



58TH ASMS CONFERENCE ON MASS SPECTROMETRY
MAY 23 – 27, 2010 • SHORT COURSES: MAY 22 - 23, 2010
Salt Lake City, Utah

LOCATION. The conference and short courses will be held at the Salt Palace Convention Center, 100 South West Temple, Salt Lake City, UT 84101. All oral sessions, poster sessions, exhibit booths and hospitality suites will be located in the convention center.

REGISTRATION. On-site conference registration will open 2:00 pm, Saturday, May 22 in the convention center. There is no on-site registration for short courses.

For more information: www.asms.org

American Society for Mass Spectrometry

2019 Galisteo Street, Building I-1, Santa Fe, NM 87505

Phone: (505) 989-4517 Fax: (505) 989-1073 office@asms.org www.asms.org



Vice President for Programs: Scott A. McLuckey

TABLE OF CONTENTS

New This Year	S2
ASMS Awards	S3
Research Awards	S4
Program Overview	S5
Workshops	S7
Sunday Program.....	S10
Monday Morning Oral Sessions	S10
Monday Afternoon Oral Sessions	S13
Tuesday Morning Oral Sessions	S15
Tuesday Afternoon Oral Sessions.....	S17
Wednesday Morning Oral Sessions	S20
Wednesday Afternoon Oral Sessions.....	S22
Thursday Morning Oral Sessions.....	S25
Thursday Afternoon Oral Sessions	S27
Monday Posters.....	S31
Tuesday Posters	S61
Wednesday Posters	S92
Thursday Posters.....	S122
Author Index	S152
Corporate Members	S217

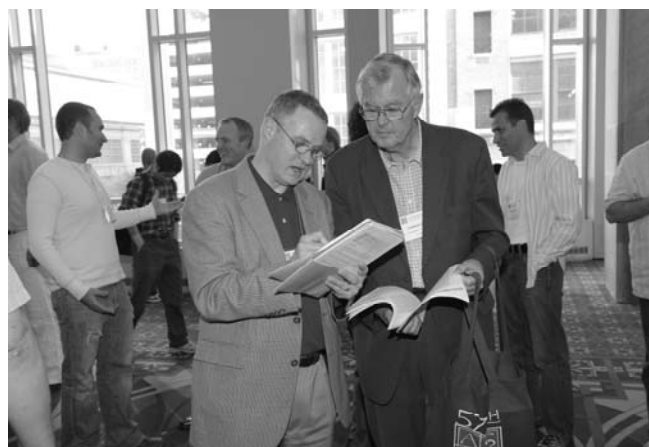
DON'T MISS ANOTHER GREAT CONFERENCE!

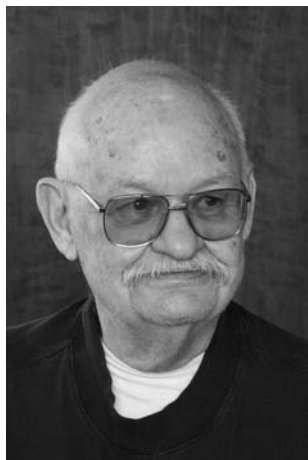
The Salt Palace Convention Center is in the heart of downtown Salt Lake City surrounded by many restaurants and shops.

www.asms.org

**New this
year!**

- Use the online abstract viewer to create your personal program.
- There will be no conference bag – let's minimize waste.
- As workshops become more popular, they have expanded to three nights – Monday, Tuesday and Wednesday. More refreshments will be offered before the start of workshops - look for a theme each evening.
- Be sure to visit the Interest Group pages on the ASMS web site to view their workshop plans.
- There will be a one-hour break between the end of workshops and the opening of corporate hospitality suites. Use the time to explore restaurants – both “fast” and “fine” in the area surrounding the convention center.
- Hospitality suites will be in the convention center – so convenient!
- Some corporate members will host breakfast seminars in the convention center. Drop by an exhibit booth to reserve a seat.
- There will be no “off-site” finale – we will have a farewell toast immediately following the closing plenary lecture.
- The conference Proceedings will be online by June 30 – no more DVD that formerly was mailed in September.



Award for a Distinguished Contribution in Mass Spectrometry**2010 Recipient: Marvin L. Vestal****Award Lecture: 4:45 – 5:30 pm, Monday, Hall 4**

The different components of a mass spectrometer need to be carefully integrated for optimum design and performance. The focused efforts of **Marvin L. Vestal** on the development of practical MALDI-TOF and TOF-TOF mass spectrometers culminated in the first commercial MALDI-TOF instrumentation – the Voyager series. More than one half of MALDI-TOF instruments in use are based on Dr. Vestal's designs. A significant accomplishment of his work is the development of a comprehensive theoretical model for the various components of a TOF analyzer with a view toward optimizing performance of a complete system for particular applications. Dr. Vestal implemented this theoretical approach to design a family of MALDI-TOF instruments that employed delayed extraction, and through further refinements, the construction of a tandem time-of-flight instrument introduced commercially as the 4700 Proteome Analyzer and later the 4800 TOF-TOF by Applied Biosystems. Advances in related technology have been combined with Dr. Vestal's theoretical predictions to provide MALDI-TOF MS and MS-MS systems that out-perform earlier instruments by orders of magnitude. The MALDI-TOF MS and MS-MS systems designed by Dr. Vestal have had and are continuing to have an enormously positive impact on many important areas of research, including proteomics, glycomics, cell signaling, structural biology, tissue imaging, and polymer science.

Dr. Marvin L. Vestal is Founder, CEO, and CSO of Virgin Instruments.

The Biemann Medal**2010 Recipient: David C. Muddiman****Award Lecture: 4:45 – 5:30 pm, Tuesday, Hall 4**

Mass spectrometric analysis requires analytes to be introduced as gaseous ionized species into the mass analyzer of choice. However, signal abundance is not a direct function of analyte concentration but depends on numerous instrumental and chemical parameters. **David C. Muddiman** discovered that one strand of a PCR amplicon appears more intense than the complementary strand in an electrospray ionization (ESI) mass spectrum. He understood that the extent of hydrophobicity contributed to this effect and his research group was able to obtain a sensitivity gain of one order of magnitude by adding a hydrophobic alkyl chain. Dr. Muddiman has extended this "hydrophobic tagging" approach to also improve the ESI response of peptides. In another major research direction, Dr. Muddiman has developed alternative ion sources for FT-ICR mass spectrometry, including the dual ESI source, matrix-assisted laser desorption electrospray ionization (MALDESI), liquid MALDESI, and an "air amplifier" for more efficient ESI. The significance of these advances is that they allow generation of multiply charged species, which are uniquely suited for FT-ICR MS due to the inverse relationship between frequency and m/z . Dr. Muddiman has published over 150 papers in peer-reviewed journals and is recognized for his unusual combination of depth and breadth in the field of biological mass spectrometry.

Dr. David C. Muddiman is Professor of Chemistry at North Carolina State University.

**Ron A. Hites Award for Outstanding Research Publication in JASMS****Award Presentation: ASMS Meeting, Wednesday 4:45 – 5:30 pm, Ballroom ACE**

The Ron Hites Award recognizes a high quality presentation of outstanding 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 Ronald A. Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS.

The 2010 award is presented to **Prof. Facundo Fernández** for the article "Direct Quantitation of Active Ingredients in Solid Artesunate Antimalarials by Noncovalent Complex Forming Reactive Desorption Electrospray Ionization Mass Spectrometry;" Leonard Nyadong, Sameer Late, Michael D. Grren, Ajay Banga, and Facundo Fernández; *JASMS* 2008, Vol. 19, 380-388. Prof. Fernández is in the School of Chemistry and Biochemistry, Georgia Institute of Technology.



2010 Recipients

Sponsored by
Thermo Scientific



Hao Chen
Ohio University

Sponsored by
Waters Corporation



Sarah Trimpin
Wayne State University

CALL FOR 2011 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 faculty or equivalent position within a North American university. Applicants may not have previously received an award under this program.

APPLICATION Applicants should submit **SEVEN** collated sets of the following

1. One-page fiscal proposal and justification
2. List of current research support
3. Three-page proposal, including references, figures, etc.
4. *Curriculum vitae*
5. Two letters of recommendation (may be sent directly to ASMS)

DEADLINE Application materials, including letters of recommendation, must be received in the ASMS office by November 30. Send to:
ASMS, 2019 Galisteo Street, Building I-1, Santa Fe, NM 87505

FISCAL The awards of \$25,000 each will be made to a university in the name of the selected individual and for the researcher's exclusive use. In accepting this award, the institution will agree not to charge overhead on the funds.

INFORMATION Contact ASMS. Telephone: (505) 989-4517 • office@asms.org

CONFERENCE PROGRAM OVERVIEW

SAT	9:00 am - 4:30 pm	SHORT COURSES
	2:00 - 5:00 pm	REGISTRATION
SUNDAY	9:00 am - 4:30 pm	SHORT COURSES
	10:00 am - 8:00 pm	REGISTRATION
	5:00 - 6:30 pm	TUTORIAL LECTURES, Hall 4 <ul style="list-style-type: none"> • Collision Induced Dissociation: How Does It Really Work and What It Can (or Can't) Tell You; Peter B. Armentrout, University of Utah • The Role of Mass Spectrometry in Drug Discovery and Development; Walter A. Korfmacher, Merck Research Laboratories
	6:45 - 7:45 pm	OPENING and PLENARY LECTURE, Hall 4 Systems Medicine and Emerging Technologies; Leroy Hood, Institute for Systems Biology
	7:45 - 9:30 pm	RECEPTION IN THE EXHIBIT HALL, Exhibit Hall ABCDE
MONDAY	8:30 - 10:30 am	ORAL SESSIONS - <i>Click title to view abstracts</i> <ul style="list-style-type: none"> • MOA: Fundamentals: Ion Structures and Energetics, Ballroom HJ • MOB: New Developments in Ion Traps and Hybrid Instruments, Ballroom ACE • MOC: MS of Nucleic Acids Ballroom BDF • MOD: MS Derived Peptide/Protein Biosignatures and Biomarkers, Room 155 • MOE: Increasing Throughput for ADME and PK Assays, Hall 2 • MOF: Application of LC-MS for PK Characteristics of Biologics, Hall 3 • MOG: Quantitative Intact Proteomics, Hall 4
	10:30 am - 2:30 pm	POSTER SESSION AND EXHIBITS, Exhibit Hall ABCDE
	2:30 - 4:30 pm	ORAL SESSIONS - <i>Click title to view abstracts</i> <ul style="list-style-type: none"> • MOA: Fundamentals: Supramolecular Chemistry: Non-Covalent Complexes, Ballroom HJ • MOB: Advances in Imaging, Ballroom ACE • MOC: MS of Synthetic Polymers, Ballroom BDF • MOD: Qualitative Analysis of Protein Therapeutics by MS, Room 155 • MOE: LC-MS Challenges & Solutions for Monitoring Human Metabolites in Safety Testing (MIST), Hall 2 • MOF: Quantitation of Biologics: Applications and Techniques, Hall 3 • MOG: Phosphoproteomics Applications, Hall 4
	4:45 - 5:30 pm	AWARD LECTURE, Hall 4 Recipient of the Award for a Distinguished Contribution in Mass Spectrometry
	5:45 - 7:00 pm	WORKSHOPS. See list on page S7.
	8:00 - 11:30pm	CORPORATE HOSPITALITY SUITES, Salt Palace Convention Center
TUESDAY	8:30 - 10:30 am	ORAL SESSIONS - <i>Click title to view abstracts</i> <ul style="list-style-type: none"> • TOA: Fundamentals: Biomolecular Ion Radical Chemistry, Ballroom HJ • TOB: MS of Lipids, Ballroom ACE • TOC: MS of Viruses, Ballroom BDF • TOD: MS of Protein-Ligand Complexes, Room 155 • TOE: Incurred Sample Reanalysis and Analytical Solutions, Hall 2 • TOF: Quantitation of Xenobiotic Metabolites without Reference Standard, Hall 3 • TOG: Quantitation in Proteomics: Peptides, Hall 4
	10:30 am - 2:30 pm	POSTER SESSION AND EXHIBITS, Exhibit Hall ABCDE
	2:30 - 4:30 pm	ORAL SESSIONS - <i>Click title to view abstracts</i> <ul style="list-style-type: none"> • TOA: Fundamentals: Ion Spectroscopy, Ballroom HJ • TOB: MS and Immunology, Ballroom ACE • TOC: MS of Carbohydrates, Ballroom BDF • TOD: New Developments in Ionization, Room 155 • TOE: Identification of Unusual Xenobiotic Metabolites Using MS, Hall 2 • TOF: Dealing with Phospholipids in Regulated Bioanalysis, Hall 3 • TOG: Bioinformatics in Proteomics, Hall 4
	4:45 - 5:30 pm	AWARD LECTURE, Hall 4; Recipient of the Biemann Medal Research Award Presentations
	5:45 - 7:00 pm	WORKSHOPS. See list on page S8.
	8:00 - 11:30pm	CORPORATE HOSPITALITY SUITES, Salt Palace Convention Center

CONFERENCE PROGRAM OVERVIEW

WEDNESDAY	8:30 - 10:30 am	<p>ORAL SESSIONS - <i>Click title to view abstracts</i></p> <ul style="list-style-type: none"> • WOA: Multiple Charging in MS, <i>Ballroom HJ</i> • WOB: MS and Clinical Diagnostics, <i>Ballroom ACE</i> • WOC: MS of Fuels, Biofuels and Heavy Oils, <i>Ballroom BDF</i> • WOD: Environmental MS Identification of Unknowns, <i>Room 155</i> • WOE: LC-MS Strategies for Metabolomics in Drug Discovery, <i>Hall 2</i> • WOF: Clinical Applications of Integrated Qualitative and Quantitative LC-MS, <i>Hall 3</i> • WOG: Characterizing PTMs, <i>Hall 4</i>
	10:30 am - 2:30 pm	POSTER SESSION AND EXHIBITS , <i>Exhibit Hall ABCDE</i>
	2:30 - 4:30 pm	<p>ORAL SESSIONS - <i>Click title to view abstracts</i></p> <ul style="list-style-type: none"> • WOA: Fundamentals: Ion-Molecule and Ion-Ion, Ion-Electron Interactions, <i>Ballroom HJ</i> • WOB: FTMS Instrumentation and Applications, <i>Ballroom ACE</i> • WOC: MS in Environmental Toxicology, <i>Ballroom BDF</i> • WOD: MS of Glycoproteins, <i>Room 155</i> • WOE: LC-MS of Reactive Xenobiotic Metabolites, <i>Hall 2</i> • WOF: MS of Pharmaceuticals and Personal Care Products in Water, <i>Hall 3</i> • WOG: MS and Systems Biology, <i>Hall 4</i>
	4:45 - 5:30 pm	ASMS MEETING , <i>Ballroom ACE</i>
	5:45 - 7:00 pm	WORKSHOPS . <i>See list on page S9.</i>
	8:00 - 11:30 pm	CORPORATE HOSPITALITY SUITES , <i>Salt Palace Convention Center</i>

THURSDAY	8:30 - 10:30 am	<p>ORAL SESSIONS - <i>Click title to view abstracts</i></p> <ul style="list-style-type: none"> • ThOA: Electron and Photon-Based Ion Activation/Dissociation (PD, ECD, ETD, EDD), <i>Ballroom HJ</i> • ThOB: H/D Exchange for Protein Structure and Folding, <i>Ballroom ACE</i> • ThOC: Recent Developments in Ion Mobility MS, <i>Ballroom BDF</i> • ThOD: Metabolomics: Bioinformatics and Metabolite Identification, <i>Room 155</i> • ThOE: Automated and Post-Acquisition Software Tools for Xenobiotic Metabolites, <i>Hall 2</i> • ThOF: Dried Blood Spot Analysis, <i>Hall 3</i> • ThOG: MS and Cellular Pathways, <i>Hall 4</i>
	10:30 am - 2:30 pm	POSTER SESSION AND EXHIBITS , <i>Exhibit Hall ABCDE</i>
	2:30 - 4:30 pm	<p>ORAL SESSIONS - <i>Click title to view abstracts</i></p> <ul style="list-style-type: none"> • ThOA: Fundamentals: Ion-Surface Interactions and Preparative MS, <i>Ballroom HJ</i> • ThOB: Biomolecular Structure, <i>Ballroom ACE</i> • ThOC: Peptide Ion Fragmentation, <i>Ballroom BDF</i> • ThOD: Novel Developments in Instrumentation, <i>Room 155</i> • ThOE: Quantitation of Endogenous Analytes in Regulated Bioanalysis, <i>Hall 2</i> • ThOF: Laser/Surface Desorption Techniques for ADME, <i>Hall 3</i> • ThOG: MS of Membrane Proteins, <i>Hall 4</i>
	4:45 - 5:30 pm	PLENARY LECTURE , <i>Hall 4</i> Svante Pääbo , <i>Max Planck Institute for Evolutionary Anthropology</i>
	5:30 - 6:00 pm	CONFERENCE CLOSING TOAST , <i>Hall 4</i>

MONDAY WORKSHOPS, 5:45 – 7:00 PM

**Identification of Unique Metabolites:
New MS Techniques and Strategies**

Organized by Drug Metabolism and
Pharmacokinetics Interest Group
Ragu Ramanathan, Gabriella Szekely-Klepser,
and Lucinda Cohen, presiding
Hall 3

The identification and quantification of xenobiotic metabolites in response to the MIST guidelines from the regulatory agency has sparked a lot of discussions recently amongst the practitioners of this field. A number of hot topics emerged from the quantification of metabolites without exact reference standards to utilization of various software tools. Subject matter experts will be invited to discuss these topics with the audience, focusing on a practical level of information sharing that will complement the oral and poster sessions in this area.

**Screening for Unknowns in our Environment Experience,
Ideas, and Suggestions**

Organized by Environmental Applications Interest Group
Enrico Davoli and Susan Richardson, presiding
Room 255 D

During last year's workshop we asked major MS manufacturers about their ideas for the future, for our high-end instrumentation, for automated screening, and unknown identification. High resolution and LC/MS instrumentation are extremely powerful, but a lot of work still needs to be done by "the mass spectrometrists." We would like to have environmental scientists' opinions about this difficult and important task that we are more and more frequently asked to do. We will also discuss about new software and approaches available. Come and bring your own ideas and suggestions for a fruitful discussion!

Fundamentals Interest Group

Nick Polfer and Daniel Austin, presiding
Room 255 C

In the tradition of the fundamentals workshop, we will encourage young mass spectrometrists to give short presentations on topics of interest to generate an informal discussion. While the exact topics are dependent on the choice of oral presentations at ASMS, it is expected that ion mobility and ion spectroscopy will feature prominently.

The Reliability of PTM Assignments

Katalin F. Medzihradzky, presiding
Room 255 E

Mass spectrometry has become the method of choice for analyzing post-translational modifications. Many PTM studies are carried out using targeted enrichment followed by LC/MS/MS in an automated, high throughput manner. Modified peptide identification as well as modification site assignments are performed by a variety of search engines. Though these search engines are able to deal with some aspects of PTM analysis they are challenged by the diverse nature of PTMs. We will focus on the reliability (or the lack of it) of automated site assignments, manual inspections, software tools and data presentation/publication. We will also discuss the often overlooked problem of non-biological PTMs.

Hot Topics in LC-MS Instrumentation Troubleshooting

Organized by LC/MS & Related Topics Interest Group
J. Will Thompson, presiding
Room 155

The LC-MS & Related Topics Interest Group workshop for 2010 will focus on user-defined areas of instrumentation troubleshooting. A survey of the Interest Group will be used to decide which

troubleshooting or training areas will be the most beneficial, including but not limited to LC column efficiency, column hardware problems, LC or MS software problems, and MS performance. Experts in instrument troubleshooting, maintenance and repair will be assembled to answer questions, but your expertise is highly valued and needed in order to have a valuable workshop! We are also excited to feature two to three original student research presentations at the beginning of this year's workshop.

**Undergraduate Research in Mass Spectrometry
Interest Group Meeting**

Jen Grant and Mike VanStipdonk, presiding
Room 255 A

We have formed this interest group to consider the challenges and synergies in pursuing undergraduate research from the perspective of both the mentor and mentee. As a group of peers, we will consider issues such as funding, maximizing our activities at ASMS, instrumentation access, etc. Also, we will strategize as to the future activities of this interest group.

Quantitative Intact Proteomics (QIP)

David Friedman and Julian Whitelegge, presiding
Room 255 B

We propose an open forum format where Julian and David moderate the discussion while "roaming the room" with microphones to be handed to participants. David/Julian will open the workshop with a 5 minute introduction to QIP themes, and present a short list of possible discussion points generated from a pre-survey using our existing email interest list. A small panel of 2 or 3 additional experts will be invited to give a 5-minute presentation on a topical area in the beginning, and then remain in front during the discussion. Kathryn Lilley (Cambridge) has already accepted our invitation to be on the expert panel; she is an expert on QIP-related issues, including experimental design and statistical power.

NIH Update: Funding Opportunities and Recent Policy Changes

Douglas Sheeley, presiding
Hall 2

The National Institutes of Health has recently made changes to several aspects of the application and review process, including new formats and page limits for applications, a new scoring system, and a new format for summary statements. NIH staff will provide an overview of these changes, as well as more general information on NIH policies and the grant application process. In addition, current funding opportunities related to mass spectrometry will be discussed, including small business grants. There will be time for questions and discussion.

The Role of Mass Spectrometry in Our Future Energy Supply

David Stranz and Wolfgang Schrader, presiding
Room 255 F

The world's energy supply environment is changing rapidly. The character of traditional petroleum-based fuels is becoming more complex as sweet crude oil sources become depleted and are replaced by sources that are heavier and more difficult to extract and process. At the same time, there is an explosion of new biologically-based fuels with their own characterization problems.

This workshop will feature short presentations and a panel discussion from practitioners analyzing petroleum- and biologically-based fuel sources, with focus on the analytical problems unique to each field and the requirements for improvement in technique, instrumentation, and analysis tools.

Current Topics in FTMS

Organized by FTMS Interest Group
Adam Hawkridge, presiding
Hall 3

An anonymous web-based survey was conducted in January/February 2010 to assess the experience levels and interests of the FTMS Interest Group Members that could then be used to guide the organizational structure and content of the Workshop. The number of topics covered during the Workshop will be kept to a minimum (2-3) as will the length of any presentation (< 5 slides) so as to maximize time for discussion. An outline of the topics with potential discussion points will be made available before the start of ASMS via the FTMS Interest Group webpage. An email will be sent to all FTMS Interest Group Members notifying them when the outline is posted.

Metabolomics Current Challenges and Future Directions

Organized by Metabolomics Interest Group
Lloyd W. Sumner & William R. Wikoff, presiding
Room 255 E

The objective of this workshop is to gather together active metabolomics researchers to discuss the current challenges and future directions of the field in the presence of those who wish to learn more about metabolomics. Key topics of discussion will include instrumental advances, data standards, data acquisition and processing, databases and repositories, and metabolite identification and annotation. A panel will guide the discussion, and substantial proportion of the allotted time will be allocated for audience feedback. Thus, bring your comments and we look forward to your participation

LC/MS/MS Analysis of Biomarkers and their Impact on Drug Development

Organized by Pharmaceuticals Interest Group
Carmen T. Santasania and Chris Petucci, presiding
Room 255 D

The purpose of this workshop will be to explore the role that mass spectrometry plays in the analysis of biomarkers. A panel led discussion will center around the challenges that biomarkers pose to the analyst and their impact on drug development.

Problem Solving Session

Organized by Polymeric Materials Interest Group
Michael Polce, presiding
Room 255 C

The workshop will consist of several short informal presentations (3-5 power point slides) in which speakers briefly describe a specific unresolved measurement challenge they have encountered (sample prep, ionization issues, data interpretation, etc.) and the audience provides useful comments and suggestions in an open discussion. A brief meeting will follow to discuss any technical topics of current interest to the group (ion mobility MS of polymers, MS/MS, polymer pyrolysis, new instrumentation, etc.).

Biologics Mass Spectrometry:

Best Practices and Recent Developments

Organized by Protein Therapeutics Interest Group
Guodong Chen & Jon Williams, presiding
Room 255 B

Protein Therapeutics Interest Group (PTIG) is concerned with characterization of protein therapeutics with mass spectrometry, one of rapidly growing fields in the biopharmaceutical industries. This inaugural workshop will bring together experienced scientists and newcomers in the field. Meeting will include a panel discussion on best practices in structural characterization of protein therapeutics

and recent advances in quantitative analysis of protein therapeutics in plasma samples. There will be several short informal presentations, followed by discussions. Meeting will begin with brief discussions on PTIG impact on 2010 ASMS conference program and request for suggestions on 2011 sessions as well as workshop topics.

Careers of Young Mass Spectrometrists

Organized by Young Mass Spectrometrists Interest Group
Connell Cunningham and Bich Vu, presiding
Room 255 A

The workshop will hold panel discussions which deal with issues related to the careers of young mass spectrometrists. Representatives from industry, academia, and government organizations will be invited to give advice on career prospects. The topics will be related to scientific publishing, grant writing, management, entrepreneurship, career pathways in academia and industry, as well as in government organizations.

Challenge in LC-MS/MS Bioanalysis: Scientific Investigations following Incurred Sample Reanalysis (ISR) - Failure and Different Approaches and Techniques for Phospholipids Removal

Organized by Regulated Bioanalysis Interest Group
Fabio Garofolo, Stephen Lowes, and Patrick Vallano, presiding
Hall 2

This year workshop will focus on the following 2 “hot topics:”

1. Conducting **Incurred Sample Reanalysis (ISR)** is now a well established experiment for those performing quantitative bioanalysis in support of PK determinations for regulatory submission. Subsequently, attention has turned to investigating ISR failure to meet reproducibility acceptance criteria and other unexpected outcomes. During this discussion we will explore practical ISR out-of-specification investigations (OOSI) conducted in support of pre-clinical/clinical studies. The debate will step through established and implemented approaches to the investigation process, the associated conclusions and investigation reporting for support of regulated bioanalytical studies.
2. **Phospholipids** are present in biological matrices to a great extend. The presence of phospholipids in sample extracts may produce severe matrix effect and significantly impact the chromatography. We will discuss the extraction conditions that remove phospholipids and the recent approaches used by the industry to handle the effects produced by phospholipids.”

Rearrangement Reactions in Peptide Fragmentation: From Fundamentals to Applications

Organized by Peptide Fragmentation Interest Group
Gavin Reid & Bela Paizs, presiding
Room 155

Rearrangement reactions in peptide fragmentation have received significant attention in the last few years. Typical examples include head-to-tail cyclization and reopening (scrambling) reactions of *b*-type fragments formed by CID, migration of phosphate groups in phosphorylated peptides upon CID, and radical-driven rearrangements upon ECD/ETD of peptide ions. This workshop will provide a forum for researchers studying these rearrangement reactions using both fundamental and statistical methodologies to discuss the application of the related chemistries for peptide sequencing. To facilitate discussion presenters will be allowed to give only short (flash) introduction to their approaches.

Ion Mobility-Mass Spectrometry for Structural Biology

Organized by Ion Mobility MS Interest Group
John A. McLean and Brandon T. Ruotolo, presiding
Room 255 B

The utility of structural separations on the basis of ion mobility-mass spectrometry (IM-MS) has recently shown considerable promise in structural biology research. This workshop will be a forum for discussing the level of structural insight that can be obtained through IM-MS measurements, what additional technology would be necessary to elevate the impact of these measurements in the field of structural biology, and finally the challenges and limitations of IM-MS based studies relative to other structural probes. This workshop attempts to align the commonalities of IM-MS structural and allied studies to better enumerate both the present state-of-the-art as well as future directions for promoting the wider use of IM-MS in structural biology.

Challenges in MS Data Analysis

Organized by Bioinformatics for MS Interest Group
Marc Kirchner, presiding
Hall 2

The workshop will feature two 6min40s "starter/provocation" talks (with automatically advancing slides, so no chance to lengthen the presentation time) on current challenges in two MS Bioinformatics fields: (i) practical application of computational methods and (ii) computational MS statistics and method development. Each talk will be followed by 25min of open discussion.

Towards an Automated Mass Spec Analyzer for Clinical Labs - What, When and How?

Organized by Clinical Chemistry Interest Group
Nigel Clarke and Russell Grant, presiding
Hall 3

Mass Spectrometry has become the new area of interest in the clinical diagnostic world over the last few years. It is growing at an astounding rate with tests such as testosterone and vitamin D leading the way. While the high complexity Dx labs can afford to buy, upkeep and staff these complicated instruments even they will agree that we need to simplify their operation to reduce subjectivity and errors in results. Furthermore, at present large numbers of labs that want to use this technology are sitting on the side-lines waiting for it to become more "user-friendly." We propose to put together a mix of labs and vendors and generally interested parties to discuss the needs and solutions for this situation.

Practical Aspects of New Techniques for Volatile Compound Analysis

Organized by Flavor, Fragrance and Foodstuff Interest Group
David Heller, presiding
Room 255 A

New techniques have been introduced in recent years with applicability to volatile compounds. These techniques include new mass analyzers coupled with gas chromatography, such as new GC-TOF and GC-MS/MS hybrids, and also new ionization techniques, such as ambient ionization and extractive electrospray ionization. This workshop aims to bring together developers or practitioners of such new techniques to discuss practical applications to volatile compounds important to the flavor, fragrance and foodstuff arena. Attendees are invited to share relevant challenges and problem-solving techniques in an open discussion format. We hope to use this Interest Group's Forum page at the ASMS web site for advance discussion of specific topics and techniques.

H/D Exchange and Covalent Labeling

Organized by H/D Exchange and Covalent Labeling Interest Group
Michael Chalmers and Janna Kiselar, presiding
Room 255 C

The workshop will provide a forum that is focused on the discussion of the methods/experimental parameters of HDX and covalent labeling experiments. The workshop will open with a short update on the state of the field. There will be a number of short talks to introduce new advances within the field to the attendees. The goal of the talks (5 min maximum) will be to stimulate discussion. The workshop will also contain a question and answer session with questions being submitted in advance.

Troubleshooting the Imaging Process

Organized by Imaging MS Interest Group
Michelle Rezyer, presiding
Room 155

This workshop will provide a forum for attendees to get helpful hints for getting around common problems in the imaging process. Several speakers (3-4 slides each) will present tips for overcoming challenges at any point in the image generation process, from sample preparation, to image acquisition, to image processing. This will be followed by an informal discussion on specific issues brought up by the audience.

The Great Dissociation Debate. What's Your Favorite Way to Dissociate Ions Inside an Ion Trap?

Organized by Ion Trap Mass Spectrometry Interest Group
Heather Desaire, presiding
Room 255 D

This workshop will be an informal venue for speakers to discuss the relative merits of established and new methods of ion dissociation inside ion traps. New methods such as photodissociation, HCD, and various laser dissociation methods will be explored and compared to standard CID methods, for a variety of different compound types.

Metal Ions: Bridging the Gap between the Gas Phase and Solution

Organized by the Metal Ions Interest Group
Victor Ryzhov, presiding
Room 255 F

This workshop traditionally encompasses various topics involving gas-phase metal ions (bare and coordinated), including challenges in metal ion formation, their reactivity, structure and energetics. This year, the focus of the workshop will be on bridging the gap between the solution and gas-phase data. How can the gas-phase measurements be used best to address condensed phase questions? Sample topics may include hydrated metal ions/clusters and metal ion/biomolecule complexes (originated in the gas-phase or in solution). Approaches complementary to the experimental mass spectrometry techniques (such as theoretical calculations and ion spectroscopy) will be discussed.

Glycomics and Glycoproteins

Ronald Orlando, presiding
Room 255 E

This workshop will focus on the analytical challenges associated with glycomics and glycoprotein characterization, particularly: the accurate identification of individual glycans present in isomeric mixtures; and the ability to quantitatively identify changes in glycan abundance. The workshop will open with an overview of these issues, and will be followed by several short talks (5 minutes). The workshop will conclude with an informal discussion on specific issues brought up by the audience.

**5:00 – 6:30 PM, SUNDAY
TUTORIAL LECTURES
Scott McLuckey, presiding
Room: Hall 4**

5:00 pm

Collision-Induced Dissociation: How Does It Really Work and What It Can (or Can't) Tell You



Peter B. Armentrout, University of Utah

5:45 pm

The Role of Mass Spectrometry in Drug Discovery and Development



**Walter A. Korfmacher,
Merck Research Laboratories**

**6:45 – 7:45 PM, SUNDAY
CONFERENCE OPENING AND PLENARY LECTURE
Scott McLuckey, presiding
Room: Hall 4**

6:45 pm

Welcome to the 58th ASMS Conference on Mass Spectrometry; **Gary L. Glish**, President, ASMS

7:00 pm

Systems Medicine and Emerging Technologies: Catalyzing the Transformation from Reactive to Proactive (P4) Medicine



Leroy Hood, Institute for Systems Biology

**7:45 – 9:30 PM, SUNDAY
WELCOME RECEPTION IN THE EXHIBIT HALL
Exhibit Halls ABCDE**

**8:30 – 10:30 AM, MONDAY MORNING
FUNDAMENTALS: ION STRUCTURES AND ENERGETICS
Veronica Bierbaum, presiding
Room: Ballroom HJ**

MOA am 08:30 **Hydration Energies and Solvent Shell Arrangement of Transition Metal Dications Using Collision Induced Dissociation, IR Action Spectroscopy, and Theoretical Studies;** Theresa E. Cooper¹; Jeremy T. O'Brien²; Evan R. Williams²; Peter B. Armentrout¹; ¹University of Utah, Salt Lake City, UT; ²University of California, Berkeley, CA

MOA am 08:50 **Gas Phase Alpha-Effect in SN2 and E2 Mechanisms;** John Garver¹; Veronica M. Bierbaum²; ¹University of Colorado, Boulder, Boulder, CO; ²University of Colorado, Boulder, CO

MOA am 09:10 **The Intercalation Complexes of PhePhe with Metal Cations;** Robert C. Dunbar¹; Jeffrey Steill²; Jos Oomens²; ¹Case Western Reserve Univ, Cleveland, OH; ²FOM Rijnhuizen, Nieuwegein, Netherlands

MOA am 09:30 **Sensitivity of b₃ Ion Structure to Minor Changes in Amino Acid Sequence;** Alessandra Ferzoco¹; Jeffrey Steill²; Jos Oomens²; Benjamin Bythell³; Bela Paizs³; Gary L. Glish¹; ¹University of North Carolina, Chapel Hill, NC; ²FOM Rijnhuizen, Nieuwegein, Netherlands; ³DKFZ, Heidelberg, Heidelberg, Germany

MOA am 09:50 **Origin of “Magic-Number” Stability and Chiral Selectivity for Serine Clusters in the Gas Phase;** Anthony Costa; R. Graham Cooks; *Purdue University, West Lafayette, IN*

MOA am 10:10 **Does the Structure of Electrospayed Biopolymers Resemble that in Solution?** Thomas Wytenbach; Christian Bleiholder; Chun Wu; Megan Grabenauer; Michael T. Bowers; *University of California, Santa Barbara, CA*

**8:30 – 10:30 AM, MONDAY MORNING
NEW DEVELOPMENTS IN ION TRAPS AND HYBRID INSTRUMENTS
Hao Chen, presiding
Room: Ballroom ACE**

MOB am 08:30 **Accelerating Spectral Acquisition Rate of Orbitrap Mass Spectrometry;** Oliver Lange; Alexander Makarov; Wilko Balschun; Eduard Denisov; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, GERMANY*

MOB am 08:50 **Transient Analysis of The Ion Motion Inside an Ion Trap under Dipolar AC Excitation;** Wei Xu; William Chappell; R. Graham Cooks; Zheng Ouyang; *Purdue University, West Lafayette, IN*

MOB am 09:10 **A Real-Time Data Acquisition Method for Improved Protein Quantitation on Hybrid Mass Spectrometers;** Craig D. Wenger; Doug Phanstiel; Joshua J. Coon; *University of Wisconsin, Madison, WI*

MOB am 09:30 **DC Potentials Applied to Endcap Electrodes of 3-D Ion Traps for Increased Ion Injection Efficiency and Manipulation of Ion/Ion Reactions;** Boone Prentice; Wei Xu; Zheng Ouyang; Scott A. McLuckey; *Purdue University, Lafayette, IN*

MOB am 09:50 **Design and Performance of a Hybrid Mass Spectrometer Capable of Comprehensive Linked Scans with No Scanning Losses;** Sunnie Myung¹; Andrew Kruchinsky²; David Fenyo¹;

Herbert Cohen¹; Julio Cesar Padovan¹; Brian Chait¹; ¹*The Rockefeller University, New York, NY*; ²*Andrew Kruchinsky, San Francisco, CA*
 MOB am 10:10 **Design and Performance of Coaxial Ion Trap: Transferring Ions between Two Trapping Regions in One Mass Analyzer**; Ying Peng; Zhiping Zhang; Brett J. Hansen; Miao Wang; Milton L. Lee; Aaron R. Hawkins; Daniel E. Austin; *Brigham Young University, Provo, Utah*

**8:30 – 10:30 AM, MONDAY MORNING
 MS OF NUCLEIC ACIDS
 Kathrin Breuker, presiding
 Room: Ballroom BDF**

MOC am 08:30 **A Role for the MS Analysis of Nucleic Acids in the Post-Genomics Age**; Daniele Fabris; *U. Maryland Baltimore County, Baltimore, MD*
 MOC am 08:50 **ETD, PD and Hybrid Tandem MS Techniques to Characterize DNA, RNA and DNA Adducts**; Suncerae Smith; Jennifer Brodbelt; *The University of Texas, Austin, TX*
 MOC am 09:10 **Systematic Study of the Epigenetic Pathways Perturbed by 6-Thioguanine in Human Cancer Cells**; Hongxia Wang; Yinsheng Wang; *Univeristy of California, Riverside, CA*
 MOC am 09:30 **Detection of Peptide-Oligonucleotide Heteroconjugates and Protein:RNA Cross-Links via Capillary ICPMS**; Brittany Catron¹; Joseph Caruso¹; Jacqueline Giliberti²; Gary Janssen²; Patrick A. Limbach¹; ¹*University of Cincinnati, Cincinnati, OH*; ²*Miami University, Oxford, OH*
 MOC am 09:50 **Gas-Phase Anion-Electron Reactions and Vibrational Activation of Nucleic Acids and Their Complexes**; Hangtian Song; Linjie Han; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
 MOC am 10:10 **Insights into DNA Damage by Electrochemistry/Liquid Chromatography/Mass Spectrometry**; Herbert Oberacher¹; Robert Erb¹; Sabine Plattner¹; Florian Pitterl¹; Jean-Pierre Chervet²; ¹*Medical University Innsbruck, Innsbruck, Austria*; ²*Antec (Leyden) BV, Zoeterwoude, Netherlands*

**8:30 – 10:30 AM, MONDAY MORNING
 MS DERIVED PEPTIDE / PROTEIN
 BIOSIGNATURES / BIOMARKERS
 Chris Turck, presiding
 Room 155**

MOD am 08:30 **An Overview of the Roles of Mass Spectrometry in Expanding the Clinical Plasma Proteome**; Leigh Anderson¹; Matt Pope²; Morteza Razavi²; Angela Jackson³; Terry Pearson²; ¹*Plasma Proteome Institute, Washington, DC*; ²*University of Victoria, Victoria, BC Canada*; ³*UVic Genome BC Proteomic centre, Victoria, BC*
 MOD am 08:50 **MALDI MS Imaging at Cellular Resolution Across Entire Tissue Sections of ALS Mice and Co-Registration Using YFP-Labeled Fluorescent Neurons**; Kristin J. Boggio¹; Joseph Salisbury¹; Nicole Zaia¹; Nathalie Y.R. Agar²; Jeffrey N. Agar¹; ¹*Brandeis University, Waltham, MA*; ²*Brigham & Women's Hospital, Harvard Medical School, Boston, MA*
 MOD am 09:10 **Expanding the Biomarker Discovery Pipeline from Protein Expression to Turnover**; Yaoyang Zhang¹; Stefan Reckow¹; Michaela D. Filiou¹;

Christian Webhofer¹; Michael Boehme¹; Philipp Gormanns¹; Giuseppina Maccarrone¹; Wolfgang M. Egge-Jacobsen²; Christoph W. Turck¹; ¹*Max Planck Institute of Psychiatry, Munich, Germany*; ²*IMBV, University of Oslo, Oslo, Norway*
 MOD am 09:30 **Label-Free Top-Down Quantitative Proteomics: Post-Translational Modifications as Potential Disease Biomarkers**; Ying Ge; Jiang Zhang; Moltu Guy; Lisa Xu; Xintong Dong; M. Shahriar Salamat; Ken Young; *University of Wisconsin-Madison, Madison, WI*

MOD am 09:50 **Digital Pathology: Discovering and Verifying Barretts' Disease Progression Markers in Tissue Samples Using LCM-Coupled SRM Assays**; Amol Prakash¹; Brian L Hood³; Michael Athanas²; Bryan Krastins¹; Taha Reza¹; David Sarracino¹; Melanie S Flint³; Jon M Davison⁴; Mary F Lopez¹; Thomas P. Conrads⁴; ¹*Thermo Fisher Scientific, Cambridge, MA*; ²*VAST Scientific, Cambridge, MA*; ³*The University of Pittsburgh Cancer Institute, Pittsburgh, PA*; ⁴*University of Pittsburgh, Pittsburgh, PA*
 MOD am 10:10 **Development and Application of a Biomarker Discovery through Verification Pipeline to Cardiovascular Disease**; Hasmik Keshishian¹; Terri Addona¹; Xu Shi²; Michael Burgess¹; Michael Gillette¹; DR Mani¹; Gregory Lewis²; Laurie Farrell²; Michael Fifer²; Marc S. Sabatine³; Robert E. Gerszten²; Steven A. Carr¹; ¹*Broad Institute of MIT and Harvard, Cambridge, MA*; ²*Massachusetts General Hospital, Boston, MA*; ³*Brigham and Women's Hospital, Boston, MA*

**8:30 – 10:30 AM, MONDAY MORNING
 INCREASING THROUGHPUT FOR
 ADME AND KY ASSAYS
 Christopher Holliman, presiding
 Room: Hall 2**

MOE am 08:30 **Parallel Micro-Flow LC Coupled with a Multi-Inlet ESI Source for High-Throughput LC/MS/MS in Drug Discovery**; John Janiszewski¹; Richard Schneider²; Matthew Troutman¹; Sau Lan Tang Staats⁴; Wayne Lootsma⁵; William Schramm⁵; Felix Yiu⁶; Arthur Fogiel, Jr.³; ¹*Pfizer Inc., Groton, CT*; ²*Pfizer Global R&D, Groton, CT*; ³*Phoenix S&T, Inc., Chester, PA*; ⁴*Phoenix S & T, Inc, Chester, PA*; ⁵*Sound Analytics, LLC, Niantic, CT*; ⁶*Apricot Designs, Covina, CA*
 MOE am 08:50 **Reducing Bottlenecks in ADME Sample Analysis Using Solid Phase Extraction with a Quadrupole Time-of-Flight Mass Spectrometer**; Panos Hatsis¹; Michelle Romm²; Vaughn Miller²; Jakal Amin¹; William A. Lamar²; Can "Jon" Ozbal²; Shawn Harriman¹; ¹*Novartis Institutes for Biomedical Research, Cambridge, MA*; ²*BIOCIUS Lifesciences, Woburn, MA*
 MOE am 09:10 **Evaluation of a New Prototype Accurate Mass System for Simultaneous Quantitative and Qualitative Bioanalysis and Metabolite Profiling**; Henrianna Pang¹; Hesham Ghobarah²; Tanya Gamble²; Yingbo Yang¹; Sophie Pan¹; Brad Gien¹; Douglas J. Turk¹; ¹*NoAb BioDiscoveries, Inc., Mississauga, Canada*; ²*AB SCIEX, Concord, Canada*
 MOE am 09:30 **High-Throughput LDTD384-MS/MS for Drug Metabolism and Pharmacokinetic Studies**;

Sebastien Gagne¹; Patrice Tremblay²; Francis Foczeny¹; Robert Houle¹; Eric Langlois¹; Kevin Bateman¹; Pierre Picard²; ¹Merck Canada, Kirkland, Canada; ²Phytronix Technologies, Quebec, QC

MOE am 09:50 **Automated Solid-Phase Microextraction in 96-Well Plate Format: High-Throughput Analysis and Ligand-Receptor Binding Studies;** Janusz Pawliszyn¹; Dajana Vuckovic¹; Erasmus Cudjoe¹; Dietmar Hein²; Rosa Vatino³; Carlo Zamboni³; ¹University of Waterloo, Waterloo, Canada; ²Professional Analytical Service Technology, Magdala, Germany; ³Universit' a degli Studi di Bari, Bari, Italy

MOE am 10:10 **Liquid Microjunction Surface Sampling Probe Analysis of Dried Blood Spots Using an Automated Chip-Based Nano-ESI Infusion Device;** Joseph J. Stankovich¹; Matthew J. Walworth¹; Vilmos Kertesz²; Richard King³; Gary J. Van Berkel¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²Oak Ridge National Lab, Oak Ridge, TN; ³PharmaCadence Analytical Services, LLC, Hatfield, PA

**8:30 – 10:30 AM, MONDAY MORNING
APPLICATION OF LC-MS FOR
PK CHARACTERISTICS OF BIOLOGICS
Yan-Hui Liu, presiding
Room: Hall 3**

MOF am 08:30 **Development of a Novel Sample Preparation Strategy for LC/MS/MS Quantitation of Serum Binding Domain Antibodies for PK Studies;** Mary B. Moyer; Greg Waitt; Wojciech Krol; Chris Herring; Chuck Poole; Jon Williams; GlaxoSmithKline, Research Triangle Park, NC

MOF am 08:50 **LC-ESI/MS and MALDI-MS for Monitoring of Glycoform-Related Clearance of a Complex Glycoprotein in Cynomolgus Monkeys;** Li Zang; Xiaoping L. Hronowski; Yelena Lyubarskaya; Alexander Buko; Helena Madden; Weiner Meier; Rohin Mhatre; BiogenIdec Inc., Cambridge, MA

MOF am 09:10 **Biosynthetic Concatenated Labeled Peptides: Equivalence to Whole Labeled Proteins as Internal Standards for Isotope Dilution Mass Spectrometry?** Jacquelyn Cole²; Dhaval Nanavati¹; Cai Chen²; Brian Martin²; Anthony J. Makusky; Sanford P. Markey²; ¹Northwestern University, Evanston, IL; ²NIMH/NIH, Bethesda, MD

MOF am 09:30 **Identification and Quantification of *in vitro* Protein Metabolites Using a Novel Mass Spectrometry-Based Workflow;** Scott Peterman²; Amol Prakash²; Julian Saba¹; Taha Rezaei³; Bryan Krastins¹; David Sarracino¹; ¹Thermo Fisher Scientific, San Jose, CA; ²ThermoFisher Scientific, Cambridge, MA; ³Thermo Scientific BRIMS, Cambridge, MA

MOF am 09:50 **A Bioanalytical Strategy for 20 kDa PEGylated CGRP Peptide by UPLC-MS/MS;** Hongyan Li; Mark Rose; Jerry Holder; Marie Wright; Les Miranda; Christopher James; Amgen Inc, Thousand Oaks, CA

MOF am 10:10 **Quantitative LC-MS/MS Method Development for Quantitation of Therapeutic Proteins in Plasma;** Steven T. Wu¹; Zheng Ouyang²; Timothy Olah²; Mohammed Jemal¹; ¹Bristol-

Myers Squibb, Princeton, NJ; ²Bristol-Myers Squibb Company, Princeton, NJ

**8:30 – 10:30 AM, MONDAY MORNING
QUANTITATIVE INTACT PROTEOMICS
Julian Whitelegge, presiding
Room: Hall 4**

MOG am 08:30 **Quantitative Intact Proteomics (QIP): Visualizing Variation on a Global Scale;** David B. Friedman; Sebahat Ocak; Pierre Massion; Sarah Stuart; Salisha Hill; W. Hayes McDonald; Vanderbilt University School of Medicine, Nashville, TN

MOG am 08:50 **Confident Identification and Relative Quantification of Intact Proteins from Human Embryonic Stem Cells Using SILAC;** Timothy S Collier; Prasenjit Sarkar; Balaji Rao; David C. Muddiman; North Carolina State University, Raleigh, NC

MOG am 09:10 **Absolute Intact Protein Quantification by Real-Time Measurement of Tryptophan Intrinsic Fluorescence at the ESI Interface Prior to Top-Down Mass Spectrometry;** Jason D. Russell; Ryan T. Hilger; Daniel T. Lador; Mark Tervo; Michael R. Shortreed; Mark A Scalf; Lloyd M. Smith; Joshua J. Coon; University of Wisconsin, Madison, WI

MOG am 09:30 **Fluorescent Z dye Platform for Differential Covalent Labeling of Proteins for Quantitative Intact Proteomic Analysis on 2D Gels;** Edward Dratz¹; Paul Grieco¹; Scott Laffoon¹; Ben Reeves¹; Jennifer Vance¹; Matt Shipman¹; Rand Swanson²; ¹Montana State University, Bozeman, MT; ²Resonon, Inc., Bozeman, Montana

MOG am 09:50 **The "PHASST-MS" Approach: Peptidomic Profiling Reflects Cellular and Disease State in Human Pancreatic Islet Cell Culture;** Svetlana Nikoulina; Nancy Andon; Carolyn Lowe; Steven Taylor; Amylin Pharmaceuticals Inc., San Diego, CA

MOG am 10:10 **The Identification of Protein Biomarkers Distinguishing Virus Transmission Competent and Refractive Insect Populations by Coupling Genetics with Quantitative Intact Proteomics;** Michelle Cilia¹; Tara Fish¹; Kevin Howe¹; Dawn Smith²; Theodore Thannhauser¹; Stewart Gray^{1,2}; ¹USDA-ARS, Ithaca, NY; ²Cornell University, Ithaca, NY

**10:30 AM – 2:30 PM, MONDAY
POSTER SESSION
Exhibit Hall ABCDE**

**2:30 – 4:30 PM, MONDAY AFTERNOON
FUNDAMENTALS: SUPRAMOLECULAR CHEMISTRY
AND NON-COVALENT COMPLEXES**

**Evan Williams, presiding
Room: Ballroom HJ**

- MOA pm 2:30 **Native Mass Spectrometry Provides a First Structural Model for the 405 kDa CRISPR-RNA Antiviral Defense System;** Esther Van Duijn¹; Arjan Barendregt¹; Jelle Bultema³; Matthijs M. Jore²; Magnus Lundgren²; Stan J. Brouns²; Blake Wiedenheft⁴; Jennifer A. Doudna⁴; Egbert J. Boekema³; John van der Oost²; Albert J.R. Heck¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*Wageningen University, Wageningen, Netherlands*; ³*University of Groningen, Groningen, Netherlands*; ⁴*UC Berkeley, Berkeley, CA*
- MOA pm 2:50 **Ion Mobility Spectrometry/Mass Spectrometry Reveals Conformational Conversion from Random Assembly to β -Sheet-Rich Oligomers in Amyloid Fibril Forming Peptides;** Christian Bleiholder¹; Nicholas Dupuis²; Thomas Wyttenbach³; Michael T. Bowers³; ¹*University of California, SB, Santa Barbara, CA*; ²*UC Santa Barbara, Goleta, CA*; ³*University of California San, Santa Barbara, CA*
- MOA pm 3:10 **Surface-Induced Dissociation Lends Insight on Subunit Arrangement in Non-Covalent Protein Complexes;** Anne E. Blackwell; Eric D. Dodds; Christopher M. Jones; Vicki H. Wysocki; *University of Arizona, Tucson, AZ*
- MOA pm 3:30 **Analysis of Big Macromolecular Soluble and Membrane Protein Complexes for ESI-MS;** Nina Morgner; Helena Hernandez; Min Zhou; Laura A Lane; Carol Robinson; *University of Oxford, Oxford, UK*
- MOA pm 3:50 **Supercharged HD Exchange-MS for Top-down Structural Characterization of Proteins and Complexes;** Harry J. Sterling; Evan R. Williams; *University of California, Berkeley, CA*
- MOA pm 4:10 **Noncovalent Molecular Recognition of Protonated Peptidomimetic Bases by 18-Crown-6: Structure Versus Energetics;** Mary T. Rodgers; Yu Chen; *Wayne State University, Detroit, MI*

**2:30 – 4:30 PM, MONDAY AFTERNOON
ADVANCES IN ION IMAGING**

**Michelle Reyzer, presiding
Room: Ballroom ACE**

- MOB pm 2:30 **Imaging Mass Spectrometry: Current Performance and Upcoming Challenges;** Pierre Chaurand; *University of Montreal, Montreal, Canada*
- MOB pm 2:50 **Correlation of MS, MRI, and Optical Images for 3D Assessment of the Tumor Microenvironment;** Erin H. Seeley¹; Julie A. Sterling¹; Amelie R. Gillman¹; Tuhin K. Sinha²; Rachele W. Johnson¹; Thomas E. Yankeelov¹; John C. Gore¹; Gregory R. Mundy¹; Lynn M. Matrisian¹; Richard M. Caprioli¹; ¹*Vanderbilt University, Nashville, TN*; ²*University of California San Francisco, San Francisco, CA*
- MOB pm 3:10 **Revealing Bacterial Post-Translationally Modified Cannibalistic Metabolic Exchange Factors with Imaging Mass Spectrometry;** Pieter Dorrestein; *University of California, San Diego, Skaggs School, La Jolla, CA*

MOB pm 3:30 **More Information in Less Time: Strategies for High Spatial & High Mass Spectral Resolution Imaging Utilizing a Hybrid LIT-Orbitrap MS;** David C. Perdian; Edward S. Yeung; Young Jin Lee; *Iowa State University, Ames Laboratory US DOE, Ames, IA*

MOB pm 3:50 **Going Beyond Images: Exploration of Hormone Processing Pathways in Diabetic Mouse Models via Mass Spectral Imaging and Data-Mining;** Raf Van de Plas^{1,4}; Dirk Vander Mierde²; Katleen Lemaire²; Bart De Moor^{1,4}; Peter In't Veld⁵; Frans Schuit²; Etienne Waelkens^{3,4}; ¹*K.U.Leuven - SCD-SISTA Bioinformatics, Leuven, Belgium*; ²*K.U.Leuven - Gene Expression Unit, Leuven, Belgium*; ³*K.U.Leuven - Lab of Protein Phosph. and Proteomics, Leuven, Belgium*; ⁴*K.U.Leuven - ProMeta Core Facility, Leuven, Belgium*; ⁵*Brussels Free University-Diabetes Research Center, Brussels, Belgium*

MOB pm 4:10 **Intraoperative Identification of Malignant Gastrointestinal Tumors and Proximal Metastases by Rapid Evaporative Ionization Mass Spectrometry;** Julia Balog²; Tamas Szaniszló²; Daniel Szalay²; Lajos Godorhazy²; Laszlo Sasi Szabo⁴; Karl C Schaefer¹; Miklos Toth³; Zoltan Takats¹; ¹*Justus-Liebig-University, Giessen, Germany*; ²*Medimass Inc., Budapest, Hungary*; ³*Semmelweis University, Budapest, Hungary*; ⁴*University of Debrecen, Debrecen, Hungary*

**2:30 – 4:30 PM, MONDAY AFTERNOON
MS OF SYNTHETIC POLYMERS**

**Barbara Larsen, presiding
Room: Ballroom BDF**

- MOC pm 2:30 **Characterization of Enzymatically-Catalyzed Polycaprolactones;** William E. Wallace¹; Atul Bhangale²; Santanu Kundu¹; Charles M. Guttman¹; Kathleen M. Flynn¹; Richard A. Gross²; Kathryn L. Beers¹; ¹*National Institute of Standards & Technology, Gaithersburg, MD*; ²*Polytechnic Institute of New York University, New York, NY*
- MOC pm 2:50 **Library of Polymer Architectures Examined by Ion Mobility Spectrometry-Mass Spectrometry;** Sarah Trimpin¹; Hoskins Jesika²; Kanchana Wijerathne¹; Ellen D. Inutan¹; Scott M. Grayson²; ¹*Wayne State University, Detroit, MI*; ²*Tulane University, New Orleans, LA*
- MOC pm 3:10 **Ion Mobility Mass Spectrometry of Supramolecular Polymers;** Chrys Wesdemiotis; Xiaopeng Li; Wen-Bin Zhang; Stephen Z. D. Cheng; *The University of Akron, Akron, OH*
- MOC pm 3:30 **Methylation of Pendant Groups to Enable end-Group Characterization in MAA-based Copolymers;** Rémi Giordanengo¹; Stéphane Viel¹; Manuel Hidalgo²; Béatrice Allard-Breton²; André Thévand¹; Laurence Charles¹; ¹*Universités Aix-Marseille, Marseille, France*; ²*Arkema, Pierre-Bénite, France*
- MOC pm 3:50 **Electron Induced Dissociation: A New Method of Characterising Polymers;** Michael Smith; Jackie Mosely; *Durham University, Durham, UK*
- MOC pm 4:10 **Characterization of Hydrogenation Reactions and Products of 1,4-bis(phenethyl)benzene (DEB) with High-Resolution Mass Spectrometry;** Steven Thornberg; James

Hochrein; *Sandia National Laboratories, Albuquerque, NM*

**2:30 – 4:30 PM, MONDAY AFTERNOON
QUALITATIVE ANALYSIS OF
PROTEIN THERAPEUTICS BY MS
Guodong Chen, presiding
Room 155**

- MOD pm 2:30 **Application of Mass Spectrometry in the Development of Protein Therapeutics;** Reb Russell; *Bristol-Myers Squibb Co., Princeton, New Jersey*
- MOD pm 2:50 **Disulfide Linkages of an Albumin Fusion Protein;** Andrea Meeler; Mark Hesselberg; Angie Deng; Michael Byrne; Zhuchun Wu; *Human Genome Sciences, Inc., Rockville, MD*
- MOD pm 3:10 **A Tris (2-Carboxyethyl) Phosphine (TCEP) Related Cleavage on Cysteine-Containing Proteins;** Li Tao; Peiran Liu; Bethanne Warrack; Wei Wu; Yunping Huang; Guodong Chen; Reb Russell; *Bristol-Myers Squibb Co., Pennington, NJ*
- MOD pm 3:30 **Mass Spectrometry Methods to Analyze Higher Order Structure of Protein Therapeutics;** Lisa Jones¹; Justin Sperry²; James Carroll²; Michael L. Gross¹; ¹*Washington University, St. Louis, MO*; ²*Pfizer, Chesterfield, MO*
- MOD pm 3:50 **Aglycosylation Alters Protein Conformation in Antibodies Engineered with Specific Effect or Functions;** Damian Houde^{1,3}; Christopher Reyes¹; Tiffany Chen²; Steven Berkowitz¹; Dane Wittrup²; John R. Engen³; ¹*Biogen Idec, Cambridge, MA*; ²*MIT, Cambridge, MA*; ³*Northeastern University, Boston, MA*
- MOD pm 4:10 **Characterizing Biotherapeutic Protein 3D Structures by Electrospray Ion-Mobility Mass Spectrometry: Biological Significance and Comparison with X-ray Crystallography and NMR Measurements;** Weibin Chen; Asish Chakraborty; St John Skilton; Scott Berger; Jeff Mazzeo; *Waters Corporation, Milford, MA*

**2:30 – 4:30 PM, MONDAY AFTERNOON
LC-MS CHALLENGES / SOLUTIONS FOR MONITORING
HUMAN METABOLITES IN SAFETY TESTING (MIST)
Chandra Prakash, presiding
Room: Hall 2**

- MOE pm 2:30 **How to Deal with Human Metabolites in Safety Testing (MIST): An Overview;** Natalia Penner; Lewis Klunk; Chandra Prakash; *Biogen Idec, Cambridge, MA*
- MOE pm 2:50 **Mass Spectrometry Solutions for an Overall Metabolite Monitoring Strategy;** Ragu Ramanathan; Nirmala Raghavan; Donglu Zhang; Lifei Wang; Hong Cai; S. Nilgun Comezoglu; Jonathan L. Josephs; William Humphreys; *Bristol-Myers Squibb, Princeton, NJ*
- MOE pm 3:10 **Method Development for Biological Sample Processing and Metabolite Profiling by LC-MS in Drug Development;** Joanna Pols; Swapan K. Chowdhury; Kevin Alton; *Merck Research Laboratories, Kenilworth, NJ*
- MOE pm 3:30 **To the Detection and Quantification of Drug Metabolites Using the Simultaneous Collection of MRM and MS/MS Data: A Case Study;** Warren Potts¹; Ian Wilson³; Rob Plumb²; ¹*Waters Corporation, Milford, MA*; ²*Imperial College,*

London, UK; ³*Astra Zeneca DMPK, Alderly Park Macclesfield, Manchester UK*

- MOE pm 3:50 **Semi-Quantitation of Metabolites across Species for Direct and Quantitative Evaluation of MIST Coverage;** Hongying Gao; Shibing Deng; R. Scott Obach; *Pfizer, Inc, Groton, CT*
- MOE pm 4:10 **Effect of Mobile Phase pH and Aqueous-Organic Ratio on MS/MS Fragmentation Pattern: Implications in LC-MS/MS Bioanalysis;** Jian Wang; Anne Aubry; Mark S. Bolgar; Timothy Olah; Mohammed Jamal; *Bristol-Myers Squibb, Princeton, NJ*

**2:30 – 4:30 PM, MONDAY AFTERNOON
QUANTITATION OF BIOLOGICS:
APPLICATIONS AND TECHNIQUES
Jon Williams, presiding
Room: Hall 3**

- MOF pm 2:30 **Quantitative Measurement of Biologics Using Mass Spectrometry: An Overview;** Patrick J. Rudewicz; *Elan Pharmaceuticals, South San Francisco, CA*
- MOF pm 2:50 **Integrated Label-Free Quantitative Analysis of the Lung Proteome, Secretome, and Phosphoproteome in a Model of Acute Lung Injury;** Matthew W. Foster; Erik J. Soderblom; J. Will Thompson; Harvey E. Marshall; Arthur M. Moseley; *Duke University School of Medicine, Durham, NC*
- MOF pm 3:10 **A Novel Quantitative Approach for Sulfated Cholecystokinin CCK-8 in Plasma Using Immunoprecipitation LC-MS/MS;** Scott Young¹; Samir Julka¹; Glenn Bartley²; Jeffrey Gilbert³; Brian Wendelburg³; Shao-Ching Hung¹; Kerr Anderson¹; Wallace Yokoyama²; ¹*Dow Chemical Company, Midland, MI*; ²*Western Regional Research Center, USDA, Albany, CA*; ³*Dow AgroSciences, Indianapolis, IN*
- MOF pm 3:30 **Supporting Therapeutic Antibody Programs with Total Target Biomarker Quantitation by Sensitive Immunoaffinity LC-MS/MS – Validation and Implementation in Clinical Trials;** Hendrik Neubert; *Pfizer Corporation, Sandwich, Kent, UK*
- MOF pm 3:50 **Comparison of Different Mass Spectrometry Techniques for Quantitative Analysis of Peptide Drugs at Low pg/ml Levels in Biological Samples;** Anders Sonesson; Anna-Karin Wendel; Lasse Skov Jensen; Magnus Knutsson; Alf Carlshaf; *Ferring Pharmaceuticals A/S, Copenhagen S, Denmark*
- MOF pm 4:10 **Quantitation of Therapeutic Peptides and Oligonucleotides Using High-Resolution Mass Spectrometry: Benefits and Considerations;** J.C. Yves Leblanc; J. Larry Campbell; *AB SCIEX, Concord, On, Canada*

**2:30 – 4:30 PM, MONDAY AFTERNOON
PHOSPHOPROTEOMICS APPLICATIONS
Jesper Olsen, presiding
Room: Hall 4**

- MOG pm 2:30 **System-Wide Temporal Characterization of the Proteome and Phosphoproteome of Differentiating Human Embryonic Stem Cells;** Kristoffer T. G. Rigbolt¹; Tatyana A. Prokhorova¹; Vyacheslav Akimov¹; Jeanette Henningsen¹; Irina Kratchmarova¹; Moustapha Kassem²; Matthias Mann³; Jesper V. Olsen⁴; Blagoy Blagoev¹; ¹*University of Southern*

Denmark, Odense, Denmark; ²Odense University Hospital & Medical Biotech Center, Odense, Denmark; ³Max Planck Institute for Biochemistry, D Martinsried, Germany; ⁴University of Copenhagen, Denmark

MOG pm 2:50

Activity Dependent Changes in Synaptic Composition; Jonathan C. Trinidad¹; Agnes Thalhammer²; Aenoch Lynn¹; Peter Baker¹; Ralf Schoepfer²; A.L. Burlingame¹; ¹University of California, San Francisco, San Francisco, CA; ²University College London, London, UK

MOG pm 3:10

Phosphotyrosine Proteome Analysis of *E. coli* Strains Using High Resolution Fourier Transform Mass Spectrometry; Raghothama Chaerkady^{1,2}; Jyoti Sharma²; Santosh Renuse²; Harrys Kishore J^{1,2}; Nandini Patankar²; Sneha Pinto²; Harsha HC^{1,2}; Min-Sik Kim¹; Anne-Marie Hanssen³; James B. Kaper³; Akhilesh Pandey¹; ¹Institute of Genetic Med, Johns Hopkins University, Baltimore, MD; ²Institute of Bioinformatics, Bangalore, India; ³University of Maryland School of Medicine, Baltimore, MD

MOG pm 3:30

Phosphoproteomic Survey of *in vitro* Kinase Substrates and the Phosphorylation Motif; Naoyuki Sugiyama¹; Haruna Imamura¹; Koichi Yokota²; Sumiko Ohnuma¹; Mai Tsukaha¹; Masaru Tomita¹; Yasushi Ishihama¹; ¹IAB, Keio Univ., Tsuruoka, Japan; ²Carna Biosciences Inc., Kobe, Japan

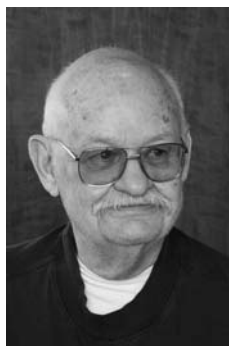
MOG pm 3:50

A Tissue-Specific Atlas of Protein Phosphorylation and Expression in the Mouse; Edward Huttlin¹; Mark Jedrychowski¹; Josh Elias²; Tapasree Goswami¹; Ramin Rad¹; Judit Villen¹; Wilhelm Haas¹; Mathew Sowa¹; Steven Gygi¹; ¹Harvard Medical School, Boston, MA; ²Stanford University, Stanford, CA

MOG pm 4:10

Multiplexed Quantitative Analysis of the Differentiating Human ES Cell Phosphoproteome via High Mass Accuracy Tandem MS; Nicole A Beauchene¹; Danielle L Swaney¹; Pengzhi Yu^{1,2}; Steven A Jackson^{1,2}; James A Thomson^{1,2}; Joshua J Coon¹; ¹University of Wisconsin, Madison, WI; ²Morgridge Institute for Research, Madison, WI

4:45 – 5:30 PM, MONDAY
AWARD LECTURE
Hall 4



Marvin L. Vestal, Recipient of the Award for a Distinguished Contribution in Mass Spectrometry

5:45 - 7:00 PM, MONDAY WORKSHOPS. See page S7

8:30 – 10:30 AM, TUESDAY MORNING
FUNDAMENTALS: BIOMOLECULAR
ION-RADICAL CHEMISTRY
Frank Turecek, presiding
Room: Ballroom HJ

TOA am 08:30 **Evidence for Internal Energy Dependent Mechanisms in the Formation of Radical Product Ions in Electron Capture Dissociation;** Natalie Thompson; Daniel A. Thomas; Takashi Baba; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*

TOA am 08:50 **Tunable Fixed-Charge Tags for Electron Transfer Dissociation of Peptides;** Thomas W. Chung; Frantisek Turecek; *University of Washington, Seattle, WA*

TOA am 09:10 **Gas-Phase Structures of the Three-Helix Bundle Protein KIX Probed by Electron Capture Dissociation;** Martin Tollinger²; Kathrin Breuker¹; ¹University of Innsbruck, Innsbruck, Austria; ²Max F. Perutz Laboratories, Vienna, Austria

TOA am 09:30 **Gas Phase Covalent Modification of Peptides via Ion/Ion Reactions: Schiff Base Formation on the Conversion of Ion Polarity;** Kerry Hassell; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*

TOA am 09:50 **Elucidating Tertiary Structure in Gaseous Proteins Using Distant Dependent Hydrogen Atom Transfer between Radical Donor-Acceptor Pairs;** Tony Ly; Ryan R. Julian; *University of California, Riverside, Riverside, CA*

TOA am 10:10 **The dGdC Radical Cation Base Pair as a Model for Oxidative Damage in DNA;** Linda Feketeova¹; Chan Bun²; George N. Khairallah¹; Leo Radom²; Richard A. J. O'Hair¹; ¹Bio21 Inst & School of Chemistry, Uni of Melbourne, Melbourne, Australia; ²School of Chemistry, University of Sydney, Sydney, Australia

8:30 – 10:30 AM, TUESDAY MORNING
MS OF LIPIDS
Amina Woods, presiding
Room: Ballroom ACE

TOB am 08:30 **Novel Fragmentation Pathways Including Regioselective Attachment and Decompositions of Anionic Adducts of Steroids Formed by Electrospray Anion Attachment;** Nalaka Rannulu; Richard B. Cole; *University of New Orleans, New Orleans, LA*

TOB am 08:50 **Mitochondrial Lipid Profiling and Identification Using High Resolution LC-MS and MS/MS;** Susan Schiavo¹; Vasant Marur⁴; Chunang (Christine) Gu²; Jules Phillips³; Bruce Kristal²; ¹Brigham and Women's Hospital, Boston, MA; ²ThermoFisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, San Jose, CA; ⁴Brigham and Women's Hosp., Boston, MA; ⁵Brigham + Women's Hospital, Boston, MA

TOB am 09:10 **Localization, Imaging and Structural Analysis of Sialylated Glycosphingolipids in Brain Tissue Sections by Mass Spectrometry;** Benoit Colsch¹; Shelley N. Jackson¹; Sucharita M. Dutta²; Amina S. Woods¹; ¹NIDA-IRP, NIH, Baltimore, MD; ²ThermoFisherScientific, San Jose, CA

TOB am 09:30 **All Gunked Up and Nowhere to Flow: Profiles of Murine Atherosclerotic Plaques by High Spatial Resolution MALDI Imaging Mass**

Spectrometry; Peggi Angel; Kevin Tompkins; Kel Vin Woo; Scott Baldwin; Richard M. Caprioli; *Vanderbilt Univ Sch of Med, Nashville, TN*

TOB am 09:50

Lipid Imaging by Matrix Implanted Laser Desorption/Ionization (MILDI) Ion Mobility-TOF MS Using Sub-Monolayer Nanoparticulate matrices; J. Albert Schultz¹; Ernest K. Lewis¹; Thomas Egan¹; Kelley Waters¹; Valerie Vaughn¹; Michael McCulley¹; Jerry F. Moore²; Jeremy Post³; Alice Delvolve³; Amina S. Woods³; ¹*Ionwerks, Inc., Houston, TX*; ²*MassThink LLC, Naperville, IL*; ³*NIDA IRP, NIH, Baltimore, MD*

TOB am 10:10

Identification of 1-Deoxy-Sphingoid Bases and N-Acyl-1-Deoxy-Sphingoid Bases by LC-ESI-MS/MS; Hyejung Park¹; Elaine Wang²; Mark Cameron Sullards²; Alfred H. Merrill²; Catherine E. Costello¹; ¹*Boston University School of Medicine, Boston, MA*; ²*Georgia Institute of Technology, Atlanta, GA*

**8:30 – 10:30 AM, TUESDAY MORNING
MS ON VIRUSES**

**Esther Van Duijn, presiding
Room: Ballroom BDF**

TOC am 08:30

Unravelling the Topology of Macromolecular Protein Complexes; Alison E. Ashcroft; Tom W. Knapman; Victoria L. Morton; Peter G. Stockley; *University of Leeds, Leeds, UK*

TOC am 08:50

Automated Limited Proteolysis and Intact Protein Hydrogen Exchange Reveals Mechanism of Action for a Novel Class of Anti-Hepatitis B Drugs; Jonathan Hilmer¹; Navid Movahed¹; Adam Zlotnick²; Brian Bothner¹; ¹*Montana State University, Bozeman, MT*; ²*Indiana University, Bloomington, IN*

TOC am 09:10

Virus Assembly and Stability Monitored by Native Electrospray and Ion Mobility Mass Spectrometry; Glen Shoemaker¹; Esther Van Duijn¹; Sue Crawford²; Charlotte Uetrecht¹; Marian Baclayon³; Wouter Roos³; Gijs Wuite³; Mary Estes²; Venkataram Prasad²; Albert J.R. Heck¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*Baylor College of Medicine, Houston, Texas*; ³*Vrije Universiteit, Amsterdam, Netherlands*

TOC am 09:30

High Throughput ESI-MS of PCR Products for the Identification of 2009 Pandemic Influenza A H1N1 Viruses; Steven Hofstadler; Jared Drader; Jose Gutierrez; Ranga Sampath; Larry Blyn; David Ecker; *Ibis Biosciences, Inc., Carlsbad, CA*

TOC am 09:50

Dynamic Evolution of the Macaque Pulmonary Proteome Response to Highly Pathogenic Avian Influenza and Spanish Flu Influenza Infections; Joseph Brown¹; Robert Palermo²; Jon Jacobs¹; Marina Gritsenko¹; Michael Katze²; Richard D. Smith¹; ¹*Pacific Northwest National Laboratories, Richland, WA*; ²*University of Washington - Dept. of Microbiology, Seattle, WA*

TOC am 10:10

Identification of Host Cell Specific Markers in HIV Particles By Mass Spectrometry; Lennard J.M. Dekker; Patrick H.M. Boers; Jeroen J.A. Van Kampen; Theo Marten Luider; Rob A. Gruters; *Erasmus Medical Center, Rotterdam, Netherlands*

**8:30 – 10:30 AM, TUESDAY MORNING
MASS SPECTROMETRY OF
PROTEIN-LIGAND COMPLEXES
Joseph Loo, presiding
Room 155**

TOD am 08:30

Quantifying Protein-Ligand Interactions with Electrospray Ionization Mass Spectrometry; Elena Kitova¹; Lan Liu¹; Lu Deng¹; Nian Sun¹; Amr El-Hawiet¹; Dhanashri Bagal²; Paul Schnier²; John Klassen¹; ¹*University of Alberta, Edmonton, Canada*; ²*Amgen, Thousand Oaks, CA*

TOD am 08:50

High-Throughput Fragment Screening by Non-Covalent Mass Spectrometry; Hannah Maple^{1,3}; Rachel Garlish^{1,2}; Matthew Crump^{1,3}; John Crosby^{1,3}; Richard Taylor^{1,2}; ¹*Bristol, UK*; ²*UCB, Slough, Berkshire, UK*; ³*School of Chemistry, University of Bristol, Bristol, UK*

TOD am 09:10

Probing the Sites of Molecular Tweezer Noncovalent Binding to Amyloid β -Protein Using Top-Down ECD-FT-ICR MS; Eric Pang^{1,2}; Sheng Yin¹; Gal Bitan²; Thomas Schrader³; Joseph A. Loo¹; David Teplow²; ¹*Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA*; ²*Department of Neurology, UCLA, Los Angeles, CA*; ³*University of Duisburg-Essen, Essen, Germany*

TOD am 09:30

Characterization of Metal Coordinated Protein-Carbohydrate Complex Conformations via Ion Mobility-Mass Spectrometry; Youjin Seo; Julie A. Leary; *UC Davis, Davis, CA*

TOD am 09:50

Investigating Protein-Peptide Binding by 'Top-Down' FT-ICR MS, Ion-Mobility MS and Hydrogen/Deuterium Exchange; David J Clarke¹; Euan Murray²; Peter A Faull²; Ted Hupp²; Perdita Barran²; Pat Langridge-Smith¹; C. Logan Mackay¹; ¹*SIRCAMs, University of Edinburgh, Edinburgh, UK*; ²*The University of Edinburgh, Edinburgh, UK*

TOD am 10:10

Characterizing Cooperative Ligand Binding to Large Protein Complexes; Liat Shimon; Amnon Horovitz; Michal Sharon; *Weizmann Institute of Science, Rehovot, Israel*

**8:30 – 10:30 AM, TUESDAY MORNING
INCURRED SAMPLE REANALYSIS AND
ANALYTICAL SOLUTIONS
Chengwei Fang, presiding
Room: Hall 2**

TOE am 08:30

Beyond Successful ISR: Case by Case Investigations for Unmatched Reassay Results When ISR Passed; Robert Massé; Aimin Tan; Sylvain Lachance; Sofi Gagnon-Carignan; Ann Levesque; *Anapharm Inc., Quebec, QC*

TOE am 08:50

Identifying Trends and Improving Outcomes from Incurred Sample Analysis Failure Investigations in a Bioanalytical CRO; Patrick Bennett; Min Meng; Scott Reuschel; *Tandem Labs, Salt Lake City, UT*

TOE am 09:10

Incurred Sample Reanalysis by a Bioanalytical Data Management System; Joel I Usansky; Mike Small; Marc Krug; *Thermo Fisher, Philadelphia, PA*

TOE am 09:30

Unexpected Event Investigation and Resolution for an ISR Test Failure for a SN-38 Assay Supporting a Clinical Study; Qin C. Ji; Lisa Iacono; Dennis Garner; Mark E. Arnold; *Bristol-Myers Squibb Co., Princeton, NJ*

- TOE am 09:50 **Application of Dried Blood Spots for the Analysis of a Novel Compound in the Presence of Liable Phase II Metabolites; Hermes Licea Perez**; Sharon Boram; Christopher Evans; *Bioanalysis, King of Prussia, PA*
- TOE am 10:10 **The Evolution and Optimization of a High-Throughput LC/MS/MS Bioanalytical Method: HPLC-MS/MS vs. UFLC-MS/MS vs. UPLC-MS/MS; Lisa Ford**; Mike Allen; Kelli Goodman; *Enthalpy Analytical, Inc., Durham, NC*

**8:30 – 10:30 AM, TUESDAY MORNING
QUANTITATION OF XENOBIOTIC METABOLITES
WITHOUT REFERENCE STANDARD
Anne Aubry, presiding
Room: Hall 3**

- TOF am 08:30 **Estimation of Metabolite Concentrations in the Absence of an Authentic Standard Based on Relative ¹²C/¹⁴C Ratios Analyzed by High-Resolution ESI-MS; Filip Cuyckens**; Nadine Pauwels; Valerie Koppen; Laurent Leclercq; *Johnson & Johnson Pharma R&D, Beerse, Belgium*
- TOF am 08:50 **A Novel Detection Technology Charged Aerosol Detection Coupled with HPLC, UV and LTQ Orbitrap MS for Drug Metabolism Study; Hong Cai**¹; Jonathan L. Josephs¹; Ragu Ramanathan¹; Christopher Crafts²; Bruce A. Bailey²; William G. Humphreys¹; *Bristol-Myers Squibb, Pennington, NJ*; *²Dionex, Sunnyvale, CA*
- TOF am 09:10 **Identification and Quantification of Reactive Metabolites and Their Adducts Using Electrochemistry Coupled to LC-MS; Uwe Karst**¹; Wiebke Lohmann¹; Anne Baumann¹; Sandra Jahn¹; Björn Meermann¹; *¹University of Münster, Münster, Germany*
- TOF am 09:30 **LC-CaptiveSpray Ionization-Mass Spectrometry for Detection, Characterization and Quantification of Circulating Human Metabolites; Nirmala Raghavan**; Ragu Ramanathan; S. Nilgun Comezoglu; William Humphreys; *Bristol-Myers Squibb, Princeton, NJ*
- TOF am 09:50 **The Performance of Accelerator Mass Spectrometry (AMS) for the Determination of ¹⁴C/¹²C Isotope Ratios Using a Newly Installed BioMICADAS AMS; Brad D. Keck**; Pete Lohstroh; Jason Giacomo; John Vogel; *Vitalea Science, Inc., Davis, CA*
- TOF am 10:10 **UPLC – ESI MSMS/ICPMS: A Tandem Tool for Quantitative Fingerprinting of Seleno-Metabolic Compounds; Johann Far**; Kasia Bierla; Brice Bouyssiere; Hugues Preud'homme; Ryszard Lobinski; *LCABIE - UMR5254 - IPREM, University of Pau, PAU, France*

**8:30 – 10:30 AM, TUESDAY MORNING
QUANTITATION IN PROTEOMICS - PEPTIDES
Michael Washburn, presiding
Room: Hall 4**

- TOG am 08:30 **Experimental and Computational Strategies in Quantitative Proteomics; Alexey Nesvizhskii**; *University of Michigan, Ann Arbor, MI*
- TOG am 08:50 **Minimally Permuted Peptide Analogs (MIPA) as Internal Standards for Relative and Absolute Quantification of Peptides and Proteins; Joerg Seidler**¹; Dominic Winter¹; Dominik Kugelstadt²; Bianca Derrer²; Barbara Kappes²; Wolf D. Lehmann¹; *¹German Cancer*

Research Center, Heidelberg, Germany;
²University of Heidelberg, Heidelberg, Germany

TOG am 09:10 **Spectral Counting Error Statistics from Nine Replicate MudPIT Samples; Bret Cooper**; *USDA-ARS, Beltsville, MD*

- TOG am 09:30 **EtEP - A Novel Method to Produce an Equimolar Mixture of Standard Peptides for Absolute Quantification and Stoichiometry Determination; Johann Holzmann**¹; Johannes Fuchs¹; Otto Hudecz²; Peter Pichler³; Mathias Madalinski¹; Robert Kurzbauer¹; Karl Mechtler^{1,2}; *¹Research Institute of Molecular Pathology, Vienna, Austria;* *²Institute of Molecular Biotechnology, Vienna, Austria;* *³Christian Doppler Laboratory for Proteome Analysis, Vienna, Austria*
- TOG am 09:50 **Detection and Correction of Interference in MRM Analysis; David Fenyo**¹; Sofia Waldemarson²; Guoan Zhang²; Asa Wahlander²; Beatrix Ueberheide¹; Sunnie Myung¹; Brian Reed¹; Kelly Molloy¹; Julio Cesar Padovan¹; Jan Eriksson³; Thomas Neubert²; Brian Chait¹; *¹The Rockefeller University, New York, NY;* *²New York University Medical Center, New York, NY;* *³Swedish University of Agricultural Sciences, Uppsala, Sweden*
- TOG am 10:10 **Development and Application of a System Suitability Standard and Protocol to Assess Data Quality in LC-MRM-MS across Multiple MS Platforms; Susan E. Abbatiello**¹; Birgit Schilling²; D. R. Mani⁴; Xingdong Feng⁸; Lisa Zimmerman⁶; Brendan Maclean⁵; Michael P. Cusack²; Terri Addona¹; Nell Sedransk⁸; Michael J. Maccoss⁵; Steven C. Hall³; Steven A. Carr¹; CPTAC Network⁷; *¹Broad Institute, Cambridge, MA;* *²Buck Institute for Age Research, Novato, CA;* *³UCSF Sandler-Moore Mass Spectrometry Core Facility, San Francisco, CA;* *⁴The Broad Institute of MIT and Harvard, Cambridge, MA;* *⁵University of Washington, Seattle, WA;* *⁶Vanderbilt University, Nashville, TN;* *⁷National Cancer Institute, Bethesda, MD;* *⁸NISS, Research Triangle Park, NC*

**10:30 AM – 2:30 PM, TUESDAY
POSTER SESSION
Exhibit Hall ABCDE**

**2:30 – 4:30 PM, TUESDAY AFTERNOON
FUNDAMENTALS: ION SPECTROSCOPY
Mary Rodgers, presiding
Room: Ballroom HJ**

- TOA pm 2:30 **Alkali Metal Cationized Aliphatic Amino Acids: Charge-Solvation Becomes More Favorable with Increasing Ion Size; Jos Oomens**^{1,2}; Miriam Drayss³; Peter B. Armentrout⁴; Mathias Schaefer³; *¹FOM Rijnhuizen, Nieuwegein, Netherlands;* *²University of Amsterdam, Amsterdam, Netherlands;* *³Inst. Organic Chemistry University of Cologne, Koeln, Germany;* *⁴University of Utah, Salt Lake City, UT*
- TOA pm 2:50 **Gas Phase Structure of Micro-Hydrated Manganese Perchlorate Salts Probed by Infrared Spectroscopy; Philippe Maitre**¹; Edith Nicol^{1,2}; Vincent Steinmetz¹; Rajeew Sinha¹; *¹Laboratoire de Chimie Physique, Orsay, France;*

²DCMR, Department of Chemistry, Ecole Polytechnique, Palaiseau, France

TOA pm 3:10 **Infrared Spectroscopic Evidence for Ring Opening of Cyclic Monosaccharides;** Sarah Stefan¹; John R. Eyler¹; Brad K. Bendiak³; Darin Brown³; Jos Oomens²; Jeffrey Steill²;

¹Department of Chemistry, University of Florida, Gainesville, FL; ²FOM Rijnhuizen, Nieuwegein, Netherlands; ³University of Colorado Health Sciences Center, Denver, CO

TOA pm 3:30 **Building and Breaking the Water Network: Thermodynamics of Hydration and Long-Range Ion Effects from Infrared Photodissociation Spectroscopy and Kinetics;** James Prell¹; Jeremy O'Brien²; Terrence Chang¹; Evan R. Williams¹; ¹University of California, Berkeley, CA; ²UC Berkeley, Berkeley, CA

TOA pm 3:50 **Structures of Bare and Hydrated Pb[AA-H]⁺ Complexes (AA=Ala, Val, Leu, Ile, Phe, Met) by IRMPD Spectroscopy and Computational Chemistry;** Michael Burt; Sarah Decker; Chad Atkins; Mark Rowsell; Travis Fridgen; Memorial University of NL, St. John's, Canada

TOA pm 4:10 **Vibrational Signatures of Zwitterionic and Charge Solvated Structures for Metal-Complexed Amino Acid Dimers;** Warren K Mino¹; John R. Eyler¹; Robert C. Dunbar²; Nicolas Polfer¹; ¹University of Florida, Gainesville, FL; ²Case Western Reserve Univ, Cleveland, OH

2:30 – 4:30 PM, TUESDAY AFTERNOON

MS AND IMMUNOLOGY

Markus Kalkum, presiding

Room: Ballroom ACE

TOB pm 2:30 **Mass Spectrometry Analysis of Natural HLA-DR Associated Peptides in Rheumatoid Arthritis or Antibiotic-Refractory Lyme Arthritis;** Chunxiang Yao¹; Elise E. Drouin²; Robert Seward^{1,2}; Allen C. Steere²; Catherine E. Costello¹; ¹Boston University School of Medicine, Boston, MA; ²MGH, Harvard Medical School, Boston, MA

TOB pm 2:50 **Sequencing and Quantification of IgG Fragments and Antigen Binding Regions by Mass Spectrometry;** Dominique de Costa¹; Ingrid Broodman²; Martijn van Duijn³; Christoph Stingl³; Lennard Dekker³; Peter Burgers³; Henk Hoogsteden¹; Peter Sillevius Smitt³; Rob van Klaveren¹; Theo Luider³; ¹Erasmus Medical Center, Dept. of Pulmonology, Rotterdam, Netherlands; ²Erasmus Medical Center, Dept. of Clinical Chemistry, Rotterdam, Netherlands; ³Erasmus Medical Center, Dept. of Neurology, Rotterdam, Netherlands

TOB pm 3:10 **Proteomic Elucidation of Intrinsic Defense Mechanisms Mediated by the Interferon Inducible Protein X;** Tuo Li; Zixuan Wang; Fang Yu; Ileana M. Cristea; Princeton University, Princeton, NJ

TOB pm 3:30 **A Mass Spectrometric Strategy to Develop Multi-Epitope Protein Vaccines against Invasive Fungal Infections;** Diana Diaz Arevalo; Teresa Hong; James Ito; Markus Kalkum; City of Hope, Duarte, CA

TOB pm 3:50 **Identification of Novel Class I MHC-Restricted Phosphopeptides for Use as Cancer Immunotherapeutics;** Jennifer Cottine; Kara

Cummings; Michelle English; Jeffrey Shabanowitz; Victor H. Engelhard; Donald F. Hunt; UVA, Charlottesville, VA

TOB pm 4:10 **Next Generation Autoimmune Disease Diagnostics: Mass Spectrometric and Peptide Chip Epitope Analysis of Autoantigens;** Michael O. Glocker¹; Jörn Kekow⁵; Reinhard Guthke²; Dirk Koczan³; Hans-Jürgen Thiesen⁴; ¹Proteome Center Rostock, Rostock, Germany; ²Hans-Knoell Institute, Jena, Germany; ³Steinbeis Transfer Center for Proteomics, Rostock, Germany; ⁴IndyMED GmbH, Rostock, Germany; ⁵Otto von Guericke University, Magdeburg, Germany

2:30 – 4:30 PM, TUESDAY AFTERNOON

MS OF CARBOHYDRATES

Joe Zaia, presiding

Room: Ballroom BDF

TOC pm 2:30 **21st Century Developments in the Mass Spectrometry of Glycans and Glycoconjugates;** Catherine E. Costello; Boston University School of Medicine, Boston, MA

TOC pm 2:50 **A Systematic Method for Comprehensive Glycome Elucidation;** Shuai Wu¹; Nannan Tao¹; Ning Tang²; Keith Waddell²; Rudi Grimm²; J. Bruce German¹; Carlito Lebrilla¹; ¹UC Davis, Davis, CA; ²Agilent Technologies, Palo Alto, CA

TOC pm 3:10 **High Performance Glycoproteome Analysis of Human and Murine Plasma Using Ion Trap Mass Spectrometry;** Katherine A. Stumpo¹; Laura Shelton²; Thomas Seyfried²; Vernon N. Reinhold¹; ¹University of New Hampshire, Durham, NH; ²Department of Biology, Boston College, Chestnut Hill, MA

TOC pm 3:30 **Method Development for the Comprehensive Compositional Analysis of Heparin/Heparan Sulfate Disaccharides from Human Serum;** Wej Wei; Milady Ninonuevo; Lieza Marie Danan; Julie A. Leary; University of California Davis, Davis, CA

TOC pm 3:50 **Toward More Structurally Informative Tandem MS of Heparan Sulfate: Chemical Modifications to Reduce Sulfate Density;** Xiaofeng Shi; Yu Huang; Joseph Zaia; Boston University School of Medicine, Boston, MA

TOC pm 4:10 **Electron Detachment Of Highly Sulfated Glycosaminoglycan Carbohydrates;** Franklin E. Leach III¹; Jeremy Wolff³; Tatiana Laremore²; Zhongping Xiao²; Sailaja Arungundram¹; Kanar Al-Mafraji¹; Andre Venot¹; Geert-Jan Boons¹; Robert J. Linhardt²; Jon Amster¹; ¹University of Georgia, Athens, GA; ²Rensselaer Polytechnic Institute, Troy, NY; ³Bruker Daltonics, Billerica, MA

2:30 – 4:30 PM, TUESDAY AFTERNOON

NEW DEVELOPMENTS IN IONIZATION

Sarah Trimpin, presiding

Room 155

TOD pm 2:30 **ESI-like MALDI Ions; Laserspray Ionization, a Powerful New Technique for API Mass Spectrometers;** Charles N. McEwen¹; Sarah Trimpin²; ¹Univ. of the Sciences in PA, Philadelphia, PA; ²Wayne State University, Detroit, MI

TOD pm 2:50 **Qualitative and Quantitative Behavior of AC Electrospray Ionization in Mass Spectrometry of Biomolecules;** Nishant Chetwani; Catherine

Cassou; David Go; Hsueh-Chia Chang; *University of Notre Dame, Mishawaka, IN*

- TOD pm 3:10 **Low-Temperature Plasma (LTP) Probe Ambient Ionization Source: Temporally and Spatially-Resolved Investigations of Plasma-Sample Interactions;** Joshua Wiley¹; Carsten Engelhard²; Ayanna Jackson¹; Jacob Shelley²; Robert Noll¹; R. Graham Cooks¹; Gary Hieftje²; ¹*Purdue University, West Lafayette, IN;* ²*Indiana University, Bloomington, IN*
- TOD pm 3:30 **Electrode-Assisted Spray Ionization Mass Spectrometry;** Abdil Ozdemir²; Chung-Hsuan Chen¹; ¹*Genomic Research Center, Taipei, Taiwan;* ²*Department of Chemistry, Sakarya University, Esentepe, Turkey*
- TOD pm 3:50 **Exploration and Developments in Nano-Electrospray Ionization Sources Operating at Atmospheric and Sub-Atmospheric Pressure;** R. Brent Dixon; Jason Page; Ioan Marginean; Nitin Agrawal; Ryan Kelly; Keqi Tang; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TOD pm 04:10 **Nanospray Desorption Electrospray Ionization Mass Spectrometry;** Patrick Roach¹; Julia Laskin¹; Alexander Laskin²; ¹*Pacific Northwest National Laboratory, Richland, WA;* ²*EMSL/PNNL, Richland, WA*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
IDENTIFICATION OF UNUSUAL XENOBIOTIC
METABOLITES USING MASS SPECTROMETRY**

**Benjamin Johnson, presiding
Room: Hall 2**

- TOE pm 2:30 **Challenges and Solutions for Detection and Identification of Metabolites of Unpredictable Structures;** Donglu Zhang¹; Benjamin M. Johnson²; ¹*Bristol-Myers Squibb, Princeton, NJ;* ²*Bristol-Myers Squibb Company, Wallingford, CT*
- TOE pm 2:50 **Metabolomics Data Processing Techniques Applied to Metabolite Identification of Xenobiotics;** Jeffrey L. Whitney; Kenneth L. Ray; Mark E. Hail; *Novatia, LLC, Monmouth Junction, NJ*
- TOE pm 3:10 **Metabolite Profiling in a Discovery Environment: A Comparison of Metabolite Profiles Following Targeted and Non-Targeted Analysis of Well Characterized Drugs;** Richard Schneider; Veronica Zelesky; Hui Zhang; *Pfizer Global R&D, Groton, CT*
- TOE pm 3:30 **Evaluation of Combined Quantitative and Qualitative Approaches for Pharmaceutical Research Using a Hybrid Quadrupole Linear Ion Trap Mass Analyzer;** Loren Olson; Richard Lauman; Renee Huang; *AB SCIEX, Foster City, CA*
- TOE pm 3:50 **Metabolism of a Vitamin C-Acrolein Adduct in Cultured Human Monocytic THP-1 Cells Studied by LC-MS/MS;** Nicholas G. Kesinger; Brandi L. Langsdorf; Cristobal L. Miranda; Jan F. Stevens; *Oregon State University, Corvallis, OR*
- TOE pm 4:10 **Hybrid Linear Ion-Trap - Orbitrap Mass Spectrometry at 100k Resolution for the Determination of the Polyether Toxins, Azaspiracids, in Shellfish;** Kevin James^{1,2}; Zuzana Skrabakova^{1,2}; John O'Halloran²; Frank van Pelt²; ¹*PROTEOBIO, Cork Institute of Technology, Cork, Ireland;* ²*Environmental Research Institute, UCC, Cork, Ireland*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
DEALING WITH PHOSPHOLIPIDS IN REGULATED
BIOANALYSIS**

**Patrick Vallano, presiding
Room: Hall 3**

- TOF pm 2:30 **Dealing with Phospholipids in Regulated Bioanalytical Methods: An Overview;** Patrick Vallano; Tina Bland; *Mylan Pharmaceuticals, Inc., Morgantown, WV*
- TOF pm 2:50 **Effect of Phospholipids on Efficiency, Reproducibility, Accuracy and Linearity of Bioanalytical Assays and Importance of Removing them during Sample Clean-Up;** Mathieu Lahaie; Jean-Nicholas Mess; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), Quebec, Canada*
- TOF pm 3:10 **Depletion of Phospholipid Matrix Interference when Dealing with Small Volume Plasma Samples;** Craig Aurand¹; David S. Bell²; Hillel K. Brandes²; Daniel Vitkuske²; ¹*Sigma Aldrich, Bellefonte, PA;* ²*Supelco/ Sigma Aldrich, Bellefonte, PA*
- TOF pm 3:30 **Evaluation of Phospholipids Effect on Ionization in LDTD-MS/MS Analysis of Human Plasma Extracts from Protein Precipitation, SPE and Liquid-Liquid Extraction;** Pierre Picard; Serge Auger; Patrice Tremblay; *Phytronix Technologies, Inc., Quebec, Canada*
- TOF pm 3:50 **Supported Liquid Extraction vs. Liquid-Liquid Extraction: Comparing Phospholipid and Analyte Recoveries under Various Extraction Conditions;** Brian T. Hoffman; Erika Moore; Daniel Mulvana; *Advion Biosciences, Ithaca, NY*
- TOF pm 4:10 **On-Line Removal of Phospholipids from Protein Precipitated Samples Using Silica Hydride-Based Trapping Column;** Katty X. Wan; Maria P. Metchkarova; Matthew J. Rieser; *Abbott Laboratories, Abbott Park, IL*

**2:30 – 4:30 PM, TUESDAY AFTERNOON
BIOINFORMATICS IN PROTEOMICS**

**Michael MacCoss, presiding
Room: Hall 4**

- TOG pm 2:30 **A New Kinetic Model of Peptide Fragmentation for Improved Discrimination in Peptide Identification;** Shaojun Sun¹; Chia-Yu Yen¹; Stephane Houel²; Natalie Ahn^{1,2}; Meredith Betterton¹; William Old¹; ¹*University of Colorado, Boulder, CO;* ²*Howard Hughes Medical Institute, Boulder, CO*
- TOG pm 2:50 **Thousandfold Faster Database Searching For Peptide Identification from Tandem Mass Spectra;** Benjamin Diament¹; William Noble²; ¹*Univ of Washington, Seattle, WA;* ²*University of Washington, Seattle, WA*
- TOG pm 3:10 **Template Proteogenomics: Sequencing Proteins Using an Imperfect Database;** Natalie E Castellana¹; Victoria Pham²; David Arnott³; Jennie Lill⁴; Vineet Bafna⁵; ¹*UCSD, La Jolla, CA;* ²*Genentech, South San Francisco, CA;* ³*Genentech, Inc., S. San Francisco, CA;* ⁴*Genentech Inc, South San Francisco, CA;* ⁵*Univ. Cal. San Diego, San Diego, CA*
- TOG pm 3:30 **Skyline Targeted Proteomics Environment: Sharing SRM/MRM Method Creation and Results Analysis across Laboratories and Instrument Platforms;** Brendan Maclean¹;

Daniela Tomazela¹; Susan E. Abbatiello²; Birgit Schilling³; Nicholas Shulman¹; Matthew Chambers⁴; David Tabb⁴; Bradford W. Gibson³; Steven A. Carr²; Daniel C. Liebler⁴; Michael J. Maccoss¹; ¹University of Washington, Seattle, WA; ²Broad Institute, Cambridge, MA; ³Buck Institute for Age Research, Novato, CA; ⁴Vanderbilt University, Nashville, TN; ⁵National Cancer Institute, Bethesda, MD

TOG pm 3:50

DirectTag-TagRecon: Sequence Tagging Reveals Ubiquity of Peptide Modifications in Clinical Cancer Samples; Surendra Dasari; Matthew Chambers; David Tabb; *Vanderbilt University, Nashville, TN*

TOG pm 4:10

Database Independent Proteomics; Ab initio Analysis of the Ostrich Proteome by a Combination of Lys-N and Electron Transfer Dissociation; A.F. Maarten Altelaar; Danny Navarro; Bas van Breukelen; Jos Boekhorst; Berend Snel; Shabaz Mohammed; Albert J.R. Heck; *Utrecht University, Utrecht, Netherlands*

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

4:45 pm

**Presentation of the Thermo Scientific Research Award
Presentation of the Waters Corporation Research Award**



4:55 pm

David C. Muddiman, Recipient of the Biemann Medal

5:45 - 7:00 PM, TUESDAY WORKSHOPS. See page S8

**8:30 – 10:30 AM, WEDNESDAY MORNING
MULTIPLE CHARGING IN MASS SPECTROMETRY
Rachel Loo, presiding
Room: Ballroom HJ**

WOA am 08:30

BIRD-Experiments on Multiply Charged Anions in a New Temperature-Controllable ICR Cell; Tatjana Karpuschkin²; Maria Massaouti¹; Eugene Nikolaev³; Oliver Hampe²; Manfred M. Kappes²; ¹Foundation for Research & Technology-Hellas Forth, Heraklion, Greece; ²Karlsruhe Institute for Technology, Karlsruhe, Germany; ³The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation

WOA am 08:50

Laserspray Using a Commercial AP-MALDI Source for Rapid Switching between Singly and Multiply Charged Ions; Barbara S. Larsen¹; Sarah Trimpin; Charles N. McEwen³; ¹The DuPont Company, Wilmington, DE; ²Wayne State University, Detroit, MI; ³Univ. of the Sciences in PA, Philadelphia, PA

WOA am 09:10

Unusual Electrospray Solvent for Protein Desorption; Nicolas Auzeil¹; Anna Warnet²; Jean-Claude Tabet²; ¹Université Paris Descartes, Paris, France; ²University Paris VI (UPMC), Paris, France

WOA am 09:30

Factors that Promote ESI Multiple Charging for Proteins; Joseph A. Loo; Shirley H. Lomeli; Rachel R. Ogorzalek Loo; *UCLA, Los Angeles, CA*

WOA am 09:50

Vapor Treatment of Electrospray Droplets for Altering Protein Charge State Distributions; Anastasia Kharlamova; Boone Prentice; Teng-Yi Huang; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*

WOA am 10:10

A Critical Evaluation of Charge Manipulation Strategies Coupled to Nano-Electrospray Ion Mobility-Mass Spectrometry; Russell Bornschein; Brandon Ruotolo; *The University of Michigan, Ann Arbor, MI*

**8:30 – 10:30 AM, WEDNESDAY MORNING
MS AND CLINICAL DIAGNOSTICS
Alan Rockwood, presiding
Room: Ballroom ACE**

WOB am 08:30

A Physician's Perspective on Clinical Mass Spectrometry; William Roberts; *University of Utah, Salt Lake City, UT*

WOB am 08:50

Quantitative Underivatized Amino Acid Analysis - Development, Dimensionality, Data Reduction and Diagnostic Utility; Brian Rappold; Russell Grant; Patricia Holland; *Labcorp, Burlington, NC*

WOB am 09:10

Derivative Design for Clinical Analysis: Free Amino Acid Quantification with MPBS and DMABS; David W. Johnson; SA Pathology/Women's and Children's Hospital, N Adelaide SA, Australia

WOB am 09:30

Top-Down Sequencing of Hemoglobin Variants with Multiple Activation Techniques; Roger Theberge¹; Mark E. McComb²; Cheng Lin³; Catherine E. Costello⁴; ¹Boston University School, Boston, MA; ²Boston University Med. School, Boston, MA; ³Boston University, Boston, MA; ⁴Boston University School of Medicine, Boston, MA

WOB am 09:50

Clinical Diagnosis of Doss Porphyria and Erythropoietic Porphyria Using Tandem Mass Spectrometry; John R. Choiniere; Frantisek Turecek; Michael H. Gelb; C. Ronald Scott; *University of Washington, Seattle, WA*

WOB am 10:10

Diagnosis and Quantification of Toxemia of Anthrax Using Mass Spectrometry; John R. Barr¹; Anne E. Boyer¹; Conrad P. Quinn¹; Maribel Gallegos²; Renato Lins²; Zsuzsanna Kuklennyik¹; James L. Pirkle¹; ¹CDC, Atlanta, GA; ²Battelle Memorial Institute, Atlanta, GA

**8:30 – 10:30 AM, WEDNESDAY MORNING
MS OF FUELS, BIOFUELS AND HEAVY OILS
Kuangan Qian, presiding
Room: Ballroom BDF**

WOC am 08:30

Ambient Analysis of Saturated Hydrocarbons Using Discharge-Induced Oxidation in Desorption Electrospray Ionization; Chunping Wu; Marcela Nefliu; R. Graham Cooks; *Purdue University, West Lafayette, IN*

WOC am 08:50

NonCovalent Aggregation: The Overriding Principle that Defines Mass Spectral Characterization of Asphaltenes; Amy M.

McKenna¹; Lynda J. Donald²; Ryan P. Rodgers¹; Kenneth G. Standing³; Alan G. Marshall¹; ¹*Natl High Magnetic Field Laboratory, Tallahassee, FL*; ²*Department of Chemistry, University of Manitoba, Winnipeg, MB*; ³*Department of Physics, University of Manitoba, Winnipeg, MB*; ⁴*Department of Chemistry and Biochemistry, FSU, Tallahassee, FL*

- WOC am 09:10 **Thermal Analysis - Modulated Fast Gas Chromatography- Single Photon Ionisation TOF-MS for Comprehensive Characterization of Crude Oil-Fractions and Polymers**; Ralf Zimmermann¹; Mohammad Saraji-Bozorgzad²; Markus Eschner²; ¹*University of Rostock, Rostock, GERMANY*; ²*Helmholtz Zentrum München, Oberschleißheim, Germany*
- WOC am 09:30 **Investigation of Deposition and Fouling in Crude Oils By Liquid Chromatography and FT-ICR Mass Spectrometry**; Wolfgang Schrader¹; Sami Lababidi¹; Julia Hesse¹; Katharina Lührig¹; Fabiane Nachtigall¹; Jan T. Andersson²; ¹*Max-Planck Inst Coal Res., Mülheim / Ruhr, Germany*; ²*Univ. Münster, Münster, Germany*
- WOC am 09:50 **Assessment of Asphaltene Structure Using Ion Mobility-Mass Spectrometry**; Sharon Munisamy¹; Kyle Fort²; Christopher Becker¹; David H. Russell²; ¹*Baylor University, Waco, TX*; ²*Texas A&M University, College Station, TX*
- WOC am 10:10 **Biodiesel Analysis - Complexity and Time**; G. John Langley¹; Christianne Wicking¹; Tom Lynch²; ¹*University of Southampton, Southampton, UK*; ²*BP Global Lubricants, Pangbourne, UK*

8:30 – 10:30 AM, WEDNESDAY MORNING
ENVIRONMENTAL MS IDENTIFICATION OF UNKNOWNNS
Enrico Davoli, presiding
Room 155

- WOD am 08:30 **Data Mining Strategies for Identification of Unknowns in Environmental Water Samples**; Imma Ferrer; Michael Thurman; *University of Colorado, Boulder, CO*
- WOD am 08:50 **Non Targeted Screening of Marine Biotoxins in Shellfish by Ultra High Resolution Mass Spectrometry**; Joseph Hui¹; Pearl Blay¹; James Chang²; Jeremy Melanson¹; ¹*NRC Institute for Marine Biosciences, Halifax, Canada*; ²*Thermo Scientific, San Jose, CA*
- WOD am 09:10 **Liquid Chromatography Tandem Mass Spectrometry Discovery of Haloquinones as Water Disinfection Byproducts**; Xing-Fang Li; Yuli Zhao; Feng Qin; Jessica Boyd; Wagner Megan; *University of Alberta, Edmonton, Canada*
- WOD am 09:30 **Metaproteomics: Phylogenomic-Based Identification of Microbes from MS/MS Environmental Samples and Unprecedented Assignment Of Peptides and Proteins Using Spectral Libraries**; William Cannon^{1,2}; Mitchell Rawlins¹; Gaurav Kulkarni¹; Douglas Baxter¹; Ananth Kalyanaraman²; Mary Lipton¹; Stephen Callister¹; ¹*Pacific NW National Lab, Richland, WA*; ²*Washington State University, Pullman, WA*
- WOD am 09:50 **Determination of Natural Pyrethrins by LC-EI-MS**; Achille Cappiello; Giorgio Famigliani; Pierangela Palma; Veronica Termopoli; Bruno Tirillini; Helga Truffelli; *Universita di Urbino, Urbino, Italy*

WOD am 10:10 **Characterization of Oligomers in Biogenic Secondary Organic Aerosol by High-Resolution Mass Spectrometry and Infrared Multi-Photon Dissociation**; Wiley A. Hall; Murray Johnston; *University of Delaware, Newark, DE*

8:30 – 10:30 AM, WEDNESDAY MORNING
LC-MS STRATEGIES FOR METABOLOMICS IN DRUG DISCOVERY

Gabriella Szekely-Klepser, presiding
Room: Hall 2

- WOE am 08:30 **Putting Metabolomics to Practice in Drug Discovery**; Michael Reily; *Bristol-Myers Squibb, Princeton, NJ*
- WOE am 08:50 **Solid-phase Microextraction for Untargeted LC-MS Metabolomics Studies Using Benchtop Orbitrap Instrument**; Dajana Vuckovic¹; Janusz Pawliszyn¹; Inés de Lannoy²; Brad Gien²; Robert Shirey³; Leonard Sidisky³; Sucharita Dutta⁴; ¹*University of Waterloo, Waterloo, Canada*; ²*NoAb BioDiscoveries, Mississauga, Canada*; ³*Supelco Inc., Bellefonte, PA*; ⁴*ThermoFisher Scientific, San Jose, CA*
- WOE am 09:10 **High Resolution Liquid Chromatography and High Resolution Mass Spectrometry for Simultaneous Qualitative and Quantitative Analysis**; Gérard Hopfgartner¹; J.C. Yves Le Blanc²; Emmanuel Varesio¹; ¹*School of Pharmaceutical Sciences, EPGL, LSMS, Geneva, Switzerland*; ²*AB-SCIEX, Toronto, Canada*
- WOE am 09:30 **HILIC-UPLC-MS for the Metabolic Profiling of Biofluids: Application to Toxicological Studies**; Elizabeth J Want¹; Konstantina Spagou^{2,3}; Perrine Masson³; ¹*Imperial College, London, UK*; ²*Aristotle University, Thessaloniki, Greece*; ³*Imperial College London, London, UK*
- WOE am 09:50 **Practical Ways to Identify Metabolite Markers in Drug Discovery Using High Resolution LC/MS-Based Metabolomics Approach**; Haiying Zhang; Thomas Harrity; Petia Shipkova; George Psaltis; Randolph Ponticciello; David Gordon; Laura Patrone; John Kozlosky; Lindsay Tomlinson; Greg Cosma; Joseph Horvath; Jonathan Josephs; William Humphreys; *Bristol-Myers Squibb R&D, Princeton, NJ*
- WOE am 10:10 **Non-Targeted Biochemical Profiling Platform Reveals Biomarkers of Sepsis, Including Those at Highest Risk for Septic Death, at Time of Presentation**; Anne M. Evans¹; Robert P. Mohny¹; Jacob Wulff¹; Raymond J. Langley²; Stephen Kingsmore²; ¹*Metabolon, Inc., Durham, NC*; ²*The National Center for Genome Research, Santa Fe, NM*

8:30 – 10:30 AM, WEDNESDAY MORNING
CLINICAL APPLICATIONS OF INTEGRATED QUALITATIVE AND QUANTITATIVE LC-MS
Mustafa Varoglu, presiding
Room: Hall 3

- WOF am 08:30 **Overcoming the Conundrums of Multi-Disciplinary Translational Proteomics – Lessons Learned from Multiple Clinical Proteomics Studies**; J. Will Thompson; Laura Dubois; Erik J Soderblom; Meredith Turner; Matt Foster; Jeanette McCarthy; Virginia Kraus; Jonathan Catterall; Victoria Christian; Arthur

- Moseley; *Duke University School of Medicine, Durham, NC*
- WOF am 08:50 **'Eye-Tracking' of Proteins from Human Intraocular Fluids – Qualitative and Quantitative Approaches Toward Understanding the Progression of Eye Disease;** Keiryn L. Bennett¹; Marion Funk²; Andreas Pollreis²; Marion Tschernutter¹; Melanie Planyavsky¹; Katja Parapatics¹; Florian P. Breitwieser¹; Ceereena Ubaida Mohien³; Andre Mueller¹; Zlatko Trajanoski³; Jacques Colinge¹; Giulio Superti-Furga^{1,1}; Ursula Schmidt-Erfurth² ¹*CeMM - Center for Molecular Medicine, Vienna, Austria*; ²*Medical University of Vienna, Vienna, Austria*; ³*Technical University of Graz, Graz, Austria*
- WOF am 09:10 **Proteome Analysis of Cerebrospinal Fluid: Monitoring Changes in Protein Abundance over the Course of Antiretroviral Therapy in HIV Infected Individuals;** Thomas Angel¹; Jon Jacobs¹; Richard Price²; Serena Spudich²; Marina Gritsenko¹; Dietmar Fuchs³; Lars Rosengren⁴; Henrik Zetterberg⁴; Dave Camp¹; Richard D. Smith¹; ¹*PNNL, Richland, WA*; ²*Department of Neurology, University of California, San Francisco, CA*; ³*Biocentre, Innsbruck Medical University, Innsbruck, Austria*; ⁴*Sahlgrenska Academy at University of Gothenburg, Gothenburg, Sweden*
- WOF am 09:30 **Quantitation by High Resolution Full Scan Accurate Mass-The Future of Discovery DMPK?** Jonathan L. Josephs; Yanou Yang; Chiuwa Emily Luk; Petia Shipkova; William Humphreys; *Bristol-Myers Squibb, Pennington, NJ*
- WOF am 09:50 **Evaluating the Intestinal Health of Premature Infants by NanoLC-MS Analysis of Excreted Oligosaccharides;** Maria Lorna A. de Leoz¹; Shuai Wu¹; Mark Underwood¹; Peggy Cheng¹; John S. Strum¹; Rudolf Grimm²; Bruce German¹; David Mills¹; Carlito B. Lebrilla¹; ¹*University of California, Davis, CA*; ²*Agilent Technologies, Santa Clara, CA*
- WOF am 10:10 **Mass Spectrometric Characterization of Arylpropionamide-Derived Selective Androgen Receptor Modulators and their *in-vitro* and *in-vivo* Generated Metabolites;** Mario Thevis¹; Enrico Gerace²; Hans Geyer¹; Wilhelm Schänzer¹; ¹*German Sport University, Cologne, Germany*; ²*University of Turin, Turin, Italy*
- 8:30 – 10:30 AM, WEDNESDAY MORNING CHARACTERIZING PTMS**
Andy Tao, presiding
Room: Hall 4
- WOG am 08:30 **Quantitative Mass Spectrometry Reveals Complexity and Function of Protein Ubiquitination;** Junmin Peng; *Emory University, Atlanta, GA*
- WOG am 08:50 **Improved Methodologies for the Identification of Ubiquitin and Ubiquitin-Like Protein (Ubl) Conjugation Sites Identifies Novel Ubl Chain Linkages;** Tharan Srikumar^{1,2}; Stanley Jeram^{1,2}; Xiang-Dong Zhang³; H. Anne Eisenhauer¹; Richard Rogers⁴; Patrick G.A. Pedrioli⁵; Michael Matunis⁶; Henry Lam⁷; Brian Raught^{1,2}; ¹*Ontario Cancer Institute, Toronto, Canada*; ²*Medical Biophysics, University of Toronto, Toronto, Canada*; ³*Dept. Biological Sciences, Wayne State University, Detroit, MI*; ⁴*Institute for Systems Biology, Seattle, WA*; ⁵*Institute of Biochemistry ETH, Zurich, Switzerland*; ⁶*Biochem. and Mol. Biol. The Johns Hopkins Univ., Baltimore, MD*; ⁷*Dept Chem Biomol Engineer. Hong Kong Univ Sci Tech, Clear Water Bay, Hong Kong*
- WOG am 09:10 **Multi-Glycomics Platform Approach for Cancer;** Carlito Lebrilla; Hyun Joo An; Scott Kronewitter; Maria Lorna A. De Leoz; Kyle Peacock; Jaehan Kim; Sureyya Ozcan; Grace Ro; *University of California, Davis, CA*
- WOG am 09:30 **Characterizing the Range of Naturally-Occurring Post-Translational Modifications in the Proteomes of Microbial Isolates and Consortia;** Robert Hettich¹; Alison Russell²; Andrew Dykstra²; Jill Banfield³; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*; ²*UTK-Oak Ridge National Lab, Knoxville, TN*; ³*University of California - Berkeley, Berkeley, CA*
- WOG am 09:50 **In-Depth Phosphoproteome Analysis Using PolyMAC;** Anton Iliuk; Victoria Martin; Bethany Alicie; Robert Geahlen; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
- WOG am 10:10 **Estimating False Discovery Rates of Post-Translational Modification Site Assignments;** Banu Dost¹; Vineet Bafna²; Nuno Bandeira³; ¹*University of California, San Diego, La Jolla, CA*; ²*Univ. Cal. San Diego, San Diego, CA*; ³*CCMS, UCSD, La Jolla, CA*
- 10:30 AM – 2:30 PM, WEDNESDAY POSTER SESSION Exhibit Hall ABCDE**
- 2:30 – 4:30 PM, WEDNESDAY AFTERNOON FUNDAMENTALS: ION/MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS**
Hilkka Kenttämää, presiding
Room: Ballroom HJ
- WOA pm 2:30 **Gas-Phase Substitution and Elimination Reactions of Vinylic and Aryl Halides;** Allison Eanes; Diogo de Oliveira; Michele Khurana; Renan Joviliano; Scott Gronert; *Virginia Commonwealth Uni, Richmond, VA*
- WOA pm 2:50 **Original Formation and Reactivity on Double Bonds of Dichlorocarbene at Atmospheric Pressure Studied by Photoionization Mass Spectrometry;** David Touboul¹; Julie Allegrand¹; Alexandre Giuliani²; Olivier Laprèvote¹; ¹*CNRS-ICSN, Gif-Sur-Yvette, France*; ²*Synchrotron Soleil, Gif-Sur-Yvette, France*
- WOA pm 3:10 **Does the 2,6-Didehydropyridinium Ion Exist?** Bartłomiej J. Jankiewicz^{1,2}; Nelson R. Vinuesa¹; Lindsey M. Kirkpatrick¹; John J. Nash¹; Hilkka I. Kenttämää¹; ¹*Department of Chemistry, Purdue University, West Lafayette, Indiana*; ²*Military University of Technology, Warsaw, Poland*
- WOA pm 3:30 **Gas Phase Reactions of Carbanions with H Atoms;** Zhibo Yang¹; Oscar Martinez Jr.¹; Brian Eichelberger²; Marshall Carpenter¹; Theodore P. Snow¹; Veronica M. Bierbaum¹; ¹*University of Colorado, Boulder, CO*; ²*John Brown University, Siloam Spring, MD*
- WOA pm 3:50 **Investigating the Role of Cation Recombination Energy as a Key Factor in ETD/ECD;** Marija Mentinova¹; David Crizer²; Takashi Baba²; Gary L. Glish³; Scott A.

Mcluckey¹; ¹Purdue University, West Lafayette, IN; ²UNC-Chapel Hill, Chapel Hill, NC;

³University of North Carolina, Chapel Hill, NC

WOA pm 4:10 **High-Throughput, Combinatorial Analysis of Cationic and Anionic Ion/Ion Reagents Using an ETD-Enabled QLT-Orbitrap Coupled to a Gas Chromatograph;** Amelia C. Peterson; Graeme McAlister; Joshua J. Coon; *University of Wisconsin, Madison, WI*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
FTMS: INSTRUMENTATION AND APPLICATIONS**

**Julia Laskin, presiding
Room: Ballroom ACE**

WOB pm 2:30 **Overview: Recent Advances in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Alan G. Marshall; *Ion Cyclotron Resonance Prog, Tallahassee, FL*

WOB pm 2:50 **Harmonization of Electric Field in FT ICR Cell. The New Approaches;** Ivan Boldin; Eugene Nikolaev; *The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation*

WOB pm 3:10 **Examining Time-Dependent Space-Charge Effects in FTICR Mass Spectrometry With Multiparticle Simulations of Ion Motion;** Jon Amster¹; Franklin E. Leach III¹; Andriy Kharchenko; Ron M.A. Heeren²; Eugene Nikolaev⁴; Konstantin Aizikov; Peter B. O'connor⁶; ¹University of Georgia, Athens, GA; ²FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands; ³BUSM, Boston, MA; ⁴The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation; ⁵FOM Inst. Atomic/Molecular Phy, Amsterdam, Netherlands; ⁶University of Warwick, Coventry, UK

WOB pm 3:30 **A Gas-Phase Reactivity Study of a $\sigma,\sigma,\sigma,\sigma$ -Tetraradical Ion – the 2,4,6-Tridehydroxyridine Radical Cation;** Vanessa Gallardo¹; Bartłomiej Jankiewicz²; Nelson Vinuesa¹; John Nash¹; Hilka Kenttamaa¹; ¹Purdue University, West Lafayette, IN; ²Military University of Technology, Warsaw, Poland

WOB pm 3:50 **Tailored Ion Spatial Distribution in FT-ICR MS for Improved Analysis of Complex Mixtures;** Nathan K. Kaiser¹; Joshua J. Savory¹; Amy M. Mckenna¹; Christopher L. Hendrickson¹; Alan G. Marshall^{1,2}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Ion Cyclotron Resonance Prog, Tallahassee, FL

WOB pm 4:10 **Top-Down Proteomic Identification of Heavy Isotope Depleted Yeast Proteins Using LC-FT-ICR MS with Funnel-Skimmer Dissociation Fragmentation;** Jennifer S. Cobb¹; Aimee M. Morris¹; Michael L. Easterling²; Jeffrey N. Agar¹; ¹Brandeis University, Waltham, MA; ²Bruker Daltonics, Inc., Billerica, MA

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MS IN ENVIRONMENTAL TOXICOLOGY**

**Xingfang Li, presiding
Room: Ballroom BDF**

WOC pm 2:30 **Linking Mass Spectrometry with Toxicology for Emerging Water Contaminants;** Susan Richardson; *US EPA, NERL, Athens, GA*

WOC pm 2:50 **Arsenic Interaction with Proteins and Detecting Arsenic-Binding Proteins in Human Cells Using Mass Spectrometry and Affinity Chromatography;** Huiming Yan¹; Michael Weinfeld¹; William Cullen²; Xiufen Lu¹; Baowei

Chen¹; Meiling Lu¹; Zhongwen Wang¹; Anthony McKnight-Whitford¹; X. Chris Le¹; ¹University of Alberta, Edmonton, Canada; ²University of British Columbia, Vancouver, Canada

WOC pm 3:10 **Quantitative Analysis of 6-Thioguanine-Induced Changes in the Proteome of Jurkat-T Cells;** Fan Zhang; Yinsheng Wang; *University of California, Riverside, CA*

WOC pm 3:30 **Quantification of the HSP 70 and HSP 90 Response to Environmental Stress in Pacific Oysters Using Orthologue-Based Multiple Reaction Monitoring;** David Cassis; Shujun Lin; Cordula Klockenbusch; Juergen Kast; *University of British Columbia, Vancouver, Canada*

WOC pm 3:50 **Inhibition of 4-Aminobiphenyl-Induced DNA Damage by Sulforaphane and 5,6-Dihydrocyclopenta[c]-Dithiole-3(4H)-Thione in Bladder Cells and Tissues;** Kristen L. Randall¹; Dayana Argoti²; Yi Ding³; Joseph D. Paonessa³; Rex Munday⁴; Yueheng Zhang³; Paul Vouros¹; ¹Northeastern University, Boston, MA; ²Protein Forest, Lexington, MA; ³Roswell Park Cancer Institute, Buffalo, NY; ⁴Ruakura Research Center, Hamilton, New Zealand

WOC pm 4:10 **Determination of Chlorpyrifos and Chlorpyrifos-Oxon in Rat Blood Using Isotope Dilution Technique by GC Quadrupole and Magnetic Sector MS;** Vyacheslav N. Fishman¹; Alaine Sledz²; Kathy A. Brzak¹; Michael J. Bartels¹; ¹The Dow Chemical Company, Midland, MI; ²Kelly Services Inc., Midland, MI

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MS OF GLYCOPROTEINS**

**Yehia Mechref, presiding
Room 155**

WOD pm 2:30 **Influence of Peptide Length on the Gas-Phase Fragmentation of Pronase-Derived Glycopeptides;** Wen Zhou; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*

WOD pm 2:50 **Development of a Hyphenated Ion Mobility - Mass Spectrometry Technique for the Characterization of Glycosylated Peptides;** Craig Dorsche^{1,2}; Jim Langridge^{1,2}; Scott Geromanos^{1,2}; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Manchester, UK

WOD pm 3:10 **Monitoring Quantitative Changes in Protein Specific Glycosylation during Lactation Using MALDI-FTICR MS and Its Effect on Interactions with Pathogenic Bacteria;** Mariana Barboza; John W. Froehlich; Janneth Pinzon; Isabelle Moeller; J. Bruce German; Bart Weimer; Carlito Lebrilla; *University of California Davis, Davis, CA*

WOD pm 3:30 **A Novel Tandem Mass Spectrometry Approach for the Detection and Identification of O-GlcNAc-Modified Peptides;** Hannes Hahne; Simone Lemeer; Bernhard Kuster; *Technical University Munich, Freising, Germany*

WOD pm 3:50 **Complementary N-Linked Glycoproteomics of Myocardial Ischemia / Reperfusion Injury Reveals Complex Changes in Extracellular Environments;** Benjamin Parker¹; Giuseppe Palmisano²; Alistair Edwards¹; Melanie White^{3,4}; Kasper Engholm-Keller²; Brett Hambly¹; Albert Lee⁵; Daniel Kolarich⁵; Nicki Packer⁵; Martin Larsen²; Stuart Cordwell^{1,3}; ¹The University of Sydney, NSW, Australia; ²The University of

Southern Denmark, Odense, Denmark; ³The University of Sydney, NSW, Australia; ⁴Johns Hopkins University; ⁵Macquarie Univ., NSW, Australia

WOD pm 4:10 **Online Release of N-Glycans from Glycoproteins/Glycopeptides Prior to LC-MS/MS Analysis for Facilitating Glycomic Profiling and Determination of Glycosylation Sites;** Yazen Jmeian; Loubna Hammad; Zaneer Segu; Yuening Zhang; Yehia Mechref; *Indiana University, Bloomington, IN*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
LC-MS OF REACTIVE XENOBIOTIC METABOLITES
JinPing Gan, presiding
Room: Hall 2**

WOE pm 2:30 **Overview of LC-MS Techniques to Characterize Reactive Xenobiotic Metabolites;** Raju Subramanian; *Pharmacokinetics and Drug Metabolism, Thousand Oaks, CA*

WOE pm 2:50 **High-Throughput Screening of Drug Reactive Metabolites Using Accurate Mass Based Background Subtraction and Noise Reduction Algorithm;** Shuguang Ma; Yuan Yuan; Xiaowen Lu; Anima Ghosal; Keun-Joong Lee; Peijuan Zhu; Wei Tong; Kevin Alton; Swapan Chowdhury; *Merck Research Laboratory, Kenilworth, NJ*

WOE pm 3:10 **Characterization of Stereo Conformation of the Reactive Metabolites of the Chlorogenic Acid by UPLC/ Ion Mobility/TOF MS;** Cen Xie¹; Kate Yu²; Xiaoyan Chen¹; Tao Yuan¹; Dafang Zhong¹; Hayley Crowe²; John P. Shockcor²; Alan L Millar²; ¹*Shanghai Inst Materia Medica, Shanghai, China*; ²*Waters Corporation, Milford, MA*

WOE pm 3:30 **Screening of Glutathione and Cyanide Adducts Using Precursor Ion and Neutral Loss Scans-Dependent Acquisition of Enhanced MS and MS/MS Spectra;** Hua-Fen Liu¹; Weiping Zhao²; Wenying Jian³; Elliott Jones¹; Mingshe Zhu²; ¹*AB SCIEX, Foster City, CA*; ²*Bristol-Myers Squibb, Princeton, NJ*; ³*Johnson & Johnson PRD, Raritan, NJ*

WOE pm 3:50 **Human Serum Albumin Cys34 Adducts as a Biomarker for Exposure to Unknown Reactive Chemicals;** Jian Cai; Frederick W. Benz; Donald E. Nerland; Harrell E. Hurst; William M. Pierce, Jr.; *University of Louisville, Louisville, KY*

WOE pm 4:10 **Reactive Intermediates in the Oxidative Pathway of Haloperidol to its Neurotoxic Pyridinium Metabolite Identified by On-Line Electrochemistry/ Mass Spectrometry;** Tove Johansson Malin^{1,2}; Lars Weidolf¹; Neal Castagnoli, Jr.³; Ulrik Jurva¹; ¹*AstraZeneca R&D Mölndal, Mölndal, Sweden*; ²*University of Gothenburg, Gothenburg, Sweden*; ³*Virginia Tech and The Edward Via Virginia College, Blacksburg, VA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MS OF PHARMACEUTICALS AND
PERSONAL CARE PRODUCTS IN WATER
Dil Ramanathan, presiding
Room: Hall 3**

WOF pm 2:30 **Pharmaceuticals and their Metabolites in Drinking-Water: Breaking the Part-Per-Trillion Concentration Barrier with**

WOF pm 2:50 **LC/MS/MS;** Michael Thurman; Imma Ferrer; *University of Colorado, Boulder, CO*

WOF pm 3:10 **Multi-Target Quantitation and General Unknown Screening for Pharmaceuticals and Personal Care Products in Water Samples Using LC/MS/MS;** Andre Schreiber; Nadia Pace; *AB SCIEX, Concord, Ontario, Canada*

WOF pm 3:30 **Analysis of Steroids in Manufacturing Plant Waste Effluent by On-Line SPE/UPLC/MS/MS;** Claude Mallet¹; Alain Carrier²; Audrey Tousignant²; ¹*Waters Corporation, Milford, MA*; ²*Sandoz Canada Inc, Boucherville, Quebec, Canada*

WOF pm 3:50 **Utilizing On-Line Pre-Concentration with LC/MS/MS for the Quantification of Pharmaceuticals and Personal Care Products in Water at the ng/L Level;** Kevin J. Mchale¹; Mark Sanders²; ¹*Thermo Fisher, Somerset, NJ*; ²*Thermo Fisher Scientific, Somerset, NJ*

WOF pm 4:10 **Improved Sensitivity of Direct Aqueous Sample Analysis with Thermally Assisted Desorption Electrospray Ionization Mass Spectrometry;** Ian Campbell; Alain Ton; Christopher Mulligan; *Illinois State University, Normal, IL*

WOF pm 4:10 **Direct Detection of Pharmaceuticals and Personal Care Products Contaminants in Water with Desorption Electrospray Ionization;** Christopher Mulligan; Ian Campbell; *Illinois State University, Normal, IL*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON
MS AND SYSTEMS BIOLOGY
Salvatore Sechi, presiding
Room: Hall 4**

WOG pm 2:30 **Quantification of Protein Copy Number and Robustness in the Store-Operated Calcium Signaling Network Using Selective Reaction Monitoring (SRM) Mass Spectrometry;** Ellen Abell¹; Paola Picotti²; Tobias Meyer¹; Ruedi Aebersold²; Mary Teruel¹; ¹*Chemical & Systems Biology, Stanford University, Stanford, CA*; ²*Institute for Molecular Systems Biology, ETH Zurich, Zurich, Switzerland*

WOG pm 2:50 **Rapid Quantitation of mRNA, Proteins, and PTMs Applied to a Systems-Level Analysis of Human ES, iPS, and Fibroblast Cells;** Doug Phanstiel¹; Justin Brumbaugh¹; Craig Wenger¹; Danielle L Swaney¹; Gloria Kreitinger¹; Mark Tervo¹; Ron Stewart²; James A Thomson^{1,2}; Joshua J. Coon²; ¹*University of Wisconsin, Madison, WI*; ²*Morgridge Institute, Madison, WI*

WOG pm 3:10 **A Global Protein Kinase and Phosphatase Interaction Network in Yeast;** Ashton Breitkreutz¹; Hyungwon Choi³; Jeff Sharom¹; Lorrie Boucher¹; Victor Neduva²; Brett Larsen¹; Zhen-Yuan Lin¹; Bobby-Joe Breitkreutz¹; Chris Stark¹; Guomin Liu¹; Alexey Nesvizhskii³; Michael Tyers^{1,2}; Anne-Claude Gingras¹; ¹*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, Canada*; ²*University of Edinburgh, Edinburgh, UK*; ³*University of Michigan, Ann Arbor, MI*

WOG pm 3:30 **Soybean Root Hairs: Proteomics and Beyond;** Ljiljana Pasa-Tolic¹; Laurent Brechenmacher²; Tran Hong Nha Nguyen²; Marc Libault²; Kim K. Hixson¹; Marina Gritsenko¹; Therese Clauss¹; Feng Yang¹; Gary Stacey²; ¹*Pacific NW Nat'l Lab,*

Richland, WA; ²National Center for Soybean Biotechnology, U of MO, Columbia, MO; ³Division of Biochemistry, University of Missouri, Columbia, MO

WOG pm 3:50 **Insight into Mammalian Protein Dynamics and Homeostasis by Characterization of Global Tissue Proteomes *in vivo* Using Stable Isotope Metabolic Labeling;** Shenheng Guan; John C. Price; Sina Ghaemmaghami; Stanley B. Prusiner; Alma L. Burlingame; *University of California, San Francisco, CA*

WOG pm 4:10 **Systems Biology of Skin Disease – Effect of UV Irradiation and Contact Sensitizers on Keratinocytes;** Giridharan Gokulrangan¹; Pratima Karnik²; Yu Liu¹; Gaurav S.J.B.Rana¹; Kevin Cooper²; Mark Chance¹; ¹Case Western Reserve University, Cleveland, OH; ²Department of Dermatology, University Hospitals, Cleveland, OH

**4:45 – 5:30 PM, WEDNESDAY
ASMS MEETING
Wine and Beer, Awards and More!!
Ballroom ACE**

5:45 - 7:00 PM, WEDNESDAY WORKSHOPS. See page S9

**8:30 – 10:30 AM, THURSDAY MORNING
ELECTRON AND PHOTON-BASED ION
ACTIVATION/DISSOCIATION-PD, ECD, ETD, EDD
Jennifer Brodbelt, presiding
Room: Ballroom HJ**

ThOA am 08:30 **Top-Down Structural Analysis of 60-150 kDa Proteins with ETD-Based Tandem Mass Spectrometry;** Yury Tsybin¹; Hisham Ben Hamidane¹; Michael Groessl¹; Paul Dyson¹; Jovan Simicevic¹; Bart Deplancke¹; Sophie Nallet¹; Florian Wurm¹; Carsten Stoermer²; Ralf Hartmer²; ¹Ecole Polytechnique Federale, Lausanne, Switzerland; ²Bruker Daltonics GmbH, Bremen, Germany

ThOA am 08:50 **Photodissociation and Activated-Electron Photodetachment Dissociation (Activated-EPD) for Structural Characterization of Sugar and Protein Polyanions;** Rodolphe Antoine¹; Vincent Larraillet¹; Aleksey Vorobyev²; Amandine Racaud¹; Claire Brunet¹; Yury O. Tsybin²; Jérôme Lemoine³; Philippe Dugourd¹; ¹LASIM CNRS Univ Lyon 1, Villeurbanne, France; ²Ecole Polytechnique Federale, Lausanne, Switzerland; ³LSA CNRS Univ Lyon 1, Villeurbanne, France

ThOA am 09:10 **Travelling Wave Ion Mobility Mass Spectrometry of Electron Transfer Dissociation Products of Phosphopeptides: Evidence of Conformational Memory?** Helen Cooper¹; Jeff Brown²; Iain D G Campuzano²; Nick Tomczyk²; Andrew Creese¹; Jonathan P. Williams²; ¹University of Birmingham, Birmingham, UK; ²Waters Micromass MS Technologies, Manchester, UK

ThOA am 09:30 **Elucidating the Mechanism of ECD by Direct Experimental Examination of Aminoketyl Intermediates;** Ryan R. Julian¹; Benjamin Moore²; Tony Ly; ¹University of California, Riverside, Riverside, CA; ²UC Riverside,

Riverside, CA; ³University of California, Riverside, CA

ThOA am 09:50 **Negative Electron Transfer Dissociation Identifies Thousands of Acidic Peptides from Complex Mixtures;** Graeme Mcalister¹; Jason Russell¹; Neil Rumachik¹; Aaron Ledvina¹; John E. P. Syka²; Joshua J. Coon¹; ¹University of Wisconsin, Madison, WI; ²Thermo Fisher Scientific, Charlottesville, VA

ThOA am 10:10 **Use of High-Energy Fragment Ions Derived from Photodissociation to Improve Peptide Identification and Sequencing;** Youyou Yang; Xiaohui Liu; Liangyi Zhang; James P. Reilly; *Indiana University, Bloomington, IN*

**8:30 – 10:30 AM, THURSDAY MORNING
H/D EXCHANGE FOR
PROTEIN STRUCTURE AND FOLDING
Thomas Jorgensen, presiding
Room: Ballroom ACE**

ThOB am 08:30 **An Overview of Hydrogen/Deuterium Exchange Mass Spectrometry;** John R. Engen; *Northeastern University, Boston, MA*

ThOB am 08:50 **Structural Consequences of Loss of Metal from ALS-Associated SOD1 Variant Characterized Using Top-Down Mass Spectrometric Hydrogen/Deuterium Exchange;** Qi Wang; Qian Liu; Jennifer S. Cobb; Jared R. Auclair; Jeffrey Agar; *Brandeis University, Waltham, MA*

ThOB am 09:10 **Hydrogen Deuterium Exchange Mass Spectrometry Applied to the Characterization of Proteins of Therapeutic Interest;** Michael J. Chalmers¹; Scott Novick¹; Xi Zhang¹; Scooter Willis¹; Bruce D. Pascal¹; Ellen Y.T. Chien²; Raymond C. Stevens²; John E. Toth³; Jeffrey A. Dodge³; Patrick R. Griffin¹; ¹Scripps Florida, Jupiter, FL; ²The Scripps Research Institute, La Jolla, CA; ³Lilly Research Laboratories, Indianapolis, IN

ThOB am 09:30 **Conformational Basis for the Drug Inhibition and Resistance Mechanism of KIT Tyrosine Kinase, Determined by H/D Exchange FT-ICR MS;** Hui-Min Zhang¹; Xiu Yu²; Michael Greig²; Ketan S. Gajiwala²; Joe C. Wu³; Elizabeth A. Lunney²; Wade Diehl²; Mark R. Emmett^{1,4}; Alan G. Marshall^{1,4}; ¹Nat'l High Magnetic Field Lab, Tallahassee, FL; ²Pfizer Global R&D- La Jolla, San Diego, CA; ³Pfizer-Cambridge, Cambridge, MA; ⁴Florida State University, Tallahassee, FL

ThOB am 09:50 **Structural Characterization of Short-Lived Protein Folding Intermediates by Hydrogen Exchange Mass Spectrometry with Top-Down Electron Capture Dissociation;** Jingxi Pan²; Jun Han³; Christoph Borchers⁴; Lars Konermann¹; ¹Univ. of Western Ontario, London, CANADA; ²University of Western Ontario, London, ON; ³University of Victoria-Genome BC Proteomics Centre, Victoria, BC; ⁴UVic-GBC Proteomics Centre, Victoria, BC

ThOB am 10:10 **Conformational Dynamics of the Full Membrane Bovine Mitochondrial ADP/ATP Carrier Revealed by HDX MS Measurements;** Martial Rey³; Petr Man^{1,2}; Gerard Brandolin³; Ludovic Pelosi³; Eric Forest¹; ¹Inst. for Structural Biology, Grenoble, France; ²Institute of Microbiology, Prague, Czech Republic; ³LBBSI, iRTSV, CEA, Grenoble, France

**8:30 – 10:30 AM, THURSDAY MORNING
RECENT DEVELOPMENTS IN ION MOBILITY MS**

**Julie Leary, presiding
Room: Ballroom BDF**

- ThOC am 08:30 **Mobility Measurement Non-Denatured Protein and Protein Cluster Ions by DMA-MS;** Chris Hogan¹; Juan Fernandez De La Mora²; ¹University of Minnesota, Minneapolis, MN; ²Yale University, New Haven, CT
- ThOC am 08:50 **Chemical Effects in Differential Mobility Spectrometry/Mass Spectrometry;** Bradley B Schneider¹; Thomas Covey¹; Stephen L Coy²; Evgeny V Krylov²; Erkinjon Nazarov³; ¹AB SCIEX, Concord, Canada; ²Sionex Corp., Bedford, MA; ³Sionex, Bedford, MA
- ThOC am 09:10 **A Novel, Modular Ion Mobility Drift Cell;** Ryan Blase; Chaminda M. Gamage; Joshua Silveira; David H. Russell; *Texas A&M University, College Station, TX*
- ThOC am 09:30 **Gas-Phase Structural Biology: Measuring and Interpreting Collision Cross Sections;** Matthew F. Bush¹; Zoe Hall¹; Kevin Giles²; John Hoyes²; Andrew J. Baldwin³; Justin L.P. Benesch¹; Brandon T. Ruotolo⁴; Carol V. Robinson¹; ¹Department of Chemistry, University of Oxford, Oxford, UK; ²Waters Corporation, Manchester, UK; ³Department of Chemistry, University of Toronto, Toronto, Canada; ⁴Department of Chemistry, University of Michigan, Ann Arbor, MI
- ThOC am 09:50 **Alternatives in IMS-MS - Total Solvent-Free Analysis and Structures of Highly Charged Laserspray Ions;** Sarah Trimpin; *Wayne State University, Detroit, MI*
- ThOC am 10:10 **Assembly and Conformational Properties of DNA- and RNA-Protein Complexes Studied by Native T-Wave Ion Mobility Mass Spectrometry;** Frank Sobott; *CeProMa, University of Antwerp, Antwerp, Belgium*

**8:30 – 10:30 AM, THURSDAY MORNING
METABOLOMICS: BIOINFORMATICS AND
METABOLITE IDENTIFICATION**

**Gary Siuzdak, presiding
Room 155**

- ThOD am 08:30 **metaXCMS - Software for Second-Order Analysis of Untargeted Metabolomics Data;** Ralf Tautenhahn; Gary J Patti; Gary Siuzdak; *The Scripps Research Institute, La Jolla, CA*
- ThOD am 08:50 **Identification of Unknown Metabolites by Accurate Mass GC-TOF MS – Based Metabolomics;** Sangeeta Kumari²; Doug Stevens¹; Tobias Kind³; Oliver Fiehn⁴; ¹WATERS *The Science of What's Possible.™, Milford, MA*; ²Metabolomics Fiehn Lab, Genome centre, UC Davis, Davis, CA; ³UC Davis - Metabolomics, Davis, CA; ⁴UC Davis, Davis, CA
- ThOD am 09:10 **A Rigorous Probabilistic Approach to the Modeling of LC-MS Metabolomic Data;** Andreas Ipsen; Elizabeth J Want; Timothy Ebbels; *Imperial College London, London, UK*
- ThOD am 09:30 **New Automated Software for Biomarker Discovery with High Resolution LC-MS Data;** Serhiy Hnatyshyn²; Michael Reily²; Petia Shipkova; Thomas McClure¹; Jules Phillips¹; Mark Sanders¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Bristol Myers Squibb, Princeton, NJ

- ThOD am 09:50 **Robotized Video-Mass Scope for Direct and Live Single-cell Molecular Exploration;** Tsutomu Masujima¹; Naohiro Tsuyama¹; Hajime Mizuno¹; Takanori Harada¹; Iwao Sakane²; ¹Hiroshima Univ. BioMed., Hiroshima, Japan; ²ITO EN Co. Ltd., Makinohara, Japan

- ThOD am 10:10 **Impact of Storage and Handling Conditions on Metabolites in a Human Plasma Standard Reference Material;** Gauthier Eppe¹; Nathan G. Dodder²; Katrice A. Lippa²; Karen W. Phinney²; Michele M. Schantz²; ¹Liege University, Liège, Belgium; ²NIST, Gaithersburg, MD

**8:30 – 10:30 AM, THURSDAY MORNING
AUTOMATED AND POST-ACQUISITION SOFTWARE
TOOLS FOR XENOBIOTIC METABOLITES**

**Jimmy Flarakos, presiding
Room: Hall 2**

- ThOE am 08:30 **Identification of Metabolites from Maropitant Using a Dual-Cell Linear Ion Trap and Mass Frontier Software;** Rose Herbold¹; Yingying Huang¹; David Nakamura²; ¹Thermo Fisher Scientific, San Jose, CA; ²Elan Pharmaceuticals, South San Francisco, CA
- ThOE am 08:50 **Fast Oxidative Metabolite Identification Using Polarity Switching of Intensity-Dependent MS/MS Spectral Acquisition and Post-Acquisition Data-Mining on an Improved Q-TRAP Instrument;** Ming Yao; Mingshe Zhu; *Bristol-Myers Squibb, Princeton, NJ*
- ThOE am 09:10 **MeTABOOLite Identification from Trap to ToF; Automated Software Tools to Get All the Answers You Need;** Gary Impey²; Tanya Gamble¹; Hesham Ghobarah²; Mark M. Garner²; J.C. Yves Leblanc¹; ¹AB SCIEX, Concord, ON, Canada; ²AB/ SCIEX, Concord, ON
- ThOE am 09:30 **Metabolite Detection and Identification Using Fragment Ion Search in Conjunction with Automated Fragment Prediction;** Juraj Lutisan¹; Yingying Huang²; Alexej Nikiforov³; Milos Suchy¹; Robert Mistrik¹; ¹HighChem, Ltd., Bratislava, Slovakia; ²Thermo Fisher Scientific, San Jose, CA; ³University of Vienna, Vienna, Austria
- ThOE am 09:50 **Positive Negative Switching on a QTOF: Application to Drug Metabolite Identification and Metabolomics;** William Fitch¹; Lester Taylor²; Kenneth Imatani²; ¹Stanford University, Palo Alto, CA; ²Agilent Technologies, Santa Clara, CA
- ThOE am 10:10 **Screening Foods for Unknown Chemical Contaminants by Non-Targeted LC/MSⁿ Analysis;** Timothy R. Croley¹; Kevin D. White¹; Jon Wong¹; John H. Callahan¹; Steve Musser¹; Margaret Antler²; Vitaly Lashin²; Graham A. McGibbon²; ¹US FDA, College Park, MD; ²ACD/Labs, Toronto, ON

**8:30 – 10:30 AM, THURSDAY MORNING
DRIED BLOOD SPOT ANALYSIS**

**Fabio Garofolo, presiding
Room: Hall 3**

- ThOF am 08:30 **Implementation of a Microfluidic LC Device for Dried Blood Spot Analysis – Driving Down the Limit of Detection;** Christopher A. Evans¹; Chester L Bowen¹; Jonathan Kehler¹; Rob Plumb²; Paul Rainville²; ¹GlaxoSmithKline, King of Prussia, PA; ²Waters, Milford, MA

ThOF am 08:50 **Application of Automated Serial Blood Sampling in Mice and Dried Blood Spot Technique Using LC-MS/MS for Pharmacokinetic Studies;** Roger Pham; *Amgen, Inc., Thousand Oaks, CA*

ThOF am 09:10 **A uHPLC-MS/MS Assay for the Analysis of Omeprazole in Rat Blood Using Dried Blood Spots;** Heidi Snapp; Guowen Liu; Qin Ji; Mark E. Arnold; *Bristol-Myers Squibb Co., Princeton, NJ*

ThOF am 09:30 **Liquid Extraction Surface Analysis (LESA) of Dried Blood Spot Cards via Chip-Based Nanoelectrospray for Drug and Drug Metabolite Monitoring Studies;** Christopher Alpha¹; Daniel Eikel¹; Jason Vega¹; Jack D. Henion²; Simon J. Prosser¹; ¹*Advion BioSystems, Inc., Ithaca, NY;* ²*Advion BioSciences, Inc, Ithaca, NY*

ThOF am 09:50 **Direct Quantitative Bioanalysis of Drugs in Dried Blood Spot Samples;** Paul Abu-Rabie¹; Neil Spooner¹; Matthias Loppacher²; ¹*GlaxoSmithKline R&D Ltd, Ware, UK;* ²*Camag, Muttenz, Switzerland*

ThOF am 10:10 **Quantitative Analysis of Dried Blood Spots by DART (Direct Analysis in Real Time) /MS/MS without Sample Preparation;** Justin Gordon¹; Elizabeth Crawford²; Jing-Tao Wu¹; Brian D. Musselman²; Ming-xiang Liao¹; Bei-Ching Chuang¹; Cindy Xia¹; David Ho³; Lily Li³; Shaoxia Yu¹; ¹*Millennium Pharmaceuticals, Inc., Cambridge, MA;* ²*IonSense, Inc., Saugus, MA;* ³*TandemLabs, Woburn, MA*

**8:30 – 10:30 AM, THURSDAY MORNING
MS AND CELLULAR PATHWAYS
Ileana Cristea, presiding
Room: Hall 4**

ThOG am 08:30 **Pathway Analysis and Characterization of Novel Downstream Effectors of the mTORC1/S6K Signaling Axis by Quantitative Phosphoproteomics;** Yonghao Yu; Sang-Oh Yoon; Qian Yang; Xiaoju Max Ma; Judit Villen; John Blenis; Steven P. Gygi; *Harvard Medical School/Department of Cell Biology, Boston, MA*

ThOG am 08:50 **Pathway Analysis Reveals Apoptosis as a Regulator of Breast Cancer Induced Myeloid-Derived Suppressor Cells;** Olesya Chornoguz¹; Lydia Grmai¹; Pratima Sinha¹; Konstantin Artemenko³; Roman Zubarev²; Suzanne Ostrand-Rosenberg¹; ¹*University of Maryland Baltimore County, Baltimore, MD;* ²*Karolinska Institutet, Stockholm, Sweden;* ³*Uppsala University, Uppsala, Sweden*

ThOG am 09:10 **Functional and Mass Spectrometric Analysis of Histone Deacetylase 5 (HDAC5) Phosphorylation and Protein-Protein Interactions;** Fang Yu; Todd M. Greco; Amanda J. Guise; Ileana M. Cristea; *Princeton University, Princeton, NJ*

ThOG am 09:30 **A Targeted Protein-Protein “Interact-ome” of Components in the Insulin Signaling Pathway in Drosophila and Compared to Human Cancer Cells;** John M Asara^{1,2}; Meghana Kulkarni²; Xuemei Yang¹; Adam Friedman²; Norbert Perrimon²; Jeffrey Engelman³; ¹*Beth Israel Deaconess Medical Center, Boston, MA;* ²*Harvard Medical School, Boston, MA;* ³*Massachusetts General Hospital, Charlestown, MA*

ThOG am 09:50 **Time-Resolved Proteomic and Genomic Studies Reveal that Replication Fork Progression is Remarkably Uniform Throughout the Yeast Genome;** Matthew Sekedat¹; David Fenyó¹; Richard Rogers²; Alan Tackett²; John Aitchison²; Brian Chait¹; ¹*The Rockefeller University, New York, NY;* ²*Institute for Systems Biolog, Seattle, WA;* ³*UAMS Biochemistry & Molecular Biology, Little Rock, AR*

ThOG am 10:10 **Quantitative Phosphoproteomics Identifies Transient Signaling in the FAK-ERK Axis as a Novel Molecular Determinant of Embryonic Stem Cell Differentiation;** Yu Lu^{1,2}; Dita Mayerova³; Scott B. Ficarro¹; Yi Zhang¹; Manor Askenazi¹; Jignesh R. Parikh¹; C. John Luckey³; Jarrod A. Marto^{1,2}; ¹*Dana-Farber Cancer Institute, Boston, MA;* ²*Harvard Medical School, Boston, MA;* ³*Brigham and Women's Hospital, Boston, MA*

**10:30 AM – 2:30 PM, THURSDAY
POSTER SESSION
Exhibit Hall ABCDE**

**2:30 – 4:30 PM, THURSDAY AFTERNOON
FUNDAMENTALS: ION-SURFACE INTERACTIONS
AND PREPARATIVE MS
Guido Verbeck, presiding
Room: Ballroom HJ**

ThOA pm 2:30 **Soft Landing of Gas-Phase Ions: An Overview;** Frantisek Turecek; *University of Washington, Seattle, WA*

ThOA pm 2:50 **Preparation of Monolayer Catalytic Materials on Surfaces in Vacuum Using Ion Soft Landing Method;** Wen-Ping Peng¹; Grant Johnson²; Peng Wang²; Omar Hadjar²; Julia Laskin²; R. Graham Cooks³; ¹*National Dong Hwa University, Shoufeng, Hualien, Taiwan;* ²*Pacific Northwest National Laboratory, Richland, WA;* ³*Purdue University, West Lafayette, IN*

ThOA pm 3:10 **Surface Ion Modification and Characterization of Muscovite by Laser Ablated Carbon and Transition Metal Clusters Using Soft Landing Ion Mobility;** Stephen Davila; William Hoffmann; David Birdwell; Guido F. Verbeck; *University of North Texas, Denton, TX*

ThOA pm 3:30 **Fundamental Studies of Molecular Depth Profiling and 3-D Imaging with ToF-SIMS and Cluster Ions;** Caiyan Lu; Nick Winograd; *Penn State University, University Park, PA*

ThOA pm 3:50 **Computer Simulation of Depth Profiling in Secondary Ion Mass Spectrometry (SIMS);** Barbara J. Garrison; *Penn State University, University Park, PA*

ThOA pm 4:10 **Determinants of Surface-Induced Dissociation and Collision-Induced Dissociation Behavior in Noncovalent Protein Ensembles;** Eric D. Dodds; Anne E. Blackwell; Christopher M. Jones; Vicki H. Wysocki; *University of Arizona, Tucson, AZ*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
BIOMOLECULAR STRUCTURE
Mark Chance, presiding
Room: Ballroom ACE**

ThOB pm 2:30 **Structural Analysis of Macro-Molecular Protein Complexes Using Chemical Cross-Linking and Mass Spectrometry;** Franz

	<u>Herzog</u> ¹ ; Alexander Leitner ¹ ; Thomas Walzthöni ¹ ; Friedrich Förster ² ; Roman Jakob ³ ; Timm Maier ³ ; Martin Beck ⁴ ; Ruedi Aebersold ¹ ; ¹ <i>Swiss Institute of Technology, IMSB, Zurich, Switzerland</i> ; ² <i>Max Planck Institut, Munich, Germany</i> ; ³ <i>Swiss Institute of Technology, IMB, Zurich, Switzerland</i> ; ⁴ <i>European Molecular Biology Laboratory, Heidelberg, Germany</i>	Jeremy Balsbaugh; Jeffrey Shabanowitz; Donald F. Hunt; <i>University of Virginia, Charlottesville, VA</i>
ThOB pm 2:50	The Gating Mechanism of a Potassium Channel Probed by Structural Mass Spectrometry ; <u>Sayan Gupta</u> ¹ ; Rhijuta D'Mello ¹ ; Vassiliy N. Bavro ² ; Stephen J. Tucker ² ; Catherine Vénien-Bryan ² ; Mark R. Chance ¹ ; ¹ <i>Case Western Reserve University, Upton, NY</i> ; ² <i>University of Oxford, Oxford, UK</i>	ThOC pm 3:30 Fragmentation Chemistry of Phosphorylated and De-Phosphorylated, Protonated Peptides ; <u>Benjamin J. Bythell</u> ² ; Sam Molesworth ¹ ; Sarah Young ¹ ; Christopher L. Hendrickson ³ ; Alan G. Marshall ³ ; Michael J. Van Stipdonk ¹ ; Bela Paizs ² ; ¹ <i>Wichita State University, Wichita, KS</i> ; ² <i>DKFZ, Heidelberg, Heidelberg, Germany</i> ; ³ <i>National High Magnetic Field Laboratory, Tallahassee, FL</i>
ThOB pm 3:10	Exploring the Mechanisms of Protein Folding and Subunit Assembly by Pulsed Oxidative Labeling and ESI-MS ; <u>Bradley B. Stocks</u> ; Lars Konermann; <i>Univ of Western Ontario, London, Canada</i>	ThOC pm 3:50 Insights into Histidine-Containing Peptide b₂+Ion Formation and Structure Using IRMPD Spectroscopy and Fragment Ion Hydrogen-Deuterium Exchange ; <u>Ashley Gucinski</u> ¹ ; Julia Chamot-Rooke ² ; Arpad Somogyi ¹ ; Brittany R. Perkins ¹ ; Sung Hwan Yoon ¹ ; Vicki H. Wysocki ¹ ; ¹ <i>The University of Arizona, Tucson, AZ</i> ; ² <i>CNRS, Palaiseau, France</i>
ThOB pm 3:30	Structural Similarities and Differences of Human Apolipoprotein E2, E3, and E4, Determined by Chemical Footprinting and Mass Spectrometry ; <u>Brian C. Gau</u> ¹ ; Richard Yu-Cheng Huang ¹ ; Kanchan Garai ² ; Carl Frieden ² ; Michael L. Gross ¹ ; ¹ <i>Washington University, St. Louis, MO</i> ; ² <i>Washington University School of Medicine, St. Louis, MO</i>	ThOC pm 4:10 Cyclization and Rearrangement Reactions of a_n Ions of Protonated Peptides ; <u>Bela Paizs</u> ¹ ; Benjamin Bythell ³ ; Philippe Maitre ² ; ¹ <i>DKFZ, Heidelberg, Heidelberg, Germany</i> ; ² <i>Laboratoire de Chimie Physiq, Orsay, France</i> ; ³ <i>NHMFL/FSU, Tallahassee, FL</i>
ThOB pm 3:50	Analysis of a 670 kDa Multiprotein Complex by Cross-Linking and Mass Spectrometry ; <u>Zhuo Chen</u> ¹ ; Lutz Fischer ¹ ; Anass Jawhari ² ; Claudia Buchen ² ; Salman Tahir ¹ ; Tomislav Kamenski ² ; Morten Rasmussen ¹ ; Laurent Larivière ² ; Jimi-Carlo Bukowski-Wills ^{1,3} ; Michael Nilges ⁴ ; Patrick Cramer ² ; Juri Rappsilber ¹ ; ¹ <i>Wellcome Trust Centre for Cell Biology, Edinburgh, UK</i> ; ² <i>Ludwig-Maximilians-Universität, Munich, Germany</i> ; ³ <i>Centre for Systems Biology, Edinburgh, UK</i> ; ⁴ <i>Institut Pasteur, Paris, France</i>	<p>2:30 – 4:30 PM, THURSDAY AFTERNOON NOVEL DEVELOPMENTS IN INSTRUMENTATION Zheng Ouyang, presiding Room 155</p>
ThOB pm 4:10	A Stable Isotope Labeling Strategy for Protein-Ligand Binding Analysis in Multi-Component Protein Mixtures ; <u>Patrick D. Dearmond</u> ; Graham M. West; Michael C. Fitzgerald; <i>Duke University, Durham, NC</i>	ThOD pm 2:30 Elemental Analysis by Distance-of-Flight MS and Array Detection ; <u>Christie G. Enke</u> ¹ ; Steven Ray ² ; Alexander W. Graham ² ; Gary M. Hieftje ² ; David W. Koppenaal ³ ; Charles J. Barinaga ³ ; ¹ <i>University of New Mexico, Albuquerque, NM</i> ; ² <i>Indiana University, Bloomington, IN</i> ; ³ <i>Pacific Northwest Nat'l Laboratory, Richland, WA</i>
		ThOD pm 2:50 Discontinuous Atmospheric Pressure Interface for Mass Spectrometry Instrumentation: Theory, Development and Application ; <u>Wei Xu</u> ; Matthew Kirleis; Nickolas Charipar; Yu Xia; William Chappell; Zheng Ouyang; <i>Purdue University, West Lafayette, IN</i>
		ThOD pm 3:10 Time-Resolved Liquid Jet Desorption Electrospray Ionization-Mass Spectrometry (DESI-MS) ; <u>Zhixin Miao</u> ; Hao Chen; <i>Ohio University, Athens, OH</i>
		ThOD pm 3:30 Development of a Portable Mass Spectrometer for Operation at 1 Torr ; Glen Jackson; <i>Ohio University, Athens, OH</i>
		ThOD pm 3:50 Transmission Geometry Profiling / Imaging Mass Spectrometry with Sub-Cellular Resolution ; <u>Andrey I Zavalin</u> ; Richard M. Caprioli; <i>Vanderbilt Univ Sch of Med, Nashville, TN</i>
		ThOD pm 4:10 Sub-Attomole Detection Limits Using Enhanced Ion-Funnel Technology on a Triple Quadrupole Mass Spectrometer ; <u>George Stafford</u> ^{1,2} ; Tim Schlabach ¹ ; Anabel Fandino ¹ ; ¹ <i>Agilent Technologies, Santa Clara, CA</i>
	<p>2:30 – 4:30 PM, THURSDAY AFTERNOON PEPTIDE ION FRAGMENTATION Michael Van Stipdonk, presiding Room: Ballroom BDF</p>	
ThOC pm 2:30	Threshold Collision Induced Dissociation Measurements of Protonated Peptides ; <u>Peter B. Armentrout</u> ² ; Abhigya Mookherjee ² ; Stephanie Curtice ¹ ; Drew Heide ¹ ; Michael J. Van Stipdonk ¹ ; ¹ <i>Wichita State University, Wichita, KS</i> ; ² <i>University of Utah, Salt Lake City, UT</i>	
ThOC pm 2:50	Dependence of Head-to-Tail Cyclization on Primary Structure of Peptides in Collision-Induced Dissociation: The Case of QWFGML b₆ ; <u>Xian Chen</u> ¹ ; Jeffrey Steill ² ; Jos Oomens ^{2,3} ; Nicolas Polfer ¹ ; ¹ <i>University of Florida, Gainesville, FL</i> ; ² <i>FOM Rijnhuizen, Nieuwegein, Netherlands</i> ; ³ <i>University of Amsterdam, Amsterdam, Netherlands</i>	
ThOC pm 3:10	Exploration and Enhancement of Enzymatic and Chemical Peptide Modification Strategies for Optimizing Fragmentation by Electron Transfer Dissociation ; <u>A. Michelle English</u> ;	

**2:30 – 4:30 PM, THURSDAY AFTERNOON
QUANTITATION OF ENDOGENOUS ANALYTES IN
REGULATED BIOANALYSIS**

**Rick Steenwyk, presiding
Room: Hall 2**

- ThOE pm 2:30 **Challenges and Key Considerations for Mass Spectrometry-Based Quantitation of Biomarkers in the Clinical Setting;** Joe Lin; Eddie Takahashi; Rick Steenwyk; *Pfizer, Groton, CT*
- ThOE pm 2:50 **Parallelism and Response Factor Considerations for LC/MS Biomarker Assay Validation Using Surrogate Matrix and Surrogate Analyte Approaches;** Barry R. Jones²; Gary Schultz¹; Steve Lowes³; James A Eckstein⁴; Barry Lutzke⁵; Bradley L. Ackermann⁵; ¹*Advion BioServices, Inc., Ithaca, NY*; ²*Advion Biosciences, Ithaca, NY*; ³*Advion BioSciences, Inc., Ithaca, NY*; ⁴*Eli Lilly, Greenfield, IN*; ⁵*Eli Lilly & Company, Indianapolis, IN*
- ThOE pm 3:10 **Ultra-Low Detection Limits of Quinolinic Acid and Kynurenine via Gas Chromatography-Tandem Mass Spectrometry;** Francesca Notarangelo²; David Graham³; Robert Schwarcz²; Anthony Macherone¹; ¹*Agilent Technologies, Wilmington, DE*; ²*Maryland Psychiatric Research Center, Baltimore, Maryland*; ³*Johns Hopkins School of Medicine, Baltimore, Maryland*
- ThOE pm 3:30 **Application of a Conjugate Matrix and UHPLC-MS/MS Detection for the Determination of Eicosapentaenoic and Docosahexaenoic Acid in Human Plasma;** Chester L Bowen; Christopher A. Evans; Jonathan Kehler; *GlaxoSmithKline, King of Prussia, PA*
- ThOE pm 3:50 **Chemometric Optimization of LC-MS/MS Method for Quantification of the Biomarker Leukotrine B4 for Support of Gene-to-Clinic Drug Discovery Approach;** Margrét Thorsteinsdóttir¹; Baldur Bragi Sigurdsson²; Gisli Bragason²; Ólafur Magnússon³; ¹*University of Iceland, Reykjavik, Iceland*; ²*ArcticMass, Reykjavik, Iceland*; ³*deCODE genetics, Reykjavik, Iceland*
- ThOE pm 4:10 **Application of 2-D Nanospray Techniques for Improved Sensitivity in the Analysis of Adrenal Steroids in Plasma;** Kenneth Lewis¹; Thurman Allsup¹; Gary Valaskovic²; ¹*OpAns, LLC, Durham, NC*; ²*New Objective, Inc., Woburn, MA*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
LASER/SURFACE DESORPTION TECHNIQUES FOR
ADME**

**Shuguang Ma, presiding
Room: Hall 3**

- ThOF pm 2:30 **Mass Spectrometry of Organic Molecules and Laser-Induced Acoustic Desorption: Applications, Mechanisms and Perspectives;** Alexander Zinovev; Igor Veryovkin; Michael Pellin; *Argonne National Laboratory, Argonne, IL*
- ThOF pm 2:50 **Liquid Extraction Surface Analysis (LESA) Combined with nESI-MS as a Novel Tool in Early ADME Studies of Drug Candidates;** Daniel Eikel; Christopher Alpha; Geoffrey S. Rule; Simon J. Prosser; Jack D. Henion; *Advion BioSystems, Inc., Ithaca, NY*

ThOF pm 3:10 **LDTD384-MS/MS for *in vitro* Assays : Different Buffer Environment;** Patrice Tremblay¹; Pierre Picard¹; Serge Auger¹; Grégory Blachon²; ¹*Phytronix Technologies, Quebec, Canada*; ²*Université Laval, Québec, QC*

ThOF pm 3:30 **High-Sensitivity MALDI-MRM-MS Imaging Applied to Determine the Penetration of Multiple Fluoroquinolone Drugs into Tuberculosis Lung Granulomas;** Brendan Prideaux¹; Dieter Staab¹; Anne Goh²; Veronique Dartois²; Peiting Zheng²; Hui Qing Ang²; Maxime Herve²; Clifton E Barry³; Laura Via³; Danielle Weiner³; Daniel Schimel³; Emmanuel K Dayao³; Markus Stoeckli¹; ¹*Novartis Institutes for BioMedical Research, Basel, Switzerland*; ²*Novartis Institute for Tropical Diseases, Singapore, Singapore*; ³*National Institutes of Health, Bethesda, MD*

ThOF pm 3:50 **MALDI Imaging of Distribution of Xanthohumol and Its Metabolites in Rat Tissues;** Henry Y. Shion³; Dejan Nikolic¹; Birgit Dietz²; Guido Pauli²; Brian Wright¹; Ghenet Hagos²; Daniel Lantvit²; Alan L Millar³; John P. Shockcor³; Richard B. van Breemen¹; ¹*University of Illinois College of Pharmacy, Chicago, IL*; ²*University of Illinois, UIC/NIH Botanical Center, Chicago, IL*; ³*Waters Corp., Milford, MA*

ThOF pm 4:10 **Chemoslective Screening for Homocysteine and Related Endogenous Sulfhydryl Biomarkers in Blood and Urine Using Surface-Enhanced Transmission Mode Desorption Electrospray Ionization;** Joe Chipuk; Jennifer Brodbelt; *The University of Texas, Austin, TX*

**2:30 – 4:30 PM, THURSDAY AFTERNOON
MS OF MEMBRANE PROTEINS
Christine Wu, presiding
Room: Hall 4**

- ThOG pm 2:30 **Quantitatively Probing Cellular Membrane Proteome Dynamics Using Membrane-Impermeable Chemical Probes and Proteomics Analysis;** Haizhen Zhang; Wei-Jun Qian; Tao Liu; Roslyn N. Brown; Matthew E. Monroe; Samuel O. Purvine; Ronald J. Moore; Liang Shi; Margaret F. Romine; James K. Fredrickson; William B. Chrisler; Steven H. Wiley; Ljiljana Paša-Tolić; Richard D. Smith; Mary S. Lipton; *PNNL, Richland, WA*
- ThOG pm 2:50 **Glycan Determination on Human Embryonic Stem Cell Membrane Proteins;** Hyun Joo An¹; Phung Gip²; Jaehan Kim¹; Shuai Wu¹; David Schaffer²; Carolyn Bertozzi²; Carlito Lebrilla¹; ¹*University of California, Davis, Davis, CA*; ²*University of California, Berkeley, Berkeley, CA*
- ThOG pm 3:10 **A Multiplexed SRM Method to Monitor Membrane Protein Knockdown Using Viral Delivery of shRNA in Neuro 2A Cells;** Santiago E. Farias²; Amy Lasek¹; Paula L. Hoffman²; Christine C. Wu²; ¹*Ernest Gallo Clinic and Research Center, UCSF, San Francisco, CA*; ²*University of Colorado School of Medicine, Aurora, CO*
- ThOG pm 3:30 **Using MALDI-TOF-MS to Probe Protein-Ligand Interactions of G-Protein Coupled Receptors Incorporated into Stable Polymerized Planar Supported Lipid Bilayers;** Erin Johnson; James R. Joubert; S. Scott

Saavedra; Vicki H. Wysocki; *University of Arizona, Tucson, AZ*

ThOG pm 3:50 **Phospholipid Bilayer Nanodiscs as a Platform for Integral Membrane Protein Analysis by Hydrogen Exchange Mass Spectrometry;** Chris Morgan¹; Christine Hebling²; Kasper Rand¹; James Jorgenson²; Darrel Stafford²; John R. Engen¹; ¹*Northeastern University, Boston, MA*; ²*University of North Carolina, Chapel Hill, NC*

ThOG pm 4:10 **V-Type ATPases: What Can We Learn from Mass Spectrometry?** Min Zhou¹; Nelson Barrera²; Nina Morgner¹; Carol Robinson¹; ¹*University of Oxford, Oxford, UK*; ²*University of Santiago de Chile, Santiago, Chile*

**4:45 – 5:30 PM, THURSDAY
PLENARY LECTURE
Hall 4**



Svante Pääbo

Max Planck Institute for Evolutionary Anthropology

**5:30 - 6:00 PM, THURSDAY
FAREWELL TOAST
Hall 4**