Gau; Hongxia Wang; Leslie Hicks; *Donald Danforth Plant Science Center, St. Louis, MO*
- WP 664 **Optimization of the  $\beta$ -Elimination/Michael Addition Chemistry on Reversed-Phase Supports for Comprehensive Phosphoprotein Characterization by Mass Spectrometry;** Heinz Nika<sup>1</sup>; David H. Hawke<sup>2</sup>; Ruth Hogue Angeletti<sup>1</sup>; <sup>1</sup>*Albert Einstein College of Medicine, Bronx, NY*; <sup>2</sup>*UT- M.D. Anderson Cancer Center, Houston, TX*
- WP 665 **Robust Enrichment Methods for Single-Shot Phosphoproteomics of Cancer Cell Lines Enable Signaling Network Analysis;** Sander Piersma; Koen van der Mijjn; Bharath Sampadi; Inge de Reus; Jaco Knol; Richard de Haas; Thang Pham; Henk Broxterman; Henk Verheul; Connie Jimenez; *VU University Medical Center, Amsterdam, Netherlands*
- WP 666 **Comprehensive Phosphorylation Site Analysis of  $\alpha$ -S2 Casein Using Microwave-Assisted Acid Hydrolysis and Phosphopeptide Enrichment;** Zhendong Li; Nan Wang; Liang Li; *UofA, Edmonton, Canada*
- WP 667 **Maximizing Phosphoproteome Profiling Using Mascot, PEAKS Studio, Proteome Discoverer and OMSSA Software Packages;** Jayne Wiederin<sup>1</sup>; Melinda Wojtkiewicz<sup>1</sup>; Pawel Olszowy<sup>2</sup>; Pawel Ciborowski<sup>1</sup>; <sup>1</sup>*University of Nebraska Medical Center, Omaha, NE*; <sup>2</sup>*Nicolaus Copernicus University, Torun, Poland*
- WP 668 **Motif Antibody Enrichment Enables the Identification of a Large Discrete and Complementary Set Of Phosphorylation Sites ;** Anthony Possemato<sup>1</sup>; Sean Beausoleil<sup>1</sup>; Mike Aguiar<sup>1</sup>; Kim Lee<sup>1</sup>; Steven Gygi<sup>2</sup>; <sup>1</sup>*Cell Signaling Technology, Danvers, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- Advances in Separation Techniques for Proteomic Applications, 669 – 684**
- WP 669 **Detection of Biomarker of Oxidative Stress by Using HPLC-MS/MS and a Microfluidic Electrochemical Array;** Boya Song; Shenmin Pan; Chi Tang; Dandan Li; James Rusling; *University of Connecticut, Storrs, CT*

- WP 670 **Improved Sensitivity in Proteomics Experiments Using DMSO in nanoESI-LC-MS/MS;** Hannes Hahne<sup>1</sup>; Guillaume Medard<sup>1</sup>; Stefan K. Maier<sup>1</sup>; Dominic Helm<sup>1</sup>; Matthias Wilm<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technische Universität München, Freising, Germany*; <sup>2</sup>*University College Dublin, Dublin, Ireland*
- WP 671 **Zeptomole-level Proteomic Analysis of Limited Availability Clinical Samples Using Monolithic and Porous Layer Open Tubular Columns in Ultralow Flow LC/MS;** Alexander R. Ivanov; Siyang Li; Xianzhe Wang; Barry L. Karger; *Barnett Institute, Northeastern University, Boston, MA*
- WP 672 **A Comparison of Proteomic Data Sets Obtained from Varied Experimental Approaches;** Susan Slade<sup>1</sup>; James Langridge<sup>3</sup>; Nisha Patel<sup>2</sup>; Joanne B. Connolly<sup>3</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>*Univ of Warwick, Coventry, UK*; <sup>2</sup>*Department of Chemistry, University of Oxford, Oxford, UK*; <sup>3</sup>*Waters Corporation, Manchester, UK*
- WP 673 **Proteomic Studies on Enriched Cell Populations by Linking Cell Sorting with Microfluidic Online Sample Preparation and LC/MS;** Jeffrey Martin; Tomas Rejtar; Stephen Martin; *Novartis Institutes for Biomedical Research, Cambridge, MA*
- WP 674 **The BluePippin Automated Size-Fractionation System for Proteins;** Ezra Abrams; Chris Boles; *Sage Science, Inc., Beverly, MA*
- WP 675 **Comprehensive Genome-Wide Proteomic Analysis of Human Placental Tissue for the Chromosome-Centric Human Proteome Project;** Hyoung-Joo Lee<sup>1</sup>; Seul-Ki Jeong<sup>1</sup>; Keun Na<sup>1</sup>; Min Jeong Lee<sup>1</sup>; Sun Hee Lee<sup>1</sup>; Jong-Sun Lim<sup>1</sup>; Hyun-Jeong Cha<sup>1</sup>; Jin-Young Cho<sup>1</sup>; Ja-Young Kwon<sup>2</sup>; Hoguen Kim<sup>2</sup>; Si Young Song<sup>2</sup>; Jong Shin Yoo<sup>3</sup>; Young Mok Park<sup>3</sup>; Hail Kim<sup>4</sup>; William S. Hancock<sup>5</sup>; Young-Ki Paik<sup>1</sup>; <sup>1</sup>*Yonsei Proteome Research Center, Seoul, South Korea*; <sup>2</sup>*Yonsei University College of Medicine, Seoul, South Korea*; <sup>3</sup>*Korea Basic Science Institute, Ochang, South Korea*; <sup>4</sup>*Korea Advanced Institute of Science and Technology, Daejeon, South Korea*; <sup>5</sup>*Northeastern University, Boston, MA*
- WP 676 **High Sensitivity Microproteomic Analysis of Rare Samples by Porous Layer Open Tubular (PLOT) Columns Coupled with Mass Spectrometry;** Siyang Li; Xianzhe Wang; Somak Ray; Barry L. Karger; Alexander R. Ivanov; *Barnett Institute, Northeastern University, Boston, MA*
- WP 677 **Comparison of Gas-Phase Fractionation and Data-Dependent Acquisition for Identification of Post-translational Modifications in Glioma-Derived Stem-Like Cells;** Cheryl F. Lichti<sup>1</sup>; Huiling Liu<sup>1</sup>; Erick P. Sulman<sup>2</sup>; Frederick F. Lang<sup>2</sup>; Charles A. Conrad<sup>2</sup>; Carol L. Nilsson<sup>1</sup>; <sup>1</sup>*UTMB-Galveston, Galveston, TX*; <sup>2</sup>*The University of Texas MD Anderson Cancer Center, Houston, TX*
- WP 678 **Bottom-up Proteomics by Capillary Electrophoresis and Mass Spectrometry;** Antonius A.M. Heemskerk; Guinevere S.M. Kammeijer; Ekaterina Mostovenko; Bart Schoenmaker; Rico J.E. Derks; André M. Deelder; Magnus Palmblad; Oleg A. Mayboroda; *Leiden University Medical Center, Leiden, Netherlands*
- WP 679 **Fully Automatable Multidimensional Liquid Chromatography Systems for Shotgun Proteomics;** Yun Zhao<sup>1</sup>; C. H. Law<sup>1</sup>; Ricky P. W. Kong<sup>1,3</sup>; Guohui Li<sup>1</sup>; Herman C. Lam<sup>1</sup>; Jason Neo<sup>4</sup>; Simon M. Y. Lee<sup>2</sup>; C.Y. Ma<sup>1</sup>; Ivan K. Chu<sup>1</sup>; <sup>1</sup>*The University of Hong Kong, Hong Kong, China*; <sup>2</sup>*The University of Macau, Macau, China*; <sup>3</sup>*AB SCIEX Hong Kong, Hong Kong, China*; <sup>4</sup>*AB SCIEX Singapore, Singapore, Singapore*
- WP 680 **Bottom-Up Proteome Analysis of E. coli Using Capillary Zone Electrophoresis-Tandem Mass Spectrometry with an Electrokinetic Sheath-Flow Electrospray Interface;** Xiaojing Yan; David Essaka; Liangliang Sun; Guijie Zhu; Norman Dovichi; *University of Notre Dame, Notre Dame, U.S.*
- WP 681 **Single-Shot Capillary Zone Electrophoresis Electrospray Ionization-Tandem Mass Spectrometry Produces More Than 1,250 E. coli Peptide Identifications in a 50-Minute Separation;** Guijie Zhu; Liangliang Sun; Xiaojing Yan; Norman Dovichi; *University of Notre Dame, Notre Dame, IN*
- WP 682 **Integrated CZE-ESI-MS/MS System with Immobilized Trypsin Microreactor for Picogram of RAW 264.7 Cell Lysate Analysis;** Liangliang Sun; Guijie Zhu; Norman J. Dovichi; *University of Notre Dame, South Bend, IN*
- WP 683 **Precise Column Temperature Control Enables Improved Protein Identifications in Proteomics Shotgun Sequencing Applications;** Xiaoyue Jiang; Yi Zhang; Andreas Huhmer; *Thermo Fisher Scientific, San Jose, CA*
- WP 684 **CE-ESI-MS for Top Down Proteomics;** Yihan Li; John C. Tran; Ioanna Ntai; Kenneth R. Durbin; Adam D. Catherman; Philip D. Compton; Paul M. Thomas; Neil L. Kelleher; *Northwestern University, Evanston, IL*
- Interactions and Pathway Analysis, 685 – 706**
- WP 685 **Rapid Identification of Differential Interactomes by Affinity Purification Coupled with Data Independent Mass Spectrometry Acquisition (AP-SWATH™);** Jean-Philippe Lambert<sup>1</sup>; Amber L. Couzens<sup>1</sup>; Gordana Ivosev<sup>2</sup>; Brett Larsen<sup>1</sup>; Mikko Taipale<sup>3</sup>; Zhen-Yuan Lin<sup>1</sup>; Quan Zhong<sup>4</sup>; Susan Lindquist<sup>3</sup>; Marc Vidal<sup>4</sup>; Ruedi Aebersold<sup>5</sup>; Tony Pawson<sup>1</sup>; Ron Bonner<sup>2</sup>; Stephen Tate<sup>2</sup>; Anne-Claude Gingras<sup>1</sup>; <sup>1</sup>*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, Canada*; <sup>2</sup>*AB Sciex, Concord, Canada*; <sup>3</sup>*Whitehead Institute for Biomedical Research, Cambridge, MA*; <sup>4</sup>*Dana-Farber Cancer Institute, Boston, MA*; <sup>5</sup>*Institute of Molecular Systems Biology, ETH, Zurich, Switzerland*
- WP 686 **Temporal Proteomics Unveils *Ignicoccus hospitalis*'s Response to the Superficial Attachment and Growth Progression of Its Commensal Partner, *Nanoarchaeum equitans*;** Richard J. Giannone; Louie L. Wurch; Mircea Podar; Robert L. Hettich; *Oak Ridge National Laboratory, Oak Ridge, TN*
- WP 687 **High-Resolution Interactome of the HSP90 Machinery Reveals Specificity for Targets;** Brett Larsen<sup>1</sup>; Mikko Taipale<sup>2</sup>; Zhen-Yuan Lin<sup>1</sup>; George Tucker<sup>3</sup>; Guoci Teo<sup>4</sup>; Hyungwon Choi<sup>4</sup>; Susan Lindquist<sup>2,3</sup>; Anne-Claude Gingras<sup>1,5</sup>; <sup>1</sup>*SLRI, Toronto, Canada*; <sup>2</sup>*Whitehead Institute for Biomedical Research, Cambridge, MA*; <sup>3</sup>*MIT, Cambridge, MA*; <sup>4</sup>*National University of Singapore, Singapore, Singapore*; <sup>5</sup>*Mount Sinai Hospital, Toronto, Canada*
- WP 688 **Towards a Deep and Temporal Representation of Protein Interaction Networks via AP-SWATH;** Ben C. Collins<sup>1</sup>; Ludovic C. Gillet<sup>1</sup>; George Rosenberger<sup>1</sup>; Hannes L. Röst<sup>1</sup>; Matthias Gstaiger<sup>1</sup>; Ruedi Aebersold<sup>1,2</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*University of Zurich, Zurich, Switzerland*
- WP 689 **Dynamic Analysis of HIV-Human Protein-Protein Interactions During Infection;** Jeffrey Johnson<sup>1</sup>; Shannon Eliuk<sup>2</sup>; Amnon Golan<sup>1</sup>; Tasha Johnson<sup>1</sup>; Vlad Zabrouskov<sup>2</sup>; Nevan Krogan<sup>1</sup>; <sup>1</sup>*UCSF, San Francisco, CA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- WP 690 **Quantitative Analysis of 6-Thioguanine-Induced Changes in the Proteome of Jurkat-T Human Leukemia Cells;** Fan Zhang; Yinsheng Wang; *University of California, Riverside, CA*

- WP 691 **Quantitative Proteomic Analysis Reveals Chromium-induced Perturbation of Multiple Cellular Pathways in GM00637 Human Skin Fibroblast Cells;** Lei Guo; Yinsheng Wang; *University of California, Riverside, CA*
- WP 692 **Sphingosine-1-Phosphate Mediated Chemotaxis of Osteoclast Precursors Investigated Using Targeted Proteomics via Mass Spectrometry;** Nathan Manes; Eunkyung An<sup>1</sup>; Virginie Sjoelund<sup>1</sup>; Jing Sun<sup>1</sup>; Bastian Angermann<sup>1</sup>; Masaru Ishii<sup>2</sup>; Martin Meier-Schellersheim<sup>1</sup>; Ronald Germain<sup>1</sup>; Aleksandra Nita-Lazar<sup>1</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>Osaka University, Osaka, Japan
- WP 693 **Dynamic Pathways in Acute Autophagy Elucidated by Quantitative Label-free and SILAC-based Proteomics;** Robin Mathew<sup>1,2</sup>; Saw Kyin<sup>2</sup>; Henry Shwe<sup>2</sup>; Eileen White<sup>1</sup>; David H. Perlman<sup>2</sup>; <sup>1</sup>The Cancer Institute of New Jersey, New Brunswick, NJ; <sup>2</sup>Princeton University, Princeton, NJ
- WP 694 **Towards a Comprehensive Understanding of Platelet Activation and Platelet-Monocyte Interaction: Multiple Proteomic Approaches in the Study of Atherosclerosis;** Jiqing Huang; Chengcheng Zhang; Ru Li; Juergen Kast; *BRC, Univ. of British Columbia, Vancouver, Canada*
- WP 695 **Using Label-Free Mass Spectrometry Workflows to Quantitatively Model Signal Transduction Pathways in Cellular Systems and Clinical Samples;** Jordy J. Hsiao; Brandon H. Ng; Melinda M. Smits; Jiahui Wang; Michael E. Wright; *University of Iowa, Iowa City, IA*
- WP 696 **MS-based Quantitative Analysis of RanBP2 in Nucleocytoplasmic Transport;** Samir Karaca<sup>1</sup>; Ketan Thakar<sup>2</sup>; Ralph Kehlenbach<sup>2</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>Georg-August-University of Goettingen, Goettingen, Germany
- WP 697 **Defining the Role for miR-27a in the Regulation of Adipogenesis;** Rebecca Leon; Bruce D. Pascal; Caitlin Steckler; Patrick R. Griffin; Michael J. Chalmers; *Scripps, Jupiter, FL*
- WP 698 **Quantitative Analysis of Changes in Ubiquitination, Protein Synthesis and Degradation Caused by Protein Folding Stress Due to Inhibition of Hsp90;** Manfredo Quadroni<sup>1</sup>; Alexandra Potts<sup>2</sup>; Ivo Fierro-Monti<sup>1</sup>; Celine Hernandez<sup>1,2</sup>; Patrice Waridel<sup>1</sup>; Pablo Echeverria<sup>3</sup>; Didier Picard<sup>3</sup>; <sup>1</sup>University of Lausanne, Epalinges, Switzerland; <sup>2</sup>Swiss Institute of Bioinformatics, Lausanne, Switzerland; <sup>3</sup>University of Geneva, Geneva, Switzerland
- WP 699 **Investigation of Hepatocytes Transfected with Cytochrome P450: Data Independent LC-MS Approach to Identify and Quantify on a Multi-omic Scale;** Suzanne Geenen<sup>1</sup>; Lee A Gethings<sup>2</sup>; Cristian Cojocariu<sup>2</sup>; Janet Hammond<sup>2</sup>; Giorgis Isaac<sup>3</sup>; Lucy Fernandes<sup>2</sup>; Robert Tonge<sup>2</sup>; Johannes P.C. Vissers<sup>2</sup>; James Langridge<sup>2</sup>; Ian Wilson<sup>1</sup>; Mark McDowall<sup>2</sup>; <sup>1</sup>AstraZeneca, Macclesfield, UK; <sup>2</sup>Waters, Manchester, UK; <sup>3</sup>Waters Corp, Milford, MA
- WP 700 **Understanding Oncoprotein Networks in Cancer Cells Using Knock-In and Knock-Out AP-MS;** Jing Song; Zhenghe Wang; Rob Ewing; *Case Western Reserve University, Cleveland, OH*
- WP 701 **Integrative Systems Approach towards Elucidation of Action Mechanism for a Novel, First-In-Class ERK/AKT Dual Inhibitor Anti-Cancer Drug;** Giridharan Gokulrangan<sup>1</sup>; Daniela Schlatzer<sup>1</sup>; Neil Dhawan<sup>2</sup>; Eric Yuan<sup>3</sup>; Sahar Mazhar<sup>3</sup>; Avi Ma'ayan<sup>2</sup>; Michael Ohlmeyer<sup>2</sup>; Mark Chance<sup>1</sup>; Goutham Narla<sup>3</sup>; <sup>1</sup>Center for Proteomics and Bioinformatics, CWRU, Cleveland, OH; <sup>2</sup>Mount Sinai School of Medicine, New York, NY; <sup>3</sup>Case Comprehensive Cancer Center, Cleveland, OH
- WP 702 **Unraveling Metabolic Regulation by Real-Time Mass Spectrometry of Living Cells;** Tobias Fuhrer; Hannes Link; Andreas Kühne; Uwe Sauer; Nicola Zamboni; *ETH Zürich, Zürich, Switzerland*
- WP 703 **Proteome-Wide Analysis of Stress Response in *E. coli* Using Super-SILAC Approach;** Boumediene Soufi; Andreas Harst; Karsten Krug; Boris Macek; *Proteome Center Tuebingen, Tuebingen, Germany*
- WP 704 **Simple Quantitative Secretome Analysis of Conditioned Media from Human Endothelial Stromal Cells Under Hypoxic Conditions Characterizing Synthetic Progestin Effects;** John Shapiro<sup>3</sup>; Philip Gafken<sup>1</sup>; Michael Freitas<sup>2</sup>; Ozlem Kayisli<sup>3</sup>; Umit Kayisli<sup>3</sup>; Saeed Faramarzi<sup>3</sup>; Murat Basar<sup>3</sup>; Frederick Schatz<sup>3</sup>; Charles Lockwood<sup>3</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>Ohio State University, Columbus, OH; <sup>3</sup>Ohio State University College of Medicine, Columbus, OH
- WP 705 **Development and Application of a Multiplexed Active Small GTPase Pull-down Assay Using Multiple Reaction Monitoring;** Chengcheng Zhang; Juergen Kast; *University of British Columbia, Vancouver, Canada*
- WP 706 **Global Remodelling of Cellular Microenvironment Due to Loss of Collagen VII;** Victoria Kuettner<sup>1</sup>; Leena Bruckner-Tuderman<sup>2</sup>; Joern Dengjel<sup>1</sup>; <sup>1</sup>Freiburg University, Freiburg, Germany; <sup>2</sup>University Freiburg Medical Center, Freiburg, Germany
- Ambient Ionization: Applications II, 707 – 734**
- WP 707 **Rapid Screening of Plasticisers in Gaskets for Glass Food Jar Lids Using Atmospheric Pressure Solids Analysis Probe-High Resolution Mass Spectrometry;** Malcolm Driffield<sup>1</sup>; Dennis Speck<sup>1</sup>; Mita Parmar<sup>1</sup>; Jennifer Leak<sup>1</sup>; Liam Lister<sup>1</sup>; Emma Bradley<sup>1</sup>; Dominic Roberts<sup>2</sup>; Sara Stead<sup>2</sup>; <sup>1</sup>Food and Environmental Research Agency (Fera), York, UK; <sup>2</sup>Waters Corporation, Manchester, UK
- WP 708 **ASAP-HRMS: A Convenient Technique for Characterizing Unexpected Insoluble Materials Observed during the Development of Cosmetic Formulae;** Natali Budimir; Georges Hussler; *L'Oréal France, Aulnay Sous Bois, France*
- WP 709 **Forensic Analysis Using Rapid Ambient Ionization Techniques with High Resolution Mass Spectrometers;** Eshwar Jagerdeo; Jay Clark; Louis Reda; Jeffrey Leibowitz; *FBI, Springfield, VA*
- WP 710 **Rapid Detection of Pomegranate Juice Adulteration with Grape and Apple Juice Using DSA/TOF with Minimal Sample Preparation and No Chromatography;** Avinash Dalmia; George Perkins; Craig Whitehouse; *PerkinElmer, Shelton, CT*
- WP 711 **Tunable Desorption/Ionization with Plasma-based Ambient Mass Spectrometry: Unraveling Mysteries of Lithium-Ion Battery Degradation;** Jake Shelley; Christopher Kuhlmann; Britta Vortmann; Sascha Nowak; Carsten Engelhard; *University of Muenster, Muenster, Germany*
- WP 712 **Fast Quantitation of bisphenol-A (BPA) in Plastic Materials Using Desorption Corona Beam Ionization and Probe Tip Column Electrospray Ionization Sources;** Chao Gao<sup>1</sup>; Yanjiao Wang<sup>2</sup>; Xiaoqiang Zhang<sup>1</sup>; Xiang Li<sup>2</sup>; Wenjian Sun<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China; <sup>2</sup>Fudan University, Shanghai, China
- WP 713 **Overcoming Matrix effects: Quantitation of Explosives via Ambient Ionization with Direct Sample Analysis;** Joshua A. Wilhide; Laura M. Nevin; Gregory T. Winter; William R. LaCourse; *Univeristry of Maryland Baltimore County, Baltimore, MD*

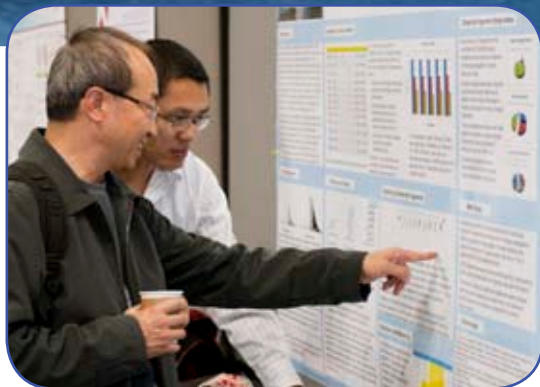


- WP 714 **Analysis of Additives in Biodegradable Polymers Using Direct Sampling Analysis (DSA) Time-of-Flight Mass Spectrometry**; Sharanya Reddy<sup>1</sup>; Rafael Auras<sup>2</sup>; Sergey Rakov<sup>1</sup>; Craig Whitehouse<sup>1</sup>; George Perkins<sup>1</sup>; <sup>1</sup>PerkinElmer, Shelton, CT; <sup>2</sup>Michigan State University, East Lansing, MI
- WP 715 **Rapid Screening of Parabens in Personal Care Products using DSA/TOF with No Sample Preparation**; Avinash Dalmia; Thomas White; Fabian Oteiza; Carl Schwarz; Blas Cerda; George Perkins; PerkinElmer, Shelton, CT
- WP 716 **Rapid Measurement of Olive Oil Adulteration with Soybean Vegetable Oil with Minimal Sample Preparation Using DSA/TOF**; Avinash Dalmia; Nicola Vosloo; George Perkins; Blas Cerda; Craig Whitehouse; PerkinElmer, Shelton, CT
- WP 717 **Rapid Differentiation Between Natural and Artificial Vanilla Flavorings Using DSA/TOF with no Sample Preparation**; Avinash Dalmia; George Perkins; Craig Whitehouse; PerkinElmer, Shelton, CT
- WP 718 **Use of Sorbent Coated Metal Probes with Direct Analysis in Real Time (DART) Ionization for Rapid Analysis of Herbal Supplements**; Joseph LaPointe; Robert Goguen; Brian Musselman; Ionsense Inc., Saugus, MA
- WP 719 **Characterizing Toothpastes: Direct Fingerprinting of Key Volatile Flavor and Marker Non-volatile Compounds by DART QToF Mass Spectrometry**; Elizabeth Crawford<sup>1</sup>; Brian Musselman<sup>2</sup>; Jerry Zweigenbaum<sup>3</sup>; <sup>1</sup>Institute of Chemical Technology Prague, Prague, Czech Republic; <sup>2</sup>Ionsense, Inc., Saugus, MA; <sup>3</sup>Agilent Technologies, Wilmington, DE
- WP 720 **Pyrolysis for Rapid Screening of Contaminated Heparin by DART Mass Spectrometry**; Peter Nemes<sup>1</sup>; William Hoover<sup>1</sup>; David Keire<sup>2</sup>; <sup>1</sup>US FDA, CDRH, Silver Spring, MD; <sup>2</sup>US FDA, CDRH, St. Louis, IL
- WP 721 **Rapid Screening of 'White Powders' for Unknown Agents Using a DART-Equipped Compact Mass Spectrometer**; Jack Henion<sup>1</sup>; Brian Musselman<sup>2</sup>; Nigel Sousou<sup>1</sup>; <sup>1</sup>Advion, Inc., Ithaca, NY; <sup>2</sup>Ionsense, Saugus, MA
- WP 722 **High Resolution Accurate Mass (HRAM) Phthalate Screening Using Direct Analysis in Real Time (DART) Ambient Ionization**; Catharina Crone<sup>1</sup>; Elizabeth Crawford<sup>2</sup>; Yue Xuan<sup>1</sup>; Markus Kellmann<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Ionsense Inc., Saugus, MA
- WP 723 **Sensitive Screening of Abused Drugs in Raw Urine and Blood by Direct Analysis in Real Time Triple Quadrupole Mass Spectrometry**; Wenfang Zhang<sup>1</sup>; Zong Yang<sup>2</sup>; Ping Li<sup>3</sup>; Yong Chen<sup>4</sup>; Dazhou Chen<sup>2</sup>; Charles C. Liu<sup>5</sup>; <sup>1</sup>Forensic Science Service Public Security Bureau, Beijing, China; <sup>2</sup>National Institute of Metrology, Beijing, China; <sup>3</sup>Lumtech Technologies Limited, Beijing, China; <sup>4</sup>Labcare Solutions, Shanghai, China; <sup>5</sup>ASPEC Technologies Limited, Beijing, China
- WP 724 **Quantitation by DART-Orbitrap Mass Spectrometer: Preliminary Analysis of Pesticides in Water by Internal Standards**; Jaewon Choi; Wonseok Choi; Jeheon Jang; Yunduck Kim; Kwater, Daejeon, South Korea
- WP 725 **Exact and Quantitative Analysis of Deuterated Pyrene: New Method for the Rapid, Convenient Hydrogen-Deuterium Exchange of Polycyclic Aromatic Hydrocarbons**; Mark Domin; Boston College, Chestnut Hill, MA
- WP 726 **Rapid Quantitative Analysis of Trimethyl Phosphate in Water with Direct Analysis in Real Time Mass Spectrometry**; Xiaowei Wang<sup>1</sup>; Liping Liu<sup>1</sup>; Bing Shao<sup>1</sup>; Jingfu Liu<sup>2</sup>; Charles C. Liu<sup>3</sup>; <sup>1</sup>Beijing Center for Disease Control and Prevention, Beijing, China; <sup>2</sup>Chinese Academy of Sciences, Beijing, China; <sup>3</sup>ASPEC Technologies Limited, Beijing, China
- WP 727 **Desorption Atmospheric Pressure Photoionization-Mass Spectrometry for the Direct Analysis of Atmospheric Aerosols Collected on Quartz Filters**; Jevgeni Parshintsev<sup>1</sup>; Anu Vaikkinen<sup>1</sup>; Vladimír Vrkoslav<sup>2</sup>; Josef Cvacka<sup>2</sup>; Risto Kostianen<sup>1</sup>; Tapio Kotiaho<sup>1</sup>; Marja-Liisa Riekkola<sup>1</sup>; Tiina J. Kauppinen<sup>1</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland; <sup>2</sup>Czech Academy of Sciences, Prague, Czech Republic
- WP 728 **Implementation of Reactive Transmission Mode Desorption Electrospray Ionization – Ketone and Aldehyde Derivatization with Girard's T Reagent**; Alex Bishop; Jennifer Brodbelt; University of Texas, Austin, TX
- WP 729 **Normal Phase Liquid Chromatography Coupled to Continuous Flow – Extractive Desorption Electrospray Ionization – Mass Spectrometry for Phospholipid Analysis**; Li Li; Kevin Schug; Univ of Texas, Arlington, TX
- WP 730 **Coupling Free-Flow Electrophoresis with Desorption Electrospray Ionization Mass Spectrometry (DESI-MS) for Proteomic Analysis**; Sarah Anciaux; Michael Bowser; University of Minnesota, Minneapolis, MN
- WP 731 **Using Desorption Electrospray Ionization Mass Spectrometry to Detect Specific Decomposition Pathways of Ruthenium Catalysts during C-H Activation Reactions**; Cornelia Flender; Jennifer Roizen; Eric McNeill; Justin Du Bois; Richard Zare; Stanford University, Stanford, CA
- WP 732 **Detection of Explosive Molecular Adduct Ions with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry**; G. Asher Newsome<sup>1,2</sup>; Lauryn E. DeGreeff<sup>3</sup>; Christopher J. Katilie<sup>1,2</sup>; Kevin J. Johnson<sup>2</sup>; <sup>1</sup>Nova Research, Inc., Alexandria, VA; <sup>2</sup>U.S. Naval Research Laboratory, Washington, DC; <sup>3</sup>National Research Council, Washington, DC
- WP 733 **Analysis of Organic Light-Emitting Diodes (OLED) Using an Atmospheric Pressure MALDI Source Coupled to an Orbitrap-based Mass Spectrometer**; Maxie Kohler<sup>1</sup>; Kerstin Strupat<sup>2</sup>; Thorsten Umbach<sup>1</sup>; Heike Klesper<sup>1</sup>; Klaus Meerholz<sup>1</sup>; <sup>1</sup>University of Cologne, Cologne, Germany; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 734 **ESI and MALDI Sample Introduction, Preparation Unified By Electric Induction?** Drew Sauter<sup>1</sup>; Andrew Sauter III<sup>1</sup>; Alexander Scheeline<sup>2</sup>; Andrew Grange<sup>3</sup>; Gary Groenewold<sup>4</sup>; <sup>1</sup>Nanoliter, LLC, Henderson, NV; <sup>2</sup>University of Illinois, Urbana, IL; <sup>3</sup>USEPA, Las Vegas, NV; <sup>4</sup>Idaho National Lab, Idaho Falls, ID

#### Ion Mobility Fundamentals, 735 – 754

- WP 735 **Separation of Isomeric Nitro-PAH by TWIM-MS Using Polarizable Drift Gases: The Effects of Ion Charge Distribution on the Resolution**; Maira Fasciotti<sup>1</sup>; Caroline Franco<sup>2</sup>; Gabriel Heerdt<sup>3</sup>; Annibal D. Perreira Netto<sup>2</sup>; Nelson H. Morgon<sup>3</sup>; Romeu J. Daroda<sup>1</sup>; Marcos N. Eberlin<sup>4</sup>; <sup>1</sup>INMETRO, Rio de Janeiro, BR; <sup>2</sup>Federal Fluminense University, Niterói, Brazil; <sup>3</sup>UNICAMP, Campinas, BR; <sup>4</sup>Thomson Mass Spectrometry Laboratory, Campinas, BR
- WP 736 **Structure of Polyphenol Clusters – An Ion Mobility Study**; Frédéric Poussigue<sup>1,2</sup>; Arnaud Vernier<sup>1,3</sup>; Jérôme Lemoine<sup>1,2</sup>; Philippe Dugourd<sup>1,3</sup>; Fabien Chiro<sup>1,2</sup>; <sup>1</sup>Université Lyon 1, Villeurbanne, France; <sup>2</sup>CNRS, UMR 5280 ISA, Villeurbanne, France; <sup>3</sup>CNRS, UMR 5306 ILM, Villeurbanne, France
- WP 737 **Ion Mobility Mass Spectrometry of Small Molecule, Polymer, and Native Protein Complex Anions**; Samuel J. Allen; Alicia M. Schwartz; Matthew F. Bush; University of Washington, Seattle, WA

- WP 738 **Travelling Wave Ion Mobility Calibration with Phosphoric Acid Clusters;** Helene Lavanant; Vincent Tognetti; Carlos Afonso; *Normandie Univ UMR 6014, FR 3038; Univ Rouen; CNRS, Mont St Aignan, France*
- WP 739 **Ion Mobility-Mass Spectrometry of Iodide Salt Cluster Ions in Air and Comparison to Density Functional Theory Structural Predictions;** Chris Hogan; Hui Ouyang; Carlos Larriba-Andaluz; Derek Oberreit; *University of Minnesota, Minneapolis, Minnesota*
- WP 740 **Determination of Collision Cross Sections for Ion Standards using a New Commercial Drift Tube for IM-MS using Nitrogen Bath Gas;** Peter Backlund<sup>1</sup>; Stephanie Cologne<sup>1</sup>; Christopher Crutchfield<sup>1</sup>; Christian Klein<sup>2</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Alex Mordehai<sup>2</sup>; Alfred L. Yergey<sup>1</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 741 **Towards Predicting Differential Mobility Based Upon Molecular Structure;** Brad Schneider<sup>1</sup>; Erkinjon Nazarov<sup>2</sup>; Goran Ristic<sup>1</sup>; Thomas Covey<sup>1</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>Draper Laboratories, Tampa, FL
- WP 742 **Calculations of Ion Mobilities for Biological Macromolecules Using the Electronic Surface Representation;** Yuri Alexeev<sup>1</sup>; Dmitri G. Fedorov<sup>2</sup>; Alexandre A. Shvartsburg<sup>3</sup>; <sup>1</sup>Argonne National Laboratory, Argonne, IL; <sup>2</sup>Nanosystem Research Institute, Tsukuba, Japan; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA
- WP 743 **A New Paradigm for Electrospray Ion Mobility-Mass Spectrometry of Proteins;** Kent Gillig; Yu-Ling Chang; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- WP 744 **Multiplexed High Pressure Ion Mobility-TOFMS: High Resolution, Sensitivity and Structural Information in One Package;** Richard Knochenmuss; Stephan Graf; Katrin Fuhrer; Marc Gonin; *Tofwerk, Seftigen, Switzerland*
- WP 745 **Selected Accumulation Ion Mobility Spectrometry (SAIMS) Hyphenated with a Fourier Transform Mass Spectrometer (FTMS);** Melvin A. Park; Desmond Kaplan; Mark Ridgeway; *Bruker Daltonics, Inc., Billerica, MA*
- WP 746 **Maximizing Gas Phase Peak Capacity while Minimizing Analysis Time through DIMS/TIMS/MS;** Mark Ridgeway; Desmond Kaplan; Kevin Dixon; Melvin Park; *Bruker Daltonics, Billerica, MA*
- WP 747 **Development of a Spatially Multiplexed 8-Channel Ion Mobility-Mass Spectrometer: Vacuum System, Ion Source, and Interfacing Ion Funnel Arrays;** Katrina L. Leaptrot; Jody C. May; John A. McLean; *Vanderbilt University, Nashville, TN*
- WP 748 **Electrical Mobilities of Near-Spherical, Multiply-Charged Ionic Liquid Nanodrops in Air: Influence of Drift-Gas Temperature and Ion-Induced Dipole Interactions;** Juan Fernández García; Juan Fernández de la Mora; *Yale University, New Haven, CT*
- WP 749 **Measuring Reduced Ion Mobilities of Tetraalkylammonium Cations in Intermediate Field Using a Double Slit Differential Mobility Analyzer (DMA);** John van Nostrand; Udo Verkerk; K. W. Michael Siu; *York University - CRMS, Toronto, Canada*
- WP 750 **The Inability of Hard Sphere Specular Scattering to Predict Ion Mobility in Diatomic Gases in the 5-100kDa Range;** Carlos Larriba Andaluz; Christopher Hogan; *University of Minnesota, Minneapolis, MN*
- WP 751 **Distance Geometry: A Time Efficient Approach for Sampling Conformational Space in Support of Ion Mobility Structural Mass Spectrometry;** Sarah M. Stow<sup>1</sup>; Cody R. Goodwin<sup>1</sup>; Michal Kliman<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Ed Darland<sup>2</sup>; Brian O. Bachmann<sup>1</sup>; Terry P. Lybrand<sup>1</sup>; John A. McLean<sup>1</sup>; <sup>1</sup>Department of Chemistry at Vanderbilt University, Nashville, TN; <sup>2</sup>Agilent Technologies Inc., Santa Clara, CA
- WP 752 **Imaging the Ion Beam Inside a Drift Tube Ion Mobility Spectrometer Using a Pixelated Detector;** Harikrishnan Sukumar<sup>1</sup>; Stephen Davila<sup>1</sup>; John Stone<sup>2</sup>; Gary Eiceman<sup>1</sup>; <sup>1</sup>New Mexico State University, Las Cruces, NM; <sup>2</sup>Queen's University, Kingston, Ontario, Canada
- WP 753 **Development of a New Ion Mobility-Quadrupole Time-of-Flight Mass Spectrometer for High-Resolution and High-Throughput Biological Sample Analyses;** Ruwan Kurulugama<sup>1</sup>; Alexander Mordehai<sup>1</sup>; Nathan Sanders<sup>1</sup>; Christian Klein<sup>1</sup>; Yehia Ibrahim<sup>2</sup>; Erin Baker<sup>2</sup>; Richard Smith<sup>2</sup>; George Stafford<sup>1</sup>; John Fjeldsted<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- WP 754 **Reduced Ion Mobilities: A Need for Parameterization of Chemical Analyte Properties?** Philipp Cochems<sup>1</sup>; Walter Wissdorf<sup>2</sup>; Yessica Brachthaeuser<sup>2</sup>; Christine Polaczek<sup>2</sup>; Thorsten Benter<sup>2</sup>; Stefan Zimmermann<sup>1</sup>; <sup>1</sup>Leibniz University Hannover, Hannover, Germany; <sup>2</sup>University of Wuppertal, Wuppertal, Germany





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

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Imaging MS: Instrumentation.....	052-072
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LC-MS Instrumentation.....	108-120
LC-MS Sample Preparation (Proteins & Peptides).....	121-139
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Informatics: Peptide Identification/Characterization II.....	669-693
Ion Spectroscopy.....	694-710
Ion Structure / Energetics.....	711-727

### Ion Mobility – FAIMS, 001 -021

- ThP 001 **Parameters Characterization and Optimization in Differential Mobility Spectrometer Relative to Uses of LDTD Ion Source;** Sarah Demers<sup>1</sup>; Réal Paquin<sup>1</sup>; Gregory Blachon<sup>2</sup>; Pierre Picard<sup>2</sup>; Serge Auger<sup>2</sup>; <sup>1</sup>Université Laval, Quebec City, Canada; <sup>2</sup>Phytronix Technologies, Quebec City, Canada
- ThP 002 **Performance Characterization of a Differential Ion Mobility Spectrometer Operated in Laminarized Low-Pressure Subsonic Flows;** Dimitris Papanastasiou<sup>1</sup>; Ioannis Orfanopoulos<sup>1</sup>; Diamantis Kounadis<sup>1</sup>; Alexander Lekkas<sup>1</sup>; Ioannis Nikolas<sup>2</sup>; Roger Giles<sup>3</sup>; Andrew Entwistle<sup>3</sup>; Emmanuel Raptakis<sup>1</sup>; <sup>1</sup>Fasmatech, Athens, GR; <sup>2</sup>Technical University of Crete, Chania, GR; <sup>3</sup>Shimadzu Research Laboratory, Manchester, UK
- ThP 003 **Application of Differential Ion Mobility Technology to Improve the Quantitation of Small Molecules by LC-MS/MS;** Richard Grater; Naveed Shaik; Ellen Rohde; Lawrence Gan; *BiogenIdec, Cambridge, MA*
- ThP 004 **Identification of Compounds in Organic Aerosols Using Differential Ion Mobility Spectrometry and High Mass Accuracy Tandem Mass Spectrometry;** Sandra Spencer; Samantha Isenberg; Gary Glish; *University of North Carolina, Chapel Hill, NC*
- ThP 005 **Investigation of Vitamin K2 Structures Using Differential Ion Mobility Spectrometry and DFT Calculations;** David Crizer; Samantha Isenberg; Beth Marbois; Gary Glish; *University of North Carolina, Chapel Hill, NC*
- ThP 006 **Comparison of Electrospray, Nano-electrospray, and Low Temperature Plasma Ionization for Use with Differential Ion Mobility Spectrometry;** Brandon Santiago; Gary Glish; *University of North Carolina, Chapel Hill, NC*
- ThP 007 **Differential Mobility Separation Pre-filtration on an Agilent ESI Mass Spectrometer;** Theresa Evans-Nguyen; Spiros Manolagos; Franci Sinatra; James Alberti; Kevin Hufford; *Draper Laboratory, Tampa, FL*
- ThP 008 **Improving the LC-MS/MS Selectivity of Hexabromocyclododecane Diastereomers with Differential Mobility Spectrometry;** Changqing Lin<sup>1</sup>; Yi Pan<sup>1</sup>; Chen Zheng<sup>2</sup>; Yongming Xie<sup>2</sup>; <sup>1</sup>Shanghai Putuo Environmental Monitoring Station, Shanghai, China; <sup>2</sup>Shanghai AB Sciex Analytical Instrument Trading Co, Shanghai, China

- ThP 009 **A Sensitive and Selective LC-Differential Mobility-Mass Spectrometric Analysis of Allopregnanolone and Its Isomers in Human Plasma;** Wen Jin<sup>1</sup>; Michael Jarvis<sup>1</sup>; Michal Weinstock<sup>1</sup>; Margaret Altemus<sup>2</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>New York Presbyterian Hospital and Cornell University, New York, NY
- ThP 010 **Improving Protein and Peptide Detection by Combining Differential Mobility and Atmospheric Proton Transfer Reaction;** J.C. Yves Leblanc; J. Larry Campbell; Igor Chernushevich; Stephen Tate; *AB SCIEX, Concord, On, Canada*
- ThP 011 **Improving Speed and Selectivity of Targeted Peptide Quantification Using FAIMS;** Susan E. Abbatiello<sup>1</sup>; Lindsay Pino<sup>1</sup>; Michael Belford<sup>2</sup>; Eric Kuhn<sup>1</sup>; Nathan Yates<sup>3</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>The Broad Institute of Harvard and MIT, Cambridge, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>University of Pittsburgh, Pittsburgh, PA
- ThP 012 **High-Throughput Analysis of Drugs in Biological Matrices with Enhanced Selectivity for Quantitation Using FAIMS SPE/MS/MS;** Michael Ugarov<sup>1</sup>; Yuqin Dai<sup>1</sup>; Kari Schlicht<sup>2</sup>; Vaughn Miller<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Wakefield, MA
- ThP 013 **Faster Reaction Monitoring of Reductive Amination Using Chip-Based FAIMS-MS;** Lauren Brown<sup>1</sup>; Celine Laine<sup>1</sup>; Danielle Toutoungi<sup>1</sup>; Shelly Li<sup>2</sup>; Gilles Goetz<sup>2</sup>; Guilong Cheng<sup>2</sup>; <sup>1</sup>Owlstone Ltd, Cambridge, UK; <sup>2</sup>Pfizer Global R&D, Groton, CT
- ThP 014 **Separation of Isomers Using Modifier Gases on Chip-based FAIMS / Triple Quadrupole MS;** Christopher Beekman<sup>1</sup>; Timothy J. Garrett<sup>1</sup>; Michael Ugarov<sup>2</sup>; George Stafford<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 015 **Electrospray/ High-field Asymmetric Waveform Ion Mobility Spectrometry/ Mass Spectrometry of Transition Metals: Potential for Environmental and Nuclear Applications;** Jared Boock; Richard Yost; *University of Florida, Gainesville, FL*
- ThP 016 **Using Gas Additives to Improve Signal Intensity and Selectivity of a Cylindrical FAIMS Device;** Randy W. Purves<sup>1</sup>; Allison R. Ozog<sup>1</sup>; Stephen J. Ambrose<sup>1</sup>; Michael Belford<sup>2</sup>; Satendra Prasad<sup>2</sup>; Jean-Jacques Dunyach<sup>2</sup>; <sup>1</sup>National Research Council, Saskatoon, Canada; <sup>2</sup>Thermo Fisher, San Jose, CA



- ThP 017 **Ion Mobility Separations of Protein Conformers with Resolving Power up to 400 Using Hydrogen-Rich Gas Buffers;** Alexandre A. Shvartsburg; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- ThP 018 **Effect of Electrode Geometry on FAIMS Gas Flow With Regard to Sensitivity and Resolution;** Michael Belford; Satendra Prasad; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- ThP 019 **Exploring the Effects of Carrier Gas Modifiers Using Chip-Based Field Asymmetric Waveform Ion Mobility Spectrometry Combined with Mass Spectrometry;** Robert Smith<sup>1</sup>; Danielle Toutoungi<sup>2</sup>; James Reynolds<sup>1</sup>; Ashley Sage<sup>3</sup>; Billy Boyle<sup>2</sup>; Colin Creaser<sup>1</sup>; <sup>1</sup>Loughborough University, Loughborough, UK; <sup>2</sup>Owlstone Ltd, Cambridge, UK; <sup>3</sup>Agilent Technologies, Stockport, UK
- ThP 020 **Identification of Amino-Sulfonamide Isomers Using Chip-Based FAIMS-MS Approaches;** Danielle Toutoungi<sup>1</sup>; Lauren Brown<sup>1</sup>; Billy Boyle<sup>1</sup>; Samantha J Barry<sup>2</sup>; Jean-Claude Wolff<sup>2</sup>; <sup>1</sup>Owlstone Ltd, Cambridge, UK; <sup>2</sup>GlaxoSmithKline, Stevenage, UK
- ThP 021 **Analysis of Intact Protein Ions by Chip-Based-FAIMS-MS;** Lauren Brown<sup>1</sup>; Danielle Toutoungi<sup>1</sup>; Billy Boyle<sup>1</sup>; Colin Creaser<sup>2</sup>; <sup>1</sup>Owlstone Ltd., Cambridge, UK; <sup>2</sup>Loughborough University, Loughborough, UK

#### Imaging MS: Large Molecules, 022 – 025

- ThP 022 **DESI Detection of Surface Proteins with MS Imaging and MVA Analysis;** Wei Rao; Adam Celiz; David Scurr; Morgan Alexander; David Barrett; *University of Nottingham, Nottingham, UK*
- ThP 023 **Quantitation of Peptides by MALDI Imaging Using Labeled Peptide;** Guillaume Hochart; David Bonnel; Gregory Hamm; Raphael Legouffe; Fabien Pamelard; Jonathan Stauber; *ImaBiotech, MS Imaging Department, Lille, France*
- ThP 024 **Imaging of Nanoparticle Biodistributions *in vivo* Using Laser Desorption/Ionization Mass Spectrometry;** Bo Yan; Sung Tae Kim; Chang Soo Kim; Krishnendu Saha; Daniel F. Moyano; Vincent M. Rotello<sup>\*</sup>; Richard W. Vachet<sup>\*</sup>; *University of Massachusetts, Amherst, MA*
- ThP 025 **MALDI Imaging and In Source Decay Identification of Glioma Biomarkers up to 80kDa;** Rima Ait-Belkacem<sup>1</sup>; Caroline Berenguer<sup>1</sup>; Claude Villard<sup>1</sup>; Sega Ndiaye<sup>1</sup>; L'Houcine Ouafik<sup>1</sup>; Dominique Figarella-Branger<sup>1</sup>; Olivier Chinot<sup>2</sup>; Daniel Lafitte<sup>1</sup>; <sup>1</sup>AIX Marseille Universite, Marseille, France; <sup>2</sup>Assistance publique hopitaux de Marseille, Marseille, France

#### Imaging MS: Quantitative Analysis, 026 – 030

- ThP 026 **Grid Method: A Novel Workflow for Dissection and LC-MS/MS Analysis to Study Ocular Drug Distribution;** Josh Rowe; Julie Whitcomb; Chris Huntington; Jinsong Ni; *Allergan, Inc., Irvine, CA*
- ThP 027 **Quantitative Bioimaging of Drugs in Thin Tissue Sections;** Olga Reifschneider<sup>1</sup>; Christoph A. Wehe<sup>1</sup>; Michael Sperling<sup>1, 2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Münster, Münster, Germany; <sup>2</sup>European Virtual Institute for Speciation Analysis, Münster, Germany
- ThP 028 **A Quantitative Study of Peptide Release by Mass Spectrometry Imaging of Microfluidic Microchannels;** Callie Croushore<sup>1, 2</sup>; Stanislav Rubakhin<sup>1, 2</sup>; Jonathan Sweedler<sup>1, 2</sup>; <sup>1</sup>Beckman Institute, UIUC, Urbana, IL; <sup>2</sup>Department of Chemistry, UIUC, Urbana, IL
- ThP 029 **Quantitative DESI & MALDI Imaging Applied on Ophthalmic Related Compound Distribution Study;** Raphael Legouffe<sup>1</sup>; Joseph H Kennedy<sup>2</sup>; Gregory Hamm<sup>1</sup>;

Fabien Pamelard<sup>1</sup>; Justin Wiseman<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>ImaBiotech, MS Imaging Department, Lille, France; <sup>2</sup>Prosolia, Inc., Indianapolis, IN

- ThP 030 **Spatially-Aware Feature-Sparse Clustering for Mass Spectrometry Imaging;** Kyle Bemis<sup>1</sup>; Livia Eberlin<sup>2</sup>; Christina Ferreira<sup>1</sup>; R. Graham Cooks<sup>1</sup>; Olga Vitek<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Stanford University, Palo Alto, CA

#### Imaging MS: Method Development II, 031 – 051

- ThP 031 **MALDI Imaging MS of Intact Pollen Grains and Pollen Mixtures;** Steffen M. Weidner<sup>1</sup>; Bernd Enthalder<sup>2</sup>; Benjamin C. Krause<sup>3</sup>; <sup>1</sup>Federal Inst. for Materials Research & Testing, 1.3, Berlin, Germany; <sup>2</sup>University of Hamburg, Institute of Food Chemistry, Hamburg, Germany; <sup>3</sup>Humboldt-University, Physical Chemistry, Berlin, Germany
- ThP 032 **Development of the Technique for Visualizing the Plant Metabolites Distribution Using MALDI-MS Imaging;** Junya Nakamura<sup>1</sup>; Maiko Kaku<sup>2</sup>; Yoshinori Fujimura<sup>2</sup>; Katsutoshi Takahashi<sup>3</sup>; Daisuke Miura<sup>2</sup>; Hiroyuki Wariishi<sup>4</sup>; <sup>1</sup>Grad. Sch. Biores. Bioenviron. Sci., Kyushu Univ., Fukuoka, Japan; <sup>2</sup>ICMRN, Kyushu Univ., Fukuoka, Japan; <sup>3</sup>AIST, Tokyo, Japan; <sup>4</sup>Fac. Arts and Sci., Kyushu Univ., Fukuoka, Japan
- ThP 033 **Pre-coated Targets with Matrix and Trypsin for *in-situ* Protein Digestion in Imaging Mass Spectrometry;** Faizan Zubair; Junhai Yang; Jeremy L. Norris; Richard M. Caprioli; Paul E. Laibinis; *Vanderbilt University, Nashville, TN*
- ThP 034 **The Challenge of On-Tissue Digestion for MALDI-IMS a Comparison of Different Protocols to Improve Imaging Experiments;** Hanna Diehl<sup>1</sup>; Julian Elm<sup>1</sup>; Judith Baronner<sup>1</sup>; Dennis Trede<sup>2</sup>; Herbert Thiele<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Corinna Henkel<sup>1</sup>; <sup>1</sup>Medizinisches Proteom-Center, Ruhr-University, Bochum, Germany; <sup>2</sup>Steinbeis Innovation Center SCiLS, Bremen, Germany
- ThP 035 **High Resolution MALDI Imaging at 25 µm Pixel Size for Peptides after On-Tissue Digestion;** Andreas Roempp; Katharina Huber; Yvonne Schober; Thorsten Schramm; Bernhard Spengler; *Justus Liebig University, Giessen, Germany*
- ThP 036 **Acquisition and Analysis of 3D MALDI Imaging Data Sets;** Shannon Cornett<sup>1</sup>; Janina Oetjen<sup>2</sup>; Dennis Trede<sup>3, 4</sup>; Michaela Aichler<sup>5</sup>; Jan Strehlow<sup>6</sup>; Stefan Heldmann<sup>7</sup>; Judith Berger<sup>8</sup>; Michael Gottschalk<sup>9</sup>; Klaus Steinhörst<sup>3</sup>; Jan Hendrik Kobarg<sup>3, 4</sup>; Stefan Wirtz<sup>6</sup>; Stefan Schifferle<sup>3, 4</sup>; Herbert Thiele<sup>3</sup>; Axel Walch<sup>5</sup>; Peter Maass<sup>3, 4</sup>; Theodore Alexandrov<sup>3, 4</sup>; Detlev Suckau<sup>9</sup>; Michael Becker<sup>9</sup>; <sup>1</sup>Bruker Daltonics, Billerica, MA; <sup>2</sup>University of Bremen, MALDI Imaging Lab, Bremen, Germany; <sup>3</sup>Steinbeis Innovation Center SCiLS, Bremen, Germany; <sup>4</sup>Univ. Bremen, Center for Industrial Mathematics, Bremen, Germany; <sup>5</sup>Helmholtz-Zentrum München, Dept. of Pathology, Munich, Germany; <sup>6</sup>Fraunhofer MEVIS Inst. for Medical Image Computing, Bremen, Germany; <sup>7</sup>Fraunhofer MEVIS Project Group Image Registration, Lübeck, Germany; <sup>8</sup>Bruker Biospin MRI GmbH, Ettlingen, Germany; <sup>9</sup>Bruker Daltonik GmbH, Bremen, Germany
- ThP 037 **Polyhydroxyflavonoids as a Novel Family of Matrices for MALDI Tissue Imaging;** Xiaodong Wang<sup>1</sup>; Jun Han<sup>1</sup>; Albert Chou<sup>1</sup>; Juncong Yang<sup>1</sup>; Jingxi Pan<sup>1</sup>; Christoph Borchers<sup>1, 2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Dept of Biochemistry and Microbiology, U Victoria, Victoria, Canada
- ThP 038 **2D Graphene as a MALDI IMS Matrix for Brain Tissue;** William Friesen; Brian Schultz; Joe Steet; Sarbajit Banerjee; Troy Wood; *SUNY at Buffalo, Buffalo, NY*

- ThP 039 **Imaging MALDI Mass Spectrometry in Microscope Mode with Infrared Lasers – Breaking the Diffraction Limit on Biological Samples;** Jens Soltwisch; Julia Jungmann; Donald F. Smith; Andras Kiss; Shane Ellis; Ron Heeren; *FOM Institute AMOLF, Amsterdam, the Netherlands*
- ThP 040 **Correlated Imaging Mass Spectrometry and Raman Spectroscopy for Oncology and Drug Resistance;** Dorothy Ahlf; Eric Weaver; Rachel Masyuko; Haohang Li; Paul Bohn; Amanda Hummon; *University of Notre Dame, Notre Dame, IN*
- ThP 041 **Silver Assisted LDI for High Spatial Resolution Imaging MS of Olefins from Thin Tissue Sections;** Martin Dufresne<sup>1</sup>; Aurelien Thomas<sup>1</sup>; Julien Breault-Turcot<sup>2</sup>; Jean-François Masson<sup>2</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>*Pierre Chaurand Group, Montréal, Canada*; <sup>2</sup>*Jean-François Masson, Montreal, Canada*
- ThP 042 **Novel Bioinformatics Platform for Interactive Interrogation of DESI-mass Spectrometry Imaging Datasets in Clinical Research Settings;** Kirill Veselkov<sup>1</sup>; Reza Mirnezami<sup>1</sup>; Nicole Strittmatter<sup>1</sup>; James Kinross<sup>1</sup>; Robert Goldin<sup>1</sup>; Abigail Speller<sup>1</sup>; Tigran Abramov<sup>2</sup>; Ara Darzi<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>*Imperial College London, London, UK*; <sup>2</sup>*Sevastopol National Technical University, Streletskaya Bay, Crimea, Ukraine*
- ThP 043 **Characterizing and Imaging Glycerophosphocholine Lipids by Lithiation and C60-SIMS;** Anita Durairaj; Lauren M. Jackson; Nicholas Winograd; *The Pennsylvania State University, University Park, PA*
- ThP 044 **Blotting Assisted by Heating and Solvent Extraction for DESI-MS Imaging of Biological Tissues;** Elaine Cristina Cabral<sup>1</sup>; Mario Francesco Mirabelli<sup>2</sup>; Consuelo J. Perez<sup>1</sup>; Demian Rocha Ila<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*; <sup>2</sup>*University of Calabria, Cosenza, Italy*
- ThP 045 **The Evolution of 3D Biological Imaging to FIB-TOF Tomography;** Gregory L. Fisher; John S. Hammond; Scott R. Bryan; *Physical Electronics, Chanhassen, MN*
- ThP 046 **High-Sensitivity Bio-Molecular Imaging and Protein Identification with a C<sub>60</sub> Ion Microprobe;** John Hammond<sup>1</sup>; Gregory Fisher<sup>1</sup>; Mark Jansen<sup>2</sup>; Luke MacAleese<sup>2</sup>; Ron Heeren<sup>2</sup>; <sup>1</sup>*Physical Electronics, Chanhassen, MN*; <sup>2</sup>*FOM/AMOLF, Amsterdam, The Netherlands*
- ThP 047 **Molecular Imaging and Analysis of Drugs by Laser Ablation Atmospheric Pressure Chemical Ionization Mass Spectrometry (LA/APCI-MS);** Christina Herdering; Christoph A. Wehe; Olga Reifschneider; Michael Sperling; Uwe Karst; *University of Münster, Münster, Germany*
- ThP 048 **Visualization of Lipid Species on Human Retina Using Mass Microscope;** Takahiro Hayasaka<sup>1</sup>; Naoko Goto-Inoue<sup>2</sup>; Noritaka Masaki<sup>1</sup>; Mitsutoshi Setou<sup>1</sup>; <sup>1</sup>*Hamamatsu University School of Medicine, Hamamatsu, Japan*; <sup>2</sup>*Tokyo Metropolitan University, Hachioji, Japan*
- ThP 049 **Mass Spectrometry Analysis and Imaging of Lipids and Proteins in Human Liver via MALDI and Liquid Extraction Surface Analysis;** Joscelyn Sarsby; Rian L. Griffiths; Rory Steven; Alan Race; Emily Guggenheim; Trish Lalor; Helen J. Cooper; Josephine Bunch; *University of Birmingham, Birmingham, UK*
- ThP 050 **Microscope Mode Mass Spectrometry – An Approach for Improved Imaging over Multiple Mass Ranges;** Benjamin Winter; Edward Halford; Simon-John King; Alexandra Lauer; Claire Vallance; Mark Brouard; *University of Oxford, Oxford, UK*
- ThP 051 **Laserspray Ionization on an Orbitrap Exactive : Performing Imaging Mass Spectrometry at Ultra High Mass Resolution;** Andrew F. Harron; Khoa Hoang; Charles McEwen; *USP, Philadelphia, PA*
- Imaging MS: Instrumentation, 052 – 072**
- ThP 052 **Robotic Plasma Probe Ambient Ionization Mass Spectrometry Imaging of Non-Planar Surfaces;** Ezequiel M. Morzan<sup>1,2</sup>; Rachel V. Bennett<sup>2</sup>; Facundo M. Fernandez<sup>2</sup>; <sup>1</sup>*Universidad de Buenos Aires, Buenos Aires, Argentina*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*
- ThP 053 **Near-Field Laser Ablation for Mass Spectrometry of Single Cells;** Yonathan Merid; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- ThP 054 **Rapid Imaging of Unprocessed Chicken Bone Marrow by LAESI-MS with T-Wave Ion Mobility Separation Using a Synapt G2-S;** Emmanuelle Claude<sup>1</sup>; Michel W.F. Nielen<sup>2,3</sup>; Brent R. Reschke<sup>4</sup>; Hilary Major<sup>1</sup>; <sup>1</sup>*Waters Corporation, Manchester, UK*; <sup>2</sup>*RIKILT, Wageningen, The Netherlands*; <sup>3</sup>*Wageningen University, Lab of Organic Chemistry, Wageningen, The Netherlands*; <sup>4</sup>*Protea Biosciences, Morgantown, US*
- ThP 055 **Mass Imaging Analysis of Oligonucleotides and Peptides Microarrays by Using Microscopic MALDI Imaging Mass Spectrometry;** Joo Yeon Oh<sup>1</sup>; Sohee Yoon<sup>1</sup>; Jeong Hee Moon<sup>2</sup>; Sang Yun Han<sup>1</sup>; Tae Geol Lee<sup>1</sup>; <sup>1</sup>*Korea Res. Inst. of Standards and Science, Daejeon, South Korea*; <sup>2</sup>*Korea Res. Inst. of Bioscience and Biotechnology, Daejeon, South Korea*
- ThP 056 **Fast Survey Scan Acquisition and Multiple Detector Utilization for Elemental Mass Spectrometric Bioimaging;** Christoph Alexander Wehe<sup>1</sup>; Olga Reifschneider<sup>1</sup>; Ann-Christin Bülter<sup>1</sup>; Michael Kieshauer<sup>1</sup>; Michael Sperling<sup>1,2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>*University of Münster, Münster, Germany*; <sup>2</sup>*European Virtual Institute for Speciation Analysis, Münster, Germany*
- ThP 057 **A Method For Rapid Matrix Sublimation for MALDI Lipid Ion Imaging;** Vijanaka Fernando<sup>2</sup>; Vladimir Collado<sup>1</sup>; Victor Spicer<sup>1</sup>; Werner Ens<sup>1</sup>; <sup>1</sup>*University of Manitoba, Winnipeg, Canada*; <sup>2</sup>*The Open University of Sri Lanka, Colombo, Sri Lanka*
- ThP 058 **Atmospheric Pressure MALDI Imaging Mass Spectrometry with High Spatial Resolution;** Berk Oktem; Konstantin Novoselov; Jianhua Tang; Vladimir Doroshenko; *MassTech Inc., Columbia, MD*
- ThP 059 **The Implementation of the Time-Stamping, Multi-Hit PIMMS Sensor in Combination with a Commercially Available Time-Of-Flight Mass Spectrometer;** Edward Halford<sup>1</sup>; Samuel Coles<sup>1</sup>; Alexandra Lauer<sup>1</sup>; Benjamin Winter<sup>1</sup>; Jason W. L. Lee<sup>1</sup>; Mark Mills<sup>2</sup>; Steve Thompson<sup>2</sup>; Claire Vallance<sup>1</sup>; Mark Brouard<sup>1</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*SAI, Manchester, UK*
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- ThP 061 **Protein and Lipid Tissue Imaging at 5 µm Spatial Resolution, Using Commercial Bruker MALDI TOFMS Instrument with Gaussian Laser Beam;** Andre Zavalin<sup>1</sup>; Junhai Yang<sup>1</sup>; Andreas Haase<sup>2</sup>; Armin Holte<sup>2</sup>; Richard Caprioli<sup>3</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Vanderbilt University School of Medicine, Nashville, TN*
- ThP 062 **Differential Mobility-Enhanced Ambient Mass Spectrometry Imaging;** Chaminda M. Gamage<sup>1</sup>; Rachel V. Bennett<sup>1</sup>; Asiri S. Galhena<sup>2</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*The Coca-Cola Company, Atlanta, GA*



- ThP 063 **Rapid Prototyping of a Low-Temperature Plasma Mass Imaging System (LTP-MSI) by Using Phidgets and OpenMZxy**; Mauricio Maldonado-Torres; Pedro Jiménez-Sandoval; Robert Winkler; *CINVESTAV Unidad Irapuato, Irapuato, Mexico*
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- ThP 078 **Electro-Hydrodynamic Simulations for Mass Spectrometers in Transitional Flow Regime**; Xiaoyu Zhou; Ouyang Zheng; *Biomedical Engineering School, Purdue University, West Lafayette, IN*
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- ThP 092 **GPU Based Ion Cloud Dynamics Simulation in Orbitrap with Accounting for Space Charge Shielding by the Inner Electrode;** Pavel Ryumin; Gleb Vladimirov; Eugene Nikolaev; *The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation*
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- ThP 105 **Preparative Scale Mass Spectrometry: A Modernized Electromagnetic Isotope Separator;** Kevin Hart; Brian Egle; W. Scott Aaron; *Oak Ridge National Laboratory, Oak Ridge, TN*
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- ThP 116 **Strategies for Structure Elucidation Using Ultrafast Mass Spectrometry (UFMS): Using nMS<sup>2</sup> as an Alternative to MS<sup>3</sup>;** Paul Wynne<sup>1,2,3</sup>; Nigel Grieves<sup>1,2,3</sup>; Bruce Fraser<sup>1,2,3</sup>; <sup>1</sup>Shimadzu Australasia, Sydney, Australia; <sup>2</sup>Shimadzu Australasia, Palmerston North, New Zealand; <sup>3</sup>Shimadzu Australasia, Melbourne, Australia
- ThP 117 **On-Chip LC Separations for Inlet Ionization Based Mass Spectrometry Detection;** Berk Oktem<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; Eric L. Kendall<sup>2</sup>; Don L. DeVoe<sup>2</sup>; <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>University of Maryland, College Park, MD
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- ThP 119 **Maximizing Triple Quadrupole Mass Spectrometry Productivity Through the Automated Use of an Expanded Dual-Channel HPLC System with Online Sample Cleanup;** Kevin McCann; Sameer Nene; Doug McIntyre; Edmond Neo; Dennis Nagtalon; Dorothy Yang; Agilent Technologies, Santa Clara, CA
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- ThP 122 **Specific and Efficient N-propionylation of histones with Propionic acid N-hydroxysuccinimide Ester for Histone Marks Characterization by LC-MS;** Rijing Liao<sup>1</sup>; Yanyan Yu<sup>1</sup>; shaolian zhou<sup>1</sup>; wei yi<sup>1</sup>; huili zhai<sup>2</sup>; <sup>1</sup>China Novartis Institutes for Biomedical Research, Shanghai, China; <sup>2</sup>Novartis Institutes for BioMedical Research, Inc., Boston, MA
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- ThP 124 **An Optimized Method for Preparing Yeast and Human Protein Extracts for Mass Spectrometry Method Development and Instrument Validation;** Sergei Savelyev; Ethan Strauss; Mike Rosenblatt; Marjeta Urh; Promega Corporation, Madison, WI
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- ThP 126 **Enhanced Protein Mass Spectrometry Analysis with Trypsin/Lys-C Mix;** Marjeta Urh<sup>1</sup>; Sergei Savelyev<sup>1</sup>; Ethan Strauss<sup>1</sup>; Mike Rosenblatt<sup>1</sup>; Richard Jones<sup>2</sup>; Michael Ford<sup>2</sup>; Dave Allen<sup>2</sup>; <sup>1</sup>Promega, Madison, WI; <sup>2</sup>MSBioworks LLC, Ann Arbor, MI
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- ThP 128 **Electroelution for Sample Preparation Enabling Top Down Proteomics of Native and Denatured Proteins;** Luis Henrique Ferreira Do Vale<sup>1</sup>; Adam Catherman<sup>1</sup>; John Tran<sup>1</sup>; Philip Compton<sup>1</sup>; Paul Thomas<sup>1</sup>; Edivaldo Ximenes Filho<sup>2</sup>; Marcelo Valle de Sousa<sup>2</sup>; Neil Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Universidade de Brasilia, Brasilia, Brazil
- ThP 129 **Proteomic Analysis of the Murine Presynaptic Active Zone by Fractionation at High pH and nLC-ESI-MS/MS;** Benjamin F. Mueller<sup>1</sup>; Melanie Lassek<sup>2</sup>; Marion Rohmer<sup>1</sup>; Dominic Baeumlisberger<sup>3</sup>; Jens Weingarten<sup>2</sup>; Walter Volknandt<sup>2</sup>; Michael Karas<sup>1</sup>; <sup>1</sup>Goethe-University, Institute of Pharm. Chemistry, Frankfurt am Main, Germany; <sup>2</sup>Goethe-University, Institute of Neuroscience, Frankfurt am Main, Germany; <sup>3</sup>SunChrom GmbH, Friedrichsdorf, Germany
- ThP 130 **Effects of Matrix Age on Protein Binding Results Extracted with a Prototype Phospholipid Removal Plate and Analyzed Using MFLC-MS/MS;** Chad Christianson; Casey Johnson; Sharon Cox; Shane Needham; Alturas Analytics, Moscow, ID
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- ThP 291 **A Mass Spectrometry Based View at the Origin and Role of Tyrosine Phosphorylation in Multi-Cellularity;** A.F. Maarten Altelaar<sup>1</sup>; Jeffrey Ringrose<sup>1</sup>; Henk van den Toorn<sup>1</sup>; Michael Eitel<sup>2</sup>; Harm Post<sup>1</sup>; Pieter Neerincx<sup>1</sup>; Bernd Schierwater<sup>2</sup>; Albert Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*Tierärztliche Hochschule, Hannover, Germany*
- ThP 292 **Fuelling the Knowledge of Blood Coagulation Signaling with Time Resolved Quantitative Phosphoproteomics of Thrombin-Stimulated Endothelial Cells;** Maartje Van Den Biggelaar<sup>1</sup>; Juan-Ramon Hernandez<sup>2</sup>; Alexander B Meijer<sup>1</sup>; Koen Mertens<sup>1</sup>; Sara Zanivan<sup>2</sup>; <sup>1</sup>*Sanquin Research, Amsterdam, The Netherlands*; <sup>2</sup>*Beatson Institute for Cancer Research, Glasgow, UK*
- ThP 293 **Tyrosine Phosphoproteomics Analysis of Human Skeletal Muscle;** DanJun Ma<sup>1</sup>; Michael Caruso<sup>1</sup>; Monique Lewis<sup>1</sup>; Xiangmin Zhang<sup>1</sup>; Zaher Msallaty<sup>1</sup>; Berhane Seyoum<sup>1</sup>; Jeffrey Horowitz<sup>2</sup>; Zhengping Yi<sup>1</sup>; <sup>1</sup>*Wayne state university, Detroit, MI*; <sup>2</sup>*Division of Kinesiology, University of Michigan, Ann Arbor, MI*
- ThP 294 **Elucidation and Validation of Cell Signaling Activated by Ischemic Preconditioning in the Rat Myocardium by Phosphoproteomics: The Role of mTOR;** Kiersten Liddy; Melanie White; Benjamin Parker; Nestor Solis; Brett Hambly; Stuart Cordwell; *The University of Sydney, Sydney, Australia*
- ThP 295 **Impact of the Degree of Peptide Phosphorylation on Quantitation by Liquid Chromatography ICP- and ESI-MS;** Guillaume Ballihaut; W. Clay Davis; *NIST, Charleston, SC*
- ThP 296 **Triple SILAC Phosphoproteomics Reveals Drug Targets in Multiple Myeloma Cells: A Case for CID over HCD Using the Orbitrap Elite;** Susanne Breikopf<sup>1</sup>; Min Yuan<sup>1</sup>; John M Asara<sup>1,2</sup>; <sup>1</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- ThP 297 **Global Phosphorylation Profiling Reveals Pathways in Cardio-Protective Signaling Induced by Fibroblast Growth Factor 2 (FGF2) during Cardiac Ischemia/Reperfusion Injury;** Aruna Wijeratne; Janet Manning; Jo El Schultz; Ken Greis; *University of Cincinnati, Cincinnati, OH*
- ThP 298 **Implementing Multiplexed SID-MRM-MS Assays to Quantify Phosphorylated Peptides in the DNA Damage Response Pathway;** Jacob Kennedy; Richard Ivey; Jeffrey Whiteaker; ChenWei Lin; Uliana Voytovich; Amanda Paulovich; *Fred Hutchinson CRC, Seattle, WA*
- ThP 299 **Parallel Reaction Monitoring Assays for Phosphorylation Sites of AKT Isoforms in Patient-Derived Breast Cancer Xenografts with PI3K-AKT Pathway Aberrations;** Matthew Meyer<sup>1</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Kelly V. Ruggles<sup>2</sup>; Jeanne Rumsey<sup>1</sup>; Jeremy Hoog<sup>1</sup>; Jacqueline Snider<sup>1</sup>; Robert Kitchens<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; David Fenyo<sup>2</sup>; Brigitte Simons<sup>3</sup>; Jason Held<sup>4</sup>; Matthew J. Ellis<sup>1</sup>; R. Robert Townsend<sup>1</sup>; <sup>1</sup>*Washington University School of Medicine, St. Louis, Missouri*; <sup>2</sup>*New York University, New York, NY*; <sup>3</sup>*AB Sciex, Toronto, CA*; <sup>4</sup>*Buck Institute, Novato, CA*
- ThP 300 **A SILAC-based Phosphoproteomic Analysis of Human Cervical Cancer Cells upon Staurosporine-induced Apoptosis;** Weitao Jia<sup>1,2</sup>; Armann Andaya<sup>2</sup>; Julie Leary<sup>2</sup>; <sup>1</sup>*Campus Mass Spectrometry Facilities, U.C.Davis, Davis, CA*; <sup>2</sup>*Dept. of Molecular and Cellular Biology, U.C.Davis, Davis, CA*
- ThP 301 **Quantification of Phosphorylation on Eukaryotic Initiation Factors;** Armann Andaya; Nancy Villa; Nick Mahoney; Weitao Jia; Christopher Fraser; Julie Leary; *Dept. of Molecular and Cellular Biology, UC, Davis, CA*
- ThP 302 **Profiling the Phosphoproteome of Healthy Mouse Brain: From Discovery to Targeted Quantitation;** Jenny M Armenta<sup>1</sup>; Brad J. Williams<sup>1</sup>; Erik J. Soderblom<sup>2</sup>; Brenna M. Richardson<sup>2</sup>; Meredith E. Turner<sup>2</sup>; J. Will Thompson<sup>2</sup>; M. Arthur Moseley<sup>2</sup>; LeRoy Martin<sup>1</sup>; Michael J. Nold<sup>1</sup>; <sup>1</sup>*Waters, Beverly, MA*; <sup>2</sup>*Duke University Medical Center, Durham, NC*
- ThP 303 **Discovering Immediate-early Events of Hedgehog Signal Transduction in Tumorigenesis and Cerebellar Development;** Teresa Purzner; *Stanford University, Stanford, CA*
- ThP 304 **Capturing Native Protein States in Real-Time Using a Novel MS Compatible Phosphatase and Protease Inhibitor Formulation;** Jeff Turner; Gordon Nicol; Tina Kornmeier; Lillian Vickery; Pegah Jalili; John Dapron; Henry Duewel; *Sigma-Aldrich Corporation, St. Louis, MO*
- ThP 305 **Mass Spectrometry Analysis of c-Jun N-Terminal Kinase-Mediated Mitochondrial Protein Phosphorylation in Liver Injury;** Li-Rong Yu<sup>1</sup>; Sehwan Jiang<sup>2</sup>; Mohamed Abdelmegeed<sup>2</sup>; Yuan Gao<sup>1</sup>; Atrayee Banerjee<sup>2</sup>; Byoung-Joon Song<sup>2</sup>; <sup>1</sup>*National Center for Toxicological Research, FDA, Jefferson, AR*; <sup>2</sup>*National Institute on Alcohol Abuse and Alcoholism, Bethesda, MD*
- ThP 306 **PITRAQ, a Strategy to Simultaneously Correlate Protein Expression and Phosphorylation Stoichiometry between Different Samples: Evaluation on Different Mass Spectrometers;** Pieter Glibert<sup>1</sup>; Maarten Dhaenens<sup>1</sup>; Filip Van Nieuwerburgh<sup>1</sup>; Lennart Martens<sup>2,3</sup>; Dieter Deforce<sup>1</sup>; <sup>1</sup>*Pharmaceutical Biotechnology, Ghent University, Ghent, Belgium*; <sup>2</sup>*Department of Medical Protein Research, VIB, Ghent, Belgium*; <sup>3</sup>*Department of Biochemistry, Ghent University, Ghent, Belgium*

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- ThP 307 **Characterization of Mitochondrial Ubiquitin Substrates of Parkin and USP30 by Mass Spectrometry;** Lilian Phu; Joy Tea; Christian Cunningham; Daisy Bustos; Corey E. Bakalarski; Qinghua Song; William F. Forrest; Jacob Corn; Morgan Sheng; Baris Bingol; Donald S. Kirkpatrick; *Genentech, South San Francisco, CA*
- ThP 308 **Characterization of a Segmentally <sup>15</sup>N-Labeled Branched Ubiquitin Trimer;** Yan Wang; Emma Dixon; Carlos Castaneda; Tanuja Kashyap; David Fushman; *University of Maryland, College Park, MD*
- ThP 309 **Quantitative Assessment of Proteome and Ubiquitinome Regulation of Skeletal Muscle following Denervation-Induced Atrophy Using *in vivo* SILAC;** Sriram Aravamudan; Thomas Braun; Marcus Krüger; *Max Planck Institute for Heart and Lung Research, Bad Nauheim, Germany*
- ThP 310 **A Proteomic Investigation of Proteasome Malfunctioning in *Drosophila*;** Karen Sap; Karel Bezstarosti; Dick Dekkers; Olaf Voets; Erikjan Rijkers; Peter Verrijzer; Jeroen Demmers; *Erasmus University Medical Center, Rotterdam, Netherlands*
- ThP 311 **Novel Mass Spectrometry Approach to Reveal Oxidation-Derived Carbonyl-Groups *in vivo*;** Ralf Hoffmann; *Universität Leipzig, Leipzig, Germany*



- ThP 312 **Development of Mass Spectrometry Sample Preparation Methods for Localization and Quantitation of Protein Carbonyls in Biological Matrices;** David Simpson; Suresh Narayanasamy; Lara Lewellyn; Mike Grotewiel; Scott Gronert; *VA Commonwealth University, Richmond, VA*
- ThP 313 **Investigation of Protein Carbonylation in Human Plasma Collected from Patients with Chronic Kidney Disease on Dialysis;** Chelsea Coffey; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- ThP 314 **Streptavidin Affinity Enrichment and Mass Spectrometric Quantitation of Oxidatively Modified *Drosophila melanogaster* Proteins;** Suresh Narayanasamy<sup>1</sup>; David Simpson<sup>1</sup>; Lara Lewellyn<sup>2</sup>; Michael Grotewiel<sup>2</sup>; Scott Gronert<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Virginia Commonwealth University, Richmond, VA*; <sup>2</sup>*Department of Human & Molecular Genetics, VCU, Richmond, VA*
- ThP 315 **Protein Ascorbylation of Human Glutaredoxin-1 by a Reactive Degradation Product of Oxidized Ascorbate;** Klaus Klarskov<sup>1</sup>; Aureore Flandrin<sup>2</sup>; Francois-Olivier McDuff<sup>1</sup>; Richard J. Wagner<sup>1</sup>; <sup>1</sup>*University of Sherbrooke, Sherbrooke, Canada*; <sup>2</sup>*ENSIAC, Toulouse, France*
- ThP 316 **Mass Spectrometry Based Quantitative Redox Proteomics in Hypoxic Cardiomyocyte;** Kuan-Ting Pan<sup>1</sup>; Yi-Yun Chen<sup>2</sup>; Chun-Yi Yang<sup>1</sup>; Tzu-Ching Meng<sup>1,2</sup>; Kay-Hooi Khoo<sup>1,2</sup>; <sup>1</sup>*IBS, National Taiwan University, Taipei, Taiwan*; <sup>2</sup>*Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*
- ThP 317 **Enhanced Protein/Peptide Characterization Using Electrochemically Assisted Disulfide Bond Reduction;** Jean-Pierre Chervet; Agnieszka Kraj; Hendrik-Jan Brouwer; Nico Reinhoud; *Antec, Zoeterwoude, The Netherlands*
- ThP 318 **Unraveling Modifications of Human Skeletal Muscle Troponin by Top-down Mass Spectrometry;** Yi-Chen (Ivy) Chen<sup>1</sup>; Marius Sumandea<sup>2</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Eli Lilly and Company, Indianapolis, IN*
- ThP 319 **Identification and Quantitation of Cysteine Sulfoxidation Sites;** Chia-Fang Lee; Tanya Paull; Maria Person; *The University of Texas, Austin, TX*
- ThP 320 **Site-specific Quantitation Strategy for Characterizing the Dynamic Change of S-nitrosoproteome and Glutathionylome;** Yi-Ju Chen<sup>1</sup>; Sheng-Huang Lin<sup>2</sup>; Wen-Ying Shen<sup>2</sup>; Yu-Ju Chen<sup>1</sup>; Chun-Hung Lin<sup>2</sup>; <sup>1</sup>*Institute of Chemistry, Academia Sinica, Taipei City, Taiwan*; <sup>2</sup>*Institute of Biological Chemistry, Academia Sinica, Taipei City, Taiwan*
- ThP 321 **Iodo-based Labeling Reagent: Permanent Quantitative Labeling of S-nitrosylation Coupled with Mass Spectrometry;** Heaseung Sophia Chung<sup>1</sup>; Christopher Murray<sup>1</sup>; Ryan Bomgarden<sup>2</sup>; Vidya Venkatraman<sup>1</sup>; John Rogers<sup>2</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>*School of Medicine, Johns Hopkins University, Baltimore, MD*; <sup>2</sup>*Thermo Fisher Scientific, Rockford, IL*
- ThP 322 **A Novel Method to Detect Protein S-nitrosothiols;** Jaimeen Majmudar; Brent Martin; *University of Michigan, Ann Arbor, Michigan*
- ThP 323 **Post-Translational Nitration and Nitrosylation of Salivary Proteins Identified by Immunoprecipitation Coupled with NanoLC-ESI/MS/MS;** Wen-Peng Lin; Hauh-Jyun Candy Chen; *Natl. Chung Cheng Univ., Chia-Yi, Taiwan*
- ThP 324 **Impact of Histone Modifications on Global Protein Expression in *Saccharomyces cerevisiae*;** Linan Wang; Neha Rastogi; Mark Parthun; Michael A. Freitas; *Ohio State University, Columbus, OH*
- ThP 325 **CID and ETD Based Profiling of Posttranslational Modifications of Histones in Human Monocyte Derived Macrophages;** Pawel Olszowy<sup>1,2</sup>; Pawel Ciborowski<sup>1</sup>; <sup>1</sup>*University of Nebraska Medical Center, Omaha, NE*; <sup>2</sup>*Nicolaus Copernicus University, Torun, Poland*
- ThP 326 **Novel Language for the Histone Code: Glutamine Polyaminylation;** Chi-Chi Chou<sup>1</sup>; Cheng-Han Yu<sup>2</sup>; Geen-Dong Chang<sup>2</sup>; Kay-Hooi Khoo<sup>1,2</sup>; <sup>1</sup>*Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*National Taiwan University, Taipei, Taiwan*
- ThP 327 **Decipher the Histone Code in the Induced Pluripotent Stem Cell Reprogramming Process;** Miao Liu; Changhai Tian; Hong Peng; Shi-Jian Ding; *Univ of Nebraska Med Center, Omaha, NE*
- ThP 328 **Precursor Ion Scanning for Identification of ADP-Ribosylation Sites of CD38 Mutants;** Robert Sherwood; Hong Jiang; Xuling Zhu; Qun Liu; Hening Lin; Sheng Zhang; *Cornell University, Ithaca, NY*

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- ThP 329 **MALDI Mass Spectrometry Analysis of Sialylated Glycoprotein by in Gel Derivatization for Sialic Acids;** Kaoru Kaneshiro; Chikako Hamana; Takashi Nishikaze; Shin-ichirou Kawabata; Koichi Tanaka; *Shimadzu Corporation, Kyoto, Japan*
- ThP 330 **Enzymatic Sialylation of IgA1 Hinge-Region: Toward the Understanding of Pathogenic Role of Sialic Acid in IgA Nephropathy;** Kazuo Takahashi<sup>1</sup>; Milan Raska<sup>2</sup>; Milada Horynova-Stuchlova<sup>2</sup>; Alena Kasperova<sup>2</sup>; Stacy D. Hall<sup>3</sup>; Yoshiyuki Hiki<sup>1</sup>; Yukio Yuzawa<sup>1</sup>; Zina Moldoveanu<sup>3</sup>; Bruce A. Julian<sup>3</sup>; Matthew B. Renfrow<sup>3</sup>; Jan Novak<sup>3</sup>; <sup>1</sup>*Fujita Health University School of Medicine, Toyoake, Japan*; <sup>2</sup>*Palacky University in Olomouc, Olomouc, Czech Republic*; <sup>3</sup>*University of Alabama, Birmingham, AL*
- ThP 331 **Glycoform Determination of a Recombinant IgG Prepared from Transgenic Silkworms;** Junko Amano; Kazuko Hachisu; Takashi Shirai; *The Noguchi Institute, Itabashi, Japan*
- ThP 332 **Anti-citrullinated Protein Antibodies Show IgG-type Specific Changes Compared to Matched Controls in Human Serum and Synovial Fluid;** Susanna Lundström; Cátia Cerqueira; Elena Ossipova; Karin Lundberg; Lars Klareskog; Roman Zubarev; *Karolinska Institutet, Stockholm, Sweden*
- ThP 333 **Characterization of N-linked Glycosylation Sites of Human Clusterin in Renal Cell Carcinoma Plasma Samples Using Nano-LC-MS/MS Based Platform;** Francisca Gbormittah<sup>1</sup>; Fateme Tousi<sup>1</sup>; Marina Hancapie<sup>1</sup>; Shiao-Lin Wu<sup>1</sup>; William Hancock<sup>1</sup>; Othon Iliopoulos<sup>2,3</sup>; <sup>1</sup>*Barnett Institute, Northeastern University, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*Cancer Center, Massachusetts General Hospital, Boston, MA*
- ThP 334 **Glycoproteomics of Hepatic Metastasis in Colorectal Cancer;** Sheng-Ta Tsai<sup>1</sup>; Chein-Hung Chen<sup>1</sup>; Hsin-Yu Hsieh<sup>1</sup>; Wei-Chao Chang<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>*Genomics Research Center, Taipei, Taiwan*; <sup>2</sup>*China Medical University, Taichung, Taiwan*
- ThP 335 **Quantitative N-linked Glycoproteomic Profiling of Human Induced Pluripotent Cells, Embryonic Stem Cells, and Somatic Cells;** Putty-Reddy Sudhir; Madireddy Pavana Kumari; Hung-Chih Kuo; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- ThP 336 **Cell Surface Chemoproteomics for Capturing States of Cardiac Differentiation from Pluripotent Stem Cells;** Subarna Bhattacharya; Sandra Chuppa; Rebekah Gundry; *Medical College of Wisconsin, Milwaukee, WI*

- ThP 337 **Mass Spectrometry Characterization of a Novel Form of the Retinoic Acid Receptor Responder Protein-1; Haeri Seol**; Kristy Brown; Joseph Devaney; Brennan Harmon; Roger Packer; Yetrib Hathout; *Children's National Medical Center, Washington, DC*
- ThP 338 **MALDI MS Analysis of N-glycan Structures of a Cell Adhesion Molecule, CADM1, in Various Cancer Cells; Mika Sakurai-Yageta**<sup>1</sup>; Tomoko Maruyama<sup>1</sup>; Kaoru Kaneshiro<sup>2</sup>; Sadanori Sekiya<sup>2</sup>; Shinichi Iwamoto<sup>2</sup>; Koichi Tanaka<sup>2</sup>; Yoshinori Murakami<sup>1</sup>; <sup>1</sup>*The University of Tokyo, Tokyo, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- ThP 339 **Qualitative and Quantitative Investigation of Glycans Attached to Prostate-specific Antigen (PSA) Glycoprotein of Healthy and Cancer Samples; Ulrike Schweiger-Hufnagel**<sup>1</sup>; Kristina Marx<sup>1</sup>; Daniel Kolarich<sup>2</sup>; Wolfgang Jabs<sup>1</sup>; Anja Resemann<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Max Planck Institute of Colloids and Interfaces, Berlin, Germany*
- ThP 340 **Glycosylation Analysis of Cucumisin, a Subtilisin-Like Serine Protease from *Cucumis melo* L. Using MALDI-QIT-TOF MS; Shuuichi Nakaya**<sup>1</sup>; Yuzo Yamazaki<sup>1</sup>; Ami Sotokawauchi<sup>3</sup>; Yohei Kamiyo<sup>3</sup>; Kazutaka Murayama<sup>2</sup>; Kazunari Arima<sup>3</sup>; <sup>1</sup>*Application Development Center, Shimadzu Corp., Kyoto, Japan*; <sup>2</sup>*Tohoku University, Sendai, Japan*; <sup>3</sup>*Kagoshima University, Kagoshima, Japan*
- ThP 341 **Determination of Extensive Glycosylation on Glycoproteins and Glycolipids in High-density Lipoprotein; Jincui Huang**; Hyeoung Lee; Angela Zivkovic; Jennifer Smilowitz; Bruce German; Carlito Lebrilla; *UC, Davis, CA*
- ThP 342 **Large Scale Characterization of Intact Sialylated Glycopeptides Reveals Extensive Plasma Sialylation and Modulation of Surface Sialylation upon EGF Stimulation; Peter Højrup**; Sara Eun Lendal; Giuseppe Palmisano; Martin R. Larsen; *Univ. Southern Denmark, Odense, Denmark*
- ThP 343 **MRM Quantification of Site-Specific Core-Fucosylation of Potential Biomarkers in Liver Diseases; Haidi Yin**; Zhenxin Lin; Andy Lo; Jianhui Zhu; David M. Lubman; *University of Michigan, Medical School, Ann Arbor, MI*
- ThP 344 **Label-free Quantification of Site-Specific Core-Fucosylation of alpha-2-macroglobulin in Pancreatic Diseases; Zhenxin Lin**; Haidi Yin; Andy Lo; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- ThP 345 **Mass Spectrometry Identification of Co-Immunoprecipitated N-linked Glycoproteins from Rat Brain *in vivo*; Norelle Wildburger**<sup>1,2</sup>; Cheryl Lichti<sup>1</sup>; Mark Emmett<sup>3,4</sup>; Carol Nilsson<sup>1,3</sup>; <sup>1</sup>*Department of Pharmacology & Toxicology, Galveston, TX*; <sup>2</sup>*Neuroscience and Cell Biology, Galveston, TX*; <sup>3</sup>*Sealy Cancer Center, Galveston, TX*; <sup>4</sup>*Department of Biochemistry and Molecular Biology, Galveston, TX*
- ThP 346 **Targeted Glycoproteomic Analysis of Serum Glycoproteins Enables Site-Specific Glyco-Biomarker Discovery; Serenus Hua**<sup>1</sup>; Injung Ji<sup>1</sup>; Myung Jin Oh<sup>1</sup>; Sung-Hyeon Lee<sup>2</sup>; Rudolf Grimm<sup>1,3</sup>; Jung Hoe Kim<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*Chungnam National University, Daejeon, Korea*; <sup>2</sup>*Korea Advanced Institute of Science and Technology, Daejeon, Korea*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- ThP 347 **HCD Product Ion Triggered ETD MS/MS Facilitates the Detection of O-GlcNAc Modified Residues of Insulin Receptor Substrate 2; Lashanda Waller**; Jennifer Rutherford Bethard; Mary Berkaw; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- ThP 348 **High Efficiency LC/MS Analysis of O-GlcNAc Modified Synthetic Peptides; Barry Boyes**<sup>1,2</sup>; Alex Harvey<sup>3</sup>; Ron Orlando<sup>2</sup>; <sup>1</sup>*Advanced Materials Technology Inc, Wilmington, DE*; <sup>2</sup>*Complex Carbohydrate Research Center, Athens, GA*; <sup>3</sup>*Glycoscientific, Athens, GA*
- ThP 349 **Analysis of GalNAc-transferase Site-Specificity by ETD Tandem Mass Spectrometry; Tyler Stewart**; Kazuo Takahashi; Koshi Yamada; Milan Raska; Milada Stuchlova Horynova; Jan Novak; Matthew Renfrow; *UAB, Birmingham, AL*
- ThP 350 **Entamoeba O-phosphodiester-linked Glycans and Phosphopeptides Studied with Mass Spectrometry; Edwin M. Motari**<sup>1</sup>; John R. Haserick<sup>1,3</sup>; Andrea Carpentieri<sup>2</sup>; Catherine E. Costello<sup>3,4</sup>; Phillips W. Robbins<sup>1</sup>; John Sameulson<sup>1</sup>; <sup>1</sup>*Boston University School of Dental Medicine, Boston, MA*; <sup>2</sup>*Università di Napoli Federico II, Napoli, Italy*; <sup>3</sup>*Boston University School Medicine, Boston, MA*; <sup>4</sup>*Boston University, Boston, MA*
- ThP 351 **MS-based Characterization of Site-specific Protein O-glycosylations by Combining Glycan Release and Non-release Methods; Shu-Hui Chen**; Li-Juan Huang; *National Cheng Kung University, Tainan, Taiwan*
- ThP 352 **Simultaneous Mapping of N- and O-linked Glycosylation Sites in Renal Cell Carcinoma Cells; Xiaoying Ye**; DaRue A. Prieto; Josip Blonder; *SAIC-Frederick, Inc., Frederick, MD*
- ThP 353 **High Performance Ultraviolet Photodissociation of O-Linked Glycopeptide Anions in an Orbitrap Mass Spectrometer; Scott A. Robotham**; Jennifer S. Brodbelt; *University of Texas, Austin, TX*
- ThP 354 **MS3 (MRM3) Quantitative O-glycopeptide Analysis; Miloslav Sunda**; Julius Benicky; Radoslav Goldman; *Georgetown University, Lombardi Cancer Center, Washington, DC*
- ThP 355 **O-linked Glycopeptide Analysis by Automated Scoring of ETD Mass Spectra; Zhikai Zhu**; Eden Go; David Hua; Heather Desaire; *Chemistry Department, University of Kansas, Lawrence, KS*
- ThP 356 **Comprehensive Study of O-linked Glycans of Erythropoietin; Nannan Tao**; Ulrike Schweiger-Hufnagel; Kristina Marx; Stephanie Kaspar; Anja Resemann; *Bruker Daltonics Inc., Billerica, MA*
- ThP 357 **LC-MS/MS Identification of the O-Glycosylation and Hydroxylation of Amino Acid Residues of Collagen  $\alpha$ -1 (II) chain from Bovine Cartilage; Ehwang Song**; Yehia Mechref; *Texas Tech University, Lubbock, TX*

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- ThP 359 **Automated Identification of MS/MS Spectra from Heparan Sulfate (HS) Glycosaminoglycan; Yulun Chiu**; Rongrong Huang; Ron Orlando; Joshua S. Sharp; *CCRC, University of Georgia, Athens, GA*
- ThP 360 **Separation and Sequencing of a Synthesized Heparin-Like Tetramers Library Using Chemical Derivatization and LC-MS/MS with an In-House Developed Sequencing Program; Rongrong Huang**; Yulun Chiu; Ron Orlando; Joshua S. Sharp; *CCRC, University of Georgia, Athens, GA*
- ThP 361 **A Simple Method for Early Age Phenotype Confirmation Using Toe Tissue from a Mouse Model of MPS IIIA; Paul J. Trim**; Stephen K. Duplock; Adeline A. Lau; Kim M. Hemsley; John J. Hopwood; Marten F. Snel; *Lysosomal Diseases Research Unit, SA Pathology, North Adelaide, Australia*
- ThP 362 **Optimization of Tissue Surface Digestion by Glycosidase Enzymes; Lilla Turiak**; Chun Shao; Joseph Zaia; *Boston University School of Medicine, Boston, MA*

- ThP 363 **Development of a Chemical Inkjet Printer and Liquid Microjunction Extraction Strategy for Improving Mass Spectrometric Profiling of Glycosaminoglycans on Tissue Sections;** Chun Shao; Lilla Turiak; Yu Huang; Joseph Zaia; *CBMS, Boston University, Boston, MA*
- ThP 364 **Determination of the Effect of Depolymerization Methods on Highly-Sulfated HS Domains Using LC/MS;** Yang Mao; Yu Huang; Joseph Zaia; *Boston University School of Medicine, Boston, MA*
- ThP 365 **Efficient Electron Detachment Dissociation (EDD) of Highly Sulfated Heparin Oligosaccharides on an LC Time Scale;** Yu Huang; Xiang Yu; Yang Mao; Cheng Lin; Joseph Zaia; *Boston University School of Medicine, Boston, MA*
- ThP 366 **Structural Characterization of Chemoenzymatically Synthesized Longer (dp5-dp11) Heparan Sulfate Glycosaminoglycans Using Electron Detachment Dissociation;** Yuejie Zhao<sup>1</sup>; Isaac Agyekum<sup>1</sup>; John Muchena<sup>1</sup>; Yongmei Xu<sup>2</sup>; Jian Liu<sup>2</sup>; Lingyun Li<sup>3</sup>; Robert Linhardt<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*; <sup>3</sup>*Rensselaer Polytechnic Institute, Troy, NY*
- ThP 367 **ESI-MS Analysis of Sulfated Glycans Using Ionic Liquid;** Tianjiao Yang; Yehia Mechref; *Texas Tech University, Lubbock, Texas*
- ThP 368 **Confirming the Presence of "Charge-localization isomers" in the Disulfated GAG-Type Disaccharide;** Yoko Ohashi<sup>1</sup>; Yuya Otsuka<sup>2</sup>; Toshikazu Minamisawa<sup>2</sup>; Takashi Hirano<sup>1</sup>; <sup>1</sup>*The University of Electro-Communications, Chofu, Tokyo, Japan*; <sup>2</sup>*Seikagaku Corporation, Tokyo, Japan*
- ThP 369 **Polysaccharide Structures, Containing Charged Polysulfated/Polycarboxylated Moieties, Elucidated Using the MASSPEC Algorithm for Analysis of Exact-Mass ESI Negative Ionization MSMS Data;** Marshall M. Siegel<sup>1</sup>; Gary Walker<sup>1</sup>; Lingyun Li<sup>2</sup>; Robert J. Linhardt<sup>2</sup>; <sup>1</sup>*MS Mass Spec Consultants, Fair Lawn, NJ*; <sup>2</sup>*Rensselaer Polytechnic Institute, Troy, NY*
- ThP 370 **Quantitative Analysis of Oligosaccharides Derived from Sulfated Glycosaminoglycans by Affinity Purification and MALDI MS;** Chih-Che Wu; *Department of Applied Chemistry, National Chi Nan, Puli, Taiwan*
- ThP 371 **Biomimetic Reagents for Selective Free Radical and Acid-Base Chemistry of Glycans: Application to Glycan Structure Determination by Mass Spectrometry;** Jinshan Gao; Daniel Thomas; Chang Ho Sohn; J. L. Beauchamp; *CCE at Caltech, Pasadena, CA*
- ThP 372 **Charge Carrier Effect to the Ionization and Fragmentation Efficiency of Glycans;** Yaping Lin<sup>1</sup>; Chia-Lin Wu<sup>1</sup>; Chein-Hung Chen<sup>1</sup>; Jung-Lee Lin<sup>1</sup>; Pang-Hung Hsu<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>*Academia sinica, Taipei, Taiwan*; <sup>2</sup>*National Taiwan Ocean University, Keelung, Taiwan*
- ThP 373 **Statistical Analysis Model for Classifying Stereo Structures of Oligosaccharides;** Y. Melodie Du; Chiharu Konda; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- ThP 374 **Collision-Induced Dissociation of Reducing-End Modified Small Oligosaccharides;** Chiharu Konda<sup>1</sup>; Tammy Fang<sup>2</sup>; Jia Ren<sup>1</sup>; Brad Bendiak<sup>2</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of Colorado Denver, Aurora, CO*
- ThP 375 **Glycan Structural Elucidation On A Novel Quadrupole Dual Cell Linear Ion Trap Orbitrap Hybrid Mass Spectrometer;** Julian Saba<sup>1</sup>; Shannon Eliuk<sup>1</sup>; Sergei Snovidat<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*ThermoFisher Scientific, Rockford, IL*
- ThP 376 **Novel Bioinformatics Approaches to Glycan Profiling in Liquid Chromatography-Mass Spectrometry;** Chuan-Yih Yu<sup>1</sup>; Yunli Hu<sup>2</sup>; Anoop Mayampurath<sup>1</sup>; Yehia Mechref<sup>1,2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*Texas Tech University, Lubbock, TX*
- ThP 377 **Detailed Structural Investigation of Beta-Glucans from Yeast Cell Walls by Electron-Transfer Dissociation;** Liang Han<sup>1</sup>; Catherine E. Costello<sup>2</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*
- ThP 378 **Comparison of ETD and ECD for Analysis of Permethylated Glycans;** Mengdi Fan<sup>1</sup>; Yi Pu<sup>1</sup>; Catherine E Costello<sup>1,2</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*
- ThP 379 **Structural Characterization of Singly Charged Glycan Anions via Electronic Excitation Tandem Mass Spectrometry;** Jordan C. Ernst; Di Gao; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- ThP 380 **Ion fragility of Permethylated Glycans and Glycoconjugates in Hybrid Ion Trap-Fourier Transform Mass Spectrometers;** Ming-Yi Ho; Kay-Hooi Khoo; *Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*
- ThP 381 **Linkage and Anomeric Differentiation in Oligosaccharides by Sequential Fragmentation and Variable-wavelength Infrared Photodissociation Fingerprints;** Yanlan Tan; Nicolas Polfer; *Department of Chemistry, University of Florida, Gainesville, FL*
- ThP 382 **Determination of Isomeric Oligosaccharides by Photo Dissociation with Visible Light;** Andrea Hahn; Jurgen Grotemeyer; *Christian-Albrechts-Univ, Kiel, Germany*
- ThP 383 **Computer Assisted Algorithm for the Automated Annotation of Glycosaminoglycan MS/MS;** Jiana Duan; Jon Amster; *University of Georgia, Athens, GA*

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- ThP 384 **Isobaric Protein-Level Labeling for Serum Glycoprotein Quantification Analysis on an Orbitrap Elite;** Song Nie; Andy Lo; Jianhui Zhu; David M. Lubman; *Department of Surgery, University of Michigan, Ann Arbor, MI*
- ThP 385 **Targeted Quantification of O-Linked Glycosylation Site for Glycan Distribution Determination;** Scott Peterman<sup>1</sup>; Amol Prakash<sup>1</sup>; Julian Saba<sup>2</sup>; Mary Lopez<sup>1</sup>; Jennifer Cushing<sup>3</sup>; Audra Ann Harget<sup>3</sup>; Matthew Renfrow<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific BRIMS, Cambridge, MA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*University of Alabama Birmingham, Birmingham, AL*
- ThP 386 **Identification and Absolute Quantification of Amadori-peptides in Human Plasma as Potential Diabetes Type 2 Biomarkers;** Andrej Frolov; *Universität Leipzig, Leipzig, Germany*
- ThP 387 **Evaluation of Lyso-Gb<sub>3</sub> Analogues as Novel Biomarkers for Fabry Disease;** Pamela Lavoie; Michel Boutin; Christiane Auray-Blais; *Université de Sherbrooke/CRC-CHUS, Sherbrooke, Canada*
- ThP 388 **A Sensitive HILIC-MS/MS Method for Simultaneously Measuring Carnitine, Palmitoyl Carnitine and Stearoyl Carnitine as Potential Biomarkers of Fatty Acid  $\beta$ -Oxidation in Mice;** Xiaolin Zhang; Xiao Ding; Georgia Hatzivassiliou; Mark Merchant; Kirsten Messick; Brian Dean; *Genentech, South San Francisco, CA*
- ThP 389 **Quantification of DNA Interstrand Crosslinks Induced by CENUs in L1210 Cells Using Liquid Chromatography Electrospray Ionization Tandem Mass Spectrometry;** Lili Li; Xuechai Chen; Guohui Sun; Lijiao Zhao; Rugang Zhong; *Beijing University of Technology, Beijing, China*



- ThP 390 **Quantitation of 8-iso-PGF<sub>2</sub>α in Human Urine Using UHPLC-MS-MS**; Yongchao Li<sup>2</sup>; Jeff Dahl<sup>1</sup>; Jerry White<sup>2</sup>; Richard B. van Breenen<sup>2</sup>; <sup>1</sup>Shimadzu, Columbia, MD; <sup>2</sup>University of Illinois College of Pharmacy, Chicago, IL
- ThP 391 **Detection of Low Levels of Estradiol with the Use of Micro Flow LC Coupled to a Sensitive Mass Spectrometer System**; Alexandre Wang; Jesse Seegmiller; Hua-fen Liu; *AB SCIEX, Foster City, CA*
- ThP 392 **Monitoring Steroidal Analogues in Clinical and Environmental Chemistry: One Model for Exposomics**; Anthony Macherone; Melissa Churley; *Agilent Technologies, Wilmington, DE*
- ThP 393 **Determination of 1,25-Dihydroxylvitamine D3(DHD3) and 1,25-Dihydroxyvitamine D2 (DHD2) in Human Plasma by Immunoaffinity Extraction, Diels-Alder Derivatization and Methylamine Adduction LC/MS/MS**; Xiaohua Li; Vincent Windisch; Allan Xu; *Keystone Bioanalytical, North Wales, PA*
- ThP 394 **Quantification of 25-hydroxyvitamin D3 in Rat Serum Using Derivatization to Enhance LC-MS/MS Sensitivity**; Yinghe Li; Yifan Shi; Meng Fang; Pamela Rogers; *Alliance Pharma, Inc., Malvern, PA*
- ThP 395 **A Quantitative Stable Isotope LC-MS/MS Method to Measure Niacin in Blood and Plasma**; Lulu Yang; Ann Qin; Allan Jauchico; Justin Ly; YuZhong Deng; Brian Dean; Xiaorong Liang; *Genentech Inc., South San Francisco, CA*
- ThP 396 **Measurement of Serotonin Concentration Changes in a Rat Osteoporosis Model after Dosing a Bone Growth Promoter**; Elizabeth A. Mahan; Suzie Yeh; Emily Adarayan; Rena Zhang; Scott Fauty; Han Gerrits; Freek Bourgoudien; Benno Ingelse; *Merck & Co., West Point, PA*
- ThP 397 **Development of a High Throughput Multi-analyte Assay for the Quantification of Green Tea – Derived Catechins in Human Plasma**; John Bannister; Deborah Mawson; Keon Jeffery; Phillip Teale; Bob Gray; Phillip Grace; *LGC Health Sciences, Teddington, UK*
- ThP 398 **LC-MS/MS Quantification of Free Desmosines in Plasma**; Tasso Miliotis<sup>1</sup>; Sven Kjellström<sup>2</sup>; <sup>1</sup>AstraZeneca R&D Molndal, Molndal, Sweden; <sup>2</sup>Biochemistry and Structural Biology, Lund, Sweden
- ThP 399 **Development of an *in vivo* Quantitative Assay for Covalently Modified Serum Albumin: Monitoring Acetaminophen Toxicity**; André LeBlanc; Souade Ben Haddou; Tze Chieh Shiao; René Roy; Lekha Sleno; *UQAM, Montréal, Canada*
- ThP 400 **Screening Serum Albumin Adducts of Carcinogenic Arylamines under Different Proteolytic Digestion Systems**; Lijuan Peng; Robert Turesky; *Wadsworth Center, NYS Department of Health, Albany, NY*
- ThP 401 **Simultaneous Profiling of Sixteen Biomarkers of Occupational Exposure and Endogenous Metabolites in Urine**; Lucie Rimnacova<sup>1</sup>; Petr Simek<sup>1</sup>; Petr Husek<sup>1</sup>; Jaroslav Mraz<sup>2</sup>; <sup>1</sup>Biology Centre, Czech Academy of Sciences, Ceske Budejovice, Czech Republic; <sup>2</sup>National Institute of Public Health, Prague, Czech Republic
- ThP 402 **A LC-MS/MS Method for Determination of 1-Hydroxypyrene, 3-hydroxybenzo[a]pyrene and 3-hydroxybenz[a]anthracene: Application to Biomonitoring of Human Smoke Polycyclic Aromatic Hydrocarbon Exposure**; Hongwei Hou; Xiaotao Zhang; Wei Xiong; Qingyuan Hu; *China National Tobacco Quality Supervision & Test, Zhengzhou, China*
- ThP 403 **HPLC-ESI-MS/MS Quantification of Urinary Metabolites of 1,3-butadiene in Smokers to Identify Ethnic Differences in Metabolism**; Srikanth Kotapati<sup>1</sup>; Lani Park<sup>2</sup>; Amanda Esades<sup>1</sup>; Loic Le Marchand<sup>2</sup>; Natalia Tretyakova<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of Hawai'i, Honolulu, HI
- ThP 404 **Characterization of Aromatic Amine Exposure in U.S. Smokers and Non-Smokers: NHANES 2005-2006**; Tiffany Seyler; Elizabeth Cowan; Jenny Kim; Rey DeCastro; Benjamin Blount; Lanqing Wang; *CDC, Atlanta, GA*
- ThP 405 **Human Exposure Assessment to the Plasticizer di(isononyl)cyclohexane-1,2-dicarboxylate (DINCH) Using Urinary Metabolites Identified in Rats**; Manori Silva; Ella Samandar; James Preau; Antonia Calafat; *Centers for Disease Control and Prevention, Atlanta, GA*
- ThP 406 **Comparative Analysis of Acid, Base and Beta-Glucuronidase Hydrolysis of Conjugated 4-aminobiphenyl in Fortified Urine**; Jenny G. Kim<sup>1,2</sup>; Elizabeth A. Cowan<sup>1</sup>; Tiffany H. Seyler<sup>1</sup>; Lanqing Wang<sup>1</sup>; Benjamin Blount<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>ORISE, Oak Ridge, TN
- ThP 407 **Long Term Stability of Volatile Nitrosamines in Human Urine**; James Hodgson<sup>1,2</sup>; Tiffany Seyler<sup>2</sup>; Lanqing Wang<sup>2</sup>; <sup>1</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>2</sup>Centers for Disease Control and Prevention, Atlanta, GA
- ThP 408 **LC-MS/MS Analysis of Mercapturic Acids: Addressing Selectivity and Matrix Effect Issues**; Alan Dzerk; Veniamin Lapko; Ridha Nachi; Kirk Newland; Curtis Sheldon; *Celerion, Inc, Lincoln, NE*
- ThP 409 **Rapid Quantitation of Diastereomeric CEDG-A Potential Biomarker for Diabetes in Human Urine by LC-MS/MS**; Jing Ke<sup>1</sup>; Kelly Lam<sup>1</sup>; Yijin Xiao<sup>1</sup>; Harry Zhao<sup>1</sup>; Zhongping (John) Lin<sup>1</sup>; Daniel Tamae<sup>2</sup>; Gerald E. Wuenschell<sup>2</sup>; John Termini<sup>2</sup>; <sup>1</sup>Frontage Laboratories, Inc, Exton, PA; <sup>2</sup>City of Hope Medical Center, Duarte, CA
- ThP 410 **Validation of a Method of Measuring Amino Acids Composition of Peptides and Proteins by Gas Chromatography/Mass Spectrometry**; Ayat H. BaniRashaid; Peter de B. Harrington; Glen P. Jackson; *Ohio University, Athens, OH*

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- ThP 411 **Label-free Shotgun Proteomic Characterization of Laser Capture Microdissected Formalin Fixed Paraffin Embedded Melanoma Biopsies**; Owen E. Branson; John P. Shapiro; Joseph Markowitz; Sara B. Peters; William E. Carson III; Michael A. Freitas; *Ohio State University, Columbus, OH*
- ThP 412 **Novel Diagnostic and Prognostic Biomarker Candidates of Hepatocellular Carcinoma Revealed by a Quantitative 2D-DIGE and Label-Free Proteome Analysis**; Wael Naboulsi<sup>1</sup>; Dominik Megger<sup>1</sup>; Thilo Bracht Bracht<sup>1</sup>; Kristin Rosowski Rosowski<sup>1</sup>; Birgit Korte<sup>1</sup>; Stephanie Tautges<sup>1</sup>; Don Marvin Voß<sup>1</sup>; Michael Kohl<sup>1</sup>; Maïke Ahrens<sup>1</sup>; Sacha Hagemann<sup>2</sup>; Frank Weber<sup>4</sup>; Hideo Baba<sup>2</sup>; Jörg F. Schlaak<sup>3</sup>; Martin Eisenacher<sup>1</sup>; Christian Stephan<sup>1</sup>; Helmut Meyer<sup>1</sup>; Barbara Sitek<sup>1</sup>; <sup>1</sup>MPC, Ruhr-Universität Bochum, Bochum, Germany; <sup>2</sup>Pathologie, Universitätsklinikum Essen, Essen, Germany; <sup>3</sup>Hepatologie, Universitätsklinikum Essen, Essen, Germany; <sup>4</sup>Universitätsklinikum Essen, Essen, Germany
- ThP 413 **A Study Combining Label-Free Proteomics and 2D-DIGE Revealed Novel Biomarker Candidates for Cholangiocellular Carcinoma**; Juliet Padden<sup>1</sup>; Dominik Megger<sup>1</sup>; Thilo Bracht<sup>1</sup>; Stephanie Tautges<sup>1</sup>; Don Marvin Voss<sup>1</sup>; Kristin Rosowski<sup>1</sup>; Birgit Korte<sup>1</sup>; Michael Kohl<sup>1</sup>; Martin Eisenacher<sup>1</sup>; Hideo A. Baba<sup>2</sup>; Jörg F. Schlaak<sup>3</sup>; Christian Gerges<sup>4</sup>; Brigitte Schumacher<sup>4</sup>; Horst Neuhaus<sup>4</sup>; Helmut E. Meyer<sup>1</sup>; Barbara Sitek<sup>1</sup>; <sup>1</sup>Medizinisches Proteom-Center, Ruhr-Universität Bochum, Germany; <sup>2</sup>Institut für Pathologie, Universitätsklinikum Essen, Germany; <sup>3</sup>Klinik

für Gastroenterologie und Hepatologie, Universitätsklinikum Essen, Germany; <sup>4</sup>Evang. Krankenhaus Düsseldorf, Düsseldorf, Germany

- ThP 414 **Metabolic Profiling of Hepatocellular Carcinoma and Hepatitis C Using GC-MS, LC-TOF-MS and LC-MS/MS methods;** Hamid Baniasadi<sup>1</sup>; G. A. Nagana Gowda<sup>3</sup>; Siwei Wei<sup>1</sup>; Jeremiah Bowers<sup>1</sup>; Nicholas Skill<sup>2</sup>; Mary Maluccio<sup>2</sup>; Daniel Raftery<sup>1,3</sup>; <sup>1</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Surgery, Indiana University, Indianapolis, IN; <sup>3</sup>University of Washington, Seattle, WA
- ThP 415 **Investigation into the Mechanisms of Prostate Cancer Androgen Independence Using Label-Free Data-Independent Quantitative LC-IM-DIA-MS and Pathway Analysis;** Brian Morrisey<sup>1</sup>; Robert Tonge<sup>2</sup>; Lee A Gethings<sup>2</sup>; Johannes PC Vissers<sup>2</sup>; Stephen Pennington<sup>1</sup>; <sup>1</sup>UCD Conway Institute, University College Dublin, Dublin, Ireland; <sup>2</sup>Waters Corporation, Manchester, UK
- ThP 416 **Development of a 4 Protein Signature that Predicts Outcome to Tamoxifen Treatment in Recurrent Estrogen Receptor Positive Breast Cancer;** Tommasso De Marchi<sup>1</sup>; Ning Qing Liu<sup>1</sup>; Christoph Stingl<sup>1</sup>; Marcel Smid<sup>1</sup>; Maxime Look<sup>1</sup>; Rene Braakman<sup>1</sup>; Mark Opdam<sup>2</sup>; Sabine Linn<sup>2</sup>; Fred Sweep<sup>3</sup>; Paul Span<sup>3</sup>; John Martens<sup>1</sup>; John Foekens<sup>1</sup>; Arzu Umar<sup>1</sup>; <sup>1</sup>Erasmus University Medical Center, Rotterdam, The Netherlands; <sup>2</sup>Netherlands Cancer Institute, Amsterdam, The Netherlands; <sup>3</sup>Radboud University Nijmegen Medical Center, Nijmegen, The Netherlands
- ThP 417 **A Proteomics Profile Associated with Neoadjuvant Chemotherapy Sensitivity in Triple-Negative Breast Cancer;** Rene Braakman<sup>1,3</sup>; Christoph Stingl<sup>1</sup>; Lennart Mulder<sup>2,3</sup>; Marcel Smid<sup>1</sup>; Esther Lips<sup>2,3</sup>; John Martens<sup>1,3</sup>; Theo Luiders<sup>1</sup>; Sjoerd Rodenhuis<sup>2,3</sup>; John Foekens<sup>1,3</sup>; Arzu Umar<sup>1,3</sup>; <sup>1</sup>Erasmus Medical Center, Rotterdam, The Netherlands; <sup>2</sup>Netherlands Cancer Institute, Amsterdam, The Netherlands; <sup>3</sup>Center for Translational Molecular Medicine, Eindhoven, The Netherlands
- ThP 418 **Genome Wide Proteomics of ERBB2 and EGFR Pathways in Inflammatory Breast Cancer;** Yue Zhang<sup>1</sup>; Massimo Cristofanilli<sup>2</sup>; Fredrika Robertson<sup>3</sup>; James Reuben<sup>3</sup>; Zhaomei Mu<sup>2</sup>; Hogune Im<sup>4</sup>; Michael Snyder<sup>4</sup>; Matan Hoffree<sup>5</sup>; Trey Ideker<sup>5</sup>; Gilbert Omenn<sup>6</sup>; Susan Fanayan<sup>7</sup>; Seul-Ki Jeong<sup>8</sup>; Young-ki Paik<sup>8</sup>; Shiao-Lin Wu<sup>1</sup>; William Hancock<sup>1</sup>; <sup>1</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>2</sup>Thomas Jefferson University, Philadelphia, PA; <sup>3</sup>M D Anderson Cancer Center, Houston, TX; <sup>4</sup>Department of Genetics, Stanford University, Stanford, CA; <sup>5</sup>University of California, La Jolla, CA; <sup>6</sup>University of Michigan, Ann Arbor, MI; <sup>7</sup>Macquarie University, Sydney, Australia; <sup>8</sup>Yonsei University, Seoul, Korea
- ThP 419 **A Novel Proteomic Approach for the Routine Screening for Ovarian Cancer Using PAP samples;** Lewis Pannell<sup>1</sup>; Lindsay Schambeau<sup>1</sup>; Meghan Tanner<sup>1</sup>; Dean Billheimer<sup>2</sup>; Rodney Rocconi<sup>1</sup>; Michael Finan<sup>1</sup>; <sup>1</sup>Mitchell Cancer Institute, Mobile, AL; <sup>2</sup>University of Arizona, Tucson, AZ
- ThP 420 **Comparison of Label-Free and SILAC Quantitative Analysis of Breast Cell Lines Glycoproteomes;** Ten-Yang Yen; Alejandro Corona; Roger Yen; Chris Alleyne-Chin; Leslie Timpe; Bruce Macher; San Francisco State University, San Francisco, CA
- ThP 421 **Large-Scale Comparative Proteomic Analysis of Colon Cancer Cells Isolated from Multiple Patients Using an Extensive Ion Current –Based Approach;** Chengjian Tu; Jun Li; Shichen Shen; Eslam Nouri-Nigeh; Wilfrido Mojica; Jun Qu; University at Buffalo, Buffalo, NY
- ThP 422 **Validation of Early Serum Biomarkers of Colorectal Cancer Using Selective Reaction Monitoring Mass Spectrometry;** Melanie M. Ivancic; Amy A. Irving; Jennifer K. Pleiman; Linda Clipson; William F. Dove; Michael R. Sussman; University of Wisconsin, Madison, WI
- ThP 423 **Proteomic Analysis of Perineural Invasion in Pancreatic Adenocarcinoma Reveals Up-regulation of Neurosecretory Protein VGF in Invaded Nerves;** Richard Jones<sup>1</sup>; Wasfi Alrawashdeh<sup>2</sup>; Ravi Amunugama<sup>1</sup>; Michael Ford<sup>1</sup>; David Allen<sup>1</sup>; Nilukshi Wijesuriya<sup>3</sup>; Pedro Cutillas<sup>2</sup>; Tatjana Crnogorac-Jurcevic<sup>2</sup>; <sup>1</sup>MS Bioworks, LLC, Ann Arbor, MI; <sup>2</sup>Barts Cancer Institute, QMUL, London, UK; <sup>3</sup>Department of Pathology, Royal London Hospital, London, UK
- ThP 424 **Target Proteomic Profiling of Frozen Pancreatic CD24+ Adenocarcinoma Tissues by Immuno-Laser Capture Microdissection and Nano-LC-MS/MS;** Jianhui Zhu; Song Nie; Jing Wu; David M. Lubman; University of Michigan Medical Center, Ann Arbor, MI
- ThP 425 **Global Analysis of the Phosphoproteome of Human Blasts Reveals Predictive Phosphorylation Markers for the Treatment of Acute Myeloid Leukemia with AC220;** Christoph Schaab<sup>1,2</sup>; Felix Oppermann<sup>1</sup>; Martin Klammer<sup>1</sup>; Heike Pfeifer<sup>3</sup>; Andreas Tebbe<sup>1</sup>; Thomas Oellerich<sup>3</sup>; Jürgen Krauter<sup>4</sup>; Mark Levis<sup>5</sup>; Alexander E. Perl<sup>6</sup>; Henrik Daub<sup>1</sup>; Björn Steffen<sup>3</sup>; Klaus Godl<sup>1</sup>; Hubert Serve<sup>3</sup>; <sup>1</sup>Evotec Munich, Martinsried, Germany; <sup>2</sup>Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>3</sup>Department of Medicine, Goethe University, Frankfurt, Germany; <sup>4</sup>Medizinische Hochschule Hannover, Hannover, Germany; <sup>5</sup>Sidney Kimmel Comprehensive Cancer Center, Baltimore, MD; <sup>6</sup>Abramson Cancer Center, PA
- ThP 426 **Identification of SLPI as a Progression-Associated Protein in Oral Pre-Cancerous Lesions by Quantitative Proteomics of Non-Invasively Collected Brushed Biopsies;** Ya Yang<sup>1</sup>; Nelson Rhodus<sup>2</sup>; Frank Ondrey<sup>3</sup>; Patricia Fernandes<sup>3</sup>; YaQin Zhu<sup>1</sup>; Timothy Griffin<sup>4</sup>; <sup>1</sup>9th People's Hospital, Shanghai JiaoTong University, Shanghai, China; <sup>2</sup>School of Dentistry, University of Minnesota, Minneapolis, MN; <sup>3</sup>Dept of Otolaryngology, University of Minnesota, Minneapolis, MN; <sup>4</sup>Department of BMBB, University of Minnesota, Minneapolis, MN
- ThP 427 **Rapid Phenotyping Renal Cell Carcinoma from Fine Needle Aspirates Using DESI-MS;** Joseph H Kennedy<sup>1</sup>; Matthew T Olson<sup>2</sup>; Justin M Wiseman<sup>1</sup>; <sup>1</sup>Prosolia, Inc., Indianapolis, IN; <sup>2</sup>The John Hopkins Hospital, Baltimore, MD
- ThP 428 **CD180 : A New Marginal Zone B-cell Lymphoma Biomarker Discovered by Plasma Membrane Microparticle Proteomic Analysis;** Sarah Lennon<sup>1</sup>; Laurent Miguet<sup>2</sup>; Christine Carapito<sup>1</sup>; Luc Fornecker<sup>1</sup>; Laurent Mauvieux<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Sarah Cianféroni-Sanglier<sup>1</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse Bioorganique, Strasbourg, France; <sup>2</sup>Institut d'hématologie et d'immunologie, Strasbourg, France
- ThP 429 **Screening Biomarkers of Thyroid Cancer by a Combination of Tissue Imaging and Serum Metabolites Profiling Using MALDI-FTICR MS;** Shuai Guo; Hui Liu; Yumei Guo; Yaping Zhang; Fang Li; Zhili Li; IBMS, CAMS&PUMC, Beijing, China
- ThP 430 **Selective Sampling Strategy and Quantitative Proteomic Analysis Reveals New Mechanisms of Oxygen-Regulated Solid Tumor Growth in Mouse Model;** Shujia Dai<sup>1</sup>; Dmitriy Lukashev<sup>2</sup>; Somak Ray<sup>1</sup>; Barry Karger<sup>1</sup>; Michail Sitkovsky<sup>2</sup>; <sup>1</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>2</sup>Bouve College of Health Sciences Northeastern Univ, Boston, MA



- ThP 431 **Quantitative Proteomic Analysis Reveals a Molecular Triad Signature as Biomarker Candidates for Astrocytomas and Oligodendrogliomas;** Jose Cesar Rosa<sup>4</sup>; Suely Kazue Nagahashi Marie<sup>1</sup>; Sueli Oba-Shinjo<sup>1</sup>; João Bosco de Oliveira<sup>2</sup>; Andreia Otake<sup>3</sup>; Roger Chammas<sup>3</sup>; Clarice Izumi<sup>4</sup>; Anelisa Ramao<sup>4</sup>; Helen Julie Laure<sup>4</sup>; Marcela Gimenez<sup>4</sup>; <sup>1</sup>Dept. of Neurology, Medical School of Sao Paulo, Sao Paulo, Brazil; <sup>2</sup>Dept. of Laboratory Medicine, Clinical Center, NIH, Bethesda, MD; <sup>3</sup>Experimental Oncology, Medical School of Sao Paulo, Sao Paulo, Brazil; <sup>4</sup>Cell & Molecular Biology, FMRP-Univ. Sao Paulo, Ribeirao Preto, Brazil
- ThP 432 **CSF Proteome Characterisation: Dynamics of Plasma Proteins and CNS Specific Proteins;** Jill Anette Opsahl<sup>1,2</sup>; Elise Aasebø<sup>2</sup>; Yngvild Bjørlykke<sup>2</sup>; Hilde Garberg<sup>1</sup>; Astrid Guldbrandsen<sup>2</sup>; Frode S. Berven<sup>1,2</sup>; <sup>1</sup>Proteomics Unit at University of Bergen, Bergen, Norway; <sup>2</sup>The KG Jebsen Centre for MS-Research, Bergen, Norway
- ThP 433 **Comparison of Cuprizone and Experimental Autoimmune Encephalomyelitis Multiple Sclerosis Models Using TMT and Label-Free Quantitative Proteomics and Translation to Patients;** Eystein Oveland<sup>2,3</sup>; Stig Wergeland<sup>1,3</sup>; Harald Barsnes<sup>1,2</sup>; Kjell-Morten Myhr<sup>1,3</sup>; Lars Bø<sup>1,3</sup>; Frode Berven<sup>2,3</sup>; <sup>1</sup>University of Bergen, Bergen, Norway; <sup>2</sup>Proteomics Unit at University of Bergen, Bergen, Norway; <sup>3</sup>Haukeland University Hospital, Bergen, Norway
- ThP 434 **Selection and Quantification of Neurotrauma Markers in Cerebrospinal Fluid (CSF) by Mass Spectrometry;** Sean Shen; Ina Wanner; Gregg Czerwiec; Joseph A. Loo; University of California, Los Angeles, CA
- ThP 435 **Using Neuroblastoma as an Alzheimer's Disease Model to Study the Effect of Angiotensin Converting Enzyme Inhibitors;** Yu-Chang Tyan<sup>1</sup>; Ming-Hui Yang<sup>2</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>National Yunlin University of Science & Technology, Yunlin, Taiwan
- ThP 436 **MALDI-TOF MS Investigation of Analyte Release from Regions of the Mammalian Peripheral Sensory-Motor System;** Stanislav Rubakhin<sup>1</sup>; Jonathan Sweedler<sup>2</sup>; <sup>1</sup>Beckman Institute, UIUC, Urbana, IL; <sup>2</sup>Department of Chemistry, UIUC, Urbana, IL
- ThP 437 **Proteomic Investigation of Saliva from Children with Autism Spectrum Disorder (ASD) and Matched Controls during Circadian Rhythmicity;** Katherine M. Beglinger<sup>1</sup>; Armand G. Ngounou Wetie<sup>1</sup>; Kelly L. Wormwood<sup>1</sup>; Jarrod W. Mattingly<sup>1</sup>; Urmi Roy<sup>1</sup>; Jeanne P. Ryan<sup>2</sup>; Alisa G. Woods<sup>1</sup>; Costel Darie<sup>1</sup>; Sokolowska Sokolowska<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>State University of New York, Plattsburgh, NY
- ThP 438 **A TransOmics study of the Saliva of Children with Autism Spectrum Disorder Using High Definition Mass Spectrometry;** Alisa G. Woods<sup>1</sup>; Joanne B. Connolly<sup>2</sup>; Lee Gethings<sup>2</sup>; Armand G. Ngounou Wetie<sup>1</sup>; Cristian Cojocariu<sup>2</sup>; Janet Hammond<sup>2</sup>; Jeanne P. Ryan<sup>3</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>Waters, Manchester, UK; <sup>3</sup>State University of New York, Plattsburgh, NY
- ThP 439 **Proteomic Investigation of Sera and Saliva from Children with Autism Spectrum Disorder and Matched Controls;** Kelly L. Wormwood<sup>1</sup>; Armand G. Ngounou Wetie<sup>1</sup>; Izabela Sokolowska<sup>1</sup>; Katherine M. Beglinger<sup>1</sup>; Jarrod W. Mattingly<sup>1</sup>; Urmi Roy<sup>1</sup>; Jeanne P. Ryan<sup>2</sup>; Alisa G. Woods<sup>1</sup>; Costel Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>State University of New York, Plattsburgh, NY
- ThP 440 **Proteomic Quantification of Characteristic Markers of Human Oligodendrocyte Differentiation;** Raghothama Chaerkady<sup>1</sup>; Candace Kerr<sup>1,2</sup>; Robert Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Department of Biochemistry, University of Maryland, Baltimore, MD
- ThP 441 **Quantitative Proteomic Techniques: Exploring Protein Pathways and Potential Biomarkers in Dorsal Region of Rat Spinal Cord Associated with Neuropathic Pain;** Ping Sui; Hiroyuki Watanabe; Georgy Bakalkin; Konstantin Artemenko; *Uppsala University, Uppsala, Sweden*
- ThP 442 **Mass Spectrometry-Based Biomarker Discovery: toward the Development of Fundamental Neurochemistry Knowledge Essential for the Development of New Pain Medicines;** Floriane Pailleux<sup>1,2</sup>; Pascal Vachon<sup>1</sup>; Jérôme Lemoine<sup>2</sup>; Francis Beaudry<sup>1</sup>; <sup>1</sup>Université de Montréal, Saint-Hyacinthe, Canada; <sup>2</sup>Université de Lyon, Villeurbanne, France
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- ThP 443 **miR-27b-regulated TCTP as a Novel Plasma Biomarker for Oral Cancer: From Quantitative Proteomics to Post-Transcriptional Study;** Wan-Yu Lo<sup>1</sup>; Huang-Joe Wang<sup>1</sup>; Chih-Wei Chiu<sup>2</sup>; Sung-Fang Chen<sup>2</sup>; <sup>1</sup>China Medical University, Taichung, Taiwan; <sup>2</sup>National Taiwan Normal University, Taipei, Taiwan
- ThP 444 **Direct ESI-LC-MS/MS Microorganism Identification and Monitoring in Endotracheal Samples from VAP Suspected Patient;** Chloé Bardet<sup>1</sup>; Christelle Compagnon<sup>1</sup>; Marie Cécile Ploy<sup>2</sup>; Jérôme Lemoine<sup>3</sup>; Marc Rodrigue<sup>1</sup>; Tanguy Fortin<sup>1</sup>; <sup>1</sup>Biomerieux, Marcy L'étoile, France; <sup>2</sup>UMR-S 1092, INSERM Université de Limoges, Limoges, France; <sup>3</sup>UMR 5180, CNRS Université de Lyon 1, Lyon, France
- ThP 445 **Changes in the Human Hippocampus Proteome during Alzheimer's Disease;** David C. Hondius<sup>1,2</sup>; Roel C. van der Schors<sup>2</sup>; Jeroen J.M. Hoozemans<sup>1</sup>; Pim van Nierop<sup>2</sup>; Saskia M. van der Vies<sup>1</sup>; Ka Wan Li<sup>2</sup>; Annemieke J.M. Rozemuller<sup>1</sup>; August B. Smit<sup>2</sup>; <sup>1</sup>Dept. of Pathology, VU University Medical Center, Amsterdam, NL; <sup>2</sup>Neuroscience Campus Amsterdam, VU University, Amsterdam, NL
- ThP 446 **Creating Reference Materials for Clinically-Relevant Proteins via QconCAT Peptides;** Tyler A Zimmerman; Mark Lowenthal; Meiyao Wang; Karen Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
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- ThP 448 **Top-Down Proteomics of Chronic Lymphocytic Leukemia: A Pilot Project;** Emma Doud<sup>1</sup>; Vivian Bin Liu<sup>2,3</sup>; Shuo Ma<sup>2,3</sup>; Steven Rosen<sup>2,3</sup>; Paul Thomas<sup>1</sup>; Neil Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, Illinois; <sup>2</sup>Robert H. Lurie Comprehensive Cancer Center, Chicago, IL; <sup>3</sup>Feinberg School of Medicine, Chicago, IL
- ThP 449 **Towards the Mechanism of EGFR Inhibitor Resistance in Non-Small Lung Cancer Cells;** Michael Blank<sup>1</sup>; Ryan Bomgarden<sup>2</sup>; John Rogers<sup>2</sup>; Ryan Jacobs<sup>3</sup>; Jason Fong<sup>3</sup>; Neelu Puri<sup>3</sup>; Vlad Zabrouskov<sup>1</sup>; Rosa Viner<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Rockford, IL; <sup>3</sup>University of Illinois at Chicago, Rockford, IL
- ThP 450 **Proteomic Analysis of Oxidative Stress-Induces Monocyte Necrosis;** Haiping Tang<sup>1</sup>; Enbing Tian<sup>2</sup>; Shan Feng<sup>1</sup>; Qingtao Wang<sup>2</sup>; Chongdong Liu<sup>2</sup>; Haiteng Deng<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>Chaoyang Hospital Affiliated to Capital Medical Un, Beijing, China
- ThP 451 **Oxacillin Resistance Study on Methicillin Resistant and Susceptible *Staphylococcus aureus* by Label Free Quantitative Proteomics;** Xiao-Fen Liu<sup>1</sup>; Ying-Wei Hu<sup>1</sup>; Pei-Jing Pai<sup>1</sup>; Dai-Jie Chen<sup>2</sup>; Henry Lam<sup>1</sup>; <sup>1</sup>Hong Kong



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<sup>2</sup>China State Institute of Pharmaceutical Industry, Shanghai, China

- ThP 452 **In-depth Characterization of the Cerebrospinal Fluid Proteome including Glycosylation Patterns and Molecular Weights as a Resource for Targeted Proteomics Assays;** Astrid Guldbrandsen; Heidrun Vetthe; Yehia Farag; Hilde Garberg; Magnus Berle; Eystein Oveland; Jill Anette Opsahl; Harald Barsnes; Frode Berven; University of Bergen, Bergen, Norway
- ThP 453 **Comparison of Five Serum Depletion or Fractionation Methods Applied for Clinical Biomarkers Discovery Studies;** Gabriel Mazzucchelli<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Dominique Baiwir<sup>2</sup>; Edouard Louis<sup>3</sup>; Edwin De Pauw<sup>1</sup>; Marie-Alice Meuwis<sup>3</sup>; <sup>1</sup>MS Lab, GIGA-R, University of Liege, Liege, Belgium; <sup>2</sup>GIGA proteomic facility, Liege, Belgium; <sup>3</sup>Dpmt of Gastroenterology, University Hospital, CHU, Liege, Belgium
- ThP 454 **Skin Aging - Identification of Protein Factors Secreted by Human Dermal Fibroblasts Using a Quantitative Proteome Approach;** Daniel Waldera-Lupa<sup>1</sup>; Gereon Poschmann<sup>1</sup>; Faiza Khalfallah<sup>2</sup>; Fritz Boege<sup>2</sup>; Kai Stühler<sup>1</sup>; <sup>1</sup>Heinrich-Heine Universität Düsseldorf, Düsseldorf, Germany; <sup>2</sup>Universitätsklinikum Düsseldorf, Düsseldorf, Germany
- ThP 455 **Dried Blood Spot Proteomics: Automated Surface Sampling and Sample Preparation;** Nicholas J. Martin; Josephine Bunch; Helen J. Cooper; University of Birmingham, Birmingham, UK
- ThP 456 **Super-SILAC Based Quantitative Proteomics for Comparison of Different Acute Myeloid Leukaemia Cell Lines;** Elise Aasebø<sup>1</sup>; Gro Gausdal<sup>2</sup>; Olav Mjaavatten<sup>1</sup>; Arthur van der Burgh<sup>1</sup>; Bjørn Tore Gjertsen<sup>3</sup>; Stein Ove Døskeland<sup>2</sup>; Øystein Bruserud<sup>3</sup>; Frode Selheim<sup>1</sup>; Frode S. Berven<sup>1</sup>; <sup>1</sup>Proteomics Unit, IBM, University of Bergen, Bergen, Norway; <sup>2</sup>Department of Biomedicine, University of Bergen, Bergen, Norway; <sup>3</sup>Institute of Medicine, University of Bergen, Bergen, Norway
- ThP 457 **Comparative Proteomics of Androgen and Anti-androgen Treatment in Prostate Cells;** Arum Park<sup>1</sup>; Jiyeong Lee<sup>1</sup>; Hee-Joung Lim<sup>2</sup>; Byung Heun Cha<sup>1</sup>; Tag Keun Yoo<sup>3</sup>; HooKeun Lee<sup>4</sup>; Hee-Gyoo Kang<sup>1</sup>; <sup>1</sup>Eulji University, Seongnam, Korea; <sup>2</sup>Korea University, Seoul, Korea; <sup>3</sup>Department of Urology and Pathology, Eulji University, Daejeon, Korea; <sup>4</sup>Lee Gil Ya Cancer and Diabetes Institute, Incheon, Korea
- ThP 458 **Compare the Change of Proteome Profiling in Prostate Cells by Disulfiram and Bicalutamide Using In-gel Digestion;** Anne Seok<sup>1</sup>; Hee-Joung Lim<sup>2,3</sup>; JuHwan Lee<sup>1</sup>; JiYeong Lee<sup>1</sup>; Sung Hee Hyun<sup>4</sup>; Jong-Hoon Kim<sup>2</sup>; Kwang Ho Kim<sup>3</sup>; Hee-Gyoo Kang<sup>1</sup>; <sup>1</sup>Eulji University, Seongnam, Korea; <sup>2</sup>Korea University, Seoul, Korea; <sup>3</sup>Kairos Co. Ltd, Seongnam, Korea; <sup>4</sup>Department of Biomedical Laboratory Science, Eulji University, Daejeon, Korea
- ThP 459 **Sarcomere Protein Expression Studies Suggest Mutation-Specific Disease Mechanisms in Human Hypertrophic Cardiomyopathy;** Richard Jones<sup>1</sup>; Michael Ford<sup>1</sup>; Ravi Amunugama<sup>1</sup>; David Allen<sup>1</sup>; Frank Davis<sup>2</sup>; Adam Helms<sup>2</sup>; Sarah Bartolone<sup>2</sup>; Sharlene Day<sup>2</sup>; <sup>1</sup>MS Bioworks, LLC, Ann Arbor, MI; <sup>2</sup>University of Michigan, Ann Arbor, MI
- ThP 460 **The Peptidome and the Degradome of the Juvenile Idiopathic Arthritis (JIA) Synovial Fluid;** Cristina Clement; Ginger Janow; Myrasol Callaway; Edward Nieves; Steven Porcelli; Laura Santambrogio; Albert Einstein College of Medicine, Bronx, NY
- ThP 461 **Cellular Senescence and an Inflammatory Senescence-Associated Secretory Phenotype in Human Preadipocytes;** Yi Zhu; Mayo Clinic, Rochester, MN
- ThP 462 **Top-Down Sequencing via MALDI-MS/MS for Clinical Determination of Protein Variants;** Roger Theberge; Christian Heckendorf; Stephen Whelan; Catherine E Costello; Mark E McComb; Boston University School of Medicine, Boston, MA
- ThP 463 **Smooth Muscle Cell TGF-beta Signaling Study and Multi-Target Quantification upon TGF-beta Stimulation;** Xiaoguan Liu<sup>1</sup>; Sarah Parker<sup>1</sup>; Harry (Hal) Dietz<sup>1</sup>; Brigitte Simons<sup>2</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>AB SCIEX, Concord, ON
- ThP 464 **Clinical Proteomics Improves Subtyping of Pituitary Adenomas;** Jason D Theis; Surendra Dasari; Julie Vrana; Ken Johnson; Catarina Giannini; Mark Jentoft; Ahmet Dogan; Mayo Clinic, Rochester, MN
- ThP 465 **Optimization of Mass Spectrometry-based Detection of Beta-Amyloid Variants and the Proteome Profiles from Alzheimer's Disease Senile Plaques;** Ko-Yi Chien; Ina Caesar; Sam Gandy; Rong Wang; Mount Sinai Medical Center, New York, NY
- ThP 466 **Proteome Measurement Repeatability and Depth of Protein Coverage in Lymphoma Cell Lines;** Kenneth L. Johnson; Carrie J. Heppelmann; Surendra Dasari; Jason D. Theis; Roman Zenka; H. Robert Bergen, III; Andrew L. Feldman; Ahmet Dogan; Mayo Clinic, Rochester, MN
- ThP 467 **Preliminary Large Scale Quantitative Proteomic Analysis of Bortezomib Resistant Multiple Myeloma;** Zhiping Wu<sup>1</sup>; Xusheng Wang<sup>1</sup>; Haiyan Tan<sup>1</sup>; Megan Schertzer<sup>1</sup>; Dharminder Chauhan<sup>2</sup>; Kenneth Anderson<sup>2</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>ST. Jude, Memphis, TN; <sup>2</sup>Dana-Farber Cancer Institute, Harvard Medical Sch, Boston, MA
- ThP 468 **Quantitative Proteomics Analysis of Human Central Memory T Cells for Assessing Protein Expression Profile of HIV-Infected subjects on HAART;** Sausan Azzam; Daniela Schlatter; Douglas Bazdar; Jill Barnholtz-Sloan; Yanwen Chen; Mark Chance; Scott Sieg; Case Western Reserve University, Cleveland, OH
- ThP 469 **Comparative Phosphoproteomic Analysis of 106 Human Liver Tissues by 2-dimensional Image-Converted Analysis of Liquid Chromatography and Mass Spectrometry (2DICAL);** Masaya Ono<sup>1</sup>; Masahiro Kamita<sup>1</sup>; Tomohiro Sakuma<sup>2</sup>; Miho Banno<sup>2</sup>; Tesshi Yamada<sup>1</sup>; <sup>1</sup>Natl Cancer Ctr Research Institute, Tokyo, Japan; <sup>2</sup>Mitsui Knowledge Industry Co., Ltd., Tokyo, Japan
- ThP 470 **Label-free Quantitative Proteomics of Biopsy Tissue from Breast Cancer Patients Reveals Inflammatory Activation of the Tumor Microenvironment;** Michael Groessl<sup>1</sup>; Kerstin Gloessmann<sup>2</sup>; Georg Pfeiler<sup>2</sup>; Christopher Gerner<sup>1</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Medical University of Vienna, Vienna, Austria
- ThP 471 **Classification of MALDI-FTICR Serum Peptide and Protein Profiles of Patients with Pancreatic Cancer;** Simone Nicolardi; Berit Velstra; Bart J. Mertens; Bert A. Bonsing; Rob A.E.M. Tollenaar; André M. Deelder; Wilma E. Mesker; Yuri E.M. van der Burgt; Leiden University Medical Center (LUMC), Leiden, Netherlands
- ThP 472 **Development of Analytical Methods for the Measurement of Thyroglobulin by Mass Spectrometry in Human Serum;** Brittany Catron; W. Clay Davis; Stephen Long; NIST, Charleston, SC
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ThP 474 **Bronchoalveolar Lavage Fluid Protein Profiling In ARDS: Early Differences Between Survivors And Non-Survivors**; Maneesh Bhargava; Trisha Becker; LeeAnn Higgins; Pratik Jagtap; Sanjoy Dey; Michael Steinbach; Baolin Wu; Vipin Kumar; Peter Bitterman; David Ingbar; Wendt Chris; *University of Minnesota, Minneapolis, MN*

ThP 475 **Proteomic Approach for the Diagnosis of Nephropathic Cystinosis Using LC-MRM-MS**; Sunhee Jung<sup>1</sup>; Thierry Vilboux<sup>2</sup>; William Gahl<sup>2</sup>; Si Houn Hahn<sup>1,3</sup>; <sup>1</sup>Seattle Children's, Seattle, WA; <sup>2</sup>NIH, Bethesda, MD; <sup>3</sup>University of Washington, Seattle, WA

ThP 476 **Integrating Biomarker Discovery and Evaluation Using Global Semi-Quantitative and Targeted Quantitative MS Technologies**; Elodie Duriez<sup>2</sup>; Magali Court<sup>1</sup>; Cedric Mesmin<sup>2</sup>; Claire Adam<sup>1</sup>; Mourad Mellal<sup>1</sup>; Madalen Le Gorrec<sup>1</sup>; Yves Allory<sup>3</sup>; Nuria Mallats<sup>4</sup>; Antonia Vlahou<sup>5</sup>; François Radvanyi<sup>6</sup>; Markus Fisher<sup>7</sup>; Bruno Domon<sup>2</sup>; Jérôme Garin<sup>1</sup>; Christophe Masselon<sup>1</sup>; <sup>1</sup>CEA Grenoble, Grenoble, France; <sup>2</sup>CRP Santé, Luxembourg, Luxembourg; <sup>3</sup>Hôpital Mondor, Créteil, France; <sup>4</sup>CNIO, Madrid, Spain; <sup>5</sup>BRFAA, Athens, Greece; <sup>6</sup>Institut Curie, Paris, France; <sup>7</sup>Entelchon GmbH, Regensburg, Germany

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ThP 478 **Cystic Fibrosis Transmembrane Conductance Regulator Localization Studied via Targeted Quantitative Mass Spectrometry and Isotope Labeling in Cells**; Adam McShane; Bekim Bajrami; Xudong Yao; *University of Connecticut, Storrs, CT*

ThP 479 **Application of Stable Isotope Dilution Approach for Targeted Quantitation of Membrane Transporters**; Vahid Farrokhi; Bekim Bajrami; Adam McShane; Franz Rueckert; Reza Nemati; Barrett Wells; Xudong Yao; *University of Connecticut, Storrs, CT*

ThP 480 **Tuning Protease Digest Conditions for Analysis of Membrane Proteins**; Lie Min<sup>1,2</sup>; Kelvin H. Lee<sup>1,2</sup>; <sup>1</sup>Delaware Biotechnology Institute, Newark, DE; <sup>2</sup>University of Delaware, Newark, DE

ThP 481 **Comparison of Commercial Surfactants on Membrane Protein Digestion Efficiency for MS-based Proteomic Applications**; Matthew Waas; Subarna Bhattacharya; Sandra Chuppa; Xiaogang Wu; Kathleen R. Noon; Rebekah L. Gundry; *Medical College of Wisconsin, Milwaukee, WI*

ThP 482 **Examining Ligand Induced Conformational Changes in the Human Erythrocyte Glucose Transporter, GLUT1, through Chemical Crosslinking and Mass Spectrometry**; Kenneth Lloyd; Stephanie Maniatis; John D. Leszyk; Anthony Carruthers; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*

ThP 483 **Analysis of Cell Surface Membrane Proteins in a Metastatic Melanoma Cell Line**; Eric Stephens; Yinsheng Wang; *University of California, Riverside, CA*

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ThP 485 **Top-down Proteomics and High-resolution Mass Spectrometry of Mouse Mitochondrial Membrane Proteins**; Upendra K. Kar; Alexander Yoon; Chris Ryan; Kym F. Fault; Julian Whitelegge; *Pasarow Mass Spectrometry Laboratory, UCLA, Los Angeles, CA*

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ThP 487 **Novel Label Free Species-Specific Quantitation Method for Mixed Proteomes - Application to Studies of Human Infectious Disease and Bacterial Endosymbionts**; Will Thompson; Laura Dubois; Arthur Moseley; *Duke University School of Medicine, Durham, NC*

ThP 488 **SILAC Study Reveals the Significant Changes on the Cell Shape and Energy Shift after IPTG Inducing on Escherichia coli**; Ping Xu; *State Key Laboratory of Proteomics, Changping District, China*

ThP 489 **Development of Software for Detecting and Identifying Fungal Species Using GC/MS, LC/MS and IMS Data of Microbial Volatile Organic Compounds**; Takae Takeuchi<sup>1</sup>; Shoko Ichii<sup>1</sup>; Yoshitaka Nakamura<sup>2</sup>; Toshiki Sugai<sup>3</sup>; Masato Kiuchi<sup>4</sup>; Tomohiro Akashi<sup>5</sup>; <sup>1</sup>Nara Women's University, Nara, Japan; <sup>2</sup>DYNACOM Co., Ltd., Chiba, Japan; <sup>3</sup>Toho University, Funabashi, Japan; <sup>4</sup>AIST, Ikeda, Japan; <sup>5</sup>Nagoya University, Nagoya, Japan

ThP 490 **Use of an Automated Software Tool for the Evaluation of  $\beta$ -lactamase Activity by MALDI-TOF**; Gary Kruppa<sup>1</sup>; Katrin Spärbier<sup>2</sup>; Christoph Lange<sup>2</sup>; Markus Kostrzewa<sup>2</sup>; Jette Jung<sup>3</sup>; Soeren Schubert<sup>3</sup>; <sup>1</sup>Bruker Daltonics Inc., Billerica, MA; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Max-von-Pettenkofer Institute, Munich, Germany

ThP 491 **A Chemical Fingerprint Database of Marine Bacteria Based on High-Resolution LC-MS**; Liang Lu; Ji-Jie Wang; Ying Xu; Henry Lam; Pei-Yuan Qian; *Hong Kong University of Science and Technology, Hong Kong, China*

ThP 492 **Comparation of Different Methods of MALDI-TOF for Fast and Reliable Identification of *Saccharomyces cerevisiae* in the Sugarcane Fermentative Process**; Mariana Silva; Thaís Regiani; Carlos Labate; *Max Feffer Laboratory of Plant Genetics ESALQ/USP, Piracicaba, Brazil*

ThP 493 **Novel Bacterial Classification Method by MALDI-TOF MS Based on Ribosomal Protein Coding in *S10-spc-alpha* Operon at Strain level**; Hiroto Tamura<sup>1</sup>; Naomi Yamamoto<sup>1</sup>; Yudai Hotta<sup>1,2</sup>; Hiroaki Sato<sup>3</sup>; Keisuke Shima<sup>4</sup>; Shinji Funatsu<sup>4</sup>; Yuzo Yamazaki<sup>4</sup>; Helen Montgomery<sup>5</sup>; Akifumi Hosoda<sup>1,6</sup>; Noriyuki Ojima<sup>4</sup>; <sup>1</sup>Meijo University, Nagoya, Japan; <sup>2</sup>Kumiai Chemical Industry, Tokyo, Japan; <sup>3</sup>AIST, Tsukuba, Japan; <sup>4</sup>Shimadzu Corporation, Kyoto, Japan; <sup>5</sup>Shimadzu UK, Manchester, UK; <sup>6</sup>"The Knowledge Hub" of AICHI, Nagoya, Japan

ThP 494 **Parallel SIMS and MALDI MS Imaging to Visualize Biomolecule Distributions in Microbial Biofilms across Multiple Size Scales**; Eric J Lanni; Jonathan V. Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*

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- ThP 496 **Differentiation of *Borrelia* Species with MALDI-MS Using Spray Sample Deposition;** Franco Basile<sup>1</sup>; Gwendoline Toh-Boyo<sup>1</sup>; Shaun Wulff<sup>1</sup>; Claudia Molins<sup>2</sup>; <sup>1</sup>University of Wyoming, Laramie, WY; <sup>2</sup>Centers for Disease Control and Prevention, Fort Collins, CO
- ThP 497 **A Multiplexed MassCode PCR Assay for the Detection of Bacterial and Viral Agents on an APCI Single Quadrupole Mass Spectrometer;** William A. Harris<sup>1</sup>; Mark D. Burton<sup>1</sup>; Danielle N. Dickinson<sup>1</sup>; Johnny K. Ho<sup>1</sup>; Yvette R. Hudson<sup>1</sup>; Kristin M. Taylor<sup>1</sup>; Anna Kidney<sup>2</sup>; Michael J. Perry<sup>2</sup>; Christina T. Egan<sup>2</sup>; Rafal Tokarz<sup>3</sup>; Thomas Briesse<sup>3</sup>; Peter Sheffield<sup>4</sup>; Carsten Carstens<sup>4</sup>; Douglas B. Henderson<sup>1</sup>; <sup>1</sup>Northrop Grumman, Linthicum, MD; <sup>2</sup>NYS DOH - Wadsworth, Albany, NY; <sup>3</sup>Columbia University, New York, NY; <sup>4</sup>Agilent Technologies, La Jolla, CA
- ThP 498 **Rapid Organism Identification by Shotgun Proteomics: A Novel, Easy to Implement Database Search Strategy;** Dobryan Tracz; Staurt McCorrister; Patrick Chong; David Lee; Cindi Corbett; Garrett R Westmacott; Public Health Agency Canada, Winnipeg, Canada
- ThP 499 **Analysis of Bacteria by Performing *in situ* Pyrolysis on a DART ID Cube™/Time-of-Flight MS;** Yvette R. Hudson; Johnny K. Ho; Danielle N. Dickinson; William A. Harris; Douglas B. Henderson; Northrop Grumman, Linthicum, MD
- ThP 500 **Optimizing Soil Metaproteomic Methods to Capture *in situ* Microbial Community Expression;** Eun-Hae Kim<sup>1</sup>; Ben Woodcroft<sup>2</sup>; Robert Jones<sup>1</sup>; Manesh Shah<sup>4</sup>; Gene Tyson<sup>2</sup>; Nathan VerBerkmoes<sup>3</sup>; Virginia Rich<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>University of Queensland, Brisbane, Australia; <sup>3</sup>New England Biolabs, Ipswich, MA; <sup>4</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 501 **Advanced Deep Metaproteomics Methods Provide Unique Insights into the Diversity of the Human Proteome and Gut Microbiota in Healthy Adults;** Lang Ho Lee<sup>1,2</sup>; Kristen Corrier<sup>1,2</sup>; Brian Dill<sup>6</sup>; Manesh Shah<sup>2</sup>; Robert Hettich<sup>2</sup>; Janet Jansson<sup>3</sup>; Marcelo Sztein<sup>4</sup>; Nathan VerBerkmoes<sup>5</sup>; <sup>1</sup>University of Tennessee, Knoxville, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>4</sup>University of Maryland School of Medicine, Baltimore, MD; <sup>5</sup>New England Biolabs Inc., Ipswich, MA; <sup>6</sup>University of Dundee, Scotland, UK
- ThP 502 **Characterizing Microbiome Stability and Metabolic Activities in Post-Surgery Crohn's Diseased Human Gut by High Performance Mass Spectrometry;** Robert Hettich<sup>1</sup>; Alison Erickson<sup>1</sup>; Weili Xiong<sup>1</sup>; Brandi Cantarel<sup>2</sup>; Claire Fraser-Liggett<sup>2</sup>; Chongle Pan<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Maryland, Baltimore, MD
- ThP 503 **MALDI MS Investigation of Mass Fingerprints Generated Directly from Whole Cell Bacteria;** Philippa Hart<sup>1</sup>; Emmanuel Wey<sup>2</sup>; Omar Belgacem<sup>1</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>Royal Free Hospital NHS Foundation Trust, London, UK
- ThP 504 **Quantitative Proteomic Profiling of *Clostridium difficile*;** Lu Yu; Laura Deakin; Trevor Lawley; Gordon Dougan; Jyoti Choudhary; Wellcome Trust Sanger Institute, Hinxton, UK
- ThP 505 **Disease Phenotype of Juvenile and Adult CFTR-Knockout Ferrets;** T. Idil Evans; Yulong Zhang; Weihong Zhou; Hongshu Sui; John Engelhardt; R. Marshall Pope; University of Iowa, Iowa City, IA
- ThP 506 **Discriminating Pathogenic and Non-Pathogenic *Francisella* Strains with Three Proteogenomic Biomarkers;** Emie Durighello; Alain Lorphelin; Marie-Anne Roncato; Eric Ezan; Laurent Bellanger; Jean Armengaud; CEA, Bagnols Sur Ceze, France
- ThP 507 **Quantitative Proteomic and Surface Proteomic Investigation of the *Staphylococcus aureus* Response to Oxacillin Adaptation;** Nestor Solis<sup>1</sup>; Benjamin Parker<sup>1</sup>; Stephen Kwong<sup>1</sup>; Neville Firth<sup>1</sup>; Mark Graham<sup>2</sup>; Stuart Cordwell<sup>1</sup>; <sup>1</sup>The University of Sydney, Sydney, Australia; <sup>2</sup>Children's Medical Research Institute, Sydney, Australia
- ThP 508 **Protein Analysis of Host Components within Protease-Treated Influenza A Virus Particles;** Jie Zheng<sup>1</sup>; Debbie Huiling Ko<sup>1</sup>; Myint Zu Myaing<sup>1</sup>; Boon-Huan Tan<sup>2</sup>; Richard Sugrue<sup>1</sup>; Kai Tang<sup>1</sup>; <sup>1</sup>Nanyang Technological University, Singapore; <sup>2</sup>DSO national Laboratories, Singapore
- ThP 509 **Autoacetylation Sites in the *Pseudomonas syringae* Type III Secreted Effector Protein, HopZ1a, Deduced by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Jacquelyn R Jhingree<sup>1</sup>; Amy H Lee<sup>1,2</sup>; Darrell Desveaux<sup>1,2</sup>; David S Guttman<sup>1,2</sup>; <sup>1</sup>CAGEF, University of Toronto, Toronto, Canada; <sup>2</sup>Dept. of Cell and Systems Biology, University of Toronto, Toronto, Canada
- ThP 510 **Comprehensive Top-down Proteomic Analysis of the Pathogenic Bacterium *Pseudomonas aeruginosa* PAO1;** Joanna Ntai; John Tran; Archer Smith; Ryan Fellers; Bryan Early; Paul Thomas; Neil Kelleher; Northwestern University, Evanston, IL
- ThP 511 **Targeted Analysis of *Salmonella* effector Proteins Using Multiple Reaction Monitoring;** Joost Gouw; Nat Brown; Leonard Foster; University of British Columbia, Vancouver, Canada
- ThP 512 **Characterization of Flagellar Hook Protein from *Spirochetes* Using Tandem Mass Spectrometry;** Justin M. Hettick<sup>1</sup>; KellyAnn Miller<sup>2</sup>; Milinda James<sup>2</sup>; Nyles W. Charon<sup>2</sup>; Michael R. Miller<sup>2</sup>; <sup>1</sup>NIOSH, Morgantown, WV; <sup>2</sup>West Virginia University, Morgantown, WV
- ThP 513 **Proteomics for Mycosis Vaccine Development;** Jackson Chamber; Diana Diaz-Arevalo; Mayyen Wong; Miriam Chamber; Jason Yu; Molly Shannahoff; Karina Vega; James Ito; Markus Kalkum; City of Hope, Duarte, CA
- ThP 514 ***Syntrophus aciditrophicus* Triosephosphate Isomerase: What We Gain from MS-Deduced Protein Sequence Not Predicted from the Genome;** Hong Hanh Nguyen; Yanan Yang; Robert Gunsalus; Joseph Loo; Rachel Ogorzalek Loo; UCLA, Los Angeles, CA
- ThP 515 **iTRAQ Analysis of *Campylobacter jejuni* Prophage Effects on Protein Expression Associated with the Virulence and Biology of the Organism;** Stuart McCorrister; Patrick Chong; Garrett Westmacott; Clifford Clark; Public Health Agency of Canada, Winnipeg, Canada
- ThP 516 **Intact Protein Profiling and Deconvolution of Bacterial Lysates on Multiple Mass Spectrometers;** Denis Andrzejewski<sup>1</sup>; John H. Callahan<sup>1</sup>; Timothy Croley<sup>1</sup>; Peter E. Leopold<sup>2</sup>; Melinda A. McFarland<sup>1</sup>; <sup>1</sup>FDA-CFSAN, College Park, MD; <sup>2</sup>BioAnalyte, Inc., Portland, ME
- ThP 517 **Top-down Proteomic Identification of Shiga Toxin 2 Variants from Shiga Toxin-Producing *Escherichia coli* (STEC) Using MALDI-TOF-TOF-MS/MS-PSD;** Clifton K. Fagerquist; William J. Zaragoza; Omar Sultan; Nathan Woo; Beatriz Quinones; Michelle Swimley; Michael B. Cooley; Robert E. Mandrell; USDA, Albany, CA
- ThP 518 **Metabolomic Analysis of Marine Microalgae Using High Resolution Mass Spectrometry for Taxonomic Comparisons and Screening of Marine Biotoxins;** Philipp Hess<sup>1,2</sup>; Florence Mondegue<sup>1</sup>; Thomas Glauner<sup>3</sup>; Bernhard Wuest<sup>3</sup>; Manoella Sibati<sup>1</sup>; Zita Zendong<sup>1,4</sup>; Christine Herrenknecht<sup>4</sup>; Veronique Sechet<sup>1</sup>; <sup>1</sup>Ifremer, Nantes, France; <sup>2</sup>IUML, Institut Universitaire Mer et Littoral, CNRS, Nantes, France; <sup>3</sup>Agilent Technologies, Waldbronn, Germany; <sup>4</sup>LUNAM, Université de Nantes, MMS EA2160, Nantes, France



ThP 519 **Discovery and Quantitation of the Marine Microbial Metaproteome in the Central Pacific Ocean;** Mak Saito<sup>1</sup>; Matthew McIlvin<sup>1</sup>; Dawn Moran<sup>1</sup>; Tyler Goepfert<sup>1</sup>; Vlad Zabrouskov<sup>2</sup>; Justin Blethrow<sup>2</sup>; <sup>1</sup>Woods Hole Oceanographic Institution, Woods Hole, MA; <sup>2</sup>Thermo Scientific, San Jose, CA

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ThP 520 **Development of a Fieldable DART-based High Performance Ruggedized Ambient Ionization Mass Spectrometer (DART-HiPR-MS);** Danielle N. Dickinson<sup>1</sup>; William A. Harris<sup>1</sup>; Hoon Ra<sup>1</sup>; Johnny K. Ho<sup>1</sup>; Yvette R. Hudson<sup>1</sup>; Douglas B. Henderson<sup>1</sup>; Karl A. Hanold<sup>2</sup>; Robert Tysl Jr.<sup>2</sup>; Paul Chaney<sup>2</sup>; Brian D. Musselman<sup>3</sup>; Joseph Tice<sup>3</sup>; <sup>1</sup>Northrop Grumman, Linthicum, MD; <sup>2</sup>Syagen, Santa Ana, CA; <sup>3</sup>Ionsense, Saugus, MA

ThP 521 **A Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) Instrument Designed for Sensitive and Selective Monitoring in Real-Life Threat Scenarios;** Alfons Jordan<sup>1</sup>; Lukas Märk<sup>1</sup>; Thomas Kassebacher<sup>1,2</sup>; Jens Herbig<sup>3</sup>; Philipp Sulzer<sup>1</sup>; Simone Jürschik<sup>1</sup>; Matteo Lanza<sup>1</sup>; Chris A. Mayhew<sup>4</sup>; Tilmann D. Märk<sup>1,2</sup>; <sup>1</sup>IONICON Analytik GmbH., Innsbruck, Austria; <sup>2</sup>University of Innsbruck, Innsbruck, Austria; <sup>3</sup>IONIMED Analytik, Innsbruck, Austria; <sup>4</sup>University of Birmingham, Birmingham, UK

ThP 522 **Quantitative Detection of Botulinum Neurotoxins by MALDI-TOF Mass Spectrometry;** Dongxia Wang; Jakub Baudys; Joan Krilich; Suzanne R. Kalb; John R. Barr; Centers of Disease Control and Prevention (CDC), Atlanta, GA

ThP 523 **Atmospheric Pressure Chemical Ionization and Secondary Electrospray Ionization for Sensitive Detection of Explosives on the Field-Deployable Compact Ion Trap;** Victor Laiko; Berk Oktem; Thomas Souli; Vladimir Doroshenko; MassTech, Inc., Columbia, MD

ThP 524 **Auto-sampling Explosives Trace Detection Baggage Screener Using Mass Spectrometry;** Yuichiro Hashimoto; Hisashi Nagano; Yasuaki Takada; Yasutaka Suzuki; Hideo Kashima; Masakazu Sugaya; Yasunori Doi; Koichi Terada; Minoru Sakairi; Hitachi, Ltd, Central Research Lab, Kokubunji, Tokyo, Japan

ThP 525 **A High Throughput Screen for Serine-198 Adducted Butyrylcholinesterase in Human Sera by Immunomagnetic Separation and HPLC-MS/MS Analysis;** Melissa Carter<sup>1</sup>; Brian Crow<sup>1</sup>; Brooke Pantazides<sup>2</sup>; Caroline Watson<sup>2</sup>; Thomas Blake<sup>1</sup>; Rudolph Johnson<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA; <sup>2</sup>ORISE, Atlanta, GA

ThP 526 **Proteomics for Botulism Outbreak Investigations: a Powerful Tool to Track Sources of Intoxication and Commonality of Botulism Outbreaks;** John R. Barr; Suzanne Kalb; Jakub Baudys; Jon Rees; Dongxia Wang; CDC, Atlanta, GA

ThP 527 **Advances in Security Checkpoint Screening for Explosives and Narcotics Using Mass Spectrometry;** Garth Patterson; Phil Tackett; Brent Rardin; Mitch Wells; Dennis Barket; FLIR Mass Spectrometry, West Lafayette, IN

#### Food Safety - Pesticides, 528 – 558

ThP 528 **Determination of 200 Residual Pesticides in Food by Ultra High Performance Liquid Chromatography/ Triple Quadrupole Mass Spectrometry;** Hongyuan Hao<sup>1</sup>; YiKun Deng<sup>2</sup>; Jinting Yao<sup>1</sup>; Hengtao Dong<sup>1</sup>; Hui Gao<sup>1</sup>; Yueqi Li<sup>1</sup>; Taohong Huang<sup>1</sup>; Shin-ichi kawano<sup>1</sup>; Yuki Hashi<sup>1</sup>; <sup>1</sup>Shimadzu (China) Co., Ltd., Shanghai, China; <sup>2</sup>Shimadzu (Guangzhou) Analysis & Technology Service, Guangzhou, China

ThP 529 **Identification and Quantitation of Pesticides in Food Samples Using UHPLC-MS/MS with the Enhanced Scheduled MRM Functionality and MS/MS Library Searching;** Andre Schreiber<sup>1</sup>; Paul Yang<sup>2</sup>; David Cox<sup>1</sup>; Yun Yun Zou<sup>1</sup>; Jon Wong<sup>3</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>Ministry of Environment, Toronto, Canada; <sup>3</sup>U.S. Food and Drug Administration, College Park, MD

ThP 530 **Targeted Screening and Quantification of Pesticide Residuals in Tobaccos by Ultra Fast LC/MS/MS;** Jie Xing<sup>1</sup>; Zhi Wei Ting<sup>1</sup>; Yin Ling Chew<sup>2</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore; <sup>2</sup>Department of Chemistry, Faculty of Science, National University of Singapore, Singapore

ThP 531 **Rapid Analysis of Pesticides in Commercial Fruit Juices and Fruit Wine by Liquid Chromatograph/High Resolution Orbitrap Mass Spectrometer;** Kai-Chih Yang; Bo-Shen Wu; Yu-Huai Chang; Min-Wei Cheng; Ying-Ru Shen; Su-Hsiang Tseng; Ya-Min Kao; Lih-Ching Chiueh; Yang-Chih Shih; Taiwan Foods And Drugs Administration, Department, Taipei City, Taiwan

ThP 532 **Validation of an Accurate Mass Screening Method for Pesticide Residues in Food Using UPLC-QToF MS and Automated Data Processing Software;** Sara Stead<sup>1</sup>; Dominic Roberts<sup>1</sup>; Michael McCullagh<sup>1</sup>; Ramesh Rao<sup>1</sup>; Monica Lopez Garcia<sup>2</sup>; Richard Fussell<sup>2</sup>; <sup>1</sup>Waters corp, Manchester, UK; <sup>2</sup>Food and Environment Research Agency, York, UK

ThP 533 **Application of a Prototype Microfluidic Device with MS for the Screening of Pesticide Residues in Food Analyses;** Michael McCullagh<sup>1</sup>; Severine Goscinny<sup>2</sup>; David Douce<sup>1</sup>; Dominic Roberts<sup>1</sup>; Sara Stead<sup>1</sup>; Ramesh Rao<sup>1</sup>; Kenneth Rosnack<sup>3</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>WIV-ISP, Brussels, BE; <sup>3</sup>Waters Corp, Milford, MA

ThP 534 **The Use of Micro Flow UHPLC to Reduce Solvent Usage in the Pesticide Screening of Food Samples by LC-MS/MS;** Stephen J. Lock; ABSCIEX, Warrington, UK

ThP 535 **High-Throughput Determination of Carbendazim in Orange Juice Using Strong Cation Exchange SPE and LDTD-MS/MS;** Serge Auger<sup>1</sup>; Gregory Blachon<sup>1</sup>; Vincent Bédard<sup>2</sup>; Veronique Marceau<sup>2</sup>; David Dube<sup>2</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>Phytrox Technologies, Quebec, Canada; <sup>2</sup>Silicyle, Quebec, Canada

ThP 536 **Targeted/Non Targeted Screening of Pesticides in QuEChERS Extracts of Vegetables Using UHPLC-TOF and High Throughput Screening Software;** Sharanya Reddy; Sergey Rakov; Blas Cerda; George Perkins; PerkinElmer, Shelton, CT

ThP 537 **Simultaneous Analysis of 15 Pesticides in Green tea Using ASE and LC-MS/MS;** Jin Kyoung Kim<sup>1</sup>; Seon Song<sup>1</sup>; Soon-Kil Cho<sup>1</sup>; Yangmo Jeong<sup>1</sup>; Jong-Hyoun Park<sup>2</sup>; Jae-Han Shim<sup>2</sup>; <sup>1</sup>National Agricultural Products Quality Management, Gwangju, Republic of Korea; <sup>2</sup>Chonnam National University, Gwangju, Republic of Korea

ThP 538 **Rapid and Simple Approaches to Multi-residue Pesticide Analysis in Fruits and Vegetables on both GC-MS/MS and LC-MS/MS;** Helen (Qingyu) Sun; Zicheng Yang; Kefei Wang; Bruker Corporation, Fremont, CA

ThP 539 **Analysis of Multiple Pesticide Residues in Salad Using Triple Quadrupole GCMS/MS System;** Ankush Bhone<sup>1</sup>; Durvesh Sawant<sup>1</sup>; Dheeraj Handique<sup>1</sup>; Prashant Hase<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Ajit Datar<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Akshata Salve<sup>2</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India; <sup>2</sup>G. N. Khalsa College, Matunga, Mumbai, Maharashtra, India

ThP 540 **Micro Flow UHPLC-MS/MS in Pesticide Analysis of Infant Foods;** David Baker<sup>1</sup>; Neil Loftus<sup>1</sup>; Simon Hird<sup>2</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>The Food and Environment Research Agency, York, UK

- ThP 541 **Accurate Mass Screening and Confirmation of Pesticides in Fruit and Vegetable Samples with New Targeted MS/MS Data Review Workflow**; Thomas Glauner<sup>1</sup>; Guenther Kempe<sup>2</sup>; Matthieu Rault<sup>3</sup>; Vadim Kalmeyer<sup>3</sup>; Yoshimasa Tsunoi Yoshimasa Tsunoi<sup>3</sup>; Marc Tischler<sup>3</sup>; <sup>1</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>2</sup>Lua Saxony, Chemnitz, Germany; <sup>3</sup>Agilent Technologies Inc., Santa Clara, CA
- ThP 542 **Analysis of Multiresidue Pesticides Present in Ayurvedic Medicines Like Churna Using Triple Quadrupole Gas Chromatograph Mass Spectrometer (GCMS/MS)**; Dr. Manoj Surwade; Aarti Karkhanis; Manish kumar Deshmukh; *ThermoFisher Scientific India, Powai, Mumbai, India*
- ThP 543 **Applying High Speed Data Acquisition MS/MS to the Analysis of Pesticides Residues in Complex Spice Matrix**; Alan Barnes<sup>1</sup>; David Baker<sup>1</sup>; Neil Loftus<sup>1</sup>; Simon Hird<sup>2</sup>; <sup>1</sup>Shimadzu MS/BU (Overseas), Manchester, UK; <sup>2</sup>The Food and Environment Agency, York, UK
- ThP 544 **Comparison of LC and GC Triple Quadrupole MS for the Screening of 500 Pesticides in Matrix**; Juan Carmona<sup>1</sup>; Marcus Miller<sup>2</sup>; David Steiniger<sup>1</sup>; Jason Cole<sup>1</sup>; Mary Blackburn<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; Paul Silcock<sup>1</sup>; Jennifer Massi<sup>2</sup>; Charles Yang<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific Austin, Austin, TX; <sup>2</sup>Thermo Fisher Scientific San Jose, San Jose, CA
- ThP 545 **Broad Scope Pesticide Screening in Food Using GC Triple Quadrupole MS**; David Steiniger; Juan Carmona; Paul Silcock; Sergio Guazzotti; *Thermo Fisher Scientific, Austin, TX*
- ThP 546 **Maximising Information from GC/MS/MS Systems for Pesticide Analysis**; Bruce Peebles; Robert Trengove; *Murdoch University, Murdoch, Australia*
- ThP 547 **Evaluation of Matrix Effects for Dilute-and-Shoot LC-MS/MS Analysis of Carbendazim in Orange Juices and Wines**; Helen (Qingyu) Sun; Zicheng Yang; Kefei Wang; *Bruker Corporation, Fremont, CA*
- ThP 548 **Automated MS Optimization of a Modified Triple Quadrupole Mass Spectrometer Enabled Improved Multi-Residue Pesticide Analysis in Fruit and Vegetables**; Fandino Anabel<sup>1</sup>; Thomas Glauner<sup>2</sup>; Bernhard Wüst<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc, Santa Clara, CA; <sup>2</sup>Agilent Technologies R&D and Marketing GmbH & Co., Waldbronn, Germany
- ThP 549 **Quantification of Phosphorothioate Pesticides in Indian Red Chilli at Sub ppb Concentrations Using Negative Ionization APCI Technique**; Arvind Thyagarajan; Saravanan Subramanian; Raman Palvannanathan; Mohan Kasi; Venkat Manohar; *IICMS, Chennai, India*
- ThP 550 **Quantitative Analysis of Trace Level Pesticides in Vegetable Foods by GC-MS/MS**; Sun Qian; Fan Jun; Gao Peng; Huang Taohong; Hashi Yuki; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Shanghai, China*
- ThP 551 **Fast Quantitation of Carbendazim and Qualitative Analysis of Pesticides in Orange Juice Using LC/TOF**; Avinash Dalmia; Courtney Phillips; George Perkins; *PerkinElmer, Shelton, CT*
- ThP 552 **Rapid Simultaneous Screening of Multiple Pesticide Residues in Food Matrices**; Joerg Riener; *Agilent Technologies, Waldbronn, Germany*
- ThP 553 **Development of a Sensitive CE-MS/MS Method for the Quantitation of Polar Pesticides and Their Metabolites in Food Samples**; Hans Brunnert; Thomas Glauner; Martin Greiner; *Agilent Technologies GmbH, Waldbronn, Germany*
- ThP 554 **Qualitative Screening for Pesticides in Fruit and Vegetable Samples with UHPLC-QTOF-MS Employing All Ions MS/MS Acquisition**; Thomas Glauner<sup>1</sup>; Bernhard Wuest<sup>1</sup>; Joachim Thiemann<sup>1</sup>; Guenther Kempe<sup>2</sup>; <sup>1</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>2</sup>LUA Saxony, Chemnitz, Germany
- ThP 555 **Evaluation of the Data Processing and Multiresidue Determination of Pesticide Residues in Fruits by LC-QTOF-MS**; Renato Zanella<sup>1</sup>; Juliana S. Munaretto<sup>1</sup>; Mariela de S. Viera<sup>1</sup>; Celso Blatt<sup>2</sup>; Daniela Daniel<sup>2</sup>; Manoel L. Martins<sup>1</sup>; Martha B. Adaime<sup>1</sup>; <sup>1</sup>Federal University of Santa Maria, LARP, Santa Maria - RS, Brazil; <sup>2</sup>Agilent Technologies, Inc., Barueri - SP, Brazil
- ThP 556 **Direct Analysis of Pesticides from Food Commodities by Swab/Desorb Mass Spectrometry**; Sheng-Suan (Victor) Cai; Andrey Vilkov; Jack Syage; *Morpho Detection, Inc., Santa Ana, CA*
- ThP 557 **Software System for Automated Pesticide Screening**; Tim Croley<sup>1</sup>; Igor Teslya<sup>2</sup>; Graham A. McGibbon<sup>2</sup>; Ann M. Knolhoff<sup>1</sup>; Scott McDonald<sup>2</sup>; John Callahan<sup>1</sup>; Richard Lee<sup>2</sup>; <sup>1</sup>FDA/CFSAN, College Park, MD; <sup>2</sup>Advanced Chemistry Development, Toronto, Canada
- ThP 558 **Multiresidue Pesticide Analysis in Crude Food Extracts Using AOC-MEPS and LC/MS/MS**; Yuka Fujito<sup>1</sup>; Shigeaki Shibamoto<sup>2</sup>; Kiyomi Arakawa<sup>2</sup>; Ichiro Hirano<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>Shimadzu Analytical & Measuring Center Inc., Kyoto, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- Lipids: Profile Analysis, 559 – 591**
- ThP 559 **Accurate Mass Search of Candidate Individual Lipid Species from High-Resolution Mass Spectra for Shotgun Lipidomics**; Baichen Zhang<sup>1</sup>; Miao Wang<sup>1</sup>; Yingying Huang<sup>2</sup>; Xianlin Han<sup>1</sup>; <sup>1</sup>Sanford-Burnham Medical Research Institute, Orlando, FL; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- ThP 560 **In-vivo Tissue Identification Using Ambient Ionization Mass Spectrometry - Comparison of Different Multivariate Classification Workflows**; Julia Balog<sup>1</sup>; Laszlo Molnar<sup>1</sup>; Kirill Vesekov<sup>2</sup>; Zoltan Takats<sup>2</sup>; <sup>1</sup>Medimass Ltd, Budapest, Hungary; <sup>2</sup>Imperial College London, London, UK
- ThP 561 **Fecal Lipidomics Profiling and Structural Identification Using High Resolution LC-MS and HCD Fragmentation**; Susan S. Bird<sup>1,2</sup>; Katherine E. Gregory<sup>1,3</sup>; Vera S. Gross<sup>4</sup>; Vasant R. Marur<sup>1</sup>; Alexander V. Lazarev<sup>4</sup>; W. Allen Walker<sup>2,5</sup>; Bruce S. Kristal<sup>1,2</sup>; <sup>1</sup>Brigham and Women's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Boston College, Boston, MA; <sup>4</sup>Pressure BioSciences, South Easton, MA; <sup>5</sup>Massachusetts General Hospital, Boston, MA
- ThP 562 **Hyphenating Size-Exclusion Chromatography with Electrospray; Using On-Line Liquid-Liquid Extraction to Study the Lipid Composition of Lipoproteins Particles**; Albert Koulman; Michael Osei; Jules Griffin; *Medical Research Council, Cambridge, UK*
- ThP 563 **A Very Fast Triple Quadrupole Mass Spectrometer as a Tool for SRM-based Phospholipidomics**; Yoshihiro Kita<sup>1</sup>; Suzumi Tokuoka<sup>1</sup>; Masaki Yamada<sup>1,2</sup>; Takao Shimizu<sup>1</sup>; <sup>1</sup>The University of Tokyo, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 564 **Comprehensive and Quantitative Lipidome Profiling of Colorectal Adenocarcinoma Cell Lines and Their Secreted Exosomes**; Cassie Fhaner<sup>1</sup>; Hong Ji<sup>2</sup>; Richard Simpson<sup>2</sup>; Gavin Reid<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>La Trobe University, Victoria, Australia
- ThP 565 **Effects of Long- and Short-term Caloric Restriction on Serum Triglycerides Revealed by Lipidomics Analysis via High Resolution LC-MS with HCD**; Bruce S. Kristal<sup>1,2</sup>; Van S. Hubbard<sup>3</sup>; Pamela E. Starke-Reed<sup>3</sup>; Susan S. Bird<sup>1,2</sup>; Vasant R. Marur<sup>1,2</sup>; Matthew J. Sniatynski<sup>1,2</sup>; <sup>1</sup>Brigham and Women's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Division of Nutrition Research Coordination, NIH, Bethesda, MD



- ThP 566 **High-throughput Lipidomic Analysis of Arachidonic Acid Metabolites in Biological Fluids by Liquid Chromatography/Mass Spectrometry**; Natalia Belikova; Yasuhiro Yamashita; Jenny Lin; *JCL Bioassay USA, Inc., Hoffman Estates, IL*
- ThP 567 **Large-scale Screening of African Infant Plasma Lipidomic Phenotypes: Application of UPLC-MS in Dietary Interventional Epidemiology Studies**; María Gómez-Romero; Nikita Gandhi; Manuja R. Kaluarachchi; Caroline J. Sands; Hannah J. Lees; Elaine Holmes; Jeremy K. Nicholson; Anisha D. Wijeyesekera; *Imperial College London, London, UK*
- ThP 568 **Identification of Novel Metabolites of Docosahexaenoic Acid in Neural Stem Cells Using Stable Isotope Labeled Compounds and High-Resolution Mass Spectrometry**; Karl R. Kevala<sup>1</sup>; Mohammed Rashid<sup>1</sup>; Mark Sanders<sup>2</sup>; Hee-Yong Kim<sup>1</sup>; <sup>1</sup>National Institutes of Health, Bethesda, MD; <sup>2</sup>Thermo Fisher Scientific, Somerset, NJ
- ThP 569 **Effect of the Expression of the ACSL4 Enzyme on Lipid Metabolism in Cell Line Models of Human prostate and breast cancers**; Farid Jahouh<sup>2</sup>; Xinyu Wu<sup>2</sup>; Peng Lee<sup>2</sup>; Marie E. Monaco<sup>2</sup>; Rong Wang<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY; <sup>2</sup>New York University School of Medicine, New York, NY
- ThP 570 **Hopanoic Acid Containing and Intact Polar Components of the Lipidome of *Rhodospirillum rubrum* palustris TIE-1 Investigated Using UPLC-TOF-MS<sup>E</sup>**; Nathan Dalleska<sup>1</sup>; Cajetan Neubauer<sup>1</sup>; Dianne Newman<sup>1,2</sup>; <sup>1</sup>Caltech, Pasadena, CA; <sup>2</sup>Howard Hughes Medical Institute, Pasadena, CA
- ThP 571 **Determination of Ubiquinone and Related Metabolites in Zebrafish Embryos by LC-HRMS**; Claudio Medana; Federica Dal Bello; Chiara Martano; Vera Mugoni; Massimo Santoro; Claudio Baiocchi; *University of Turin, Torino, Italy*
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