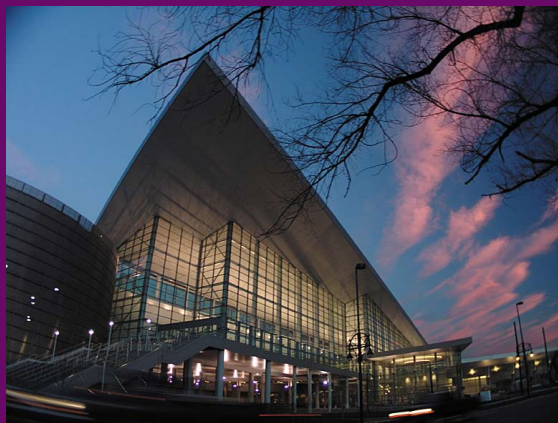


# 56th ASMS Conference on Mass Spectrometry and Allied Topics

**JUNE 1 – 5, 2008  
DENVER, COLORADO**





**56<sup>TH</sup> ASMS CONFERENCE ON MASS SPECTROMETRY**  
**JUNE 1 - 5, 2008 • SHORT COURSES: MAY 31 - JUNE 1, 2008**  
**Colorado Convention Center, Denver, Colorado**



**LOCATION.** The conference and short courses will be held at the Colorado Convention Center, 700 14<sup>th</sup> Street, Denver, Colorado. All oral sessions, poster sessions, and exhibit booths will be located in the Convention Center. Corporate Member hospitality suites will be in the Sheraton (formerly Adams Mark) Hotel.

**REGISTRATION.** Conference on-site registration will open 2:00 pm, Saturday, May 31 in the convention center. There is no on-site registration for short courses.

For more information: [www.asms.org](http://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](mailto:office@asms.org) [www.asms.org](http://www.asms.org)



**Vice President for Programs: Gary L. Glish**

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## CONFERENCE PROGRAM OVERVIEW

SAT	9:00 am - 4:30 pm	<b>SHORT COURSES</b>
	2:00 - 5:00 pm	<b>REGISTRATION</b>
SUNDAY	9:00 am - 4:30 pm	<b>SHORT COURSES</b>
	10:00 am - 8:00 pm	<b>REGISTRATION</b>
	5:00 - 6:30 pm	<b>TUTORIAL LECTURES, Korbel Ballroom 2-3</b> <ul style="list-style-type: none"> <li>• <b>Julia Laskin</b> (<i>Pacific Northwest National Laboratory</i>) Interactions of Ions with Surfaces</li> <li>• <b>R. Graham Cooks</b> (<i>Purdue University</i>) Metastable Ions</li> </ul>
	6:45 - 7:45 pm	<b>OPENING and PLENARY LECTURE: Marc Abrahams</b> ( <i>Annals of Improbable Research</i> ) Improbable Research - Spectrometric and Otherwise, <i>Wells Fargo Theatre</i>
	7:45 - 9:30 pm	<b>RECEPTION IN THE EXHIBIT HALL</b>
MONDAY	8:30 - 10:30 am	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• MOA: Label Free Quantitation of Proteins, <i>Wells Fargo Theatre</i></li> <li>• MOB: Fundamentals of Ion/Ion Reactions, <i>Korbel Ballroom 1</i></li> <li>• MOC: Developments in Ion Mobility Instrumentation, Theory, and Applications, <i>Korbel 2-3</i></li> <li>• MOD: Challenges in Elemental Analysis using Mass Spectrometry, <i>Korbel Ballroom 4</i></li> <li>• MOE: Discovering Peptide Biomarkers, <i>Four Seasons Ballroom 1-2</i></li> <li>• MOF: Endogenous Metabolite Profiling, <i>Four Seasons Ballroom 3-4</i></li> <li>• MOG: MS Characterization of Carbohydrates, <i>Rooms 601-607</i></li> </ul>
	10:30 am - 2:30 pm	<b>POSTER SESSION AND EXHIBITS</b>
	2:30 - 4:30 pm	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• MOA: Advances in Top-Down Proteomics, <i>Wells Fargo Theatre</i></li> <li>• MOB: Spectroscopy of Gaseous Ions, <i>Korbel Ballroom 1</i></li> <li>• MOC: Developments in Ion Trapping Instrumentation, <i>Korbel Ballroom 2-3</i></li> <li>• MOD: Emerging Mass Spectrometry Techniques in Environmental Analysis, <i>Korbel Ballroom 4</i></li> <li>• MOE: The Paradigm Shift in Clinical Diagnostics using Mass Spectrometry, <i>Four Seasons 1-2</i></li> <li>• MOF: Quantitation of Drug Metabolites, <i>Four Seasons Ballroom 3-4</i></li> <li>• MOG: Characterizing Protein-Ligand Interactions with Mass Spectrometry, <i>Rooms 601-607</i></li> </ul>
	4:45 - 5:30 pm	<b>AWARD LECTURE: Recipient of the Award for a Distinguished Contribution in Mass Spectrometry;</b> <i>Wells Fargo Theatre</i>
	5:45 - 7:00 pm	<b>WORKSHOPS</b>
	6:30 - 11:00pm	<b>CORPORATE HOSPITALITY SUITES, Sheraton Hotel</b>
TUESDAY	8:30 - 10:30 am	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA: Protein Quantitation using Labeling, <i>Wells Fargo Theatre</i></li> <li>• TOB: Structure and Energetics of Metal Ions Reacting with Biomolecules, <i>Korbel Ballroom 1</i></li> <li>• TOC: Novel Developments in Mass Spectrometry Instrumentation, <i>Korbel Ballroom 2-3</i></li> <li>• TOD: The Role of Mass Spectrometry in the Petroleum Field, <i>Korbel Ballroom 4</i></li> <li>• TOE: Disease Protein Biomarker Discovery by Mass Spectrometry, <i>Four Seasons Ballroom 1-2</i></li> <li>• TOF: Identification of Reactive Metabolites in Drug Discovery: Significance of Mass Spectrometry towards Detection, <i>Four Seasons Ballroom 3-4</i></li> <li>• TOG: Biological Applications of Chemical Cross Linking, <i>Rooms 601-607</i></li> </ul>
	10:30 am - 2:30 pm	<b>POSTER SESSION AND EXHIBITS</b>
	2:30 - 4:30 pm	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• TOA: The Role of Mass Spectrometry in Understanding Cellular Pathways, <i>Wells Fargo Theatre</i></li> <li>• TOB: Fundamentals of Ion/Surface Interactions, <i>Korbel Ballroom 1</i></li> <li>• TOC: Developments in TOF, <i>Korbel Ballroom 2-3</i></li> <li>• TOD: Pharmaceutical Drugs as Environmental Pollutants, <i>Korbel Ballroom 4</i></li> <li>• TOE: H/D Exchange and Protein Folding, <i>Four Season 1-2</i></li> <li>• TOF: Biomarker Applications in the Clinical Setting, <i>Four Seasons Ballroom 3-4</i></li> <li>• TOG: Advances in the Characterization of Glycoproteins, <i>Rooms 601-607</i></li> </ul>
	4:45 - 5:30 pm	<b>AWARD LECTURE: Recipient of the Biemann Medal;</b> <i>Wells Fargo Theatre</i>
	5:45 - 7:00 pm	<b>WORKSHOPS</b>
	6:30 - 11:00pm	<b>CORPORATE HOSPITALITY SUITES, Sheraton Hotel</b>

## CONFERENCE PROGRAM OVERVIEW

<b>WEDNESDAY</b>	8:30 - 10:30 am	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• WOA: New Approaches to Metabolomics, <i>Wells Fargo Theatre</i></li> <li>• WOB: Fundamentals and Applications of Ion Activation: Alternatives to CID, <i>Korbel Ballroom 1</i></li> <li>• WOC: New Developments in Hybrid MS-MS Instruments, <i>Korbel Ballroom 2-3</i></li> <li>• WOD: Imaging of Polymers/Materials and Surfaces, <i>Korbel Ballroom 4</i></li> <li>• WOE: LC-MS Techniques for Discovering Biomarkers of Toxicity and Efficacy, <i>Four Seasons Ballroom 1-2</i></li> <li>• WOF: Protein Gas Phase Structure, <i>Four Seasons Ballroom 3-4</i></li> <li>• WOG: Applications of Ion Mobility Spectrometry, <i>Rooms 601-607</i></li> </ul>
	10:30 am - 2:30 pm	<b>POSTER SESSION AND EXHIBITS</b>
	2:30 - 4:30 pm	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• WOA: Characterization of Membrane Proteins, <i>Wells Fargo Theatre</i></li> <li>• WOB: Understanding Peptide Fragmentation: Theory and Experiment, <i>Korbel Ballroom 1</i></li> <li>• WOC: Developments and Application of APPI, <i>Korbel Ballroom 2-3</i></li> <li>• WOD: Mass Spectrometry in Biodefense, <i>Korbel Ballroom 4</i></li> <li>• WOE: Lipid Analysis by Mass Spectrometry, <i>Four Seasons Ballroom 1-2</i></li> <li>• WOF: Metabolites and Degradation Products of Environmental Contaminants, <i>Four Seasons Ballroom 3-4</i></li> <li>• WOG: Imaging Mass Spectrometry for Small Molecule Applications, <i>Rooms 601-607</i></li> </ul>
	4:45 - 5:30 pm	<b>ASMS BUSINESS MEETING</b>
	5:45 - 7:00 pm	<b>WORKSHOPS</b>
	6:30 - 11:00 pm	<b>CORPORATE HOSPITALITY SUITES</b>

<b>THURSDAY</b>	8:30 - 10:30 am	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• ThOA: Novel Applications of Bioinformatics, <i>Wells Fargo Theatre</i></li> <li>• ThOB: Metal Ion Activated Dissociation, <i>Korbel Ballroom 1</i></li> <li>• ThOC: Ion Trap Applications, <i>Korbel Ballroom 2-3</i></li> <li>• ThOD: Structural Biology and Biophysics of Nucleic Acids, <i>Korbel Ballroom 4</i></li> <li>• ThOE: Characterizing Post-Translational Modifications, <i>Four Seasons Ballroom 1-2</i></li> <li>• ThOF: Increasing LC-MS Sample Throughput for Pharmacokinetic Assays, <i>Four Seasons Ballroom 3-4</i></li> <li>• ThOG: Analyte "Fingerprinting" with No Sample Preparation, <i>Rooms 601-607</i></li> </ul>
	10:30 am - 2:30 pm	<b>POSTER SESSION AND EXHIBITS</b>
	2:30 - 4:30 pm	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• ThOA: New Developments in Bioinformatics, <i>Wells Fargo Theatre</i></li> <li>• ThOB: Polymer/Material Ionization and Structural Elucidation, <i>Korbel Ballroom 1</i></li> <li>• ThOC: Developments in Imaging Instrumentation and Methodology, <i>Korbel Ballroom 2-3</i></li> <li>• ThOD: Characterizing DNA, RNA, and Adducts, <i>Korbel Ballroom 4</i></li> <li>• ThOE: Ionization and Characterization of Macromolecules and Complexes, <i>Four Seasons Ballroom 1-2</i></li> <li>• ThOF: Matrix Effects: LC-MS Challenges and Solutions, <i>Four Seasons Ballroom 3-4</i></li> <li>• ThOG: Application of ETD/ECD, <i>Rooms 601-607</i></li> </ul>
	4:45 - 5:30 pm	<b>PLENARY LECTURE: Charlie Bamforth; University of California, Davis</b> The Beauty of Beer: Sublime Science Meets Art and Humanity, <i>Wells Fargo Theatre</i>
	5:45 - 8:00 pm	<b>GALA RECEPTION, Hyatt Regency Hotel</b>

Workshops are organized on topics of special interest with a focus on new technology.  
There is no additional charge for workshops – they are open to all as a forum for discussion.

### MONDAY WORKSHOPS, 5:45 – 7:00 PM

#### The Clinical Mass Spectrometry Space - Who's Driving?

Korbel Ballroom 1

*Clinical Chemistry Interest Group*

Russell Grant and Donald Chace, presiding

Workshop discussions will include the various models employed in the discovery, developmental and clinical utility axis to define the clinical mass spectrometry space. Which research based MS workflows have made the transition to clinical practice and why. The value of MS in evidence based medicine and how to close the communication gap to clinicians. Input will be garnered from academia, industry and manufacturers.

#### New LC-MS Techniques and Strategies for Drug Metabolism

Korbel Ballroom 2-3

*Drug Metabolism and Pharmacokinetics Interest Group*

Ragu Ramanathan and Jonathon Josephs, presiding

Some of the newest high resolution LC-MS techniques and their applications in drug metabolism and pharmacokinetics will be discussed.

#### FTMS: The Perspectives

Korbel Ballroom 4

*FTMS Interest Group; Yury Tsybin, presiding*

What should be the next step in FTMS method and technique development? What are the unique FTMS application areas? How far could we push the mass accuracy? You are welcome to share your vision on these and other FTMS hot topics!

#### Review of the Basics and New Progress in the Field

Four Seasons Ballroom 1-2

*H/D Exchange & Covalent Labeling Interest Group*

John R. Engen and Robert L. Hettich, presiding

This workshop is designed for both newcomers to the field and those who have been in the area for a while. Two mini tutorials covering hydrogen exchange and covalent labeling methods will be given. The latest developments in both areas will also be discussed, including several short presentations and an open Q&A session.

#### Metal Complexes and Clusters: Structure and Reactivity

Four Seasons Ballroom 3-4

*Metal Ions Interest Group; Gary S. Groenewold, presiding*

The workshop will focus on the current state of the art for examining the chemistry of metal coordination complexes and clusters in the gas phase. Discussions will focus on the appeal of investigations of metal species in the gas phase, ion formation approaches, developments in ion structure determination, synergy between vibrational measurements and computational methods. Further topics will include the use of dissociation and condensation reactions for determining quantitative properties and qualitative reactivity behavior.

#### Scientific Record Keeping: Pitfalls and Protocols

Rooms 601-607

Michael Asam, Kenneth Busch and Anthony Craig, presiding

This workshop will endeavor to provide guidance for distinguishing between the types of scientific records that should be retained and records that can be discarded as well as the circumstances that might impact retain/discard decisions. We will also provide some discussion on the differences between authorship and patent inventorship and what can be expected in various venues where record keeping becomes important such as patent interference proceedings, patent or trade secret litigation, and scientific fraud investigations.

### TUESDAY WORKSHOPS, 5:45 – 7:00 PM

#### Key Challenges to Success with Metabolomics

Korbel Ballroom 1

*Metabolomics Interest Group*

Eric Milgram and Anders Nordstrom, presiding

With interest in metabolomics growing rapidly, many organizations have begun to explore the technique, either by implementing the technology in-house or working with companies who specialize in this technology. However, despite an ever growing body of literature on the potential of the technique, there have been no examples where metabolomics has led to a major, novel insight that has been rigorously validated. Rather, there have been many examples where the potential of metabolomics has been "demonstrated" by "independently discovering" a relevant finding that is already known. During this workshop, a panel of scientists who routinely use metabolomics as a means to an end, not as an interesting technology, will be convened to give their perspective on the potential of the technique along with its key challenges. An interactive discussion will follow.

#### Current Practices in Fast and Ultra-Fast Chromatography using Sub-2um Particles

Korbel Ballroom 2-3

*LC-MS and Pharmaceutical Interest Groups; Chris Petucci,*

Wyeth and Carmen Santasania, and Shane Needham, presiding

The recent interest in using sub-2 um particles for HPLC-MS applications in the pharmaceutical industry has led us to sponsor a combined workshop of the Pharmaceutical and LC-MS Related Topics Interest Groups. This workshop will be an open forum to discuss the current applications of sub-2 um particles with HPLC-

MS in the pharmaceutical industry. The advantages, disadvantages, and acceptance of the technology will be discussed.

#### Recent Triumphs in the Development and Applications of Ion Trap Mass Spectrometry

Korbel Ballroom 4

*Ion Trap MS Interest Group; Gavin E. Reid, presiding*

The Ion Trap Mass Spectrometry workshop in 2008 will consist of a number of short informal presentations (3-5 slides each) for graduate students or other young scientists working in ion trap mass spectrometry research areas to briefly describe their single most exciting result for the year. Topics of interest could include the development, modification or miniaturization of novel ion trap instrumentation, or applications demonstrating for example, the highest mass ion that was analyzed, the most sequential stages of ion manipulation, the most innovative ion-molecule, ion-photon, ion-ion reaction, etc.

#### Cascading Reactions in the Gas Phase

Four Seasons Ballroom 1-2

*Fundamentals Interest Group; Ryan Julian, presiding*

This workshop will focus on the ability of mass spectrometry or related techniques to observe and unravel chemistry occurring in multiple-step reactions. Both reactions where multiple rapid rearrangements occur and sequential MS<sup>n</sup> type reactions where intermediates are observable are suitable for discussion. Reactions may involve covalent or noncovalent rearrangements.

**TUESDAY WORKSHOPS CONTINUED, 5:45 – 7:00 PM****Presenting Proteomics Data in Accordance with the 'Paris Guidelines'**

Four Seasons Ballroom 3-4

Kati Medzihradzky and Robert J. Chalkley presiding

This workshop will discuss the "Paris Guidelines" for reporting protein identification, post-translational modifications as well as quantitative proteomics data. Examples for data submission will be given.

**Polymers and Materials**

Rooms 601-607

*Polymer Interest Group*; Mark Arnould, presiding

The workshop will encompass the polymeric materials interest group meeting. The discussion will include topics having to do with the organization of the interest group, suggestions to the society and technical information on polymer and materials mass spectrometry.

**Hydrocarbons and Other Compounds from Petroleum: Are We Ready for Alternative Sources?**

Rooms 702-706

*Hydrocarbon & Chemical Processes Interest Group*

Michael Cheng, presiding

World demand for energy is increasing, particularly liquid transportation fuels, it is necessary to seek out alternative sources. In addition to petroleum, we will discuss the analyses of fuel and intermediates derived from sources such as coal, shale, tar sand, and biomass.

**Flavor, Fragrance and Foodstuff Interest Group Meeting**

Rooms 708-712

Indarpal Singh, presiding

Mass Spec Users Meeting to share challenges and solutions with issues related to quantitation, ionization, matrix effects, ion suppression, ion enhancement, and sampling techniques in the analysis of flavor, fragrance, and food.

**WEDNESDAY WORKSHOPS, 5:45 – 7:00 PM****Signal Suppression in LC-MS Determination of Environmental Contaminants**

Korbel Ballroom 1

*Environmental Applications Interest Group*

Susan Richardson, presiding

Ionization process using electrospray source is susceptible to interference from the matrix. In the majority of cases the signal is suppressed and in some instance it has been enhanced. Environmental samples have complex matrix which can affect the ionization process. As LC-MS based methods for determination of environmental contaminants are becoming more popular, more problems associated with signal suppression have been encountered. In this workshop signal suppression observed in various procedures along with potential solution will be discussed.

**Ion Mobility-Mass Spectrometry: Strategies for Interpreting Structural Information**

Korbel Ballroom 2-3

*Ion Mobility Interest Group*

John McLean, presiding

Attendant with the recent commercial availability of IM-MS instrumentation, in a variety of forms, this workshop will be a forum for discussion of how to calibrate and interpret structural information from IM-MS separations. Different calibration and interpretation strategies are necessary when processing drift tube, differential mobility, and t-wave IM-MS data for structural information. Furthermore, different strategies are best suited for small biological molecules relative to massive protein complexes and nanomaterials. The aim of this workshop is to discuss the merits and challenges of various calibration strategies that are presently used, in an effort to establish more generally accepted procedures.

**Peptide Fragmentation and Sequencing: How to Narrow the Gap?**

Korbel Ballroom 4

Bela Paizs and Michael Van Stipdonk, presiding

*Peptide Fragmentation Interest Group*

The primary goal of gas-phase peptide dissociation studies is to improve the existing fragmentation models implemented in sequencing tools of MS-based proteomics. Currently, the information gap between the peptide fragmentation and sequencing communities is wide. Recent mechanistic insights into peptide fragmentation hardly infiltrate the most popular sequencing softwares that are mainly based on peptide mechanisms described in the mid 90s. This workshop attempts to narrow this gap by discussing recent mechanisms and peptide MS-MS spectra that are particularly difficult to assign at present.

**The Costs of Maintaining Modern Mass Spectrometers: Creative Solutions Needed?**

Korbel Ballroom 4

*Analytical Laboratory Managers Interest Group*

Richard Kondrat, presiding

Instrument maintenance issues such as costs, service contracts, and technical support will be discussed by representatives from several instrument manufacturers, NSF, industrial and academic workshop participants. The generation of creative solutions to current problems is strongly encouraged by all so that instrument operations can be maintained while holding costs to reasonable levels.

**Perspectives on the Changing Role of Mass Spectrometry in Academia**

Four Seasons Ballroom 1-2

*Young Mass Spectrometrists Interest Group*

Steven M. Patrie, presiding

A growth in academic positions in systems biology may lead a young mass spectrometrists into a department of biology or medicine as opposed to a more traditional physical science program. This will undoubtedly present unique challenges in establishing oneself as an independent investigator. Our panel will discuss the merging fields of biology, medicine and mass spectrometry and help us to understand the future roles/demands that a young mass spectrometrists will face in an applications-based world. Aspects of the discussion will generally focus upon working in academics; working with collaborators in biology and medicine whose expectations of technologies may be exceedingly high; running core facilities while performing one's own research; grant writing; and opportunities for a mass spectrometrists at smaller institutions.

**Progress in Field Forensics**

Four Seasons Ballroom 3-4

*Forensics Interest Group*

Brian Eckenrode, presiding

This workshop will address several key challenge areas in field forensics. There will be a focus primarily on new developments in the use of canines at crime scenes and during investigative efforts. Additionally, subject areas will include microbial forensics, microarrays and MS in DNA analysis, ricin methods, and instrumentation improvements in relation to trace VOCs analysis.

**MONDAY POSTER TOPICS**

Instrumentation: New Concepts 1  
Direct Ionization 1  
Instrumentation: Ion Sources, ESI-related  
APPI  
Ion Structures/Energetics 1  
Environmental Analysis  
Atmospheric/Aerosol Chemistry  
Imaging MS for Small Molecules and Lipids  
Computer Applications: General  
Homeland Security  
Small Molecule Analysis: Pharmaceuticals  
Quantitation of Small Molecules: Pharmaceutical Focus  
Toxicology  
Drug Metabolism: High Throughput  
Drug metabolism: Xenobiotic Metabolite Profiling  
Metabolomics 1  
Peptides: Quantitation  
Peptides: Fragmentation  
LC-MS Sample Prep: Protein Analysis  
Phosphoproteins: Characterizations  
PTMs: Histones  
Proteins: Cross Linking  
Proteins: Membranes  
Protein Conformation  
Protein Quantitation 1  
Protein Sequencing  
Proteomics: Plasma  
Proteomics: New Approaches for Sample Preparation  
Proteomics: Biomarker Discovery 1  
Proteomics: Clinical Applications  
Bioinformatics 1  
Systems Biology: Quantitative

**TUESDAY POSTER TOPICS**

Instrumentation: FTMS  
Direct Ionization 2  
MALDI: Sample Prep  
MALDI/Tandem MS  
ECD/ETD/EDD  
Emerging Contaminants 1  
Imaging MS Instrumentation and Sample Prep  
High Throughput Analysis/Robotics  
Carbohydrates/Oligosaccharides: General  
Lipids: Biochemistry & Steroids 1  
Lipid Structural Analysis  
Non-Covalent Interactions 1  
Microbial Analysis  
Small Molecule Analysis: Biologically Relevant Compounds  
Quantitation of Small Molecules/Plasma Matrix  
Drug Metabolism: Pharmacokinetics  
Drug Metabolism: Quantitation 1  
Drug Metabolism: Accelerating Metabolite Identification  
Metabolomics 2  
Neuropeptides  
Peptides: General  
Peptides: Sequencing  
LC-MS Sample Prep: Phospholipid Removal  
Phosphoproteins: Methods  
PTMs: Methylation, Acetylation, Glycosylation, Ubiquitination  
Proteins: General 1  
Protein Conformation: Oxidative and Covalent Labeling  
Protein Quantitation 2  
Proteins: Modified, Methodology and *in vitro* Modifications  
Proteomics: New Approaches to Data Analysis  
Proteomics: Biomarker Discovery 2  
Bioinformatics 2  
Systems Biology: Discovery

**WEDNESDAY POSTER TOPICS**

Instrumentation: TOF  
Instrumentation: Quadrupoles and Traps 1  
Ion Mobility  
Elemental Analysis and Speciation  
Agriculture  
Ion Activation  
Ion Molecule Reactions 1  
Emerging Contaminants 2  
Hydrocarbon & Petrochemical  
Imaging MS Proteins & Peptides  
Computer Applications: Proteomics  
Materials and Polymers  
Carbohydrates/Oligosaccharides: Structural Characterization  
Non-Covalent Interactions 2  
Nucleic Acids  
LC-MS 1  
Clinical Chemistry: Small Molecule  
Small Molecule Analysis: Data Processing/Instrumentation  
Quantitation of Small Molecules  
Immunology  
Drug Metabolism: Quantitation 2  
Drug Metabolism: Reactive Metabolites  
PTMs: Sulfation, Nitration and Strategies  
Phospho-Proteomics  
Proteins: Glycoproteins  
Protein Conformation HD Exchange 1  
Protein Quantitation 3  
Proteins: Modified, Biological Applications  
Proteomics: Biomarker Assays 1  
Proteomics: New Approaches to Instrumentation  
Proteomics: Biomarker Discovery 3  
Bioinformatics 3  
Systems Biology: Interactions

**THURSDAY POSTER TOPICS**

Instrumentation: New Concepts 2  
Instrumentation: Quadrupoles and Traps 2  
Ion Mobility Applications  
Instrumentation: Ion Sources General  
Ionization Mechanisms  
Ion Structures Energetics 2  
Ion Molecule Reactions 2  
Analysis of Pesticides and Herbicides  
Natural Products  
GC-MS  
Forensics  
Micro-Scale Separation MS  
Carbohydrates/Oligosaccharides: Biomarker Discovery  
Lipids: Biochemistry & Steroids 2  
LC-MS 2  
Clinical Chemistry: Large Molecule  
Small Molecule Analysis Food-Related and Other  
Quantitation of Small Molecules/Bioanalysis  
Metabolomics 3: Methods  
Peptides: Glycopeptides  
LC-MS Sample Preparation  
Phosphopeptide Enrichment  
PTMs: Deamidation, Disulfides  
Proteins: General 2  
Proteins: Recombinant  
Protein Conformation HD Exchange 2  
Proteins: General, Methods  
Proteomics: Biomarker Assays 2  
Proteomics: Applications  
Proteomics: Biomarker Discovery 4  
Proteomics: Tissue  
Bioinformatics 4



## SUNDAY, JUNE 1

5:00 – 6:30 pm  
TUTORIAL LECTURES

Korbel Ballroom 2-3

5:00 pm **Interactions of Ions with Surfaces**

Julia Laskin, Pacific NW National Laboratory

5:45 pm **Metastable Ions**

R. Graham Cooks, Purdue University

## 6:45 – 7:45 pm

## CONFERENCE OPENING AND PLENARY LECTURE

Wells Fargo Theatre

6:45 pm Welcome to the 56<sup>th</sup> ASMS Conference on Mass Spectrometry

Barbara S. Larsen, President, ASMS  
 Presentation of the Thermo Scientific Research Award  
 Presentation of the Waters Corp. Research Award  
 Presentation of the ASMS Research Award

7:00 pm **Improbable Research, Spectrometric and Otherwise**Marc Abrahams, *Annals of Improbable Research*

## 7:45 – 9:30 pm

## WELCOME RECEPTION IN THE EXHIBIT HALL

## MONDAY MORNING, JUNE 2

## 8:30 – 10:30 am

## LABEL FREE QUANTITATION OF PROTEINS

Wells Fargo Theatre

Chair: Arthur Moseley

- MOA am 08:30 **Workflow Checkpoints in Label-Free Quantitative Proteomics: An Applied Biomarker Investigation for Renal Cell Carcinoma from Tissue Interstitial Fluid;** Susan E. Abbatiello<sup>1</sup>; Jennifer Nina Sutton<sup>2</sup>; Brian L. Hood<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>University of Pittsburgh Cancer Institute, Pittsburgh, PA; <sup>2</sup>Thermo Fisher Scientific, Cambridge, MA
- MOA am 08:50 **Differential Analysis and Annotation of the CHO Cytosolic Proteome using a Label-Free LC-MS Strategy;** Leo E. Bonilla<sup>2</sup>; Christopher Farnsworth<sup>2</sup>; Allison Bianchi<sup>1</sup>; Wen Yu<sup>2</sup>; Kimberly Lee<sup>2</sup>; Christopher Russell<sup>2</sup>; <sup>1</sup>Amgen, Seattle, WA; <sup>2</sup>Molecular Sciences-Amgen, Seattle, WA
- MOA am 09:10 **Absolute Quantification Based on Ion Accounting: Technical Considerations and Biological Implications;** J. Will Thompson<sup>1</sup>; Scott Geromanos<sup>2</sup>; Martha Stapels<sup>2</sup>; Wenle Xia<sup>1</sup>; Niel Spector<sup>1</sup>; Michael Forrester<sup>1</sup>; Arthur Moseley<sup>1</sup>; <sup>1</sup>Duke University School of Medicine, Durham, NC; <sup>2</sup>Waters Corporation, Milford, MA
- MOA am 09:30 **A Refined Label-Free Method for Quantitative Proteomic Genetic Linkage Analysis;** Eric Foss<sup>3</sup>; Dragan Radulovic<sup>2</sup>; Scott A. Shaffer<sup>1</sup>; Antonio Bedalov<sup>3</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Florida Atlantic University, Boca Raton, FL; <sup>3</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MOA am 09:50 **Proteome-Wide Accurate Label-Free Quantitation of Cell Lines and Tissues;** Juergen Cox; Christian Luber; Boris Macek; Ana Velic; Matthias Mann; *Max-Planck-Institute of Biochemistry, Martinsried, Germany*
- MOA am 10:10 **Absolute and Relative Quantitation of Proteins in Mouse and Rat Brains;** Martha D. Stapels<sup>1</sup>; Chelsea Piper<sup>2</sup>; An Zhou<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Legacy Research, Portland, OR

## 8:30 – 10:30 am

## FUNDAMENTALS OF ION/ION REACTIONS

Korbel Ballroom 1

Chair: Yu Xia

- MOB am 08:30 **Gas-Phase Bio-Ion/Ion Reactions: The Hows and Whys of Reagent Selection;** Scott A. Mcluckey; *Purdue University, West Lafayette, IN*
- MOB am 08:50 **Theoretical Study of ETD/ECD Mechanisms;** Jack Simons; *Univ. of Utah, Salt Lake City, UT*
- MOB am 09:10 **Charge State Dependence of Proton Transfer Versus Electron Transfer in a Gas-Phase Ion/Ion Electron Transfer Dissociation Process on Tryptic Peptides;** Jian Liu; Teng-Yi Huang; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*
- MOB am 09:30 **Crown-Ether Alkane-1,n-Diammonium Complexes. Electron Capture, Femtosecond Electron Transfer and Theory;** Anne S. I. Holm<sup>2</sup>; Mikkel K. Larsen<sup>2</sup>; Subhasis Panja<sup>2</sup>; Preben Hvelplund<sup>2</sup>; Steen Brondsted Nielsen<sup>2</sup>; Ryan D. Leib<sup>3</sup>; William A. Donald<sup>3</sup>; Evan R.

- Williams<sup>3</sup>; Chan; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*University of Aarhus, Aarhus, Denmark*; <sup>3</sup>*University of California, Berkeley, CA*
- MOB am 09:50 **Ion/Ion Reactions Between Chelators and Nucleic Acid Substrates Induce Gas-Phase Transfer of Metal Ions**; Kevin B. Turner; Sarah A. Monti; Daniele Fabris; *University of Maryland Baltimore County, Baltimore, MD*
- MOB am 10:10 **How to Maximize the ETD MS-MS Duty Cycle for Shotgun Proteomics**; Jason D. Russell; Danielle L. Swaney; Joshua J. Coon; *University of Wisconsin, Madison, WI*

8:30 – 10:30 am

**DEVELOPMENTS IN ION MOBILITY:  
INSTRUMENTATION, THEORY, AND APPLICATIONS**
*Korbel Ballroom 2-3*

Chair: Facundo Fernandez

- MOC am 08:30 **Overview of Ion Mobility Mass Spectrometry Applications and Instrumentation**; Herbert H Hill; Prabha Dwivedi; Bill Siems; *Washington State University, Pullman, WA*
- MOC am 08:50 **New Structural Measurement Strategies using Ion Mobility-Mass Spectrometry**; John A. McLean; Larissa S. Fenn; Randi Gant; Thomas J. Kerr; Ablatt Mahsut; Sevugarajan Sundarapandian; *Vanderbilt University, Nashville, TN*
- MOC am 09:10 **A Cryogenic Ion Mobility-Mass Spectrometer: Theory and Applications**; Jody C. May; Kent J. Gillig; David H. Russell; *Texas A&M University, College Station, TX*
- MOC am 09:30 **Fundamentals of Collisional Heating and Dipole Alignment of Macromolecular Ions in FAIMS and Implications for Differential Mobility Analyses (DMA)**; Alexandre A. Shvartsburg<sup>1</sup>; Ridha Mabrouki<sup>1</sup>; Errol W. Robinson<sup>1</sup>; Erin S. Baker<sup>1</sup>; Sergei Y. Noskov<sup>2</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*USDoE PNNL, Richland, WA*; <sup>2</sup>*University of Calgary, Calgary, Alberta, Canada*
- MOC am 09:50 **Design and Operation of a New High Resolution Ion Mobility Mass Spectrometer**; Nicholas Dupuis; Paul Kemper; Michael T. Bowers; *University of California Santa Barbara, Santa Barbara, CA*
- MOC am 10:10 **Signal to Noise Ratio Gains in Digitally-Multiplexed Atmospheric Pressure Drift Tube Ion Mobility Spectrometry**; Mark Kwasnik; Facundo Fernandez; Joe Caramore; *Georgia Institute of Technology, Atlanta, GA*

8:30 – 10:30 am

**CHALLENGES IN ELEMENTAL ANALYSIS USING  
MASS SPECTROMETRY**
*Korbel Ballroom 4*

Chair: Joe Caruso

- MOD am 08:30 **Elemental Analysis of Laboratory and Ambient Organic Aerosols using Electron Ionization Mass Spectrometry**; Allison C. Aiken<sup>1</sup>; Peter F. DeCarlo<sup>2</sup>; Jesse H. Kroll<sup>3</sup>; Douglas R. Worsnop<sup>3</sup>; Kenneth Docherty<sup>1</sup>; Ingrid M. Ulbrich<sup>1</sup>; Edward Dunlea<sup>1</sup>; Claudia Mohr<sup>2</sup>; J. Alex Huffma; <sup>1</sup>*University of Colorado at Boulder, Boulder, CO*; <sup>2</sup>*Paul Scherrer Institut, Villigen, Switzerland*; <sup>3</sup>*Aerodyne Research Inc., Billerica, MA*; <sup>4</sup>*State University of New York, Albany, NY*; <sup>5</sup>*University of Calif*

- MOD am 08:50 **Off-Line Coupling of Capillary Electrophoresis to Laser Ablation Inductively Coupled Plasma Mass Spectrometry for Elemental Speciation**; Jan Preisler; Ondrej Peš; Pavla Foltynová; Radek Vyhnanek; Tomáš Vaculovic; Viktor Kanický; *Masaryk University, Brno, Czech Republic*
- MOD am 09:10 **An Investigation of Xenon as a Universal ICP-MS Collision Cell Gas via Sulfur Optimization with Application to Bottled Water Contaminants**; Scott E. Afton; Joseph A. Caruso; *University of Cincinnati, Cincinnati, OH*
- MOD am 09:30 **Collision/Reaction Cell ICP-MS with Shielded Torch and High Resolution ICP-MS for the Determination of Selenium Isotope Ratios in Different Matrices**; Khalid A. Al-Saad<sup>1</sup>; Mohammed A. Amr<sup>1</sup>; Abdulfatah I. Helal<sup>2</sup>; Nagwa F. Zahran<sup>2</sup>; <sup>1</sup>*Central Laboratories Unit, Qatar University, Doha, QATAR*; <sup>2</sup>*Atomic Energy Authority 13759, Cairo, Egypt*
- MOD am 09:50 **Characterization of an Inductively Coupled Plasma/Electrospray Ionization Dual-Source Time-of-Flight Mass Spectrometer for Metallomic and Speciation Analysis**; Duane A. Rogers; Steven Ray; Gary M. Hieftje; *Indiana University, Bloomington, IN*
- MOD am 10:10 **Imaging Mass Spectrometry By LA-ICP-MS In Life Sciences**; Sabine Johanna, Dr. Becker; *Research Centre Juelich, Germany*

8:30 – 10:30 am

**DISCOVERING PEPTIDE BIOMARKERS**
*Four Seasons Ballroom 1-2*

Chair: Tim Griffin

- MOE am 08:30 **Class II MHC Restricted Phosphopeptides as Cancer Immunotherapeutics or Diagnostics**; Jie Qian<sup>1</sup>; Florence A. Depontieu<sup>2</sup>; Angela L. Zarlign; Andrew Norris<sup>1</sup>; Dina Bai<sup>1</sup>; Victor H. Engelhard<sup>1</sup>; Suzanne Topalian<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, VA*; <sup>2</sup>*Johns Hopkins School of Medicine, Baltimore, MD*
- MOE am 08:50 **Novel Mass Spectrometric Immunoassay for the Structural Characterization of C-Peptide within Healthy and Diabetes Mellitus Type 2 Populations**; Paul E. Oran; Jason W. Jarvis; Chad Borges; Randall Nelson; *Arizona State University, Tempe, AZ*
- MOE am 09:10 **Neuropeptidomic Approaches for Specific and Sensitive Identification of Endogenous Peptides**; Maria Fälth<sup>1</sup>; Anna Nilsson<sup>1</sup>; Karl Skold<sup>1</sup>; Marcus Svensson<sup>1</sup>; Mats Boren<sup>2</sup>; David Fenyo<sup>3</sup>; Malin Andersson<sup>1</sup>; Per Svenningsson<sup>4</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*; <sup>2</sup>*Denator, Uppsala, Sweden*; <sup>3</sup>*The Rockefeller University, New York, NY*; <sup>4</sup>*Karolinska Institutet, Stockholm, Sweden*
- MOE am 09:30 **Development of Independent Urinary Biomarker Panels for Differential Diagnosis and Evaluation of ANCA-Associated Vasculitis Disease Activity**; David Good<sup>1</sup>; Marion Haubitz<sup>2</sup>; Harald Mischak<sup>4</sup>; Joshua J. Coon<sup>3</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Medizinische Hochschule Hannover, Hannover, Germany*; <sup>3</sup>*University of Wisconsin-madi, Madison, WI*; <sup>4</sup>*Mosaiques Diagnostics, Hannover, Germany*
- MOE am 09:50 **Designed by Mass Spectrometry: Structural Reporter Peptides for the Early Diagnosis of**

- Invasive Aspergillosis**; Teresa Hong; Khue Truong; Diana Diaz Arevalo; Karine Bagramyan; Joesph M. Lyons; James I. Ito; Markus Kalkum; *City of Hope, Duarte, CA*
- MOE am 10:10 **Isoform Distribution and Reduced Levels of Apolipoprotein C1 in Persons with a T45S Polymorphism: Determined by MALDI-TOF Profiles**; Stephen B. Harvey<sup>1</sup>; Matthew Stone<sup>1</sup>; Raj Kasthuri<sup>1</sup>; Gary Nelsestuen<sup>1</sup>; Kenneth McMillian<sup>2</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*American Indian Community Development Corp., Minneapolis, MN*

8:30 – 10:30 am

## ENDOGENOUS METABOLITE PROFILING

*Four Seasons Ballroom 3-4*

Chair: Joshua D. Rabinowitz

- MOF am 08:30 **LC-MS Approach for Comprehensive Metabolomics Analysis**; Kara Pearson<sup>1</sup>; Yutai Li<sup>1</sup>; Amy F. Loughlin<sup>1</sup>; Caroline K Ferraro<sup>1</sup>; Qiuwei xu<sup>1</sup>; Ethan Xu<sup>1</sup>; Peter Askovich<sup>2</sup>; Andrey Bondarenko<sup>2</sup>; Eric Minch<sup>1</sup>; Jeffrey; <sup>1</sup>*Merck & Co., Inc., West Point, PA*; <sup>2</sup>*Rosetta Biosoftware, Seattle, WA*
- MOF am 08:50 **Absolute Quantitation of Intracellular Metabolites in *Escherichia coli***; Bryson D. Bennett; Elizabeth Kimball; Joshua D. Rabinowitz; *Princeton Univeristy, Princeton, NJ*
- MOF am 09:10 **The Effects of Drought and Heat Stress Combination on Arabidopsis Plants: A Metabolomics Analysis**; Vladimir Shulaev<sup>1</sup>; Donna L. Wilson<sup>2</sup>; Anne Ferguson<sup>2</sup>; <sup>1</sup>*Va Bioinformatics Inst., Blacksburg, VA*; <sup>2</sup>*Thermo Fisher, San Jose, CA*
- MOF am 09:30 **Biochemical Mapping of Metabolic Alterations in Lungs of Rat Embryos**; Oliver Fiehn; Dinesh Kumar; Gert Wohlgeuth; Jesse Joad; Carol Hood; Kent Pinkerton; Tobias Kind; *UC Davis, Davis, CA*
- MOF am 09:50 **Using Metabolomics of Animal Models to Understand Complex Human Biochemistry and Disease**; William Wikoff; Howard Fox; Gary Siuzdak; *The Scripps Research Intitute, San Diego, CA*
- MOF am 10:10 **Metabolite Profiles for Phenotyping: Lipidomics of Healthy Twins**; Thomas Hankemeier<sup>1</sup>; Harmen HM Draisma<sup>1</sup>; Jacqueline J Meulman<sup>1</sup>; Ivana Bobeldijk-Pastorova<sup>2</sup>; Dorret I Boomsma<sup>3</sup>; Jan van der Greef<sup>1</sup>; <sup>1</sup>*Leiden University, Leiden, Netherlands*; <sup>2</sup>*TNO Quality of Life, Zeist, Netherlands*; <sup>3</sup>*Free University, Amsterdam, The Netherlands*

8:30 – 10:30 am

## MS CHARACTERIZATION OF CARBOHYDRATES

*Rooms 601-607*

Chair: Ron Orlando

- MOG am 08:30 **Quantitation of Glycans for Disease Marker Discovery in Breast Cancer**; Carlito Lebrilla<sup>1</sup>; Hyun Joo An<sup>1</sup>; Nannan Tao<sup>1</sup>; Scott Kronewitter<sup>1</sup>; Maria Lorna De Leoz<sup>1</sup>; Jaehan Kim<sup>1</sup>; Helen Chew<sup>2</sup>; Suzanne Miyamoto<sup>2</sup>; Kit Lam<sup>2</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*Uc Davis Cancer Center, Sacramento, CA*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- MOG am 08:50 **Targeted Glycomics from High Energy CID MALDI-MS-MS to Nanospray-Based Total Ion Mapping and MS<sup>n</sup> Analysis**; Sz-Wei Wu<sup>1</sup>; Chia-Wei Lin<sup>2</sup>; Shui-Hua Wang<sup>2</sup>; Kay-Hooi Khoo<sup>1</sup>;

- <sup>1</sup>*Inst Biol Chem, Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Inst Biochemical Sciences, Natl Taiwan U, Taipei, Taiwan*
- MOG am 09:10 **Ion-Mobility Separation Coupled with Negative Ion Fragmentation of N-Linked Carbohydrates**; David J. Harvey<sup>1</sup>; James Scrivens<sup>2</sup>; Richard Holland<sup>3</sup>; Jonathan Williams<sup>3</sup>; Mark R Wormald<sup>1</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*Univ of Warwick, Coventry, UK*; <sup>3</sup>*University of Warwick, Coventry, United Kingdom*
- MOG am 09:30 **A Glycomics Approach for Characterization of Bacterial Lipopolysaccharides**; Chow Ming Tsai; Miznur Rahman; Ewa Jankowska; John F Cipollo; *Food and Drug Administration CBER, Bethesda, MD*
- MOG am 09:50 **Tandem Mass Spectrometry Analysis of Glycosaminoglycan Oligosaccharides using EID, EDD, and IRMPD**; Jeremy Wolff<sup>1</sup>; Tatiana Laremore<sup>2</sup>; Robert J. Linhardt<sup>2</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*Rensselaer Polytechnic Institute, Troy, NY*
- MOG am 10:10 **Mass Spectrometric Analysis of Glycosaminoglycan Domain Structure**; Nancy Leymarie; Alicia M. Hitchcock; Hicham Naimy; Gregory O Staples; Michael J. Bowman; Joseph Zaia; *Boston University, Boston, MA*

## MONDAY AFTERNOON

2:30 – 4:30 pm

## ADVANCES IN TOP-DOWN PROTEOMICS

*Wells Fargo Theatre*

Chair: Kathrin Breuker

- MOA pm 02:30 **What Can Top-Down Proteomics Do for You?** Fred W. McLafferty<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Honghai Jiang<sup>1</sup>; Mahmud Hossain<sup>1</sup>; <sup>1</sup>*Cornell University, Ithaca, NY*; <sup>2</sup>*University of Innsbruck, Innsbruck, AUSTRIA*
- MOA pm 02:50 **Optimization of Intact Protein Funnel-Skimmer Dissociation for FT-ICR Mass Spectrometry**; Jennifer S. Cobb<sup>1</sup>; Michael L. Easterling<sup>2</sup>; Jeffrey N. Agar<sup>1</sup>; <sup>1</sup>*Brandeis University, Waltham, MA*; <sup>2</sup>*Bruker Daltonics, Inc., Billerica, MA*
- MOA pm 03:10 **Isotopic Resolution MS and MS-MS Analysis of Intact Human Serum Albumin**; Jianzhong Chen<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Hollie Huff<sup>2</sup>; Yvonne Carella<sup>2</sup>; James E. Bruce<sup>1</sup>; <sup>1</sup>*Washington State University, Pullman, WA*; <sup>2</sup>*Inverness Medical Innovations, Inc, Louisville, CO*
- MOA pm 03:30 **Top Down Disease Proteomics: Deciphering Protein Modifications for Understanding and Diagnosis of Human Diseases**; Ying Ge<sup>1</sup>; Lisa Xu<sup>1</sup>; Inna Rybakova<sup>1</sup>; Vlad Zabrouskov<sup>2</sup>; Richard, L. Moss<sup>1</sup>; Jeffery Walker<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- MOA pm 03:50 **Top-Down Protein Characterization: Comparison of MALDI-TOFMS versus ESI-FTMS**; Viswanatham Katta; Mary Zhu; Jennifer Zhang; *Genentech, Inc., South San Francisco, CA*
- MOA pm 04:10 **Top Down Proteomics: The Teenage Years**; Jonathan T. Ferguson; Craig D. Wenger; John F. Kellie; Haylee M. Thomas; Ji Eun Lee; Shannee Babai; Neil L. Kelleher; *University of Illinois Urbana-Champaign, Urbana, IL*

**2:30 – 4:30 pm**  
**SPECTROSCOPY OF GASEOUS IONS**

*Korbel Ballroom 1*

Chair: Rebecca Jockusch

- MOB pm 02:30 **IR Spectroscopy of Deprotonated Amino Acid and Peptide Anions**; Jos Oomens; Jeffrey D. Steill; *FOM Rijnhuizen, Nieuwegein, Netherlands*
- MOB pm 02:50 **Structure of ECD Fragments from Charge-Tagged Peptides Probed by Tunable IRMPD**; Gilles Frison<sup>1</sup>; Alexander Bull<sup>1</sup>; Guillaume Van Der Rest<sup>1</sup>; Frantisek Turecek<sup>2</sup>; Thierry Besson<sup>3</sup>; Joel Lemaire<sup>3</sup>; Philippe Maitre<sup>3</sup>; Julia Chamot-Rooke<sup>1</sup>; <sup>1</sup>*CNRS - Ecole Polytechnique, Palaiseau, France*; <sup>2</sup>*University of Washington, Seattle, WA*; <sup>3</sup>*CNRS - Université Paris Sud Orsay, Orsay, France*
- MOB pm 03:10 **Implementation of a Continuous Wave (cw) Optical Parametric Oscillator (OPO) Laser to Obtain Infrared (IR) Spectra of Gaseous Ions**; Wright Pearson; Cesar Contreras; John R. Eyler; *University of Florida, Gainesville, FL*
- MOB pm 03:30 **Vibrational and Electronic Spectroscopy of Intermediates of Methane to Methanol Conversion by Transition Metal Oxide Cations**; Gokhan Altinay; Murat Citir; Ricardo Metz; *University of Massachusetts, Amherst, MA*
- MOB pm 03:50 **Infrared and Ultraviolet Spectroscopy of Gas-Phase Helical Peptides**; Jaime A. Stearns; Caroline Seaiby; Monia Guidi; Oleg V. Boyarkin; Thomas R. Rizzo; *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
- MOB pm 04:10 **Infrared Action Spectroscopy of Hydrated Multiply Charged Ions in the Gas Phase**; Matthew Bush; Richard J. Saykally; Evan R. Williams; *University of California, Berkeley, CA*

**2:30 – 4:30 pm**  
**DEVELOPMENTS IN ION TRAPPING INSTRUMENTATION**

*Korbel Ballroom 2-3*

Chair: Peter B. O'Connor

- MOC pm 02:30 **Optimized Image Current Detection Geometry for Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Chris Hendrickson<sup>1</sup>; Steve Beu<sup>2</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*S C Beu Consulting, Austin, TX*
- MOC pm 02:50 **A Dual Reaction Cell, ETD-Enabled Orbitrap Mass Spectrometer for Top-Down Proteomics**; Graeme McAlister<sup>1</sup>; Joshua J. Coon<sup>2</sup>; <sup>1</sup>*The University of Wisconsin, Madison, WI*; <sup>2</sup>*University of Wisconsin-madi, Madison, WI*
- MOC pm 03:10 **How Far Can Ion Trap Miniaturization Go?** Zheng Ouyang; Liang Gao; Jason Harper; Qingyu Song; Wei Xu; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MOC pm 03:30 **A New Mass Independent Inlet for Introducing Massive Ions into Mass Spectrometers without Expansion-Induced Kinetic Energy**; Peter TA Reilly; Hideya Koizumi; William B Whitten; *Oak Ridge National Laboratory, Oak Ridge, TN*
- MOC pm 03:50 **Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Instrumentation Design and Development: Reduction of Ion Cloud De-Phasing and Time-of-Flight Discrimination**; Nathan Kaiser; Gunnar E. Skulason; Chad Weisbrod; James E. Bruce; *Washington State University, Pullman, WA*

- MOC pm 04:10 **A Novel, High Sensitivity Cryogenic Fourier Transform Ion Cyclotron Resonance Mass Spectrometer**; Raman Mathur; Cheng Lin; Konstantin Aizikov; Ronald W. Knepper; Peter B. O'Connor; *Boston University, Boston, MA*

**2:30 – 4:30 pm**  
**EMERGING MASS SPECTROMETRY TECHNIQUES IN ENVIRONMENTAL ANALYSIS**

*Korbel Ballroom 4*

Chair: Jose-Luis Jimenez

- MOD pm 02:30 **Real-Time Detection and Identification of Aqueous Chlorine Transformation Products using QTOF-MS**; Brett J. Vanderford; Doug B. Mawhinney; Fernando L. Rosario-Ortiz; Shane A. Snyder; *Southern Nevada Water Authority, Las Vegas, NV*
- MOD pm 02:50 **Advances in the Identification of Environmental Degradates using Hybrid-FTMS Combined with ULPC, IRMPD, and Chip-Based Nanospray**; Jesse Balcer; Jeffrey Gilbert; Joeline Smith-Drake; Kurt Graper; Laura Laughlin; Pete Johnson; Mark Krieger; *Dow AgroSciences, Indianapolis, IN*
- MOD pm 03:10 **Measurement of Methyl-Polycyclic Aromatic Hydrocarbon Metabolites in Human Urine by Gas Chromatography/High-Resolution Mass Spectrometry**; Lovisa C Romanoff; Zheng J Li; Erin N Porter; Debra A Trinidad; Donald G Patterson; Andreas Sjodin; *Centers for Disease Control and Prevention, Atlanta, GA*
- MOD pm 03:30 **Response of Green Algae (*Chlamydomonas reinhardtii*) to Environmental Stressors, Evaluated by High-Throughput Proteomics**; Marc J.-F. Suter; Holger Nestler; Victor J. Nesatyy; *EAWAG, Dübendorf, Switzerland*
- MOD pm 03:50 **Mass Spectrometry of Ambient Nanoparticles**; Murray Johnston; Christopher Zordan; Melissa Reinard; *University of Delaware, Newark, DE*
- MOD pm 04:10 **Chemical Ionization Mass Spectrometry Techniques for Measurements of Gas-Phase Ammonia**; John B. Nowak<sup>1</sup>; J. Andrew Neuman<sup>1</sup>; Dave J. Tanner<sup>2</sup>; L. Gregory Huey<sup>2</sup>; Thomas B. Ryerson<sup>3</sup>; Fred C. Fehsenfeld<sup>1</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>3</sup>*NOAA-Earth System Research Laboratory, Boulder, CO*

**2:30 – 4:30 pm**  
**THE PARADIGM SHIFT IN CLINICAL DIAGNOSTICS USING MASS SPECTROMETRY**

*Four Seasons Ballroom 1-2*

Chair: Russell Grant

- MOE pm 02:30 **Impact of Tandem Mass Spectrometry in Clinical Diagnostics**; Ravinder J. Singh; *Mayo Clinic, Rochester, MN*
- MOE pm 02:50 **Neonatal Diagnosis of Metachromatic Leukodystrophy in Dried Blood Spots by Tandem Mass Spectrometry**; Brian J. Wolfe<sup>1</sup>; Ladislav Kuchar<sup>2</sup>; C. Ronald Scott<sup>1</sup>; Michael H. Gelb<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Charles University, Prague, Czech Republic*
- MOE pm 03:10 **Label-Free Detection of Enzyme Activities with Self-Assembled Monolayer Desorption Ionization Time-of-Flight Mass Spectrometry (SAMDI-TOF MS)**; Steven Patrie; Milan Mrksich; *University of Chicago, Chicago, IL*

- MOE pm 03:30 **High-Throughput MRM Quantitative Targeted Proteomics Platform for Influenza Viral Particles;** Christopher M. Colangelo<sup>1</sup>; Erol E. Gulcicek<sup>1</sup>; Peter Palese<sup>2</sup>; Kenneth Williams<sup>1</sup>; Megan L. Shaw<sup>2</sup>; <sup>1</sup>*Yale University, New Haven, CT*; <sup>2</sup>*Mount Sinai School of Medicine, New York, NY*
- MOE pm 03:50 **Top-Down Lipidomics Screens for Assessing Metabolic Risk in Obesity Related Disorders;** Dominik Schwudke<sup>1</sup>; Juergen Graessler<sup>2</sup>; Ronny Herzog<sup>1</sup>; Stefan Bornstein<sup>2</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>*Max Planck Institute CBG, Dresden*; <sup>2</sup>*Faculty of Medicine, TU Dresden, Dresden, Germany*
- MOE pm 04:10 **Simultaneous High Throughput Detection and Characterization of Broad Groups of Respiratory Viruses by PCR coupled with High Throughput Mass Spectrometry;** Steven A. Hofstadler; Ranga Sampath; Lawrence B. Blyn; Mark Eshoo; Robert Lovari; Feng Li; Javier Fernandez; Heather Matthews; Rachael Melton; Kristin Sannes-Lowery; Jared Drader; James C. Hannis; Lendell L. Cummins; Thomas Hall; David J.; *Ibis Biosciences, Inc., Carlsbad, CA*

2:30 – 4:30 pm

**QUANTITATION OF DRUG METABOLITES***Four Seasons Ballroom 3-4*

Chair: Kevin Bateman

- MOF pm 02:30 **Metabolite Quantification: Why and How;** Philip Tiller<sup>1</sup>; Kevin Bateman<sup>2</sup>; Ronda Rippley<sup>1</sup>; Nancy Agrawal<sup>1</sup>; Kelem Kassahun<sup>1</sup>; Thomas A. Baillie<sup>1</sup>; <sup>1</sup>*Merck & Co., West Point, PA*; <sup>2</sup>*Merck Frosst, Montreal, QC*
- MOF pm 02:50 **Does Microdosing Produce a Metabolic Profile Indicative of a Normal Dose in Rats?;** Carmal Seto<sup>1</sup>; Daniel Lebre<sup>2</sup>; Tanya Gamble<sup>1</sup>; Gary Impey<sup>2</sup>; Takeo Sakuma<sup>1</sup>; Jinsong Ni<sup>3</sup>; Fred Ouyang<sup>3</sup>; Devin Welty<sup>3</sup>; Andrew Acheampong<sup>3</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>*Applied Biosystems, Concord, Canada*; <sup>3</sup>*Allergan, Irvine, CA*
- MOF pm 03:10 **A Rapid Approach to Quantitative *in vivo* Metabolite Profiling without the Need for Authentic Standards or Labeled Compounds;** Jonathan L. Josephs; Mary F. Grubb; Yanou Yang; William G. Humphreys; *Bristol-Myers Squibb, Hopewell, NJ*
- MOF pm 03:30 **Quantification of Metabolites using Chemiluminescent Nitrogen Detection (CLND) and MS-MS;** Laura E. Edwards; Jaleh Abedi; Alan D. Hendricker; Kenneth C. Lewis; *OpAns, LLC, Durham, NC*
- MOF pm 03:50 **Quantitative Imaging of Cocaine and Its Metabolites in Postmortem Brain Tissue by Intermediate-Pressure MALDI/Linear Ion Trap Tandem Mass Spectrometry;** Richard F. Reich; Kasia Cudzilo; Richard A. Yost; *University of Florida, Gainesville, FL*
- MOF pm 04:10 **Incurred Samples Investigation: “Sudden and Unusual Disappearance of Metabolite and its Stable-Labeled Internal Standard Response during LC-MS-MS GLP Bioanalysis”;** Troy Bradley; Marie-Andrée Mercier; Janick Boivin; Cynthia Coté; Catherine Dicaire; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, Canada*

2:30 – 4:30 pm

**CHARACTERIZING PROTEIN-LIGAND INTERACTIONS WITH MASS SPECTROMETRY***Rooms 601-607*

Chair: John Klassen

- MOG pm 02:30 **Hydrogen / Deuterium Exchange Characterization of Transmembrane Signaling Proteins;** Michael Chalmers<sup>3</sup>; Bruce Pascal<sup>3</sup>; Scott Novick<sup>3</sup>; Scott A. Busby<sup>3</sup>; Mark R Southern<sup>3</sup>; Ellen Chien<sup>1</sup>; Raymond C. Stevens<sup>1</sup>; David Szymkowski<sup>2</sup>; Patrick R. Griffin; <sup>1</sup>*TSRI, La Jolla, CA*; <sup>2</sup>*Xencor, Monrovia, CA*; <sup>3</sup>*The Scripps Research Institute - Florida, Jupiter, FL*
- MOG pm 02:50 **Hyphenation of Surface Plasmon Resonance Imaging to Mass Spectrometry by On-Chip MALDI MS Analysis;** Sophie Bellon<sup>1</sup>; William Buchmann<sup>2</sup>; Florence Gonnet<sup>2</sup>; Nathalie Jarroux<sup>2</sup>; Philippe Kerouredan<sup>1</sup>; Marielle Anger-Leroy<sup>1</sup>; Regis Daniel<sup>2</sup>; <sup>1</sup>*Genoptics Bio Interactions, Orsay, France*; <sup>2</sup>*Universite d'Evry, Evry, France*
- MOG pm 03:10 **Functional Consequences of Conformational Changes in the ClpP N-Terminus and Ligand-Driven ClpA Hexamer Formation: Structural MS of a Molecular Machine;** Jen Bohon<sup>1</sup>; Laura D. Jennings<sup>2</sup>; Christine M. Phillips<sup>2</sup>; Stuart Licht<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>*Case Western Reserve University, Upton, NY*; <sup>2</sup>*Massachusetts Institute of Technology, Cambridge, MA*
- MOG pm 03:30 **Ion Mobility-Mass Spectrometry Reveals Subtle Stability Differences in Multi-Protein Complex Ligand Assemblies;** Suk-Joon Hyung; Brandon Ruotolo; Carol Robinson; *Department of Chemistry, University of Cambridge, Cambridge, UK*
- MOG pm 03:50 **A Protein-Ligand Binding Assay with Proteomic Potential;** Michael C. Fitzgerald; Graham M. West; Victor Anbalagan; Liangjie Tang; *Duke University, Durham, NC*
- MOG pm 04:10 **Temperature Dependent Cooperativity in Donor-Acceptor Substrate Binding to the Human Blood Group Glycosyltransferases;** Glen K. Shoemaker<sup>1</sup>; Naoto Soya<sup>1</sup>; Monica M Palcic<sup>2</sup>; John S Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*; <sup>2</sup>*Carlsberg Laboratory, Copenhagen, Denmark*

4:45 – 5:30 pm

**AWARD LECTURE***Wells Fargo Theatre*

- 4:45 pm **Recipient of the Award for a Distinguished Contribution in Mass Spectrometry**

<b>TUESDAY MORNING, June 3</b>
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**8:30 – 10:30 am**

**PROTEIN QUANTITATION USING LABELING**

*Wells Fargo Theatre*

Chair: Susan T. Weintraub

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- TOA am 08:30 **A perspective on protein quantitation and quantitative proteomics**; Simon J. Gaskell; *University of Manchester, Manchester, UK*
- TOA am 08:50 **How Reproducible is iTRAQ? Triplicate LC-MS-MS Analysis of Normal Colon Tissue Tryptic Peptides Labeled with iTRAQ; 4-Plex Reagents**; Leeann Higgins<sup>1</sup>; Libang Yang<sup>1</sup>; Lorraine Anderson<sup>1</sup>; Thomas F. McGowan<sup>2</sup>; Cavan S. Reilly<sup>1</sup>; Bruce Witthuhn<sup>2</sup>; Glenn R. Gourley<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*U of Mn St Paul, St Paul, MN*
- TOA am 09:10 **Rapid 18O Labeling for Quantitative Proteomics by Microwave-Assisted Enzymatic Proteolysis**; Miquel Antoine<sup>1</sup>; Nathan Hagan<sup>2</sup>; Plamen A. Demirev<sup>3</sup>; <sup>1</sup>*JHU-APL, Laurel, MD*; <sup>2</sup>*Jhu Applied Physics Laborato, Laurel, MD*; <sup>3</sup>*Johns Hopkins Univ., Laurel, MD*
- TOA am 09:30 **ANIBAL, Stable-Isotope-Based Quantitative Proteomics by ANiline and Benzoic Acid Labeling of Amino and Carboxylic Groups**; Alexandre Panchaud<sup>1</sup>; Jenny Hansson<sup>2</sup>; Michael Affolter<sup>2</sup>; Rachid Bel Rhlid<sup>2</sup>; Stéphane Piu<sup>1</sup>; Philippe Moreillon<sup>1</sup>; Martin Kussmann<sup>2</sup>; <sup>1</sup>*University of Lausanne, Lausanne, Switzerland*; <sup>2</sup>*Nestle Research Center, Lausanne, Switzerland*
- TOA am 09:50 **Development of Defined SILAC Media Conditions to Prevent Arginine to Proline Conversion**; Chris Hughes; Sean C Bendall; Gilles Lajoie; *University of Western Ontario, London, ON*
- TOA am 10:10 **High Throughput Multiplexed Absolute Protein Quantification**; Nick J Bond<sup>1</sup>; Amy E Bartlett<sup>2</sup>; Martin Welch<sup>3</sup>; Kathryn S Lilley<sup>1</sup>; <sup>1</sup>*Cambridge Center for Proteomics, Cambridge, UK*; <sup>2</sup>*Waters Corporation, Milford, MA*; <sup>3</sup>*University of Cambridge, Cambridge, UK*

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**8:30 – 10:30 am**

**STRUCTURE AND ENERGETICS OF METAL IONS REACTING WITH BIOMOLECULES**

*Korbel Ballroom 1*

Chair: Jennifer Brodbelt

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- TOB am 08:30 **The Versatility of Mass Spectrometry Applied to Metal-Biomolecule Interactions**; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TOB am 08:50 **Structure of Metal-Biomolecule Complexes Probed by Ion Mobility Methods**; Thomas Wytenbach<sup>1</sup>; Bing Gao<sup>1</sup>; Megan Grabenauer<sup>1</sup>; Dengfeng Liu<sup>1</sup>; Konstantinos Thalassinos<sup>2</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>*University of California Santa Barbara, Santa Barbara, CA*; <sup>2</sup>*University of Warwick, Coventry, UK*
- TOB am 09:10 **IRMPD Spectroscopy of Doubly Charged Metal Ion/Tryptophan Complexes**; Robert C. Dunbar<sup>1</sup>; Nicolas Polfer<sup>2</sup>; Jeffrey Steill<sup>3</sup>; Jos Oomens<sup>3</sup>; <sup>1</sup>*Case Western Reserve Univ, Cleveland, OH*; <sup>2</sup>*University of Florida, Gainesville, FL*; <sup>3</sup>*Fom Rijnhuizen, Nieuwegein, Netherlands*

- TOB am 09:30 **Structures of Hydrated Metalated DNA Bases by IRMPD Spectroscopy**; Khadijeh Rajabi; Elizabeth Gillis; Travis Fridgen; *Memorial University, St. John's, Canada*
- TOB am 09:50 **Infrared Multiphoton Dissociation Spectroscopy of Cationized Serine and Threonine: Effects of Alkali-Metal Cation Size on Gas-Phase Conformation**; Mary T. Rodgers<sup>1</sup>; Peter B. Armentrout<sup>2</sup>; Jos Oomens<sup>3</sup>; Jeffrey D. Steill<sup>3</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*University of Utah, Salt Lake City, UT*; <sup>3</sup>*Fom Rijnhuizen, Nieuwegein, Netherlands*
- TOB am 10:10 **Interaction of Lead(II) Ions with 5'-Mononucleotides: Tandem Mass Spectrometry and IRMPD Spectroscopy**; Jean-Yves Salpin<sup>1</sup>; Thierry Besson<sup>2</sup>; Joël Lemaire<sup>2</sup>; Debora Scuderi<sup>2</sup>; Sébastien Guillaumont<sup>1</sup>; Jeanine Tortajada<sup>1</sup>; <sup>1</sup>*CNRS - Université d'Evry Val d'Essonne, Evry, France*; <sup>2</sup>*CNRS- Université Paris XI, Orsay, France*

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**8:30 – 10:30 am**

**NOVEL DEVELOPMENTS IN MASS SPECTROMETRY INSTRUMENTATION**

*Korbel Ballroom 2-3*

Chair: Mark E. Bier

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- TOC am 08:30 **Application of Superconducting Detectors to Ionization Cross Section Measurements of Doubly Charged Monoisotopic Diatomic Molecules**; Shigetomo Shiki<sup>1</sup>; Masahiro Ukibe<sup>1</sup>; Masataka Ohkubo<sup>1</sup>; Yuki Sato<sup>2</sup>; Shigeo Hayakawa<sup>3</sup>; Shigeo Tomita<sup>2</sup>; <sup>1</sup>*AIST, Research inst. of Inst. Tsukuba, JAPAN*; <sup>2</sup>*University of Tsukuba, Tsukuba, Japan*; <sup>3</sup>*Osaka Prefecture University, Osaka, Japan*
- TOC am 08:50 **Current-Controlled Nanospray for the Analysis of Less than Ideal Samples**; Alexei Gapeev; Aberto Berton; Daniele Fabris; *U. Maryland Baltimore County, Baltimore, MD*
- TOC am 09:10 **Low Temperature Plasma (LTP) Probe for Ambient Desorption Ionization**; Jason D. Harper<sup>1</sup>; Nicholas A. Charipar<sup>1</sup>; Christopher C. Mulligan<sup>1</sup>; Xinrong Zhang<sup>2</sup>; R. Graham Cooks<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Tsinghua University, Beijing, China*
- TOC am 09:30 **Reverse-Taylor-Cone Electrospray Ionization for Transient Imaging in Solution**; Peter Kottke; Andrei Fedorov; F. Levent Degertekin; *Georgia Institute of Technology, Atlanta, GA*
- TOC am 09:50 **Novel MALDI Ion Trap Mass Spectrometer for Large Biomolecule Detection**; Chien-Hsun Chen; Jung-Lee Lin; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- TOC am 10:10 **Nanostructure-Initiator Mass Spectrometry for Metabolomics and Enzyme Activity Profiling**; Trent Northen<sup>1</sup>; Oscar Yanes<sup>1</sup>; Jinq-Chyi Lee<sup>1</sup>; Linh Hoang<sup>1</sup>; Anders Nordstrom<sup>2</sup>; Chi-Huey Wong<sup>1</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*Karolinska Institutet, Stockholm, Sweden*

**8:30 – 10:30 am**  
**THE ROLE OF MASS SPECTROMETRY IN THE**  
**PETROLEUM FIELD**

*Korbel Ballroom 4*

Chair: Hilikka Kenttämaa

TOD am 08:30	<b>Petroleomics: Chemistry from the Underworld;</b> <u>Ryan P. Rodgers</u> <sup>1</sup> ; Brandie Ehrmann <sup>2</sup> ; Priyanka Juyal <sup>1</sup> ; Mmilili Myles Mapolelo <sup>2</sup> ; Amy Mckenna <sup>2</sup> ; Jeremiah M. Purcell <sup>1</sup> ; Tanner M. Schaub <sup>1</sup> ; Alan G. Marshall <sup>1</sup> ; <i>Nat'l High Magnetic Field Laboratory, Tallahassee, FL</i> ; <sup>2</sup> <i>Florida State Univ, Dept of Chemistry and Biochem., Tallahassee, FL</i>
TOD am 08:50	<b>Moving towards Accurate Molecular Compositions of Petroleum Products using Ion Mobility-Mass Spectrometry;</b> <u>Christopher Becker</u> ; Francisco Alberto Fernandez Lima; David H. Russell; <i>Texas A&amp;M University, College Station, TX</i>
TOD am 09:10	<b>Analysis of Asphaltenes by Laser-Induced Acoustic Desorption/Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;</b> <u>David Pinkston</u> <sup>1</sup> ; Penggao Duan <sup>1</sup> ; Mingkun Fu <sup>1</sup> ; Steven Habicht <sup>1</sup> ; Hilikka Kenttämaa <sup>2</sup> ; <sup>1</sup> <i>Purdue University, West Lafayette, IN</i> ; <sup>2</sup> <i>Chemistry Department, West Lafayette, IN</i>
TOD am 09:30	<b>Atmospheric-Pressure-Laser-Ionization Fourier-Transform Ion Cyclotron Resonance Mass Spectrometer (APLI-FT-ICRMS): A New Approach to Analyze Non-Volatile Components from Complex Crude Oil Mixtures;</b> <u>Wolfgang Schrader</u> <sup>1</sup> ; Klaus J. Brockmann <sup>3</sup> ; Thorsten Benter <sup>3</sup> ; Saroj Panda <sup>2</sup> ; <sup>1</sup> <i>Max-Planck Inst Coal Res., Mülheim / Ruhr, Germany</i> ; <sup>2</sup> <i>Max-Planck-Institute of Coal Research, Muelheim, Germany</i> ; <sup>3</sup> <i>Bergische University of Wuppertal, Wuppertal, Germany</i>
TOD am 09:50	<b>Combining Chip-ESI with APLI (cESILI) as a Multimode Source for the Analysis of Complex Mixtures with Ultrahigh Resolution Mass Spectrometry;</b> <u>Philippe Schmitt-Kopplin</u> <sup>1</sup> ; Matthias Englmann <sup>1</sup> ; Ramon Rossello-Mora <sup>3</sup> ; Ralf Schiewek <sup>2</sup> ; Klaus Brockmann <sup>2</sup> ; Thorsten Benter <sup>2</sup> ; Oliver J Schmitz <sup>2</sup> ; <sup>1</sup> <i>Helmholtz Zentrum München, Neuherberg, Germany</i> ; <sup>2</sup> <i>University of Wuppertal, Wuppertal, Germany</i> ; <sup>3</sup> <i>Institut Mediterrani d'Estudis Avançats, Esporles, Spain</i>
TOD am 10:10	<b>Elemental Mass Spectrometry (ICP MS) Detection and µHPLC for Speciation Analysis of Metals in Petroleum;</b> <u>Guilhem Caumette</u> <sup>1</sup> ; Brice Bouyssiere <sup>1</sup> ; Isabelle Merdrignac <sup>2</sup> ; Charles-Philippe Lienemann <sup>2</sup> ; Ryszard Lobinski <sup>1</sup> ; <sup>1</sup> <i>LCABIE, Pau, France</i> ; <sup>2</sup> <i>IFP, Lyon, France</i>

**8:30 – 10:30 am**  
**DISEASE PROTEIN BIOMARKER DISCOVERY BY**  
**MASS SPECTROMETRY**

*Four Seasons Ballroom 1-2*

Chair: Thomas P. Conrads

TOE am 08:30	<b>Progress toward a Biomarker Discovery-to-Development Pipeline in Clinical Proteomics;</b> <u>Steven A. Carr</u> ; Michael Gillette; Terri Addona; Hasmik Keshishian; Michael Burgess; Veronica Saenz-Vash; Karl R. Clauser; Eric Kuhn; <i>Broad Institute, Cambridge, MA</i>
TOE am 08:50	<b>Proteomic Analysis of Lung Tumor Tissue Interstitial Fluid for Biomarker Discovery;</b> <u>Brian L. Hood</u> <sup>1</sup> ; Jennifer N. Sutton <sup>2</sup> ; Manda J.

Welsh<sup>1</sup>; Wanda Brown<sup>3</sup>; Mary F. Lopez<sup>2</sup>; James D. Luketich<sup>3</sup>; William L. Bigbee<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>*The University of Pittsburgh Cancer Institute, Pittsburgh, PA*; <sup>2</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>3</sup>*The University of Pittsburgh, Pittsburgh, PA*

TOE am 09:10	<b>Using Proteomic Tools to Identify Markers of Fatty Liver Disease;</b> <u>Julie Weisz</u> <sup>2</sup> ; Kathleen Grant <sup>2</sup> ; Hidekazu Tsukamoto <sup>1</sup> ; Christine Wu <sup>2</sup> ; <sup>1</sup> <i>UCLA, Los Angeles, CA</i> ; <sup>2</sup> <i>University of Colorado, Aurora, CO</i>
TOE am 09:30	<b>Processing of Urinary Proteins as Biomarkers for Diabetic Complications;</b> <u>Daniela M Schlatter</u> <sup>1</sup> ; George Christ <sup>2</sup> ; Jean-Eudes Dazard <sup>1</sup> ; Rob Ewing <sup>1</sup> ; Sergei Ilchenko <sup>1</sup> ; Mark Chance <sup>1</sup> ; <sup>1</sup> <i>Case Western Reserve University, Cleveland, OH</i> ; <sup>2</sup> <i>Wake Forest University School of Medicine, Winston-Salem, NC</i>
TOE am 09:50	<b>Combining MALDI FTMS, Comparative Glycoproteomics, and Bioinformatics for the Discovery of Biomarkers in Prion Disease;</b> <u>Lingjun Li</u> ; Xin Wei; Allen Herbst; Sean McIlwain; Joshua Schmidt; Robert Cunningham; David Page; Judd Aiken; <i>University of Wisconsin, Madison, WI</i>
TOE am 10:10	<b>Absolute Protein Quantitation for Biomarker Studies in Cancer Cell Lines: Discovery, Verification, and Database Compilation;</b> Will Thompson <sup>1</sup> ; Scott Geromanos <sup>2</sup> ; Catalin Doneanu <sup>2</sup> ; Martha Staples <sup>2</sup> ; Neil Spector <sup>1</sup> ; Wenle Xia <sup>1</sup> ; <u>Arthur Moseley</u> <sup>1</sup> ; <sup>1</sup> <i>Duke University Medical Center, Durham, NC</i> ; <sup>2</sup> <i>Waters Corporation, Milford, MA</i>

**8:30 – 10:30 am**  
**IDENTIFICATION OF REACTIVE METABOLITES IN**  
**DRUG DISCOVERY: SIGNIFICANCE OF MASS**  
**SPECTROMETRY TOWARDS DETECTION**

*Four Seasons Ballroom 3-4*

Chair: Elizabeth M. Joshi

TOF am 08:30	<b>High-Throughput Screening and Characterization of Reactive Metabolites using Polarity Switching of Hybrid Triple Quadrupole Linear Ion Trap Mass Spectrometry;</b> <u>Bo Wen</u> <sup>1</sup> ; William L Fitch <sup>1</sup> ; Li Ma <sup>2</sup> ; Mingshe Zhu <sup>2</sup> ; Sidney D. Nelson <sup>3</sup> ; <sup>1</sup> <i>Roche Palo Alto, Palo Alto, CA</i> ; <sup>2</sup> <i>Bristol-Myers Squibb, Princeton, NJ</i> ; <sup>3</sup> <i>University of Washington, Seattle, WA</i>
TOF am 08:50	<b>UHPLC-MS-MS with On-Line Fraction Collection in Glass Coated Plates: Advantages for Reactive Metabolite Profiling in the Drug Development Process;</b> <u>Simon J. Prosser</u> ; Daniel Eikel; <i>Advion BioSystems, Ithaca, NY</i>
TOF am 09:10	<b>Generation and Identification of Reactive Metabolites and Protein Adducts by Electrochemistry Coupled On-Line to Liquid Chromatography/Mass Spectrometry;</b> <u>Uwe Karst</u> ; Wiebke Lohmann; <i>University of Münster, Münster, Germany</i>
TOF am 09:30	<b>Detection and Identification of Depurinating DNA Adducts by Electrophilic Metabolites of p-Cresol and its Related 4-Alkylphenols from Prempro;</b> <u>Long Yuan</u> ; Judy L. Bolton; Richard B. van Breemen; <i>University of Illinois, College of Pharmacy, Chicago, IL</i>
TOF am 09:50	<b>Ultra-Sensitive Glutathione Conjugate Screening in Biological Samples using Accurate</b>

**Mass Measurement;** Sean Yu; Philip Tiller; Donghui (dan) Cui; Thomas A. Baillie; *Merck & Co., West Point, PA*

TOF am 10:10 **A Novel Methodology for Screening Reactive Metabolites using Isotope Pattern Filtering of High Resolution Mass Spectrometry Data;** Qian Ruan<sup>1</sup>; Marco Ruijken<sup>2</sup>; Mingshe Zhu<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*Msmatrix, Maarssen, Netherlands*

8:30 – 10:30 am

**BIOLOGICAL APPLICATIONS OF CHEMICAL CROSS LINKING**

*Rooms 601-607*

Chair: Andrea Sinz

TOG am 08:30 **Ionic Cross-Linking Reagents and Multistage Tandem Mass Spectrometry for Mapping Protein-Protein Interactions;** Yali Lu; Marina Tanasova; Babak Borhan; Gavin E. Reid; *Michigan State University, East Lansing, MI*

TOG am 08:50 **Novel Collision-Induced Dissociative Chemical Crosslinking Reagents and Methodology to Characterize Protein-Protein Interactions using Tandem Mass Spectrometry;** Erik J. Soderblom; Michael B. Goshe; *NC State University, Raleigh, NC*

TOG am 09:10 **Novel Subunit Specific Protein Footprinting Method Reveals HIV Integrase Contacts with Viral DNA;** Zhuojun Zhao; Christopher McKee; Jacques Kessl; Jocelyn Norris; Nick Shkriabai; Mamuka Kvaratskhelia; *The Ohio State University, Columbus, OH*

TOG am 09:30 **Profiling Protein-Protein Interactions *in vivo* by Cross-Linking and Mass Spectrometry;** Saiful M. Chowdhury<sup>1</sup>; Liang Shi<sup>1</sup>; Xiuxia Du<sup>1</sup>; Uljana M. Mayer-Cumblidge<sup>1</sup>; Nikola Tolic<sup>1</sup>; Yoon Hyunjin<sup>2</sup>; Ronald J. Moore<sup>1</sup>; Norbeck D. Angela<sup>1</sup>; Fred Heffron<sup>2</sup>; <sup>1</sup>*Pacific North West National Laboratory, Richland, WA*; <sup>2</sup>*Oregon Health & Science University, Portland, OR*

TOG am 09:50 **Identification of Cross-Linked Peptides in Proteomic-Scale Experiments;** Morten Rasmussen; Salman Tahir; Zhuo Chen; Juri Rappsilber; *Wellcome Trust Centre for Cell Biology, Edinburgh, UK*

TOG am 10:10 **Identification of Cross Linked Peptides by an “Open-Modification” Search Tool;** Pragya Singh<sup>1</sup>; Scott A. Shaffer<sup>1</sup>; Alexander Scherl<sup>1</sup>; Ted L. Freeman<sup>1</sup>; Carole Holman<sup>1</sup>; Richard A. Pfuetzner<sup>1</sup>; Samuel I. Miller<sup>1</sup>; Patricia Hernandez<sup>2</sup>; Ron D; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Swiss Institute of Bioinformatics, Geneva, Switzerland*

**TUESDAY AFTERNOON**

2:30 – 4:30 pm

**THE ROLE OF MASS SPECTROMETRY IN UNDERSTANDING CELLULAR PATHWAYS**

*Wells Fargo Theatre*

Chair: Rong Wang

TOA pm 02:30 **Charting Cellular Pathways and Networks using Mass Spectrometry;** Lan Huang; *University of California, Irvine, CA*

TOA pm 02:50 **Proteomic Insights Into Autophagosomal Composition;** Joern Dengjel<sup>1</sup>; Maria Hoyer-Hansen<sup>2</sup>; Soeren Schandorff<sup>1</sup>; Anders Kristensen<sup>1</sup>; Jakob Bunkenborg<sup>1</sup>; Marja Jaattela<sup>2</sup>; Jens S. Andersen<sup>1</sup>; <sup>1</sup>*Center of Experimental Bioinformatics, Odense, Denmark*; <sup>2</sup>*Danisch Cancer Society, Copenhagen, Denmark*

TOA pm 03:10 **Protein Profiling of Specific Synapses in Specific Cell Types in the Mammalian Brain;** Ileana M. Cristea<sup>2</sup>; Fekrije Selimi<sup>1</sup>; Elizabeth Heller<sup>1</sup>; Nathaniel Heintz<sup>1</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>*Rockefeller University, New York, NY*; <sup>2</sup>*Princeton University, Princeton, NJ*

TOA pm 03:30 **An Integrated Mouse Genetic-Proteomic Approach to Uncover and Characterize Novel Protein Complexes and Their Involved Cellular Pathways in Living Animals;** Qingjun Wang<sup>1</sup>; Yun Zhong<sup>1</sup>; Xianting Li<sup>2</sup>; Nathaniel Heintz<sup>1</sup>; Zhenyu Yue<sup>2</sup>; Brian Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*Mount Sinai School of Medicine, New York, NY*

TOA pm 03:50 **Protein and Phosphorylation Expression at the Synapse;** Jonathan C. Trinidad<sup>1</sup>; Agnes Thalhammer<sup>2</sup>; Aenoch J Lynn<sup>1</sup>; Peter Baker<sup>1</sup>; Ralf Schoepfer<sup>2</sup>; Alma L Burlingame<sup>1</sup>; <sup>1</sup>*University of California, San Francisco, San Francisco, CA*; <sup>2</sup>*University College London, London, UK*

TOA pm 04:10 **Signaling Pathways Driving the Differentiation of Neural Stem Cells;** Judit Villen; Nuria de la Iglesia; Corey E Bakalarski; Steven Gygi; *Harvard Medical School, Boston, MA*

2:30 – 4:30 pm

**FUNDAMENTALS OF ION/SURFACE INTERACTIONS**

*Korbel Ballroom 1*

Chair: Vicki H. Wysocki

TOB pm 02:30 **Deciphering Protein-Protein Assemblies: Just Hitting the Surface;** Christopher Jones<sup>1</sup>; Richard Beardsley<sup>2</sup>; Asiri Galhena<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*University of Arizona, Tucson, AZ*; <sup>2</sup>*Hoffman-la Roche, Nutley, NJ*

TOB pm 02:50 **Immobilization of a-Helical Peptides on Self-Assembled Monolayer Surfaces using Soft-Landing and Reactive Landing of Mass-Selected Ions;** Peng Wang; Julia Laskin; *Pacific Northwest National Laboratory, Richland, WA*

TOB pm 03:10 **Reactive and Soft Landing of Horseradish Peroxidase Cations on *in situ* Plasma Treated Dry Metal Surfaces;** Matthew Diener<sup>1</sup>; Michael Volny<sup>2</sup>; Karl E. Jackson<sup>1</sup>; W.T. Elam<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Purdue University, Lafayette, IN*

TOB pm 03:30 **Control of Chemical Bond Scission by Site-Specific Core Excitation of Ester Terminated Self-Assembled Monolayer;** Shin-ichi Wada; Tetsuji Sekitani; Kenichiro Tanaka; *Hiroshima University, Higashi-Hiroshima, Japan*



TOB pm 03:50	<b>Directed Energy Deposition in Laser Desorption Ionization from Laser-Induced Silicon Microcolumn Arrays;</b> <u>Bennett N Walker</u> <sup>1</sup> ; Trust Razunguzwa <sup>2</sup> ; Matthew Powell <sup>3</sup> ; Richard Knochenmuss <sup>4</sup> ; Akos Vertes <sup>5</sup> ; <sup>1</sup> GWU, Washington, DC; <sup>2</sup> Protea Biosciences, Morgantown, WV; <sup>3</sup> Protea Biosciences, Morgantown, WV; <sup>4</sup> Novartis, Basel, Switzerland; <sup>5</sup> George Washington University, Washington, DC	TOD pm 03:10	<b>Identification of New Biodegradation Products of Atenolol and Glibenclamide in Sewage Sludge by UPLC-QqToF and HPLC-QqLIT;</b> <u>Damia Barcelo</u> <sup>1</sup> ; Mira Petrovic <sup>2</sup> ; Jelena Radjenovic <sup>1</sup> ; <sup>1</sup> Ministerio de Ciencia y Tecnologia, Barcelona, Spain; <sup>2</sup> Catalan Institution for Research & Advanced Study, Barcelona, Spain
TOB pm 04:10	<b>SIMS on Nano-Objects: Evidence of Sample Size Dependent Secondary Ion Response;</b> <u>Veronica T. Pinnick</u> ; Sidhartharaja Rajagopalachary; Stanislav V. Verkhoturov; Emile A. Schweikert; Texas A&M, College Station, TX	TOD pm 03:30	<b>Illicit Drugs from Wastewaters to Tap Water?: An UPLC-MS-MS Study;</b> <u>Maria Huerta</u> ; Dra.M <sup>a</sup> Teresa Galceran; Dr. Francesc Ventura; <i>Aigües de Barcelona, University of Barcelona, Barcelona, Spain</i>
<b>2:30 – 4:30 pm</b> <b>DEVELOPMENTS IN TOF</b> <i>Korbel Ballroom 2-3</i> Chair: Michael Karas		TOD pm 03:50	<b>Determination of Steroid Hormones in Environmental Samples by GC-MS-MS with Isotope Dilution;</b> <u>James L. Gray</u> ; William T. Foreman; Chris E. Lindley; Larry B. Barber; <i>US Geological Survey, Denver, CO</i>
TOC pm 02:30	<b>New MALDI-TOF MS with Very High Resolving Power and Mass Accuracy;</b> <u>Marvin Vestal</u> <sup>1</sup> ; Kevin Hayden <sup>2</sup> ; <sup>1</sup> Virgin Instruments Corp., Sudbury, MA; <sup>2</sup> Virgin Instruments Corporation, Sudbury, MA	TOD pm 04:10	<b>Analysis of Emerging Contaminants in Drinking Water by On-Line SPE/LC-MS-MS;</b> Claude Mallet; <i>Waters Corporation, Milford, MA</i>
TOC pm 02:50	<b>Automated de novo Sequencing of Complex Peptide Mixtures by LC-MALDI-Photodissociation TOF-TOF Mass Spectrometry;</b> <u>Liangyi Zhang</u> ; William R Alley; William Running; James P. Reilly; <i>Indiana university, Bloomington, IN</i>	<b>2:30 – 4:30 pm</b> <b>H/D EXCHANGE AND PROTEIN FOLDING</b> <i>Four Seasons Ballroom 1-2</i> Chair: Lars Konermann	
TOC pm 03:10	<b>Accessing Collision Energies of up to 500V per Charge on a QqTOF Instrument: Structure Characterization of Fullerenes and Large Peptides;</b> Suzanne Ackloo; Igor Chernushevich; Alexandre Loboda; Robert E. Haufler; <u>Bruce Thomson</u> ; <i>MDS Analytical Technologies, Concord, Canada</i>	TOE pm 02:30	<b>Resolving Protein Folding Mechanisms with Mass Spectrometry;</b> Patrick Wintrode; <i>Case Western Reserve University, Cleveland, OH</i>
TOC pm 03:30	<b>Development of a New API-Qq-TOF Mass Spectrometer with Ultra-High Mass Resolution and Mass Accuracy at High Scan Speed;</b> Oliver Raether <sup>1</sup> ; Melvin A. Park <sup>2</sup> ; Suetering Juergen <sup>1</sup> ; Stoermer Carsten <sup>1</sup> ; Sebastian Goetz <sup>1</sup> ; Markus Lubeck <sup>1</sup> ; Armin Holle <sup>1</sup> ; Michael Schubert <sup>1</sup> ; <u>Carsten Baes</u> ; <sup>1</sup> Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup> Bruker Daltonics, Inc., Billerica, MA	TOE pm 02:50	<b>Probing the Conformation and Dynamics of a Monoclonal Antibody by Hydrogen-Deuterium Exchange Mass Spectrometry;</b> <u>Damian Houde</u> <sup>2</sup> ; Steven Berkowitz <sup>2</sup> ; Marek Kloczewiak <sup>2</sup> ; Rohin Mhatre <sup>2</sup> ; Thomas Wales <sup>1</sup> ; John R. Engen <sup>1</sup> ; <sup>1</sup> Northeastern University, Boston, MA; <sup>2</sup> Biogen Idec, Inc., Cambridge, MA
TOC pm 03:50	<b>Effects of Background Gas Type and Pressure on the Fragmentation of Laser-Generated Ions in an Elevated Pressure MALDI Ion Source;</b> <u>Jens Soltwisch</u> <sup>1</sup> ; Stefan Berkenkamp <sup>2</sup> ; Klaus Dreisewerd <sup>1</sup> ; <sup>1</sup> University of Muenster, Muenster, Germany; <sup>2</sup> Sequenom, Hamburg, Germany	TOE pm 03:10	<b>Conformational Dynamics of Hsp90 Chaperones Measured by Amide Hydrogen Exchange Mass Spectrometry;</b> Christian Graf; Marta Stankiewicz; Günter Kramer; <u>Matthias P. Mayer</u> ; <i>Zentrum für Molekulare Biologie der Universität He, Heidelberg, Germany</i>
TOC pm 04:10	<b>Nanosecond Time-Resolved Ion Imaging System;</b> <u>James Milnes</u> <sup>1</sup> ; Panagiotis Kapentanopoulos <sup>2</sup> ; <sup>1</sup> Photek Ltd, St Leonards on Sea, UK; <sup>2</sup> University of Leeds, Leeds, UK	TOE pm 03:30	<b>Conformational Consequences of Covalent Modification of Protein Pharmaceuticals Under Stress-Like Conditions: ESI MS Study of Interferon Beta;</b> Cedric Bobst <sup>1</sup> ; Rinat R. Abzalimov <sup>1</sup> ; Damian Houde <sup>2</sup> ; Steven A. Berkowitz <sup>2</sup> ; <u>Igor A. Kaltashov</u> <sup>1</sup> ; <sup>1</sup> University of Massachuset, Amherst, MA; <sup>2</sup> Biogen Idec, Inc., Cambridge, MA
<b>2:30 – 4:30 pm</b> <b>PHARMACEUTICAL DRUGS AS ENVIRONMENTAL POLLUTANTS</b> <i>Korbel Ballroom 4</i> Chair: Edward T. Furlong		TOE pm 03:50	<b>Structural Mechanism of HK97 Capsid Expansion Monitored by X-Ray Crystallography and Hydrogen Deuterium Exchange Coupled with Mass Spectrometry;</b> <u>Ilya Gertsman</u> ; Jack Johnson; <i>Scripps Research Institute, La Jolla, CA</i>
TOD pm 02:30	<b>Pharmaceuticals as Environmental Pollutants: Issues Regarding Analysis;</b> Tammy L Jones-Lepp; <i>U.S. Environmental Protection Agency, Las Vegas, NV</i>	TOE pm 04:10	<b>Are the Conformational Dynamics of Enzymes Enhanced During Catalytic Turnover? A Hydrogen/Deuterium Exchange ESI-MS Study;</b> <u>Yu-Hong Liu</u> ; Lars Konermann; <i>The University of Western Ontario, London, Canada</i>
TOD pm 02:50	<b>Direct, Trace Level, Environmental Drug Residues Analysis by Orbitrap MS;</b> <u>Enrico Davoli</u> ; Sara Casigliani; Renzo Bagnati;		

<b>2:30 – 4:30 pm</b>	
<b>BIOMARKER APPLICATIONS IN THE CLINICAL SETTING</b>	
<i>Four Seasons Ballroom 3-4</i>	
Chair: Timothy D. Veenstra	
TOF pm 02:30	<b>Prognostic Significance of Head-and-Neck Cancer Biomarkers Previously Discovered and Identified Using iTRAQ-Labeling and Multidimensional Liquid Chromatography – Tandem Mass Spectrometry;</b> Ajay Matta <sup>1</sup> ; Leroi Desouza <sup>1</sup> ; Nootan Kumar Shukla <sup>2</sup> ; Siddhartha D. Gupta <sup>2</sup> ; Ranju Ralhan <sup>1</sup> ; <u>K W Michael Siu</u> <sup>1</sup> ; <sup>1</sup> York University, Toronto, Canada; <sup>2</sup> All India Institute of Medical Sciences, New Delhi, India
TOF pm 02:50	<b>Concurrent Proteomic Profiling of Human Tissues and Peripheral Blood Specimens for Cancer Biomarker Discovery;</b> DaRue A. Prieto <sup>1</sup> ; Donald J. Johann Jr. <sup>2</sup> ; Paul A. Rudnick <sup>3</sup> ; King C. Chan <sup>1</sup> ; Xiaoying Ye <sup>1</sup> ; Zhen Xiao <sup>1</sup> ; Stephen E. Stein <sup>3</sup> ; Haleem J. Issaq <sup>1</sup> ; <u>Josip Blonder</u> <sup>1</sup> ; <sup>1</sup> SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup> NIH, Bethesda, MD; <sup>3</sup> NIST, Gaithersburg, MD
TOF pm 03:10	<b>Evaluation of Performance Characteristics of Peptide Immunoaffinity Enrichment for Protein Quantitation using a Panel of Candidate Cancer Biomarkers;</b> <u>Jeffrey Whiteaker</u> ; Lei Zhao; Travis Lorentzen; Amanda Paulovich; <i>Fred Hutchinson Cancer Research Center, Seattle, WA</i>
TOF pm 03:30	<b>A Lectin Glyco-Array Platform for Biomarker Discovery in Colon Cancer;</b> <u>David M. Lubman</u> ; Yinghua Qiu; Kerby Shedden; Tasneem H Patwa; Dean Brenner; <i>University of Michigan, Ann Arbor, MI</i>
TOF pm 03:50	<b>Breath Analysis as a Method for Breast Cancer Detection;</b> <u>Charlene Bayer</u> <sup>1</sup> ; Sheryl G. Grabram <sup>3</sup> ; Brani Vidakovic <sup>2</sup> ; Robert J. Hendry <sup>1</sup> ; Boris Mizaikoff <sup>4</sup> ; <sup>1</sup> Georgia Tech Research Institute, Atlanta, GA; <sup>2</sup> Georgia Institute of Technology, Atlanta, GA; <sup>3</sup> Emory University School of Medicine, Atlanta, GA; <sup>4</sup> University of Ulm, Ulm, Germany
TOF pm 04:10	<b>Identification and Validation of a Tamoxifen Therapy-Response Protein Profile in Breast Cancer by nanoLC-FTICR MS;</b> <u>Arzu Umar</u> <sup>1</sup> ; Hyuk Kang <sup>2</sup> ; Robert-Jan Lamers <sup>3</sup> ; Marion E. Meijer-van Gelder <sup>3</sup> ; A. Mieke Timmermans <sup>1</sup> ; Theo M Luiders <sup>3</sup> ; John A Foekens <sup>1</sup> ; Ljiljana Pasa-Tolic <sup>4</sup> ; <sup>1</sup> Josephine Nefkens Institute, Medical Oncology, Rotterdam, Netherlands; <sup>2</sup> Ajou University, Suwon, Korea; <sup>3</sup> Erasmusmc, Rotterdam, Netherlands; <sup>4</sup> Pacific Nw Nat'l Lab, Richland, WA
<b>2:30 – 4:30 pm</b>	
<b>ADVANCES IN THE CHARACTERIZATION OF GLYCOPROTEINS</b>	
<i>Rooms 601-607</i>	
Chair: Douglas M. Sheeley	
TOG pm 02:30	<b>IDAAG: in vivo Isotopic Labeling of Glycans for Comparative Glycomics/Glycoproteomics;</b> <u>Ron Orlando</u> ; Lei Cheng; Gerardo Alvarez-Manilla; James A Atwood III; Kelley Moremen; Michael Pierce; Michael Tiemeyer; Stephen Dalton; Lance Wells; <i>University of Georgia, Athens, GA</i>
TOG pm 02:50	<b>Tags with a Unique Isotopic Signature for Glycoprotein Identification and Quantitation</b>
TOG pm 03:10	<b>Integrated Methodology for Proteomics Analysis of Glycoproteins;</b> <u>Christine Carapito</u> ; Lukas Mueller; Clementine Klemm; Ruedi Aebersold; Bruno Domon; <i>Institute of Molecular Systems Biology, Zurich, Switzerland</i>
TOG pm 03:30	<b>Dynamic Analysis of Protein N-glycosylations in Complex Samples using Liquid Chromatography Tandem Mass Spectrometry;</b> <u>Yin Wu</u> ; Haixu Tang; Yehia Mechref; Iveta Klouckova; Milos Novotny; <i>Indiana University, Bloomington, IN</i>
TOG pm 03:50	<b>Differential Analysis of Influenza Hemagglutinin Glycosylation by LC-MS-MS;</b> <u>Thomas A. Blake</u> ; Tracie L. Williams; James L. Pirkle; John R. Barr; <i>Centers for Disease Control and Prevention, Atlanta, GA</i>
TOG pm 04:10	<b>Mining the Plasma Glycoproteome for Epithelial Ovarian Cancer Biomarker Discovery;</b> <u>Taufika Islam Williams</u> <sup>1</sup> ; William A. Cliby <sup>2</sup> ; Kimberly R. Kalli <sup>2</sup> ; David C. Muddiman <sup>1</sup> ; <sup>1</sup> North Carolina State University, Raleigh, NC; <sup>2</sup> Department of Obstetrics & Gynecology, Mayo Clinic, Rochester, MN
<b>4:45 – 5:30 pm</b>	
<b>AWARD LECTURE</b>	
<i>Wells Fargo Theatre</i>	
4:45 pm	<b>Recipient of the Biemann Medal</b>
<b>WEDNESDAY MORNING, June 4</b>	
<b>8:30 – 10:30 am</b>	
<b>NEW APPROACHES TO METABOLOMICS</b>	
<i>Wells Fargo Theatre</i>	
Chair: Gary Siuzdak	
WOA am 08:30	<b>Structural Annotation of Small Molecules by Mass Spectral Libraries, Substructure Information and Accurate Mass GC-MS Data;</b> <u>Tobias Kind</u> ; Gert Wohlgemuth; Yun Lu; Mine Palazoglu; Martin Scholz; Oliver Fiehn; <i>UC Davis - Metabolomics, Davis, CA</i>
WOA am 08:50	<b>Spatially Resolved and Integrated Transcriptomics, Proteomics, and Metabolomics of Medicago Border Cells;</b> <u>Lloyd W. Sumner</u> <sup>1</sup> ; Bonnie S. Watson <sup>1</sup> ; Ewa Urbanczyk-Wochniak <sup>1</sup> ; David V. Huhman <sup>1</sup> ; Cesar M. Moreira <sup>2</sup> ; <sup>1</sup> The Noble Foundation, Ardmore, OK; <sup>2</sup> University of Florida, Gainesville, FL
WOA am 09:10	<b>mzROCK: Automating Analysis of Targeted Metabolomics Data;</b> <u>Eugene Melamud</u> ; Joshua D. Rabinowitz; <i>Princeton University, Princeton, NJ</i>
WOA am 09:30	<b>Neurometabolomics a cell at a time;</b> <u>Jonathan Sweedler</u> ; Theodore E. Lapainis; Stanislav Rubakhin; <i>University of Illinois, Urbana, IL</i>
WOA am 09:50	<b>A High Throughput and Exhaustive Analysis of Diverse Lipids by using Supercritical Fluid Chromatography - Mass Spectrometry for Metabolomics;</b> <u>Takeshi Bamba</u> ; Atsuki Matsubara; Kazumasa Hirata; Eiichiro Fukusaki; <i>Osaka University, Suita, Japan</i>

WOA am 10:10 **Novel Global, Non-Targeted Metabolomics Platform Utilizing UPLC and MS-MS Spectral Library Matching for Rapid Compound Identification;** Anne Evans; Tom Barrett; Matthew W. Mitchell; Michael V. Milburn; Eric Milgram; *Metabolon, Inc., Durham, NC*

**8:30 – 10:30 am**

**FUNDAMENTALS AND APPLICATIONS OF ION ACTIVATION; ALTERNATIVES TO CID**

*Korbel Ballroom 1*

Chair: Karinna Campbell

WOB am 08:30 **Intercluster Chemistry of Cationic Betaine Clusters Upon Collision Induced Dissociation and Electron Induced Dissociation;** Linda Feketeová; George N. Khairallah; Richard A. J. O'hair; *Bio21 Institute, The University of Melbourne, Victoria, Australia*

WOB am 08:50 **Peptide Fragmentation Induced by Low Temperature Plasma Activated Surface;** Yu Xia; Zheng Ouyang; R. Graham Cooks; *Purdue University, West Lafayette, IN*

WOB am 09:10 **[60]Fullerene Complexes and Fullerene Reversible Hydrogenation Studies in the Gas Phase;** Jean-Francois Greisch<sup>1</sup>; Edwin De Pauw<sup>2</sup>; <sup>1</sup>*University of Liège, Liège, Belgium*; <sup>2</sup>*Liege University, Liege, BELGIUM*

WOB am 09:30 **Kinetics of Surface-Induced Dissociation (SID) of N(CH<sub>3</sub>)<sub>4</sub><sup>+</sup>, N(CD<sub>3</sub>)<sub>4</sub><sup>+</sup>, and Substituted Benzyl-Pyridinium Ions using Silicon Nanoparticle Assisted Laser Desorption/Ionization (SPALDI);** Sung Hwan Yoon<sup>1</sup>; Chaminda M. Gamage<sup>2</sup>; Kent Gillig<sup>3</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*University of Arizona, Tucson, AZ*; <sup>2</sup>*Masstech, Inc., Columbia, MD*; <sup>3</sup>*Texas A&M University, College Station, TX*

WOB am 09:50 **Characterization of ECD of Multiply Charged Proteolytic Peptides from Lys N, Lys C and Glu-C Digestion;** Anastasia Kalli; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*

WOB am 10:10 **Enhancement of Photodissociation in a Quadrupole Ion Trap by Selective Derivatization Strategies;** Jennifer Brodbelt; Jeff Wilson; Lisa A Vasicek; *The University of Texas, Austin, TX*

**8:30 – 10:30 am**

**NEW DEVELOPMENTS IN HYBRID MS-MS INSTRUMENTS**

*Korbel Ballroom 2-3*

Chair: Christie G. Enke

WOC am 08:30 **Parts-per-Billion Mass Accuracy for Proteomic Studies: Toward Zero Mass Error with Broadband FT-ICR MS Analysis;** Jeremiah Tipton; Tanner M. Schaub; Chris Hendrickson; Alan G. Marshall; *National High Magnetic Field Laboratory, Tallahassee, FL*

WOC am 08:50 **Electron Capture Dissociation in a Radio Frequency Ion Trap versus a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer;** Jared M. Bushey<sup>1</sup>; Takashi Baba<sup>2</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*University of North Carolina and Hitachi, Ltd., Tokyo, Japan*

WOC am 09:10 **MALDI Produced Ions Inspected with a Linear Ion Trap - Orbitrap Mass Analyzer;** Kerstin Strupat<sup>1</sup>; Huy Bui<sup>2</sup>; Viatcheslav V. Kovtoun<sup>2</sup>; Rosa Viner<sup>2</sup>; Maria C. Prieto

Conaway<sup>2</sup>; Nick Izgarian<sup>2</sup>; Oliver Lange<sup>1</sup>; George Stafford<sup>2</sup>; Ste; <sup>1</sup>*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*

WOC am 09:30 **Decision Tree-Driven Tandem Mass Spectrometry for Shotgun Proteomics;** Danielle L Swaney; Graeme Mcalister; Joshua J. Coon; *University of Wisconsin, Madison, WI*

WOC am 09:50 **Using Dynamic Ejection of High Abundance Ions to Enhance the Dynamic Range of LTQ-FT Proteomics Measurements;** Errol Robinson; Mikhail Belov; Andrei Liyu; David Prior; Richard D. Smith; *PNNL / Battelle Northwest, Richland, WA*

WOC am 10:10 **Alignment and Combination of LC-MS and LC-MS-MS Datasets in Bottom-Up Proteomics;** Magnus Palmblad; Yuri E van der Burgt; André M Deelder; *Leiden University Medical Center, Leiden, Netherlands*

**8:30 – 10:30 am**

**IMAGING OF POLYMERS/MATERIALS AND SURFACES**

*Korbel Ballroom 4*

Chair: Mark Arnold

WOD am 08:30 **Imaging Samples via Molecular Printing;** Fiona Plows; Mariana Rusa; Vanitha Thulasiraman; Steven Gu; Steve Roth; *Bio-Rad Laboratories, Inc., Fremont, CA*

WOD am 08:50 **Bringing Imaging Mass Spectrometry from Biology to Synthetics;** Leendert A. Klerk<sup>1</sup>; Patricia Y.W. Dankers<sup>2</sup>; Gert B. Eijkel<sup>1</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM Inst. for Atomic and Molecular Physics AMOLF, Amsterdam, Netherlands*; <sup>2</sup>*University Medical Center Groningen, Groningen, Netherlands*

WOD am 09:10 **PDMS Transfer in Microcontact Printing as a Contrast Agent for TOF-SIMS Imaging;** Li Yang<sup>1</sup>; Naoto Shirahata<sup>2</sup>; Matthew Linford<sup>1</sup>; <sup>1</sup>*Brigham Young University, Provo, UT*; <sup>2</sup>*National Institute for Materials Science, Tsukuba, Japan*

WOD am 09:30 **Construction of Complex Two- and Three-Dimensional Molecular Devices: Combined Time-of-Flight Secondary Ion Mass Spectrometry and Electron Microscopy Studies;** Chuanzhen Zhou; Brian Reale; Peng Lu; Amy V. Walker; *Washington University in St. Louis, St. Louis, MO*

WOD am 09:50 **Human Fingerprint Imaging by Direct Laser Desorption Mass Spectrometry;** Andrew B. Feldman; Nathan Hagan; Jeffrey S. Lin; Plamen A. Demirev; *Johns Hopkins Univ., Laurel, MD*

WOD am 10:10 **Functional Nanomaterial Arrays for Imaging LDI-MS of Biomolecules and Pharmaceuticals;** Edward T Castellana; Stacy Sherrod; David H. Russell; *Texas A&M University, College Station, TX*

**8:30 – 10:30 am**

**LC-MS TECHNIQUES FOR DISCOVERING BIOMARKERS OF TOXICITY AND EFFICACY**

*Four Seasons Ballroom 1-2*

Chair: Amanda Paulovich

WOE am 08:30 **Discovery and Translation of Biomarkers for Early Clinical Development Studies;** Scott D. Patterson; *Amgen Inc., Thousand Oaks, CA*

WOE am 08:50 **Proteomics: From Basic Research to the Clinic;** Ronald Hendrickson; *Merck Research Laboratories, Rahway, NJ*

- WOE am 09:10 **Protein Damage by Reactive Electrophiles and its Consequences**; Jeremy S Myers; Hansen L. Wong; Simona G. Codreanu; Chris R. Orton; Daniel C. Liebler; *Vanderbilt Univ. School of Medicine, Nashville, TN*
- WOE am 09:30 **Targeted and Robust Analysis of the Plasma Metabolome using Automated Sample Preparation and Fast Fia-Ms Detection**; Wolfgang Guggenbichler; Carmen Burgmeier; Bernd Haas; Steven Ramsay; Klaus M. Weinberger; Sascha Dammeier; *Biocrates Life Sciences AG, Innsbruck, Austria*
- WOE am 09:50 **A Novel UPLC-MS Approach for the Investigation of Galactosamine-Mediated Liver Damage through Specific Serum Bile Acid Changes**; Elizabeth J Want<sup>1</sup>; Muireann Coen<sup>1</sup>; Michael Reily<sup>2</sup>; Donald Robertson<sup>2</sup>; John Lindon<sup>1</sup>; Elaine Holmes<sup>1</sup>; Jeremy Nicholson<sup>1</sup>; <sup>1</sup>*Imperial College, London, UK*; <sup>2</sup>*Bristol-Myers Squibb, Princeton, NJ*
- WOE am 10:10 **Monitoring Changes in Drug-to-Antibody Ratio Distributions of Antibody Drug Conjugates *in vivo* by Affinity Mass Spectrometry**; Keyang Xu; Luna Liu; Ola M. Saad; Ben Shen; Douglas Leipold; Kelly Flagella; Surinder Kaur; *Genentech, Inc., South San Francisco, CA*

8:30 – 10:30 am

**PROTEIN GAS PHASE STRUCTURE***Four Seasons Ballroom 3-4*

Chair: Yury Tsybin

- WOF am 08:30 **From Solution to Gas Phase: How Protein Structure Evolves after Desolvation**; Kathrin Breuker<sup>1</sup>; Michal Z. Steinberg<sup>2</sup>; R. Benny Gerber<sup>2</sup>; Fred W. McLafferty<sup>3</sup>; <sup>1</sup>*University of Innsbruck, Innsbruck, Austria*; <sup>2</sup>*Hebrew University, Jerusalem, Israel*; <sup>3</sup>*Cornell University, Ithaca, NY*
- WOF am 08:50 **Gas Phase Protein Structure: Biological Significance and Comparison with X-Ray and NMR Measurements**; James Scrivens; Konstantinos Thalassinou; Charlotte Scarff; Gillian Hilton; Vibhuti Patel; *University of Warwick, Coventry, UK*
- WOF am 09:10 **Structural and Functional Analysis of Viral Protein Complexes by Native Mass Spectrometry**; Esther Van Duijn; Charlotte Utrecht; Arjan Barendregt; Kristina Lorenzen; Albert Heck; *Utrecht University, Utrecht, Netherlands*
- WOF am 09:30 **Fluorescence Quenching Mechanism of Dye-Derivatized Peptides: Experiment and Simulation**; Joel H Parks; Xiangguo Shi; *Rowland Institute at Harvard, Cambridge, MA*
- WOF am 09:50 **Amino Acid Nature Role in Electron Capture/Transfer Dissociation of Peptides: Primary versus Secondary Structure Effects**; Hisham Ben Hamidane; Aleksey Vorobyev; Adrian Schmid; Yury Tsybin; *Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*
- WOF am 10:10 **Gas Phase Small Angle X-Ray Scattering from Trapped Ions**; Bryan J. McCullough<sup>1</sup>; Andrew Entwistle<sup>2</sup>; Steve G. Buffey<sup>3</sup>; Francesco Brancia<sup>2</sup>; S. Samar Hasnain<sup>3</sup>; Ikuo Konishi<sup>2</sup>; J. Guenter Grossmann<sup>3</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>*The University of Manchester, Manchester, UK*; <sup>2</sup>*Shimadzu*

*Research Laboratory Ltd, Manchester, United Kingdom*; <sup>3</sup>*STFC Daresbury Laboratory, Warrington, United Kingdom*

8:30 – 10:30 am

**APPLICATIONS OF ION MOBILITY SPECTROMETRY***Rooms 601-607*

Chair: Erin Baker

- WOG am 08:30 **Overtone Mobility Spectrometry**; David E. Clemmer; *Indiana University, Bloomington, IN*
- WOG am 08:50 **Profiling Histone Modifications in Response to HDAC Inhibitors using FAIMS on an Orbitrap Mass Spectrometer**; Julian Saba; Paul Drogaris; Christelle Pomies; Eric Bonneil; Pierre Thibault; *University Of Montreal, Montreal, Canada*
- WOG am 09:10 **Aggregation in Amyloid Systems: The Amylin Peptide in Diabetes Type II using IMS-MS Methods**; Michael T. Bowers; Nicholas Dupuis; *University of California, Santa Barbara, CA*
- WOG am 09:30 **High-Throughput Proteomics Platform Based on Ion Mobility Time-of-Flight Mass Spectrometry**; Mikhail Below; Brian Clowers; Prior David; William Danielson; Daniel Orton; Eric Livesay; Brianna O. Petritis; Richard Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WOG am 09:50 **Coulombic Denaturing of Gas Phase Proteins Electrospayed from Neutral Aqueous Solutions Studied by IMS (DMA) MS**; Juan Fernandez de la Mora; *Yale University - Mechanical Engineering Department, New Haven, CT*
- WOG am 10:10 **Role of Charge State on Protein Conformation and Protein Complexes Probed by Ion Mobility and Mass Spectrometry**; Catherine Kaddis; Sheng Yin; Eric Pang; Shirley Lomeli; Rachel O. Loo; Joseph A. Loo; *UCLA, Los Angeles, CA*

**WEDNESDAY AFTERNOON**

2:30 – 4:30 pm

**CHARACTERIZATION OF MEMBRANE PROTEINS***Wells Fargo Theatre*

Chair: Kevin L. Schey

- WOA pm 02:30 **Post-Translational Modifications in Transmembrane Domains of Integral Membrane Proteins Resolved by Top-Down Fourier-Transform Mass Spectrometry**; Julian Whitelegge; Christopher M. Ryan; Sara Bassilian; Puneet Souda; Kym F. Faull; *University of California LA, Los Angeles, CA*
- WOA pm 02:50 **Identification of Posttranslationally Modified Membrane Proteins in HEK293 Cells**; Thomas Borrmann<sup>1</sup>; Anke Schiedel<sup>2</sup>; Ruihua Fang<sup>1</sup>; Christa Müller<sup>2</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>*Caltech, Pasadena, CA*; <sup>2</sup>*University of Bonn, Bonn, Germany*
- WOA pm 03:10 **Proteomic Pipeline for the Topology of Integral Membrane Proteins: the Leucine and Dopamine Transporters**; Adele Blackler<sup>1</sup>; Christine Wu<sup>2</sup>; <sup>1</sup>*University of Colorado HS, Aurora, CO*; <sup>2</sup>*University of Colorado, Aurora, CO*
- WOA pm 03:30 **Global Topology Analysis of Pancreatic Zymogen Granule Membrane Proteins**; Xuequn Chen; Peter Ulintz; Eric Simon; John Williams; Philip Andrews; *The University of Michigan, Ann Arbor, MI*

- WOA pm 03:50 **Automated Analysis of Complex Protein Mixtures using Online Digestion Prior to  $\mu$ LC-MS-MS**; Edward J. Hsieh; Michael J. Maccoss; *University of Washington, Seattle, WA*
- WOA pm 04:10 **Maximizing Protein Identification Efficiency in 2D-LC ESI QTOF MS-MS for Large Scale Membrane Proteome Analysis**; Nan Wang; Liang Li; *Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*

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2:30 – 4:30 pm

**UNDERSTANDING PEPTIDE FRAGMENTATION: THEORY AND EXPERIMENT**

*Korbel Ballroom 1*

Chair: Michael J. Van Stipdonk

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- WOB pm 02:30 **Peptide Ion Fragmentation Mechanisms: an Overview**; Bela Paizs; *DKFZ, Heidelberg, Heidelberg, Germany*
- WOB pm 02:50 **Surface Induced Dissociation of Peptide Radical Anions**; Zhibo Yang<sup>1</sup>; Corey Lam<sup>2</sup>; Ivan K. Chu<sup>2</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*University of Hong Kong, Hong Kong*
- WOB pm 03:10 **Probing H Atom Transfer and Fragmentation of a Model Peptide using a Tandem Mass Spectrometry and Density Functional Theory Calculations**; Sam P Molesworth; Idia Tukonboh; Christopher Leavitt; Erach Talaty; Michael J. Van Stipdonk; *Wichita State University, Wichita, KS*
- WOB pm 03:30 **Peptide Fragmentation Modeling from Low Energy CID Data through the Use of an Iterative Database Search**; Hui Wei<sup>1</sup>; Martha D. Stapels<sup>1</sup>; Jeffrey C. Silva<sup>2</sup>; <sup>1</sup>*Waters Corporation, Beverly, MA*; <sup>2</sup>*Cell Signaling Technology, Danvers, MA*
- WOB pm 03:50 **The effect of Phosphorylation on the Electron Capture Dissociation of Peptide Ions**; Andrew Creese; Helen Cooper; *University of Birmingham, Birmingham, UK*
- WOB pm 04:10 **To B or not to B: Unique Fragmentation Chemistry of  $\beta$ -Alanine and its Peptides**; Adrian Lam; Sri H Ramarathinam; Anthony W Purcell; Richard A.J. O'Hair; *Bio21 Institute, University of Melbourne, Melbourne, Australia*

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2:30 – 4:30 pm

**DEVELOPMENTS AND APPLICATION OF APPI**

*Korbel Ballroom 2-3*

Chair: Thorsten Benter

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- WOC pm 02:30 **Atmospheric Pressure Photoionization (APPI) for LC-MS: State-of-the-Art and Future Prospects**; Damon Robb; Michael W. Blades; *University of British Columbia, Vancouver, Canada*
- WOC pm 02:50 **Unique High-Sensitivity Approach to Quantitatively Resolving Steroids in Plasma**; Sheng-Suan (Victor) Cai<sup>1</sup>; Karl A. Hanold<sup>1</sup>; Jack A. Syage<sup>1</sup>; Michael P. Balogh<sup>2</sup>; John Van Antwerp<sup>2</sup>; <sup>1</sup>*Syagen Technology, Inc., Tustin, CA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- WOC pm 03:10 **Photoionization at Atmospheric Pressure: Interaction Between UV Radiation with a Spray of Biomolecules**; Aïcha Bagag<sup>1</sup>; Alexandre Giuliani<sup>2</sup>; Olivier Laprèvote<sup>1</sup>; <sup>1</sup>*Laboratoire de spectrométrie de masse, ICSN-CNRS, Yvette, France*; <sup>2</sup>*Disco Beamline, Soleil Synchrotron, Yvette, France*
- WOC pm 03:30 **Trace Level Analysis of Nitroaromatics and Nitroamines by Liquid**

**Chromatography/Negative Ion Atmospheric Pressure Photoionization Mass Spectrometry (LC-NI-APPI-MS)**; Liguo Song; John Bartmess; Amber Wellman; Huifang Yao; *University of Tennessee, Knoxville, TN*

- WOC pm 03:50 **Single Drop Laser Ionization (SDLI) Combined with Ultrahigh Resolution Mass Spectrometry (ICR-FT/MS)**; Philippe Schmitt-Kopplin<sup>1</sup>; Klaus Brockmann<sup>2</sup>; Oliver J Schmitz<sup>2</sup>; Matthias Englmann<sup>1</sup>; Istvan Gebefuegi<sup>1</sup>; <sup>1</sup>*Helmholtz Zentrum München, Neuherberg, Germany*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*
- WOC pm 04:10 **CE-MS Through APPI: Achieving Mixed-Mode Ionization on a Single-Mode Source**; Paul Hommerson<sup>1</sup>; Amjad M. Khan<sup>2</sup>; Gerhardus J. de Jong<sup>1</sup>; Govert W. Somsen<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*AstraZeneca, Macclesfield, UK*

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2:30 – 4:30 pm

**MASS SPECTROMETRY IN BIODEFENSE**

*Korbel Ballroom 4*

Chair: Plamen A. Demirev

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- WOD pm 02:30 **Detection, Differentiation, Quantification and Subtyping of Botulinum Neurotoxins with Mass Spectrometry**; John R Barr<sup>1</sup>; Suzanne R Kalb<sup>1</sup>; Hercules Moura<sup>1</sup>; David M Schieltz<sup>1</sup>; Adrian R Woolfitt<sup>1</sup>; James L Pirkle<sup>1</sup>; James D Marks<sup>2</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, GA*; <sup>2</sup>*UCSF, San Francisco, CA*
- WOD pm 02:50 **Intact Protein Liquid Chromatography Mass Spectrometry for Bacteria Strain Differentiation and Bacterial Toxin Detection**; John H. Callahan; Denis Andrzejewski; Rebecca Bell; Eric Brown; Steve Musser; *FDA/CFISAN, College Park, MD*
- WOD pm 03:10 **Top Down Analysis of Biological Threat Agents using DESI and ETD Mass Spectrometry**; Jonathan L. Bundy<sup>1</sup>; Maureen K. Bunger<sup>1</sup>; James Stephenson<sup>1</sup>; Susanne Hering<sup>2</sup>; Benjamin Cargile<sup>1</sup>; <sup>1</sup>*Research Triangle Institute, RTP, NC*; <sup>2</sup>*Aerosol Dynamics, Berkeley, CA*
- WOD pm 03:30 **Atmospheric Pressure MALDI-MS-MS Based High Throughput Automated Multiplexed Assay System for Rapid Detection and Identification of Bioagents**; Appavu K. Sundaram; Seshu K. Gudlavalleti; Berk Oktem; Jane Razumovskaya; Chaminda M. Gamage; Robert M. Serino; Vladimir M. Doroshenko; *Science & Engineering Services, Inc., Columbia, MD*
- WOD pm 03:50 **A Metaproteomic Approach for Phylogenetic Classification of Bacterial Mixtures using LC-MS-MS Analysis of Tryptic Peptides and SEQUEST Outputs**; Jacek P. Dworzanski<sup>1</sup>; Samir V. Deshpande<sup>2</sup>; Rabih E. Jabbour<sup>1</sup>; Mary M. Wade<sup>3</sup>; Alan W. Zulich<sup>3</sup>; Charles H. Wick<sup>3</sup>; <sup>1</sup>*SAIC, Aberdeen Proving Ground, MD*; <sup>2</sup>*Science and Technology Corporation, Edgewood, MD*; <sup>3</sup>*U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD*
- WOD pm 04:10 **Simultaneous Detection and Characterization of Multiple Bacterial and Viral Bioweapons Agents in a Multiplexed PCR Assay with High Throughput ESI-MS**; Lawrence B. Blyn; Ranga Sampath; Rachael Meltion; Robert Lovari;

Thomas A. Hall; Feng Li; Cristina Ivy; Javier Fernandez; Heather Matthews; Kristin A. Sannes-Lowery; Jared Drader; James C. Hannis; Lendell L. Cummins; Mark Eshoo; David J. Ecker; S; *Ibis Biosciences, Inc., Carlsbad, CA*

2:30 – 4:30 pm

**LIPID ANALYSIS BY MASS SPECTROMETRY**

*Four Seasons Ballroom 1-2*

Chair: Thomas J. Brenna

- WOE pm 02:30 **Systems Biology Approach for Molecular Characterization of the *Saccharomyces cerevisiae* Lipidome**; Christer Ejsing<sup>1</sup>; Julio Sampaio<sup>1</sup>; Robin Klemm<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Vineeth Surendranath<sup>1</sup>; Kai Simons<sup>1</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Molecular Cell Biology and, Dresden, Germany*; <sup>2</sup>*MDS Sciex, Concord, Canada*
- WOE pm 02:50 **Lipidome Profiling with Ion Mobility Spectrometry-Mass Spectrometry**; Sarah Trimpin; Bo Tan; Brian C. Bohrer; Sam I. Merenbloom; David E. Clemmer; J. Michael Walker; *Indiana University, Bloomington, IN*
- WOE pm 03:10 **Modulation of Glycolipidomics of NS11 Glioblastoma Stem Cells after Induced Differentiation**; Huan He<sup>1</sup>; Mark R. Emmett<sup>2</sup>; Carol Nilsson<sup>3</sup>; Alan G. Marshall<sup>2</sup>; Roger A. Kroes<sup>5</sup>; Joseph R. Moskal<sup>5</sup>; Howard Colman<sup>4</sup>; Charles A. Conrad<sup>4</sup>; <sup>1</sup>*Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL*; <sup>2</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL*; <sup>3</sup>*Pfizer, Inc., San Diego, CA*; <sup>4</sup>*M.D. Anderson Cancer Center, Houston, TX*; <sup>5</sup>*The Falk Ctr*
- WOE pm 03:30 **A Novel and Flexible LC-MS-MS-Based Enzymatic Assay to Analyze Activity and Substrate Preference of Lysophospholipid Acyltransferases**; Miguel A. Gijon; Simona Zarini<sup>1</sup>; Wayne R. Riekhof<sup>2</sup>; Dennis R. Voelker<sup>2</sup>; Robert C. Murphy<sup>1</sup>; <sup>1</sup>*University of Colorado Denver, Aurora, CO*; <sup>2</sup>*National Jewish Medical and Research Center, Denver, CO*
- WOE pm 03:50 **Formation of Oxidized Bioactive Lipids During Carcinogen Activation by Human Lung Cells**; Stacy Gelhaus<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Univ. of Pennsylvania Center for Cancer, Philadelphia, PA*
- WOE pm 04:10 **Imaging Mass Spectrometry of Electrophoretically Separated Membrane Bound Species**; Stacy D. Sherrod; Arnaldo Diaz; Hudson Pace; Paul S. Cremer; David H. Russell; *Texas A&M University, College Station, TX*

2:30 – 4:30 pm

**METABOLITES AND DEGRADATION PRODUCTS OF ENVIRONMENTAL CONTAMINANTS**

*Four Seasons Ballroom 3-4*

Chair: Damià Barceló

- WOF pm 02:30 **Environmental Contaminants That Degrade in the Environment: Do They Really Disappear?** Susan Richardson; *US EPA, Athens, GA*
- WOF pm 02:50 **Investiations of the Metabolism of Fluorinated Alkylsulfonates Utilizing Different LC-MS-MS Methods**; Thomas P. Knepper<sup>1</sup>; Manuela Peschka<sup>1</sup>; Tobias Frömel<sup>1</sup>; Wolfgang Hierse<sup>2</sup>; <sup>1</sup>*University of Applied Sciences Fresenius, Idstein, Idstein, Germany*; <sup>2</sup>*Merck KGaA, Darmstadt, Germany*

- WOF pm 03:10 **Analysis of Pesticides and their Metabolites in Environmental Samples by Liquid Chromatography Coupled to Time-of-Flight Mass Spectrometry**; Imma Ferrer; Michael Thurman; *University of Colorado, Boulder, CO*
- WOF pm 03:30 **Accurate Mass Databases for Comprehensive Screening of Pesticide Residues in food by LC-TOFMS**; Juan F Garcia-Reyes<sup>1</sup>; Octavio Malato<sup>2</sup>; Milagros Mezcuca<sup>2</sup>; Antonio Molina-Diaz<sup>1</sup>; Amadeo R Fernandez-Alba<sup>2</sup>; <sup>1</sup>*University of Jaen, Jaen, Spain*; <sup>2</sup>*University of Almeria, Almeria, Spain*
- WOF pm 03:50 **Analysis of Polar Organic Compounds in Surface Waters Collected Near Lead-Zinc Mine and Milling Operations by Electrospray Ionization/Mass Spectrometry**; Colleen E. Rostad<sup>1</sup>; Christopher J. Schmitt<sup>2</sup>; John G. Schumacher<sup>3</sup>; Thomas J. Leiker<sup>4</sup>; <sup>1</sup>*USGS, WRD, NRP, Lakewood, CO*; <sup>2</sup>*US Geological Survey, BRD, Columbia, MO*; <sup>3</sup>*US Geological Survey, WRD, Rolla, MO*; <sup>4</sup>*USGS, WRD, NWQL, MRDP, Lakewood, CO*
- WOF pm 04:10 **Identification of PBDE 47, 99, and 153 Metabolites from Human Liver Microsomes by Gas Chromatography Mass Spectrometry**; Sara J. Lupton<sup>1</sup>; Barbara McGarrigle<sup>1</sup>; James Olson<sup>1</sup>; Troy D. Wood<sup>2</sup>; Diana Aga<sup>1</sup>; <sup>1</sup>*University At Buffalo, Buffalo, NY*; <sup>2</sup>*University At Buffalo/Nanogenesys, Inc., Buffalo, NY*

2:30 – 4:30 pm

**IMAGING MASS SPECTROMETRY FOR SMALL MOLECULE APPLICATIONS**

*Rooms 601-607*

Chair: Michelle Reyzer

- WOG pm 02:30 **Imaging Mass Spectrometry for the Investigation of Individual Small Molecule Tissue Distributions**; Sheerin Khatib-Shahidi; Cornelis Hop; Patrick J. Rudewicz; *Genentech, Inc., South San Francisco, CA*
- WOG pm 02:50 **Strategies for Small Molecule Imaging by MALDI-MSI**; Malcolm Clench<sup>1</sup>; Mike Burrell<sup>2</sup>; Paul J Trim<sup>1</sup>; Caroline Earnshaw<sup>1</sup>; Simona Francese<sup>1</sup>; Tasneem Muharib<sup>1</sup>; David M. G. Anderson<sup>1</sup>; Sally Atkinson<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*University of Sheffield, Sheffield, United Kingdom*
- WOG pm 03:10 **Imaging Drugs and Metabolites in Tissue using Fourier Transform Mass Spectrometry**; Dale S. Cornett; Sara L. Frappier; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- WOG pm 03:30 **Imaging Mass Spectroscopy of Mouse Lung Following Ozone Exposure**; Kyle Johnson; Joseph A. Hankin; Robert C. Murphy; *University of Colorado-Denver, Aurora, CO*
- WOG pm 03:50 **Two- and Three-Dimensional Molecular Imaging of Live Tissues by Infrared Laser Ablation Electrospray Ionization Mass Spectrometry**; Peter Nemes; Yue Li; Alexis A. Barton; Akos Vertes; *George Washington University, Washington, DC*
- WOG pm 04:10 **UV-LDI-o-TOF MS Imaging of Hydrocarbons from Single, Intact Fruit Flies**; Joanne Yew<sup>1</sup>; Klaus Dreisewerd<sup>2</sup>; Stefan Berkenkamp<sup>3</sup>; Edward Kravitz<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*University of Muenster, Muenster, Germany*; <sup>3</sup>*Sequenom GmbH, Hamburg, Germany*

4:45 – 5:30 pm  
**ASMS BUSINESS MEETING**  
**Wine and Beer, Prizes and More!!**  
*Wells Fargo Theatre*

**THURSDAY MORNING, June 5**

8:30 – 10:30 am  
**NOVEL APPLICATIONS OF BIOINFORMATICS**  
*Wells Fargo Theatre*  
 Chair: Karl R. Clauser

- ThOA am 08:30 **Validation and Expansion of the Arabidopsis Gene Annotation**; Natalie E Castellana<sup>1</sup>; Samuel Payne<sup>1</sup>; Zhouxin Shen<sup>1</sup>; Mario Stanke<sup>2</sup>; Steven P. Briggs<sup>1</sup>; Vineet Bafna<sup>1</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>UCSC, Santa Cruz, CA
- ThOA am 08:50 **Comparative Proteogenomics: Combining Mass Spectrometry and Comparative Genomics to Analyze Multiple Genomes**; Nitin Gupta<sup>1</sup>; Jamal Benhamida<sup>1</sup>; Vipul Bhargava<sup>1</sup>; Daniel Goodman<sup>1</sup>; Elisabeth Kain<sup>1</sup>; Ian Kerman<sup>1</sup>; Ngan Nguyen<sup>1</sup>; Noah Ollikainen<sup>1</sup>; Jesse Rodriguez<sup>1</sup>; Jia; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>PNNL/Battelle Northwest, Richland, WA
- ThOA am 09:10 **Identification of Dominant Signaling Pathways from Independent Proteomics Expression Datasets**; Yi Man Eva Fung; Roman Zubarev; *Uppsala University, Uppsala, Sweden*
- ThOA am 09:30 **Unique Ion Signature Mass Spectrometry: a Deterministic Method for Peptide Identification and its Implications**; Jamie Sherman; Matthew McKay; Mark Molloy; Keith Ashman; *APAF@Macquarie University, Sydney, Australia*
- ThOA am 09:50 **Measuring Run-to-Run and Lab-to-Lab Variability in Shotgun Proteomics Experiments**; Stephen Stein; Lisa E. Kilpatrick; Dmitrii Tchekhovskoi; Paul Rudnick; Eric Yan; *NIST, Gaithersburg, MD*
- ThOA am 10:10 **Dimensionality Reduction and Visualisation in Principal Component Analysis as Applied to an LC-MS Metabolomics Study**; Lyle Burton; Ron Bonner; Gordana Ivosev; *MDS Sciex, Concord, Canada*

8:30 – 10:30 am  
**METAL ION ACTIVATED DISSOCIATION**  
*Korbel Ballroom 1*  
 Chair: Diethard K. Bohme

- ThOB am 08:30 **Key Issues in Metal-Ion Activated Dissociation**; Peter B. Armentrout; *University of Utah, Salt Lake City, UT*
- ThOB am 08:50 **ECD and CID of Metal/Peptide Complexes**; Carlos Afonso; Jean-claude Tabet; *Université Paris 6, Paris, France*
- ThOB am 09:10 **Gas-Phase Activation Study of the Coordination of Lead Dications with Amino Acids**; Laura Banu; Voislav Blagojevic; Diethard K. Bohme; *York University, Toronto, Canada*
- ThOB am 09:30 **Dissociation Studies of Alkali Metal Cation Complexes of Aspartic Acid, Glutamic Acid, Asparagine, and Glutamine**; Amy L. Heaton<sup>1</sup>; Robert M. Moision<sup>2</sup>; Peter B. Armentrout<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>University of California, San Diego, San Diego, CA

- ThOB am 09:50 **Sodium Induces Unimolecular Decay Pathways in the Metastable Decay of Protonated Oligonucleotides in the Gas Phase**; Helga Dögg Flosadóttir<sup>1</sup>; Michal Stano<sup>2</sup>; Oddur Ingólfsson<sup>1</sup>; <sup>1</sup>University of Iceland, Reykjavik, Iceland; <sup>2</sup>Comenius University, Bratislava, Slovakia
- ThOB am 10:10 **The Mg(I) Reagent Anion, [MgCl<sub>2</sub>]<sup>-</sup>, Forms Coordinated Ketyl Radical Anions which Fragment via Radical Driven Pathways**; George N. Khairallah<sup>1</sup>; Charlene Thum<sup>1</sup>; Richard A. J. O'Hair<sup>2</sup>; <sup>1</sup>University of Melbourne, Victoria, Australia; <sup>2</sup>Bio21 Institute, Parkville, Australia

8:30 – 10:30 am  
**ION TRAP APPLICATIONS**  
*Korbel Ballroom 2-3*  
 Chair: Elaine Marzluff

- ThOC am 08:30 **Data-Independent Outperforms Data-Dependent Gas-Phase Fractionation Based Shotgun Proteomics**; Alexander Scherl; Scott A. Shaffer; Priska Von Haller; David R. Goodlett; *University of Washington, Seattle, WA*
- ThOC am 08:50 **Dinosaur Sequences and Their Evolutionary Tale**; John M Asara<sup>1</sup>; Mary Schweitzer<sup>2</sup>; <sup>1</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>2</sup>North Carolina State University, Raleigh, NC
- ThOC am 09:10 **Multistage-Fragmentation Analysis for Phosphopeptide Identification on an Ion-Trap Mass Spectrometer**; Shama P. Mirza<sup>1</sup>; Romina Rompietti<sup>2</sup>; Brian D. Halligan<sup>1</sup>; Gilbert C. White II<sup>2</sup>; Andrew S. Greene<sup>1</sup>; Michael Olivier<sup>1</sup>; <sup>1</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>2</sup>Blood Center of Southeastern Wisconsin, Milwaukee, WI
- ThOC am 09:30 **A New Approach to Infrared Multiphoton Photodissociation for Controlled Dissociation in a Quadrupole Ion Trap Mass Spectrometer**; G. Asher Newsome; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- ThOC am 09:50 **Investigation of Gas-Phase Reactions of Charged Aromatic s,s-Biradicals with Dipeptides in a Fourier-Transform Ion Cyclotron Resonance Mass Spectrometer**; Mingkun Fu; Sen Li; Enada F Archibold; Nishi Rochelle; Mike Yurkovich; John Nash; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*
- ThOC am 10:10 **Slow Energy Transfer: A Fluorescence and Spectrometry Study of Rhodamine 575 Cations Confined to a Paul Trap**; Nicholas A. Sassin; Stephanie C. Everhart; Beni Dangi; Joseph I. Cline; Kent M. Ervin; *University of Nevada, Reno, NV*

8:30 – 10:30 am  
**STRUCTURAL BIOLOGY AND BIOPHYSICS OF NUCLEIC ACIDS**  
*Korbel Ballroom 4*  
 Chair: Daniele Fabris

- ThOD am 08:30 **Approaches, Applications and Future Directions in the Structural Biology and Biophysics of Nucleic Acids as Studied by MS**; Henning Urlaub; *Max Planck Institute, Goettingen, Germany*
- ThOD am 08:50 **DNA-Mediated Ref1 Conformational Changes: Possible Mechanism for Protein Recruitment IN Base Excision Repair (BER) Pathway**; Eizadora T. Yu<sup>1</sup>; Sara P. Gaucher<sup>2</sup>; Kenneth Sale<sup>1</sup>; Masood Z. Hadi<sup>1</sup>; <sup>1</sup>Sandia National

- Laboratories, Livermore, CA; <sup>2</sup>Amoyris Biotechnologies, Emeryville, CA
- ThOD am 09:10 **Modeling Stable Conformers of the 5' Non-Coding Region of HIV-1 Genome using Sparse Constraints Provided by MS-Based Strategies;** Jiarong Xia; Dong Yang; Alberto Berton; Daniele Fabris; *Univeristy of Maryland Baltimore County, Baltimore, MD*
- ThOD am 09:30 **Top-Down Analysis Reveals a Complete Subunit Interaction Map for the 13-Subunit eIF3 Complex and its Interaction with RNA;** Min Zhou<sup>1</sup>; Alan M. Sandercock<sup>1</sup>; Christopher S. Fraser<sup>2</sup>; Matthew Schenauer<sup>3</sup>; Julie A. Leary<sup>3</sup>; John W. Hershey<sup>4</sup>; Jennifer Doudna<sup>2</sup>; Carol Robinson<sup>1</sup>; <sup>1</sup>*University of Cambridge,, Cambridge,, UK*; <sup>2</sup>*University of California, Berkeley, CA*; <sup>3</sup>*UC Davis, Davis, CA*; <sup>4</sup>*School of Medicine, University of California, Davis, CA*
- ThOD am 09:50 **Influence of Zwitterions on Salt Bridge Stabilisation on Single- and Double Stranded DNA/Peptide Complexes;** Ludovic Muller<sup>1</sup>; Sandra Alves<sup>1</sup>; Amina S. Woods<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>*Université Pierre et Marie Curie, Paris, France*; <sup>2</sup>*Nida Irp, Nih, Baltimore, MD*
- ThOD am 10:10 **IR and UV Spectroscopic Signatures of DNA Higher-Order Structures in the Gas Phase;** Valérie Gabelica<sup>1</sup>; Frédéric Rosu<sup>1</sup>; Gilles Grégoire<sup>2</sup>; Jean-Pierre Schermann<sup>2</sup>; Charles Desfrancois<sup>2</sup>; Joël Lemaire<sup>3</sup>; Thibault Tabarin<sup>4</sup>; Rodolphe Antoine<sup>4</sup>; Mic; <sup>1</sup>*University of Liege, Liège, Belgium*; <sup>2</sup>*University Paris 13, Villetaneuse, France*; <sup>3</sup>*Laboratoire De Chimie Physique, Orsay, France*; <sup>4</sup>*Université Lyon, Villeurbanne, France*

8:30 – 10:30 am

## CHARACTERIZING POST-TRANSLATIONAL MODIFICATIONS

Four Seasons Ballroom 1-2

Chair: Lan Huang

- ThOE am 08:30 **Mapping Protein Post-Translational Modifications with Mass Spectrometry;** Natalie Ahn; *Univ. of Colorado, Boulder, CO*
- ThOE am 08:50 **Phosphoproteome Analysis of the Tumor Suppressor Syk Induction in Breast Cancer Cells by a Novel Soluble Nanopolymer-Based Phosphopeptide Enrichment Method;** Anton Iliuk; Bethany Alicie; Minjie Guo; Robert Geahlen; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
- ThOE am 09:10 **Efficient Identification of Phosphorylation by Mass Spectrometric Phosphopeptide Fingerprinting;** Eileen Woo; David Fenyo; Benjamin Kwok; Brian Chait; *The Rockefeller University, New York, NY*
- ThOE am 09:30 **PTMap --- a Software for Identifying Full-Spectrum PTMs with High Accuracy and Low False Positives;** Yue Chen; Yingming Zhao; *UT Southwestern Medical Center, Dallas, TX*
- ThOE am 09:50 **Unbiased and Comprehensive Mapping of Chromatin Post-Translational Modifications and Simultaneous Determination of *in vivo* Methylation Kinetics;** Michael L. Nielsen; Tiziana Bonaldi; Juergen Cox; Matthias Mann; *Max-Planck-Institute of Biochemistry, Martinsried, Germany*
- ThOE am 10:10 **Analysis of ADP-Ribosylated Peptides using Electron Capture Dissociation High Resolution**

**Mass Spectrometry and Ion Mobility Analysis;** Shawna M. Hengel<sup>1</sup>; Michael Daly<sup>2</sup>; Scott A. Shaffer<sup>1</sup>; Priska Von Haller<sup>1</sup>; Laura M. Icenogle<sup>1</sup>; Carleen M. Collins<sup>1</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Waters Corporation, Oakland, CA*

8:30 – 10:30 am

## INCREASING THROUGHPUT FOR PHARMACOKINETIC ASSAYS THROUGH MASS SPECTROMETRY

Four Seasons Ballroom 3-4

Chair: Lucinda Cohen

- ThOF am 08:30 **Strategies for Increasing Throughput when using LC-MS-MS for PK Assays: A Short Overview;** Walter Korfmacher; *Schering-Plough, Kenilworth, NJ*
- ThOF am 08:50 **Improving the Reproducibility and Practicability of DART for the Direct Quantification of Drugs in Biological Fluids;** Shaoxia Yu<sup>1</sup>; Elizabeth Crawford<sup>2</sup>; Joe Tice<sup>2</sup>; Brian Musselman<sup>2</sup>; Jing-Tao Wu<sup>1</sup>; <sup>1</sup>*Millennium Pharmaceuticals, Cambridge, MA*; <sup>2</sup>*IonSense, Inc., Saugus, MA*
- ThOF am 09:10 **Full Scan Data Acquisition for Rapid Quantitative and Qualitative Analysis using a Benchtop Non-Hybrid ESI-Orbitrap Mass Spectrometer;** Kevin Bateman<sup>1</sup>; Helmut Muenster<sup>2</sup>; Markus Kellmann<sup>3</sup>; Philip Tiller<sup>4</sup>; Robert Papp<sup>1</sup>; Lester C. Taylor<sup>3</sup>; <sup>1</sup>*Merck Frosst, Montreal, QC*; <sup>2</sup>*Thermo Fisher Scientific (bremen) GmbH, Bremen, Germany*; <sup>3</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>4</sup>*Merck & Co., West Point, PA*
- ThOF am 09:30 **Opportunities in the Evolution of Multiplexed LC-MS-MS Assay Methodology for Increased PK/PD Productivity;** Erick K Kindt; *Pfizer, San Diego, CA*
- ThOF am 09:50 **Using MALDI Triple Quadrupole Mass Spectrometry for the High-Throughput Quantitative Analysis of Antidepressants in Human Plasma Samples;** Jean-Francois Alary<sup>1</sup>; Daniel Lebre<sup>1</sup>; Siew Wan<sup>2</sup>; Feng Zhong<sup>1</sup>; Pauline J. Vollmerhaus<sup>1</sup>; Timothy Sangster<sup>2</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>*Huntingdon Life Science, East Mettlers, NJ*
- ThOF am 10:10 **Solid Phase Extraction Enhanced Desorption Electrospray Ionization;** Zoltan Takats; Julia Denes; Maria Katona; *Semmelweis University, Budapest, Hungary*

8:30 – 10:30 am

## ANALYTE "FINGERPRINTING" WITH NO SAMPLE PREP

Rooms 601-607

Chair: Marcos N. Eberlin

- ThOG am 08:30 **Extractive Electrospray Ionization Mass Spectrometry in Metabolomics and Medical Diagnostics;** Renato Zenobi; Huanwen Chen; Gerardo gamez; Liang Zhu; *ETH Zurich, Switzerland*
- ThOG am 08:50 **Identifying Materials, Formulations, and Other Complex Substances by Direct Analysis and Exact Mass Measurements;** Robert B. Cody; *JEOL USA, Inc., Peabody, MA*
- ThOG am 09:10 **Endogenous Metabolites Excreted Through the Skin Analyzed by Geometry Independent Desorption Electrospray Ionization;** Andre Venter; Ayanna Jackson; Nari Talaty; Sheran Oradu; Abraham Badu-Tawiah; R. Graham Cooks; *Purdue University, West Lafayette, IN*



- ThOG am 09:30 **Real-Time Mass Spectrometric Monitoring of a Continuous Flow Micro Reactor for Organic Synthesis Optimization**; Jack D. Henion; Andrew Hague; Geoffrey S. Rule; Christopher G. Alpha; *Advion BioSciences, Inc, Ithaca, NY*
- ThOG am 09:50 **Development of a New Ionization Source Liquid Matrix-Assisted Laser Desorption Electrospray Ionization and Investigation of the MALDESI Ionization Mechanism**; Jason S. Sampson; R. Brent Dixon; Adam M. Hawkrige; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- ThOG am 10:10 **Fingerprinting Quality Control of Media for *in vitro* Bovine Embryo Production using Direct Infusion Automated Chip-Based Nano-Electrospray Mass Spectrometry**; Christina Ramires Ferreira<sup>1</sup>; Gustavo Henrique M. Ferreira Souza<sup>2</sup>; Maria Francesca Riccio Fonsêca<sup>4</sup>; Gustavo Braga Sanvido<sup>2</sup>; Andrea Cristina Brasso<sup>3</sup>; José Henrique Fortes Pontes<sup>3</sup>; Jos; <sup>1</sup>*In Vitro Brasil Ltda, ThoMson Laboratory Unicamp, Campinas - SP, Brazil*; <sup>2</sup>*ThoMson Mass Spectrometry Laboratory - Unicamp, Campinas-SP, Brazil*; <sup>3</sup>*In Vitro Brasil Ltda, Mogi Mirim-SP, Brazil*; <sup>4</sup>*ThoMson Mass Spectro*

THURSDAY AFTERNOON
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2:30 – 4:30 pm

## NEW DEVELOPMENTS IN BIOINFORMATICS

*Wells Fargo Theatre*

Chair: Ronald C. Beavis

- ThOA pm 02:30 **RAID\_DbS: Peptide Identification with Knowledge Integration using Database Searches with Realistic Statistics**; Gelio Alves; Aleksey Y Ogurtsov; Yi-Kuo Yu; *National Center for Biotechnology Information, NLM, Bethesda, MD*
- ThOA pm 02:50 **The Peptide Fragment Mass Information Required to Identify Peptides and Their Post-Translational Modifications**; David Fenyo<sup>1</sup>; Elena Ossipova<sup>2</sup>; Jan Eriksson<sup>2</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*Swedish University of Agricultural Sciences, Uppsala, Sweden*
- ThOA pm 03:10 **Combining Peptide Identification Results**; Jimi-Carlo Bukowski-Wills; Lau Sennels; Bjorn R. Paulson; Juri Rappsilber; *Wellcome Trust Centre for Cell Biology, Edinburgh, UK*
- ThOA pm 03:30 **A Statistical Approach to Quantifying Uncertainties in the AMT tag Pipeline**; Navdeep Jaitly<sup>1</sup>; Joshua Adkins<sup>1</sup>; Alan R. Dabney<sup>2</sup>; Matthew E. Monroe<sup>1</sup>; Angela D. Norbeck<sup>1</sup>; Heather M. Mottaz<sup>1</sup>; Mary S Lipton<sup>1</sup>; Gordon A. Anderson<sup>1</sup>; Richa; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Texas A&M University, College Station, TX*
- ThOA pm 03:50 **Quantification of Correlations Within and Between Imaging Mass Spectrometry Datasets**; Liam McDonnell<sup>1</sup>; Alexandra van Remoortere<sup>1</sup>; René J.M. van Zeijl<sup>1</sup>; Ron M.A. Heeren<sup>2</sup>; André M. Deelder<sup>1</sup>; <sup>1</sup>*LUMC, Leiden, Netherlands*; <sup>2</sup>*Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands*
- ThOA pm 04:10 **The Knowledge Exchange KnowEX : Sharing Resources for Data Intensive Collaborative Mass Spectrometric Projects in the Amsterdam Virtual Laboratory**; Ron M.A. Heeren; Basak

Kaletas; Ivo Klinkert; Marco Konijnenburg; Gert Eijkel; Andrey Kharchenko; *FOM Inst. Atomic/Molecular Physics, Amsterdam, Netherlands*

2:30 – 4:30 pm

## POLYMER/MATERIAL IONIZATION AND STRUCTURAL ELUCIDATION

*Korbel Ballroom 1*

Chair: Connell Cunningham

- ThOB pm 02:30 **Reactive MALDI Mass Spectrometry of Polyolefins**; William E. Wallace; *National Institute of Standards & Technology, Gaithersburg, MD*
- ThOB pm 02:50 **Surface Mediated Laser Desorption/Ionization Time-of-Flight MS of Low Molecular Weight Polymers**; Justin Engle; S. Kim R. Williams; *Colorado School of Mines, Golden, CO*
- ThOB pm 03:10 **ESI-MS Studies of Exchange Mechanisms in Zeolite Precursors: Isomorphous Substitution of Silicon Against Germanium or Gallium**; Bernd Bastian Schaaek; Ferdi Schüth; Wolfgang Schrader; *Max-Planck Inst Coal Res., Mülheim / Ruhr, Germany*
- ThOB pm 03:30 **Analysis of Polymers, Polymer Additives and Petroleum using the ASAP Method on Synapt® and Orbitrap® Mass Spectrometers**; Violeta Petkovska<sup>1,2</sup>; Charles N. McEwen<sup>1,2</sup>; <sup>1</sup>*Dupont, Philadelphia, PA*; <sup>2</sup>*DuPont, Wilmington, DE*
- ThOB pm 03:50 **Characterization of In-Chain Functionalized Copolymers by Tandem Mass Spectrometry**; David Dabney<sup>1</sup>; Michael J. Polce<sup>2</sup>; Jon Janoski<sup>1</sup>; Roderic Quirk<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*University of Akron, Akron, OH*; <sup>2</sup>*Lubrizol Advanced Materials, Brecksville, OH*
- ThOB pm 04:10 **Utilising Ion Mobility and Tandem Mass Spectrometry for the Characterisation of Polyethers**; Tony Jackson<sup>1</sup>; Gillian R. Hilton<sup>2</sup>; Konstantinos Thalassinou<sup>2</sup>; James Scrivens<sup>3</sup>; <sup>1</sup>*ICI CARG, Songjiang Industrial Estate, China*; <sup>2</sup>*University of Warwick, Coventry, United Kingdom*; <sup>3</sup>*Univ of Warwick, Coventry, UK*

2:30 – 4:30 pm

## DEVELOPMENTS IN IMAGING INSTRUMENTATION AND METHODOLOGY

*Korbel Ballroom 2-3*

Chair: Ron M. A. Heeren

- ThOC pm 02:30 **Ion Mobility Imaging Mass Spectrometry: A New Tool for In Situ Identification**; Jonathan Stauber<sup>1</sup>; Basak Kükrer Kaletas<sup>1</sup>; Ingrid M. van der Wiel<sup>1</sup>; Marten F. Snel<sup>2</sup>; Emmanuelle Claude<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- ThOC pm 02:50 **A Laser Desorption and VUV Postionization Imaging TOF MS**; Jerry F. Moore<sup>1</sup>; Gerald Gasper<sup>2</sup>; Artem Akhmetov<sup>2</sup>; Melvin Blaze<sup>2</sup>; Luke Hanley<sup>2</sup>; <sup>1</sup>*MassThink LLC, Naperville, IL*; <sup>2</sup>*University of Illinois, Chicago, IL*
- ThOC pm 03:10 **Toward Nanoscale Chemical Imaging: Investigation of Tip-Enhanced, Near-Field Optical Methods for Desorption/Ionization Mass Spectrometry at Atmospheric Pressure**; Douglas E. Goeringer<sup>1</sup>; Kent A. Meyer<sup>1</sup>; Olga S. Ovchinnikova<sup>1</sup>; Kin Ng<sup>2</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*California State University Fresno, Fresno, CA*

- ThOC pm 03:30 **Mass Spectrometry Imaging of MRI Contrast Agents in Histopathological Sections;** Josephine Bunch<sup>1</sup>; John A.T. Pugh<sup>1</sup>; Cameron W. Mcleod<sup>1</sup>; Li-Wen Lee<sup>2</sup>; Po-Wah So<sup>2</sup>; Jimmy D. Bell<sup>2</sup>; <sup>1</sup>The University of Sheffield, Sheffield, UK; <sup>2</sup>Imperial College London, Hammersmith Hospital, London, UK
- ThOC pm 03:50 **Development of Fundamental Technology for Phosphoimaging Mass Spectrometry;** Susumu Y. Imanishi<sup>1</sup>; Petri Kouvonon<sup>2</sup>; Jan-Henrik Smått<sup>3</sup>; Soeren-Oliver Deininger<sup>4</sup>; Emilia Peuhu<sup>2</sup>; Andrey Mikhailov<sup>1</sup>; Mika Lindén<sup>3</sup>; Garry Corthals<sup>2</sup>; John E; <sup>1</sup>Åbo Akademi University / Centre for Biotechnology, Turku, Finland; <sup>2</sup>University of Turku / Centre For Biotechnology, Turku, Finland; <sup>3</sup>Åbo Akademi University, Turku, Finland; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany
- ThOC pm 04:10 **Specific MALDI Imaging: The Missing Link that Brings MALDI Imaging to Biomolecules Validation;** Isabelle Fournier<sup>1</sup>; Mohamed El-Ayed<sup>1</sup>; Jonathan Stauber<sup>2</sup>; Maxence Wisztorski<sup>1</sup>; Michel Deschamps<sup>3</sup>; Ivo Rudlof<sup>3</sup>; Gottfried Proess<sup>3</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>University of Lille 1, Villeneuve d'Ascq Cedex, FRANCE; <sup>2</sup>Fom/amolf, Amsterdam, Netherlands; <sup>3</sup>Eurogentec, Eurogentec Biologics Department, Liège, Belgique

2:30 – 4:30 pm

## CHARACTERIZING DNA, RNA, AND ADDUCTS

Korbel Ballroom 4

Chair: Natalia Tretyakova

- ThOD pm 02:30 **Mass Spectrometry for DNA and RNA Adduct Analysis: An Overview;** Yinsheng Wang; University of California, Riverside, CA
- ThOD pm 02:50 **Non-Covalent Adducts of Small Molecule Ligands Affect the Stability of Conformer Specific Interactions in HIV-1 5'-UTR;** Sonnet Davis; Daniele Fabris; Univ. Maryland Baltimore County, Baltimore, MD
- ThOD pm 03:10 **Developing Approaches for Quantitative LC-MS-MS of Nucleic Acids;** Colette Castleberry<sup>1</sup>; Renee N Kepler<sup>1</sup>; Larry Sallans<sup>1</sup>; Rachel M Selby<sup>2</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>Rose-Hulman Institute of Technology, Terre Haute, IN
- ThOD pm 03:30 **Adenosine Methylations of Ribosomal RNA Characterized by Ion Trap Nano LC-MS<sup>3</sup>;** Anders MB Giessing; Finn Kirpekar; Birte Vester; Lykke H. Hansen; Anette Rasmussen; University of Southern Denmark, Odense, Denmark
- ThOD pm 03:50 **Stable Isotope Labeling HPLC-ESI-MS-MS Approach to Investigate DNA Sequence Preferences for the Formation of Oxidative DNA Lesions;** Brock Matter<sup>1</sup>; Jianwei Zhao<sup>2</sup>; Roger Jones<sup>2</sup>; Natalia Tretyakova<sup>3</sup>; <sup>1</sup>University of Minnesota Cancer Center, Minneapolis, MN; <sup>2</sup>Rutgers, New Brunswick, NJ; <sup>3</sup>University of Minnesota, Minneapolis, MN
- ThOD pm 04:10 **Analysis of the Formation and Mutagenesis of N<sup>2</sup>-(1-Carboxyethyl)-2'-Deoxyguanosine in vivo by LC-MS-MS;** Huachuan Cao; Bifeng Yuan; Yong Jiang; Yinsheng Wang; University of California, Riverside, Riverside, CA

2:30 – 4:30 pm

## IONIZATION AND CHARACTERIZATION OF MACROMOLECULES AND COMPLEXES

Four Seasons Ballroom 1-2

Chair: Esther van Duijn-Keizers

- ThOE pm 02:30 **Modularity of the Human Signalosome Complex Revealed by Mass Spectrometry;** Michal Sharon<sup>1</sup>; Haibin Mao<sup>2</sup>; Elisabetta Erba<sup>3</sup>; Elaine Stephens<sup>3</sup>; Ning Zheng<sup>2</sup>; Carol Robinson<sup>3</sup>; <sup>1</sup>Weizmann Institute of Science, Rehovot, ISRAEL; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>University of Cambridge, Cambridge, UK
- ThOE pm 02:50 **The Influence of Small Charge Carrier Field Emission on the Charge States of Proteins in ESI;** Christopher J. Hogan<sup>1</sup>; James Carroll<sup>2</sup>; Henry W. Rohrs<sup>1</sup>; Michael L. Gross<sup>1</sup>; Pratim Biswas<sup>1</sup>; <sup>1</sup>Washington University, Saint Louis, MO; <sup>2</sup>Pfizer, Chesterfield, MO
- ThOE pm 03:10 **Characterization of 800 kDa Macromolecular Complexes from Hela Cells: Effects of Collision Activation and Solvent Disruption using Ion Mobility MS;** Julie A. Leary; Matthew Schenauer; Armann Andaya; Raluca Stefanescu; UC Davis, Davis, CA
- ThOE pm 03:30 **Identification of Proteins Essential for Human Telomerase Function using Affinity Purification and Mass Spectrometry;** Zhaojing Meng<sup>1</sup>; Andrew S. Venteicher<sup>2</sup>; Philip J. Mason<sup>3</sup>; Timothy D. Veenstra<sup>1</sup>; Steven E. Artandi<sup>2</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>Stanford School of Medicine, Stanford, CA; <sup>3</sup>Washington University School of Medicine, St Louis, MO
- ThOE pm 03:50 **Combined Covalent Labeling Methods for Studying  $\beta$ 2m Oligomer Assembly by MS;** Vanessa Leah Mendoza; Srikanth Rapole; Mark R. Olbris; Richard W. Vachet; University of Massachusetts, Amherst, MA
- ThOE pm 04:10 **Structure Analysis of Acrylic Copolymers by LC / MS<sup>n</sup>;** Junkan Song<sup>1</sup>; Jan W. van Velde<sup>2</sup>; Ron M.A. Heeren<sup>2</sup>; Oscar F. Van Den Brink<sup>1</sup>; <sup>1</sup>Akzo Nobel Chemicals, Arnhem, Netherlands; <sup>2</sup>Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands

2:30 – 4:30 pm

## MATRIX EFFECTS: LC-MS CHALLENGES AND SOLUTIONS

Four Seasons Ballroom 3-4

Chair: Scott A. Miller

- ThOF pm 02:30 **Matrix Effects in LC-MS-MS Analyses of Biological Samples: An Overview;** Amit K Ghoshal<sup>2</sup>; Richard E Reitz<sup>1</sup>; Nigel, J Clarke<sup>2</sup>; <sup>1</sup>Quest Diagnostics Inc, San Juan Capistrano, DE; <sup>2</sup>Quest Diagnostics Nichols Research Inst., San Jaun Capistrano, CA
- ThOF pm 02:50 **A Study of the Matrix Enhancement of Streptomycin's Electrospray LC-MS Response in Honey Extracts;** David N. Heller; Mayda Lopez; FDA/CVM, Laurel, MD
- ThOF pm 03:10 **Reduction of Ion Suppression and Interference using Turbulent Flow Chromatography and FAIMS for Drug Discovery Bioanalysis;** Melis Arslan Coraggio; Young Shin; Patrick J. Rudewicz; Genentech, Inc., South San Francisco, CA
- ThOF pm 03:30 **Ion Suppression Due to the Locking Solution Used in the Cannulation of Rodents;** Daniel G. Morgan<sup>1</sup>; Jennifer G. Pizzano<sup>1</sup>; Kimberly A.

Widmann<sup>1</sup>; Sarah J. Taylor<sup>1</sup>; Marc R. Browning<sup>1</sup>;  
Timothy V. Olah<sup>2</sup>; <sup>1</sup>*Bristol-Myers Squibb,*  
*Wallingford, CT;* <sup>2</sup>*Bristol-Myers Squibb*  
*Company, Lawrenceville, NJ*

ThOF pm 03:50 **Sample Matrix Effects in Quantitative Small Molecule MALDI Mass Spectrometry;** Pauline J. Vollmerhaus<sup>1</sup>; Kc Van Horne<sup>2</sup>; Sylvie Beaudet<sup>1</sup>; Lexy Scott<sup>2</sup>; Ryan Kuntz<sup>2</sup>; Ryan Brough<sup>2</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada;* <sup>2</sup>*Tandem Labs, Salt Lake City, UT*

ThOF pm 04:10 **A High Throughput LC-IMS-MS Platform for Sensitive and Quantitative Proteomics Analysis;** Keqi Tang; Erin S. Baker; Eric A. Livesay; Daniel J. Orton; William F. Danielson III; David C. Prior; Anoop M. Mayampurath; Ryan T. Kelly; Jason S. Page; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*

**2:30 – 4:30 pm**

**APPLICATION OF ETD/ECD**

*Rooms 601-607*

Chair: Helen Cooper

ThOG pm 02:30 **New Trends in ECD/ETD Applications;** Roman Zubarev; Mikhail M. Savitski; Eva M. Fung; *Uppsala University, Uppsala, Sweden*

ThOG pm 02:50 **Liquid Chromatography-Tandem Mass Spectrometry using Ion Trap Based Electron Capture Dissociation;** Gary L. Glish<sup>1</sup>; Shinya Ito<sup>2</sup>; Takashi Baba<sup>3</sup>; Jared Bushey<sup>1</sup>; Naomi Manri<sup>4</sup>; Hiroyuki Satake<sup>4</sup>; Takeshi Sakamoto<sup>4</sup>; Masaki Watanabe<sup>5</sup>; Kuriko Yamada; <sup>1</sup>*University of North Carolina, Chapel Hill, NC;* <sup>2</sup>*University of North Carolina and Hitachi High-Tech, Hitachinaka-shi, Japan;* <sup>3</sup>*University of North Carolina and Hitachi Ltd., Tokyo, Japan;* <sup>4</sup>*Central Research Laboratory*

ThOG pm 03:10 **ETD Has a Sweet Tooth: A Mass Spectrometric Method for Characterizing O-GlcNAc Sites on a Chromatographic Timescale;** Namrata D. Udeshi<sup>1</sup>; Michael P. Housley<sup>2</sup>; Young-Cheon Kim<sup>3</sup>; Neil Olszewski<sup>3</sup>; Gerald W. Hart<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, VA;* <sup>2</sup>*Johns Hopkins University School of Medicine, Baltimore, MD;* <sup>3</sup>*University of Minnesota, St. Paul, MN*

ThOG pm 03:30 **ECD Beyond Proteomics: Application to Phosphate-Containing Metabolites via Metal Adduction;** Haichuan Liu<sup>2</sup>; Hyun Ju Yoo<sup>1</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI;* <sup>2</sup>*UC San Francisco, San Francisco, CA*

ThOG pm 03:50 **Towards Full Proteomics Coverage of RNA Polymerase II and III using a Combination of Multiple Proteases and Multiple MS-MS Techniques;** Shabaz Mohammed<sup>1</sup>; Kristina Lorenzen<sup>1</sup>; Alessandro Vannini<sup>2</sup>; Robert Kerkhoven<sup>1</sup>; Bas van Breukelen<sup>1</sup>; Patrick Cramer<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands;* <sup>2</sup>*Ludwig-Maximilians-Universität München, Munich, Germany*

ThOG pm 04:10 **On-Line Liquid Chromatography Electron Capture Dissociation for Phosphoproteomics;** Steve M. Sweet; Chris M Bailey; Debbie L Cunningham; John K Heath; Helen J Cooper; *University of Birmingham, Birmingham, UK*

**4:45 - 5:30 pm**  
**PLENARY LECTURE**  
*Wells Fargo Theatre*

**The Beauty of Beer: Sublime Science Meets Art and Humanity**



**Charlie Bamforth;** *University of California, Davis*

## MONDAY POSTERS

INSTRUMENTATION: NEW CONCEPTS 1, 004 - 023	
MP 004	<b>High-Capacity Ion Trap for Two-Dimensional Mass Spectrometry;</b> <u>Yuichiro Hashimoto</u> ; Hideki Hasegawa; Masuyuki Sugiyama; <i>Hitachi, Ltd, Central Research Lab, Kokubunji, Tokyo, Japan</i>
MP 005	<b>Single Particle Charge Detection for Nanoparticle Aerosol Mass Spectrometry and X-Ray Diffractive Imaging;</b> <u>Mike Bogan</u> <sup>1</sup> ; W. Henry Benner <sup>1</sup> ; Urs Rohner <sup>1</sup> ; Sebastien Boutet <sup>2</sup> ; Matthias Frank <sup>1</sup> ; <sup>1</sup> <i>Lawrence Livermore National Laboratory, Livermore, CA;</i> <sup>2</sup> <i>Stanford Linear Accelerator Center, Menlo Park, CA</i>
MP 006	<b>Continuous Time-of-Flight Mass Spectrometer Based on Ion Modulation, Ion Imaging, and Kinetic Energy Analysis;</b> <u>Oh Kyu Yoon</u> ; Matthew Robbins; Ignacio Zuleta; Griffin Barbula; Richard N. Zare; <i>Stanford University, Stanford, CA</i>
MP 007	<b>Development and Utilization of Aerodynamic Devices for Ambient Ionization in Mass Spectrometry;</b> <u>Robert Dixon</u> ; Jason Sampson; Adam Hawkrige; David C. Muddiman; <i>North Carolina State University, Raleigh, NC</i>
MP 008	<b>Planar Resistive Electrode Ion Traps;</b> <u>Ying Peng</u> <sup>1</sup> ; Ivan W. Miller <sup>1</sup> ; Zhiping Zhang <sup>1</sup> ; Brett J. Hansen <sup>1</sup> ; Miao Wang <sup>1</sup> ; Samuel Tolley <sup>2</sup> ; Milton L. Lee <sup>1</sup> ; Aaron R. Hawkins <sup>1</sup> ; Daniel E Austin <sup>1</sup> ; <sup>1</sup> <i>Brigham Young University, Provo, UT;</i> <sup>2</sup> <i>Torion Technologies Inc., Pleasant Grove, UT</i>
MP 009	<b>Ion Extraction from Linear Quadrupole Ion Trap using Excitation Gate and Axial Gradient Fields;</b> <u>Bruce B. Reinhold</u> ; Derin B Keskin; Ellis L Reinherz; <i>Dana Farber Cancer Institute, Boston, MA</i>
MP 010	<b>Development of a Novel Analytical Platform Incorporating a Digital Ion Trap Interfaced with a Synchrotron Radiation Source for SAXS Experiments;</b> <u>Francesco L Brancia</u> <sup>1</sup> ; Bryan McCullogh <sup>2</sup> ; Andrew Entwistle <sup>1</sup> ; Steve G Buffey <sup>3</sup> ; Samar Hasnain <sup>3</sup> ; Ikuo Konishi <sup>1</sup> ; J Gunter Grossmann <sup>3</sup> ; Simon J Gaskell <sup>2</sup> ; <sup>1</sup> <i>SRL, Manchester M17 1GP, UK;</i> <sup>2</sup> <i>Department of Chemistry, University of Manchester, Manchester, UK;</i> <sup>3</sup> <i>STFC Daresbury Laboratory, Daresbury, UK</i>
MP 011	<b>Macromolecule Measurement using MALDI-DITMS;</b> <u>Koichi Tanaka</u> ; Sadanori Sekiya; Masafumi Jinno; Makoto Hazama; Kei Kodera; Shinichi Iwamoto; <i>Shimadzu Corporation, Kyoto, JAPAN</i>
MP 012	<b>Miniature Differential Mobility Ion Pre-Filtration in API-MS for Rapid, Non-Invasive Radiation-Exposure Biodosimetry;</b> <u>Erkinjon G. Nazarov</u> <sup>1</sup> ; Stephen L. Coy <sup>1</sup> ; Evgeny V. Krylov <sup>1</sup> ; David J. Brenner <sup>2</sup> ; Kristopher W. Krausz <sup>3</sup> ; John B. Tyburski <sup>3</sup> ; Andrew D. Patterson <sup>3</sup> ; Josef Slavik <sup>4</sup> ; Albert J. Fornace, Jr. <sup>3</sup> ; Frank J. Gonzalez <sup>5</sup> ; Jeffrey R. Idle <sup>4</sup> ; <sup>1</sup> <i>Sionex Corp., Bedford, MA;</i> <sup>2</sup> <i>Center for Radiological Research, N-Y, NY;</i> <sup>3</sup> <i>Lab of Methabolism, National Cancer Institute, Bethesda, MD;</i> <sup>4</sup> <i>Institute of Clinical Pharmacology, Univ. of Bern, 3010 Bern, Switzerland;</i> <sup>5</sup> <i>Lombardi Comprehensive Cancer Center, Washington, DC</i>
MP 013	<b>Bridging the Gap between Theoretical and Experimental Mass Spectrum;</b> <u>Donald Kuehl</u> ; Yongdong Wang; <i>Cerno Bioscience, Danbury, CT</i>
MP 014	<b>Ion Camera: Fusing a Confocal Mass Spectrometer with an Ion-CCD;</b> <u>Gottfried Kibelka</u> ; Omar Hadjar; Chad Cameron; Scott Shill; <i>O.I. Analytical, Pelham, AL</i>
MP 015	<b>An Advanced Concept for Mass Spectrometry Simulations - The Ion Trajectory Simulation Program ITSIM 6;</b> <u>Wolfgang R. Plass</u> ; Timo Dickel; Benjamin Fabian; Emma Haettner; <i>Justus-Liebig-Universitaet Giessen, Giessen, GERMANY</i>
MP 016	<b>Quadrupole Rod Sets with Added Decapole Fields;</b> <u>Chuan-Fan Ding</u> <sup>1</sup> ; Yu Xiao <sup>1</sup> ; Chan Luo <sup>1</sup> ; Gong-yu Jiang <sup>1</sup> ; Zejiang Huang <sup>2</sup> ; You Jiang <sup>2</sup> ; Xiang Fang <sup>2</sup> ; <sup>1</sup> <i>Fudan University, Shanghai, Shanghai;</i> <sup>2</sup> <i>National Institute of Metrology, Beijing, Beijing</i>
MP 017	<b>Custom Data Acquisition with LTQInstControl COM Library of Functions for Thermo Fisher Scientific LTQ Mass Spectrometers;</b> Aleksey Nakorchevskiy; <i>TSRI, La Jolla, CA</i>
MP 018	<b>A Mass Separating Travelling Wave Ion Guide;</b> Daniel J Kenny; <i>Waters Corporation, Manchester, UK</i>
MP 019	<b>A New Ion Mobility Based Method Utilising Time Varying Collision Energy to Improve the Fragmentation Efficiency of Multiple Precursor Ions;</b> <u>Steven D Pringle</u> ; Jason L Wildgoose; Kevin Giles; Chris Hughes; <i>Waters Corporation, Manchester, UK</i>
MP 020	<b>Simulation of a Square Electrode MEMS Quadrupole Mass Filter Operating in Stability Zones 1 and 3;</b> Thomas Hogan <sup>1</sup> ; <u>Stephen Taylor</u> <sup>1</sup> ; Kerry Cheung <sup>2</sup> ; Luis Velasquez-Garcia <sup>2</sup> ; Akintunde I Akinwande <sup>2</sup> ; <sup>1</sup> <i>University of Liverpool, Liverpool, UK;</i> <sup>2</sup> <i>MIT, Cambridge, MA</i>
MP 021	<b>Radio Frequency Power Supply for the Production of High Amplitude Asymmetric Waveforms;</b> <u>Mark E. Ridgeway</u> ; Philip M Remes; Collin McKinney; Gary L. Glish; <i>University of North Carolina, Chapel Hill, NC</i>
MP 022	<b>Simulations of a New Mass-Selected Ion Separation and Transmission Method between Linear Ion Traps;</b> <u>Gong-Yu Jiang</u> <sup>1</sup> ; Chan Luo <sup>1</sup> ; Xiao-xu Li <sup>1</sup> ; Chuan-fan Ding <sup>1</sup> ; Li Ding <sup>2</sup> ; <sup>1</sup> <i>Fudan University, Shanghai, China;</i> <sup>2</sup> <i>Shimadzu Research Lab (shanghai), Shanghai, China</i>
MP 023	<b>Development and Applications of a New Non-Hybrid Orbitrap Mass Spectrometer;</b> <u>Andreas Wieghaus</u> ; Alexander Makarov; Ulf Froehlich; Markus Kellmann; Oliver Lange; <i>Thermo Fisher Scientific, Bremen, Germany</i>
DIRECT IONIZATION 1, 024 - 044	
MP 024	<b>Comparison of Mass Spectrometric Methods for the Detection of Phosphodiesterase-5 Inhibitor Prescription Drugs in Dietary Supplements;</b> <u>Martha L. Gay</u> ; John A.G. Roach; Gregory O. Noonan; <i>FDA, College Park, MD</i>
MP 025	<b>Laser-Assisted Desorption Electrospray Ionization with a Wavelength Tunable Infrared Source;</b> <u>Mark Little</u> <sup>1</sup> ; Eli Margalith <sup>1</sup> ; Kermit K. Murray <sup>2</sup> ; Yohannes Rezenom <sup>3</sup> ; <sup>1</sup> <i>Opotek, Inc., Carlsbad, CA;</i> <sup>2</sup> <i>Louisiana State Univ., Baton Rouge, LA;</i> <sup>3</sup> <i>Louisiana State University, Baton Rouge, LA</i>
MP 026	<b>Identification of Fluorochemical Paper Coatings and Characterization of Packaging by LC-MS-MS and DART-MS;</b> <u>Gregory O. Noonan</u> ; Timothy H. Begley; Luke K. Ackerman; Gregory W. Diachenko; John A.G. Roach; <i>US Food &amp; Drug Administration, College Park, MD</i>
MP 027	<b>Recent Progresses of Extractive Electrospray Ionization Mass Spectrometry (EESI-MS) for Ambient Applications;</b> <u>Huanwen Chen</u> <sup>1</sup> ; Shuiping Yang <sup>1</sup> ; Konstantin Chingin <sup>2</sup> ; Gerardo Gamez <sup>2</sup> ; Liang Zhu <sup>5</sup> ; Jianhua Ding <sup>1</sup> ; Arno Wortmann <sup>2</sup> ; Renato Zenobi <sup>2</sup> ; <sup>1</sup> <i>East China Institute of Technology, Fuzhou, CHINA;</i> <sup>2</sup> <i>ETH Zurich, Zurich, Switzerland</i>

## MONDAY POSTERS

- MP 028 **Evaluation of Desorption Electrospray Ionization (DESI) for Quantification of Small Molecules;** Brandy Young; Dariusz Janecki; Justin Wiseman; *Prosolia, Inc., Indianapolis, IN*
- MP 029 **Field Optimization of Data Collection using DART/DESI Mass Spectrometry;** Ronny C Robbins; William M. Lagna; *US Army, Gunpowder, MD*
- MP 030 **Development of Probe Electrospray using a Solid Needle;** Kenzo Hiraoka; Lee Chui Chen; Kentaro Nishidate; Daiki Asakawa; Kunihiko Mori; Takeo Kubota; Sen Takeda; Hirokazu Hori; *University of Yamanashi, Kofu, Japan*
- MP 031 **Evaluation of DART Analytical Figures of Merit on Various Surfaces using High Resolution Mass Spectrometry;** Julia L. Rummel; John R. Eyster; David H. Powell; *University of Florida, Gainesville, FL*
- MP 032 **On-Line Monitoring and Mechanistic Studies of Chemical Reactions by Direct And Instant Analysis using Extractive Electrospray Ionization Mass Spectrometry;** Liang Zhu<sup>1</sup>; Gerardo Gamez<sup>1</sup>; Huanwen Chen<sup>2</sup>; Haoxi Huang<sup>1</sup>; Konstantin Ching<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*College of Chemistry, Jilin University, Changchun, China*
- MP 033 **Quantitative and Qualitative Analysis using ASAP Ionization Combined with SPME Sample Introduction on an Orbitrap Mass Spectrometer;** Bogdan Szostek; Charles McEwen; *DuPont CRD/CCAS, Wilmington, DE*
- MP 034 **Applications of Carbon Dioxide Induced Atmospheric Sample Desorption and Analysis;** Michael Toman; Joseph A. Jarrell; *Waters Corporation, Milford, MA*
- MP 035 **Additive Analysis in Plastic Materials by DESI;** Sander Koster<sup>1</sup>; Leon Coulier<sup>1</sup>; Brian Laughlin<sup>2</sup>; William Dongen<sup>1</sup>; <sup>1</sup>*TNO Quality of Life, Zeist, Netherlands*; <sup>2</sup>*Prosolia, Indianapolis, IN*
- MP 036 **Direct Analysis in Real Time/Mass Spectrometry for Continuously Monitoring the States of Ongoing Chemical Reactions Involved with Volatile Compounds;** Yi-Tzu Cho; Che-Hsin Lin; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 037 **Desorption Electrospray Ionization Reactions between Host Crown Ethers and the Influenza Neuraminidase Inhibitor Oseltamivir for Screening of Potentially Counterfeit Tamiflu®;** Leonard Nyadong<sup>1</sup>; Kristin R. Johnson<sup>1</sup>; Edward G. Hohenstein<sup>1</sup>; David C. Sherrill<sup>1</sup>; Michael D. Green<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Center for Disease Control and Prevention, Atlanta, GA*
- MP 038 **Automated High Throughput Analyses using the Atmospheric Solids Analysis Probe (ASAP) Method;** Barbara S. Larsen<sup>1</sup>; Richard G. McKay<sup>2</sup>; <sup>1</sup>*The Dupont Company, Wilmington, DE*; <sup>2</sup>*M and M Mass Spec Consulting, Hockessin, DE*
- MP 039 **Optimizing DART-MS Sampling for Quadrupole MS-MS Analysis of Food Contaminants;** Luke K. Ackerman; Gregory O. Noonan; Timothy H. Begley; *FDA Center for Food Safety & College Park, MD*
- MP 040 **Direct Characterization of Polymer and Chemical Compounds in Strong Acids and Bases by Ambient Liquid Mass Spectrometry;** Li-Hua Lo; Min-Zong Huang; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 041 **DART-TOF Validation and Applications in Forensic Science;** Yongyi Jiang; Stephen Houck; Mark Dixon; Ashraf Mozayani; *Harris County MEO, Houston, TX*
- MP 042 **Rapid, Automated Determination of Elemental Compositions of Ions in Mass Spectra Obtained with an Open-Air Ion Source;** Andrew H. Grange; G. Wayne Sovocool; *U.S EPA, Environmental Chemistry Branch, Las Vegas, NV*
- MP 043 **Desorption Electrospray Ionization of Flame Particulate;** Jianan Dong; Yohannes Rezenom; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- MP 044 **Direct Probe-Atmospheric Pressure Chemical Ionization (DP-APCI) For Analysis of the Polyurethane Compounds;** Sara E. Whitson<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; Robert P. Lattimer<sup>2</sup>; <sup>1</sup>*The University of Akron, Akron, OH*; <sup>2</sup>*Lubrizol Advanced Materials, Cleveland, OH*
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- INSTRUMENTATION: ION SOURCES, ESI-RELATED, 045 - 063**
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- MP 045 **Synchronized Dual-Polarity Ion Production using Electrospray Ionization Method;** Yi-Sheng Wang<sup>1</sup>; Han-Kwang Chen<sup>2</sup>; Min-Chia Huang<sup>1</sup>; Chih-Che Wu<sup>2</sup>; <sup>1</sup>*Academia Sinica, Taipei, TAIWAN*; <sup>2</sup>*Chi Nan University, Nantou Hsien, Taiwan*
- MP 046 **Chemometric Study of the Effects of Instrumental Parameters on Analyte Response across Three Commercial ESI-MS Instruments using Factorial Design;** Misjudeen Raji; Kevin Schug; *University of Texas, Arlington, TX*
- MP 047 **Design and Performance of a New Combination Electrospray and Atmospheric Pressure Chemical Ionization Source;** Victor Laiko<sup>1</sup>; Craig M. Whitehouse<sup>2</sup>; <sup>1</sup>*Analytica of Branford, In, Branford, CT*; <sup>2</sup>*Analytica of Branford, Inc., Branford, CT*
- MP 048 **Observation of Unstable Binding Compounds in Aqueous Solution on CSI-TOF-MS;** Haruo Hosoda; Noriyuki Iwasaki; Kazunori Saito; Shinichi Miki; Takashi Nirasawa; Jouji Seta; *Bruker Daltonics KK, Yokohama, Japan*
- MP 049 **Continuously Monitoring the States of Ongoing Chemical Reactions by Ambient Liquid Mass Spectrometry (ALMS);** Min-Zong Huang; Cheng-Hui Yuan; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 050 **Elastomeric Microchip Electrospray Emitters for Stable Cone-Jet Mode Operation in the Nano-Flow Regime;** Ryan T. Kelly<sup>1</sup>; Keqi Tang<sup>1</sup>; Daniel Irimia<sup>2</sup>; Mehmet Toner<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Massachusetts Gen. Hospital/Harvard Medical School, Boston, MA*
- MP 051 **Signal Enhancement in Negative Ion Polarity Electrospray using an Electrospray Membrane Probe;** Shida Shen; Thomas White; Craig M. Whitehouse; *Analytica of Branford, Inc., Branford, CT*
- MP 052 **A New Ionization Source for Mass Spectrometry: Subambient Pressure Ionization with Nanoelectrospray (SPIN);** Jason S. Page; Keqi Tang; Ryan T. Kelly; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- MP 053 **New Nano-Electrospray Tip with Platinum Wire to Improve Spraying Stability;** Yunjo Chung<sup>1</sup>; Joseph Kwon<sup>2</sup>; Sunghwan Kim<sup>3</sup>; <sup>1</sup>*Chonbuk National University, Chon-Ju, South Korea*; <sup>2</sup>*Korea Basic Science Institut, Kwangju, South Korea*; <sup>3</sup>*Korean Basic Science Institute, Ochang-myun, South Korea*

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- MP 054 **Means and Mechanism for Non-disruptive Calibrant Addition to an LC-MS Interface Designed for High Flow Rate Operation;** Bradley B. Schneider; Thomas R. Covey; *MDS Sciex, Concord, CANADA*
- MP 055 **Characterization of Spraying Modes from Microfabricated Nozzles on a Nanoelectrospray Chip;** Akos Vertes<sup>1</sup>; Gary A. Schultz<sup>2</sup>; Jack D. Henion<sup>2</sup>; Jelena Lusic<sup>1</sup>; Peter Nemes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, DC*; <sup>2</sup>*Advion Biosciences, Inc, Ithaca, NY*
- MP 056 **Nanoporous Alumina as a Dual Ionization LDI-DESI Platform for Increased Peptide Coverage in Shotgun Proteomic Analysis;** Ranu Nayak<sup>1,2</sup>; Ashis K Sen<sup>1,2</sup>; Daniel R. Knapp<sup>3</sup>; <sup>1</sup>*Med Univ of South Carolina, Charleston, SC*; <sup>2</sup>*Med Univ of South Carolina, Charleston, SC*; <sup>3</sup>*Medical University of Sc, Charleston, SC*
- MP 057 **Imaging of Nanoelectrospray Spray Current with an Automated Digital Control Positioning System;** Gary Valaskovic<sup>1</sup>; Mike S. Lee<sup>2</sup>; <sup>1</sup>*New Objective, Inc., Woburn, MA*; <sup>2</sup>*Milestone Development Services, Newtown, PA*
- MP 058 **Internal Energy Deposition of a Venturi-Assisted Array of Micromachined Ultrasonic Electrospays;** Christina Y. Hampton; Catherine J. Silvestri; Thomas P. Forbes; Mark J. Varady; J. Mark Meacham; F. Levent Degertekin; Andrei G. Fedorov; Facundo M. Fernandez; *Georgia Institute of Technology, Atlanta, GA*
- MP 059 **Exploring Mechanisms of Analyte Ionization in AMSUE (Array of Micromachined UltraSonic ElectroSpray) Ion Source Combined with an FT-ICR Mass Spectrometer;** Thomas P. Forbes<sup>1</sup>; R. Brent Dixon<sup>2</sup>; David C. Muddiman<sup>2</sup>; F. Levent Degertekin<sup>1</sup>; Andrei G. Fedorov<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*North Carolina State University, Raleigh, NC*
- MP 060 **Analysis of Large Surface Areas by DESI;** Gary Abdiel Salazar; Richard H. Perry; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MP 061 **Ultrasonic nebulizer Ionization Mass Spectrometry (UNI-MS) for Biomolecule Analysis;** Chen-i Wu; Wei-San Hsu; Yi-Sheng Wang; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- MP 062 **Comparison of Electrochemistry (EC) –Electrospray (ES) Cell Designs for Investigation of Electrochemical Transformations using EC–ES–MS–MS;** Boguslaw Pozniak; Richard B. Cole; *University of New Orleans, New Orleans, LA*
- MP 063 **Injection of Intact Molecular Ions through the Ring Electrode of a 3D Ion Trap via a Cluster Source;** Jeremiah Bowers; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*
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- APPI, 064- 073**
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- MP 064 **Polymer Additives Analysis using Liquid Chromatography with Atmospheric Pressure Photoionization Mass Spectrometry (LC/APPI/MS);** Christie Bowden; *Arkema Inc., King of Prussia, PA*
- MP 065 **New Dopants for Atmospheric Pressure Photo Ionisation in Mass Spectrometry Detection;** Boutayna Rhourri Frih; Patrick Chaimbault; Michel Lafosse; *ICOA laboratory, Orléans, France*
- MP 066 **Theory and Operation of APPI for LC-MS;** Jack A. Syage; *Syagen Technology, Inc., Tustin, CA*
- MP 067 **Atmospheric Pressure Laser Ionization (APLI): Investigations on Ion Transport in Atmospheric Pressure Ion Sources;** Matthias Lorenz; Sonja Klee; René Mönnikes; Ana Lydia Mangas Suárez; Klaus J. Brockmann; Oliver J. Schmitz; Siegmär Gäß; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 068 **Ionization Labeling: A Useful Tool in GC and LC-APLI-(TOF)MS;** Ralf Schiewek; René Mönnikes; Thorsten Benter; Siegmär Gäß; Oliver J. Schmitz; *University of Wuppertal, Wuppertal, Germany*
- MP 069 **Characterization of Building Blocks of Organic LEDs with Atmospheric Pressure Laser Ionization-(TOF)MS;** Ralf Schiewek; Ana Lydia Mangas Suárez; Nan Tian; Elisabeth Holder; Askin Bilge; Ullrich Scherf; Klaus J. Brockmann; Thorsten Benter; Oliver J. Schmitz; Siegmär Gäß; *University of Wuppertal, Wuppertal, Germany*
- MP 070 **Comparison of Dopants for Charge Exchange Ionization of Nonpolar Polycyclic Aromatic Hydrocarbons with Reversed-Phase LC-APPI-MS;** Derek Smith; Damon Robb; Michael W. Blades; *University of British Columbia, Vancouver, CANADA*
- MP 071 **Measurements of REMP Spectra of Selected Ionization Labels at Reduced and Atmospheric Pressure;** René Mönnikes; Ralf Schiewek; Hendrik Kersten; Matthias Lorenz; Oliver J. Schmitz; Siegmär Gäß; Klaus J. Brockmann; Thorsten Benter; *University of Wuppertal, D-42119 Wuppertal, Germany*
- MP 072 **Ionization Mechanism of NI-DART (Negative Ion-Direct Analysis in Real Time): A Comparative Study with NI-APPI (Negative Ion-Atmospheric Pressure Photoionization);** Liguó Song; Andrew Dykstra; Huifang Yao; John Bartmess; *University of Tennessee, Knoxville, TN*
- MP 073 **Non-Uniform Isotope Patterns Produced by CID of Homogeneously Labeled Ubiquitin: Implications for Spatially-Resolved H/D Exchange Studies;** Peter L Ferguson<sup>2</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>*Univ. of Western Ontario, London, Canada*; <sup>2</sup>*Univ of Western Ontario, London, ON*
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- ION STRUCTURES/ENERGETICS 1, 074 - 088**
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- MP 074 **IRMP and DFT Investigation of Discrete, Anionic Group II Metal Nitrate Clusters;** Christopher M. Leavitt<sup>1</sup>; Jos Oomens<sup>2</sup>; Jeffrey Steill<sup>2</sup>; Gary Groenewold<sup>3</sup>; Michael J. Van Stipdonk<sup>1</sup>; <sup>1</sup>*Wichita State University, Wichita, KS*; <sup>2</sup>*FOM Rijnhuizen, Nieuwegein, Netherlands*; <sup>3</sup>*Idaho National Lab, Idaho Falls, ID*
- MP 075 **Tandem Mass Spectrometry and *ab initio* Studies of Methylene Nucleotide Triphosphate Anions;** M. Paul Chiarelli<sup>1</sup>; Eric C. Brown<sup>1</sup>; Bongsup P. Cho<sup>2</sup>; Justin B. Sperry<sup>3</sup>; <sup>1</sup>*Loyola University, Chicago, IL*; <sup>2</sup>*University of Rhode Island, Kingston, RI*; <sup>3</sup>*Washington University, St. Louis, MO*
- MP 076 **The Optical Activity of Gas Phase Fluorescein Studied using Laser Induced Fluorescence and Quadrupole Ion Trap Mass Spectrometry;** Peter D. McQueen; Qunzhou Bian; Rebecca A. Jockusch; *University of Toronto, Toronto, Canada*
- MP 077 **Mass Analyzed Threshold Ionization of Chlorine Containing Aromatic Compounds;** Mikko Riese; Frank Witte; Jürgen Grotemeyer; *Christian-Albrechts- Univ, Kiel, Germany*
- MP 078 **Investigations of the Stability of Non-Covalent Interactions between Nucleotides and Amino Acids in the Gas Phase;** John Poutsma<sup>1</sup>; Elise Dennis<sup>1</sup>; Sandra Alves<sup>2</sup>; Jean-claude Tabet<sup>2</sup>; Ludovic Muller<sup>2</sup>; <sup>1</sup>*College of William & Mary, Williamsburg, VA*; <sup>2</sup>*Université Pierre Et Marie Curie, Paris, France*

## MONDAY POSTERS

- MP 079 **Fragmentation of an Adenine-Steroid Adduct: Experimental and Theoretical Studies II;** Daryl Giblin; Qiang Zhang; Michael L. Gross; *Washington University, St Louis, MO*
- MP 080 **Negative Ion Photoelectron Spectroscopy and Thermochemistry of Formylperoxyl and Acetylperoxyl Radicals;** Stephanie M. Villano; Scott W. Wren; Shuji Kato; Veronica M. Bierbaum; W. Carl Lineberger; *University of Colorado at Boulder, Boulder, CO*
- MP 081 **Probing Anionic Zwitterion Structure via IR Spectroscopy;** Matthew M. Meyer<sup>1</sup>; Zhixin Tian<sup>1</sup>; Jeff Steill<sup>2</sup>; Jos Oomens<sup>2</sup>; Steven R. Kass<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*Fom Rijnhuizen, Nieuwegein, Netherlands*
- MP 082 **TPEPICO Study of the Low Energy Dissociation Pathways of Ortho-, Meta- and Para-Difluorobenzene Ions;** Anne-Marie Boulanger<sup>1</sup>; David M. P. Holland<sup>2</sup>; David A. Shaw<sup>2</sup>; Paul Michael Mayer<sup>1</sup>; <sup>1</sup>*University of Ottawa, Ottawa, Canada*; <sup>2</sup>*Daresbury Laboratory, Daresbury, UK*
- MP 083 **Carboxylate Coordination in Uranyl Complexes by IRMPD;** Gary Groenewold<sup>1</sup>; Michael J. Van Stipdonk<sup>4</sup>; Wibe A. de Jong<sup>2</sup>; Jos Oomens<sup>3</sup>; <sup>1</sup>*Idaho Natl. Eng. Envir. Lab, Idaho Falls, ID*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>3</sup>*FOM Institute for Plasmaphysics, Nieuwegein, The Netherlands*; <sup>4</sup>*Wichita State University, Wichita, KS*
- MP 084 **Spectroscopic Investigation of H Atom Transfer in a Gas-phase Dissociation Reaction: McLafferty Rearrangement of Model Gas-Phase Peptide Ions;** Dale R Kerstetter<sup>1</sup>; Christopher Leavitt<sup>1</sup>; Michael J. Van Stipdonk<sup>1</sup>; Jeff Steill<sup>2</sup>; Jos Oomens<sup>2</sup>; Gary Groenewold<sup>3</sup>; <sup>1</sup>*Wichita State University, Wichita, KS*; <sup>2</sup>*FOM Instituut voor Plasmafysica, Nieuwegein, The Netherlands*; <sup>3</sup>*Idaho National Laboratory, Idaho Falls, ID*
- MP 085 **Gas Phase Peptide-Peptide Interactions Probed by ECD, Energy-Resolved CID and Tunable Free-Electron Laser Infrared Spectroscopy;** Guillaume van der Rest<sup>1</sup>; Christian Malosse<sup>1</sup>; Julia Chamot-rooke<sup>1</sup>; Anne-Pascale Bouin<sup>2</sup>; Philippe Maitre<sup>3</sup>; Joel Lemaire<sup>3</sup>; <sup>1</sup>*Ecole Polytechnique, Palaiseau, France*; <sup>2</sup>*Universite Joseph Fourier, Grenoble, France*; <sup>3</sup>*Laboratoire De Chimie Physique, Orsay, France*
- MP 086 **IRMP of Ion-Molecule Reaction Products: Violation of the Even Electron Rule in the Dissociation of the [C<sub>6</sub>H<sub>4</sub>CCl<sub>2</sub>COCH<sub>3</sub>]<sup>+</sup> Ion;** Jose M. Riveros; Tatiana Giroldo; *Instituto De Quimica-USP, Sao Paulo, Brazil*
- MP 087 **Gas Phase Infrared Spectroscopy and Tandem Mass Spectrometry;** Philippe Maitre; Joel Lemaire; Debora Scuderi; Joost M Bakker; *Laboratoire de Chimie Physique, Orsay, France*
- MP 088 **ESI-ICR Investigation of Rearrangement and Fragmentation Reactions of Different Steroid Ethers;** Cristoph Freudenhammer; Jurgen Grottemeyer; *University Kiel, Kiel, Germany*
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- ENVIRONMENTAL ANALYSIS, 089 - 099**
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- MP 089 **Column-Switching Chromatography / Polarity-Switching Tandem Mass Spectrometry for Determination of Sub-ppt levels of Free and Conjugated Estrogens in Water Samples;** Feng Qin; Yuan-yuan Zhao; Michael Sawyer; Xing-Fang Li; *University of Alberta, Edmonton, Canada*
- MP 090 **An Ultra-Sensitive Method for LC-MS-MS Analyses of 3-OH-Benzo[a]Pyrene in Human Urine;** Veniamin Lapko; Ridha Nachi; Yousef Basir; Kirk Newland; *MDS Pharma Services, Lincoln, NE*
- MP 091 **Study of Cigarette Smoke by FTICRMS and FTICRMS-MS in Electrospray and Laser Desorption Modes;** Frédéric Aubriet; *LSMCL Univeristé Paul Verlaine Metz, Metz, France*
- MP 092 **Measurements of Horizontal and Vertical Gradients of Dissolved Gas Concentrations using a Calibrated Underwater Membrane Inlet Mass Spectrometer;** Ryan J. Bell<sup>1</sup>; Strawn K. Toler<sup>2</sup>; Peter G. Wenner<sup>3</sup>; R. Timothy Short<sup>2</sup>; Robert H. Byrne<sup>1</sup>; <sup>1</sup>*College of Marine Science, St Petersburg, FL*; <sup>2</sup>*SRI International, St Petersburg, FL*; <sup>3</sup>*Florida Department of Environmental Protection, Tampa, FL*
- MP 093 **Quantitative, Multi-Analyte, High Throughput, HPLC-MS-MS Method for Hemoglobin Adducts of Environmental Chemicals;** Tunde Meyers; Hubert Vesper; Magaly Mendez; Maria Ospina; Gary Myers; *CDC, Atlanta, GA*
- MP 094 **Thermally Assisted Membrane Introduction Mass Spectrometry (TAMIMS) Interfaces - Improvements for Semi-Volatile Organic Compounds in Environmental Samples;** Nicholas G. Davey; Shakour Ghafouri; Erik T. Krogh; Christopher G. Gill; *Applied Environ. Res. Labs. (AERL), Malaspina, Nanaimo, Canada*
- MP 095 **Field Measurement Applications using a New Toroidal Ion Trap GC-TMS: Separating Fact from Fiction in Complex Mixtures;** Christopher R Bowerbank; Tiffany C Wirth; Joseph L Oliphant; Edgar D Lee; Douglas W Later; *Torion Technologies, Inc., Pleasant Grove, UT*
- MP 096 **Improved Sensitivity for PAH Analysis with GC-APLI-MS;** Ian Sanders<sup>1</sup>; Thomas Arthen-Engeland<sup>1</sup>; Armin Holle<sup>1</sup>; Carsten Baesmann<sup>1</sup>; Ralf Schiewek<sup>2</sup>; Oliver J. Schmitz<sup>2</sup>; Klaus J. Brockmann<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*
- MP 097 **Determination of PAHs, Methyl-PAHs, and Nitro-PAHs in Air Filter Samples using Isotope Dilution GC-HR-MS and GC-NCI-MS;** Zheng Li<sup>1</sup>; Erin N Porter<sup>1</sup>; Lovisa C Romanoff<sup>1</sup>; Debra A Trinidad<sup>1</sup>; Jame Mulholland<sup>2</sup>; Andreas Sjodin<sup>1</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, GA*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*
- MP 098 **GC-MS Study of Microbiological Destruction of Pyridine with its Alkyl Derivatives and MALDI Characterization of the Strain Destructor;** Fatima Khasaeva; Petr Terentyev; Maria Troshina; Albert T. Lebedev; *Moscow State University, Moscow, Russian Federation*
- MP 099 **LC-MS-MS Determination of Perfluorinated Compounds (PFCs) in Fillets of Multiple Fish Species from the Cape Fear River Basin, North Carolina;** Amy D. Delinsky<sup>1</sup>; Mark J. Strynar<sup>1</sup>; Andrew B. Lindstrom<sup>1</sup>; Jerry L. Varns<sup>2</sup>; Shoji F. Nakayama<sup>3</sup>; <sup>1</sup>*U.S. EPA, RTP, NC*; <sup>2</sup>*NCBA Inc., See Program, Durham, NC*; <sup>3</sup>*ORISE, Oak Ridge, TN*
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- ATMOSPHERIC/AEROSOL CHEMISTRY, 100 - 113**
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- MP 100 **Detection of Nitrated Polycyclic Aromatic Hydrocarbons in Diesel Exhaust Particulates by GC-NCI-MS;** Cheng-Han Hung<sup>1</sup>; Hsin-Pin Ho<sup>1</sup>; Chung-Yu Chen<sup>1</sup>; Kuei-Chen Chang<sup>1</sup>; Maw-Rong Lee<sup>1</sup>; Youn-Yuen Shu<sup>2</sup>; Te-Lung Lai<sup>2</sup>; Pih Wang<sup>3</sup>; <sup>1</sup>*National Chung-Hsing University, Taichung, TAIWAN*; <sup>2</sup>*National Kaohsiung Normal University, Kaohsiung, Taiwan*;

## MONDAY POSTERS

- MP 101 <sup>3</sup>*Environmental Analysis Laboratory, Executive Yuan, Taoyuan, Taiwan*  
**Proton Transfer Reaction-Mass Spectrometry-Electroantennography to Measure Chemical Signal Dynamics (A New Insect Olfactory Ecology Tool);** Leif Abrell; Jeffrey A. Riffell; John G. Hildebrand; *University of Arizona, Tucson, AZ*
- MP 102 **On-Line Monitoring of VOC Emissions from Nanofilm Coating Products using a Handheld Membrane Inlet Mass Spectrometer;** Asger Nørgaard<sup>2</sup>; Christian Janfelt<sup>1</sup>; Peder Wolkoff<sup>2</sup>; Keld A. Jensen<sup>2</sup>; Frants R. Lauritsen<sup>1</sup>; <sup>1</sup>*University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Nat. Research Centre for the Working Environment, Copenhagen, Denmark*
- MP 103 **Proton-Transfer Reaction Ion Trap Mass Spectrometry (PIT-MS): Instrumental Improvements and Applications in Atmospheric Field Measurements;** Daniel Welsh-Bon; Carsten Warneke; Joost de Gouw; Troy Thornberry; *NOAA ESRL/CIRES/University of Colorado, Boulder, CO*
- MP 104 **Quantitative Analysis of Monoterpenes, Sesquiterpenes, and other Isomers using a Proton Transfer Reaction LIT and Triple Quadrupole Mass Spectrometry;** Levi H. Mielke<sup>1</sup>; Markus Müller<sup>2</sup>; Martin Breitenlechner<sup>2</sup>; Pawel Cais<sup>2</sup>; Armin Wisthaler<sup>2</sup>; Scott A. McLuckey<sup>1</sup>; Paul B. Shepson<sup>1</sup>; Armin Hansel<sup>2</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of Innsbruck, Innsbruck, Austria*
- MP 105 **Analysis of Organic Compounds in Aerosol Particles by Liquid Chromatography and High Resolution Mass Spectrometry;** Andreas Roempp<sup>1</sup>; Alexa Sadezky<sup>2</sup>; Richard Winterhalter<sup>2</sup>; Basem Kanawati<sup>2</sup>; Patrick Chaimbault<sup>3</sup>; Bernhard Spengler<sup>1</sup>; Geert Moortgat<sup>2</sup>; <sup>1</sup>*Justus Liebig University, Giessen, Germany*; <sup>2</sup>*Max Planck Institute for Chemistry, Mainz, Germany*; <sup>3</sup>*University of Orleans, Orleans, France*
- MP 106 **Monitoring of Fast Changes in Aerosol Chemistry with a Time-of-Flight Aerosol Mass Spectrometer;** Joel R. Kimmel; Delphine K. Farmer; Donna Sueper; Jose-Luis Jimenez; *University of Colorado, Boulder, CO*
- MP 107 **Development of a Metastable Atom Bombardment (MAB) Ionization Source for Mass Spectrometric Analysis of Aerosols;** Carly B Robinson<sup>1</sup>; Joel R Kimmel<sup>1</sup>; John T. Jayne<sup>2</sup>; Achim Trimborn<sup>2</sup>; Don David<sup>1</sup>; Douglas R. Worsop<sup>2</sup>; Jose-Luis Jimenez<sup>1</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*; <sup>2</sup>*Aerodyne Research, Inc, Billerica, MA*
- MP 108 **Characterization of Organosulfates and Nitrooxy Organosulfates from the Photooxidation of Isoprene using Liquid Chromatography/Negative Ion Electrospray Mass Spectrometry;** Magda M. Claeys<sup>1</sup>; Jason D Surratt<sup>2</sup>; Yadian Gomez-Gonzalez<sup>1</sup>; Reinhilde Vermeylen<sup>1</sup>; Arthur WH Chan<sup>2</sup>; Mona Shagholi<sup>2</sup>; Willy Maenhaut<sup>3</sup>; John H Seinfeld<sup>2</sup>; <sup>1</sup>*University of Antwerp (Campus Drie Eiken), Antwerp, Belgium*; <sup>2</sup>*California Institute of Technology, Pasadena, CA*; <sup>3</sup>*Ghent University, Gent, Belgium*
- MP 109 **Real Time Detection and Quantification of Dangerous Substances in Air without Sample Preparation using SIFT-MS;** Gregory J Francis<sup>1</sup>; Murray J. McEwan<sup>1</sup>; Vaughan S Langford<sup>2</sup>; Daniel B Milligan<sup>2</sup>; <sup>1</sup>*University of Canterbury, Christchurch, New Zealand*; <sup>2</sup>*Syft Technology Ltd, Christchurch, New Zealand*
- MP 110 **Eucalypt Smoke and Wildfires;** Simin D. Maleknia<sup>1</sup>; Tina L Bell<sup>2</sup>; Mark A Adams<sup>1</sup>; <sup>1</sup>*The University of New South Wales, Sydney, Australia*; <sup>2</sup>*University of Melbourne, Creswick, VIC, Australia*
- MP 111 **Continuous Real-Time Trace Analysis of BTEX in Ambient Air using Direct Sampling LDTD-APCI-MS2 System;** Koffi Badjagbo<sup>1</sup>; Pierre Picard<sup>2</sup>; Jean Lacoursière<sup>3</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>*Université de Montreal, Montreal, CANADA*; <sup>2</sup>*Phytronix Technologies, Inc., Quebec, QC*; <sup>3</sup>*Phytronix Technologies, Québec, QC*
- MP 112 **Structural and Mechanistic Characterization of Oligomeric Materials Found in Model Secondary Organic Aerosol (SOA) using Desorption-Electrospray Ionization (DESI) Tandem MS;** Marc Fiddler; R. Graham Cooks; Paul Shepson; *Purdue University, West Lafayette, IN*
- MP 113 **Examination of Ozone Depleting Iodine Species by Ion Chromatography in the Complex Salt Environment of Marine Aerosols;** Stacy Henday; Jinyuan Wang; William C. Schnute; *Dionex Corporation, Sunnyvale, CA*
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- MP 114 **Activity Based Imaging Mass Spectrometry with Signal Amplification;** Junhai Yang<sup>2</sup>; Pierre Chaurand<sup>2</sup>; Ned A. Porter<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt Univ Sch of Med, Nashville, TN*; <sup>2</sup>*Vanderbilt University, Nashville, TN*
- MP 115 **Mass Spectrometric Imaging of Metabolic Dynamics in the Mouse Hippocampus;** Yuki Sugiura<sup>1</sup>; Yoshiyuki Konishi<sup>2</sup>; Nobuhiro Zaima<sup>2</sup>; Hiroki Nakanishi<sup>3</sup>; Yoshiya Oda<sup>4</sup>; Ryo Taguchi<sup>3</sup>; Mitsutoshi Setou<sup>2</sup>; <sup>1</sup>*Tokyo Tech, Tokyo, Japan*; <sup>2</sup>*Mitsubishi Kagaku Institute of Life Sciences, Tokyo, Japan*; <sup>3</sup>*The University of Tokyo, Tokyo, Japan*; <sup>4</sup>*Eisai, Tsukuba, Japan*
- MP 116 **In situ Lipidomic Analysis of Non Alcoholic Fatty Liver by Cluster-TOF-SIMS Imaging;** Delphine Debois<sup>1</sup>; Marie-Pierre Bralet<sup>2</sup>; François Le Naour<sup>3</sup>; Alain Brunelle<sup>1</sup>; Olivier Laprevote<sup>1</sup>; <sup>1</sup>*ICSN / CNRS, Gif-sur-Yvette, France*; <sup>2</sup>*AP-HP Hôp. P. Brousse - Univ. Paris-Sud, UMR-S 785, Villejuif, France*; <sup>3</sup>*INSERM U602 - Univ. Paris-Sud, Institut A. Lwoff, Villejuif, France*
- MP 117 **Applications of MSI Techniques to the Study of Dermal Uptake of a Topically Treated Anti-inflammatory Acne Compound;** Brendan Prideaux<sup>1</sup>; Dieter Staab<sup>1</sup>; Andreas Billich<sup>1</sup>; Olivier Laprevote<sup>2</sup>; Alain Brunelle<sup>2</sup>; Alexandre Seyer<sup>2</sup>; Markus Stoeckli<sup>1</sup>; <sup>1</sup>*Novartis Institutes For Biomedical Research, Basel, Switzerland*; <sup>2</sup>*Icsn - Cnrs, Gif Sur Yvette, France*
- MP 118 **Automated Collection and Analysis of Desorption Electrospray Ionization (DESI) Mass Spectrometry Imaging Data;** Nicholas E. Manicke; Sanket Khandelwal; Anthony B. Costa; Thomas Kistler; Demian R. Ifa; R. Graham Cooks; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- MP 119 **Phyto-Metabolomic Spatial Profiling using MALDI Mass Spectrometric Imaging;** Rohit Shroff; Fredd Vergara; Alexander Muck; Jonathan Gershenson; Ales Svatos; *Max Planck Institute for Chemical Ecology, Jena, Germany*



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- MP 120 **LDI Mass Spectral Imaging of Plant Secondary Metabolites on *Arabidopsis thaliana* using Graphite and Silver as Matrixes;** Sangwon Cha; Zhihong Song; Hui Zhang; Hilal I. Ilarslan; Libuse Brachova; Eve S. Wurtele; Basil J. Nikolau; Edward S. Yeung; *Iowa State University, Ames, IA*
- MP 121 **Direct Identification of Small Molecules by MALDI Imaging using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Jens Fuchser<sup>1</sup>; Christian Berg<sup>2</sup>; Matthias Witt<sup>1</sup>; Michael Becker<sup>1</sup>; Christopher Thompson<sup>2</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*
- MP 122 **Examination of the Distribution of Nicosulfuron in Sunflower Plants by MALDI-MSI;** David Anderson<sup>1</sup>; Malcolm Clench<sup>1</sup>; Vikki Carolan<sup>1</sup>; Susan Crosland<sup>2</sup>; Kate Sharples<sup>2</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*Syngenta, Bracknell, UK*
- MP 123 **TLC-Imaging MALDI-MS Analysis of Phospholipids;** Beate Fuchs<sup>2</sup>; Detlev Suckau<sup>1</sup>; Martin Schürenberg<sup>1</sup>; Rosemarie Suess<sup>2</sup>; Juergen Schiller<sup>2</sup>; <sup>1</sup>*Bruker Daltonics, Bremen, GERMANY*; <sup>2</sup>*Leipzig Univ. Inst. Med. Physics and Biophysics, Leipzig, Germany*
- MP 124 **Imaging MALDI-MS: Investigation of Analyte Extraction Efficiency through Various Tissue Types;** Daniel P. Magparangan<sup>1</sup>; Dieter M. Drexler<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*; <sup>2</sup>*Bristol Myers Squibb, Wallingford, CT*
- MP 125 **TOF-SIMS of RBL-2H3 Cells: Label-Free, Molecule-Specific Imaging of Membrane Lipid Distribution in Single Cells;** Paul D. Piehowski; Angel M. Davey; Michael L. Heien; Michael E. Kurczy; Erin D. Sheets; Nicholas Winograd; Andrew G. Ewing; *The Pennsylvania State University, University Park, PA*
- MP 126 **Quantitation of Lipids in Nerve Tissue using IP-MALDI-LIT-MS;** Rachelle R Landgraf; Timothy J Garrett; Peter W Stacpoole; Richard A Yost; *University of Florida, Gainesville, FL*
- MP 127 **Following Temporal Biological Processes using Imaging MALDI MS: Phospholipid analysis in Early Mouse Pregnancy;** Kristin Burnum<sup>1</sup>; Shannon Cornett<sup>1</sup>; Satu Puolitaival<sup>1</sup>; Susanne Tranguch<sup>1</sup>; S.K. Dey<sup>1</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Vanderbilt Univ Sch of Med, Nashville, TN*
- MP 128 **TOF-SIMS Chemical Imaging of Ritual Materials from African Art Objects;** Pascale Richardin<sup>1</sup>; Vincent Mazel<sup>1</sup>; Delphine Debois<sup>3</sup>; David Touboul<sup>4</sup>; Alain Brunelle<sup>2</sup>; Philippe Walter<sup>1</sup>; Olivier Laprèvote<sup>4</sup>; <sup>1</sup>*C2RMF, Paris, FRANCE*; <sup>2</sup>*Icsn - Cnrs, Gif Sur Yvette, France*; <sup>3</sup>*Icsn / Cnrs, Gif-sur-yvette, France*; <sup>4</sup>*Cnrs-icsn, Gif-sur-yvette, France*
- MP 129 **From 2D to 3D Biomolecular Imaging with TOF-SIMS: A Study of Drug Elution from a Coronary Stent;** Greg Fisher; *Physical Electronics, Chanhassen, MN*
- MP 130 **MALDI-Ion Mobility Separation-MS Imaging of Vinblastine and its Metabolites in Rat Tissue;** Paul J Trim<sup>1</sup>; Jennie L Avery<sup>2</sup>; Andrew McEwen<sup>2</sup>; Marten F. Snel<sup>3</sup>; Emmanuelle Claude<sup>3</sup>; Peter S. Marshall<sup>4</sup>; Andrew West<sup>4</sup>; Alessandra P Princivale<sup>1</sup>; Malcolm Clench<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*BioDynamics Research Ltd, Rushden, UK*; <sup>3</sup>*Waters Corporation, Manchester, UK*; <sup>4</sup>*GlaxoSmithKline, Harlow, UK*
- MP 131 **Validation of Lipid Distribution in Images Acquired by MALDI Mass Spectrometric Imaging;** Joseph A. Hankin<sup>1</sup>; Thomas Leiker<sup>2</sup>; Robert C. Murphy<sup>3</sup>; <sup>1</sup>*University of Colorado, Aurora, CO*; <sup>2</sup>*Us Geological Survey, Denver, CO*; <sup>3</sup>*University of Colorado Hsc, Aurora, CO*
- MP 132 **Tablet Imaging using Matrix-Assisted Laser Desorption Ionisation Mass Spectrometry;** Caroline J. Earnshaw<sup>1</sup>; Don S. Richards<sup>2</sup>; Malcolm R. Clench<sup>1</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*Pfizer Global R&D, Ramsgate Road, Sandwich, Kent, UK*
- MP 133 **Visualizing Low-Mass Biomolecules using Matrix-Enhanced Surface-Assisted Laser Desorption Ionization Imaging Mass Spectrometry (ME-SALDI-IMS);** Qiang Liu<sup>1</sup>; Yongsheng Xiao<sup>1</sup>; Coral Pagan<sup>2</sup>; Yu Matthew Chiu<sup>1</sup>; Lin He<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*University of Puerto Rico, San Juan, Puerto Rico*
- MP 134 **Coupling MALDI MS with High-Efficiency Ion Mobility Spectrometry for Tissue Imaging of Low Mass Endogenous Compounds;** Emmanuelle Claude<sup>1</sup>; Paul J Trim<sup>2</sup>; Marten F Snel<sup>1</sup>; Therese McKenna<sup>1</sup>; James Langridge<sup>1</sup>; <sup>1</sup>*Waters corporation, Manchester, UK*; <sup>2</sup>*Sheffield Hallam University, Sheffield, UK*
- MP 135 **Evaluation of Multiple Preparation Methods for Biological Sample Analysis by Secondary Ion Mass Spectrometry;** Sara G. Ostrowski; Vincent S. Smentkowski; Lauraine Denault; Tracy L. Paxon; *General Electric, Niskayuna, NY*
- MP 136 **Mass Spectrometric Imaging (MSI) Revealed the Age-Related Change of Phosphatidylcholine in the Mouse Brain;** Naofumi Hosokawa<sup>1</sup>; Yuki Sugiura<sup>1</sup>; Mitsutoshi Setou<sup>2</sup>; <sup>1</sup>*Tokyo Institute of Technology, Yokohama, Japan*; <sup>2</sup>*Hamamatsu University School of Medicine, Shizuoka, Japan*
- MP 137 **Imaging Mass Spectrometry of Ubiquinone 50 in Human Muscle Tissues;** Alessandro Saba<sup>1</sup>; Andrea Raffaelli<sup>2</sup>; Gabriele Siciliano<sup>3</sup>; Doug Simmons<sup>4</sup>; Andrew James<sup>4</sup>; Robert Ellis<sup>4</sup>; Takeo Sakuma<sup>4</sup>; Piers Salvadori<sup>1</sup>; <sup>1</sup>*University of Pisa - Chemistry Dept., Pisa, ITALY*; <sup>2</sup>*Cnr Iccom, Pisa, ITALY*; <sup>3</sup>*University of Pisa - Neurosciences Dept., Pisa, Italy*; <sup>4</sup>*Applied Biosystems / Mds Sciex, Concord, ON*
- MP 138 **Electrospray-Assisted Laser Desorption Ionization (ELDI) Mass Spectrometry for Molecular Imaging of Mushroom Slices and Animal Tissues;** Hay-Yan Wang; Min-Zong Huang; Li-Hua Lo; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 139 **Simultaneous Imaging of Small Molecules from Thin Tissue Sections using MALDI Traveling Wave Ion Mobility-Mass Spectrometry;** Whitney Beth Ridenour<sup>1</sup>; Marten F. Snel<sup>2</sup>; Emmanuelle Claude<sup>2</sup>; John A. Mclean<sup>3</sup>; Sara L. Frappier<sup>3</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Department of Biochemistry, Vanderbilt University, Nashville, TN*; <sup>2</sup>*Waters Corporation, MS Technologies Centre, Manchester, M22 5PP, UK*; <sup>3</sup>*Department of Chemistry, Vanderbilt University, Nashville, TN*
- MP 140 **Relative Quantification of Phospholipid Changes in Single Cell Membranes following Lipid Incubation using Imaging MS;** Michael E. Kurczy<sup>1</sup>; Paul D. Piehowski<sup>1</sup>; Michael L. Heien<sup>1</sup>; Nicholas Winograd<sup>1</sup>; Andrew G. Ewing<sup>2</sup>; <sup>1</sup>*Penn State University, University Park, PA*; <sup>2</sup>*Goteborg University, Goteborg, Sweden*
- MP 141 **Imaging MALDI-Mass Spectrometry of Astemizole in Rat Brain Tissues;** Fangbiao Li<sup>1</sup>; Yunsheng Hsieh<sup>2</sup>; Walter Korfmacher<sup>2</sup>; <sup>1</sup>*Schering-Plough Research Institute, Kenilworth, NJ*; <sup>2</sup>*Schering-plough, Kenilworth, NJ*

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- MP 143 **Imaging Anti-Tuberculosis Drugs in Tissues using MALDI Linear Ion Trap Mass Spectrometry;** Michelle L. Reyzer<sup>1</sup>; Laura E. Via<sup>2</sup>; Clifton E. Barry, III<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*NIAD, NIH, Bethesda, MD*
- MP 144 **The Detection of Therapeutics from Marine Microbial Systems using MALDI-Imaging;** Eduardo Esquenez<sup>2</sup>; Cameron Coates<sup>1</sup>; Luke Simmons<sup>1</sup>; David Gonzalez<sup>2</sup>; William H. Gerwick<sup>1</sup>; Pieter Dorrestein<sup>2</sup>; <sup>1</sup>*Scripps Institution of oceanography, La Jolla, Ca*; <sup>2</sup>*University of California, San Diego, Skaggs school, La Jolla, Ca*
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- MP 145 **Blind Deconvolution for Representation of Delay-Line Mass Spectral Datasets;** Andriy Kharchenko; Martin Froesch; Ron M.A. Heeren; *FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands*
- MP 146 **A Novel Algorithm for Dynamic Exit in MALDI-MS-MS Analysis: Optimizing Data Accumulation Time while Minimizing Sample Consumption;** Min J. Yang; Gordana Ivosev; Suzanne Ackloo; Bill Loyd; Aaron Booy; Patrick Pribil; *MDS Analytical Technologies, Concord, Canada*
- MP 147 **Supercomputer Simulations of Interacting Ion Cloud Dynamics in FT-ICR Cells using Novel Parallel Three-Dimensional Domain Decomposition Finite Element Particle-in-Cell Code;** Alexander V. Pozdnev<sup>1</sup>; Alexander M. Popov<sup>1</sup>; Alexander S. Misharin<sup>2</sup>; <sup>1</sup>*Lomonosov Moscow State University, Moscow, Russian Federation*; <sup>2</sup>*MassTech, Inc., Columbia, MD*
- MP 148 **Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface;** Li Yang; Upakarasamy Lourderaj; William Hase; *Texas Tech University, Lubbock, TX*
- MP 149 **Enabling High-Throughput MRM Based Biomarker Validation Studies through a Vendor Neutral Application;** Joseph Simpkins; Kenneth C. Lewis; *OpAns, LLC, Durham, NC*
- MP 150 **Ab Initio Direct Dynamics Trajectory Study of the Cl + CH3I SN2 Nucleophilic Substitution Reaction;** Jiaxu Zhang; Upakarasamy Lourderaj; William Hase; *Texas Tech University, Lubbock, TX*
- MP 151 **Automatic Mass Calibration and Improved Mass Accuracy;** Tony Ferrige<sup>1</sup>; Robert Alecio<sup>1</sup>; Stuart Ray<sup>1</sup>; Hyun Joo An<sup>2</sup>; Maria Lorna de Leoz<sup>2</sup>; Scott Kronewitter<sup>2</sup>; Suzanne Miyamoto<sup>3</sup>; Carlito Lebrilla<sup>2</sup>; <sup>1</sup>*Positive Probability Limited, Ely, UK*; <sup>2</sup>*UC Davis, Davis, CA*; <sup>3</sup>*UC Davis Cancer Center, Sacramento, CA*
- MP 152 **Fully Unsupervised Automatic Assignment and Annotation of Sum Formulae for Product Ion Peaks, Neutral Losses in MS and Production Spectra;** Sandy Yates<sup>2</sup>; Ilmari Krebs<sup>1</sup>; <sup>1</sup>*Bruker Daltonik, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics, Fremont, CA*
- MP 153 **Analytical Intermolecular Potential for Protonated Peptide Ions Colliding with Fluorinated Self-assembled Monolayers;** Wenfang Hu<sup>1</sup>; William Hase<sup>2</sup>; <sup>1</sup>*Lubbock, TX*; <sup>2</sup>*Texas Tech University, Lubbock, TX*
- MP 154 **A Query Language for Retrieving Information from Raw Data Files;** Michael W. Senko; Eric C. Hemenway; *Thermo Fisher Scientific, San Jose, CA*
- MP 155 **IUPAC Standard Definitions of Terms Relating to Mass Spectrometry: Final Recommendations;** Kermit K. Murray<sup>1</sup>; Robert K. Boyd<sup>2</sup>; Marcos N Eberlin<sup>3</sup>; G. John Langley<sup>6</sup>; Liang Li<sup>4</sup>; Yasuhide Naito<sup>5</sup>; <sup>1</sup>*Louisiana State Univ., Baton Rouge, LA*; <sup>2</sup>*National Research Council, Ottawa, ON*; <sup>3</sup>*Thomson Lab Unicamp, Campinas, Brazil*; <sup>4</sup>*University of Alberta, Edmonton, AB*; <sup>5</sup>*GPI, Hamamatsu, JAPAN*; <sup>6</sup>*University of Southampton, Southampton, UK*
- MP 156 **Direct Dynamics Simulations of Surface-Induced Dissociation of N-Protonated Octaglycine;** Kyoyeon Park<sup>1</sup>; Bipasha Deb<sup>1</sup>; Kihyung Song<sup>2</sup>; William Hase<sup>1</sup>; <sup>1</sup>*Texas Tech University, Lubbock, TX*; <sup>2</sup>*Korea National University of Education, Chongwon, Chungbuk, Korea*
- MP 157 **Mass++: Universal & Plug-in Style Software for Mass Spectrometer;** Satoshi Tanaka<sup>1</sup>; Ken Aoshima<sup>2</sup>; Yuji Miura<sup>2</sup>; Tsuyoshi Tabata<sup>2</sup>; Yoshiya Oda<sup>2</sup>; <sup>1</sup>*Core Research for Evolutional Science and Technol, Saitama 332-0012, Japan*; <sup>2</sup>*Eisai Co., Ltd. Laboratory of Core Technology, Tsukuba, Ibaraki 300-2635, Japan*
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- MP 159 **Microorganism Fingerprinting by Laser Desorption Ion Mobility Mass Spectrometry;** Juaneka Hayes<sup>1</sup>; Kermit K. Murray<sup>1</sup>; Michael V. Ugarov<sup>2</sup>; J. Albert Schultze<sup>2</sup>; <sup>1</sup>*Louisiana State Univ., Baton Rouge, LA*; <sup>2</sup>*Ionwerks, Inc., Houston, TX*
- MP 160 **In vitro Detection and Absolute Quantitation of Functional Ricin;** Sara C. McGrath; David M. Schieltz; Lisa G. McWilliams; Suzanne R. Kalb; John Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- MP 161 **Ion-Molecule Chemistry of C2H5SC2H4Cl Relevant to Chemical Ionization Detection of Mustard - Experimental and Theoretical Results;** Albert Viggiano; Anthony Midey; *AFRL, Hanscom AFB, MA*
- MP 162 **Applications of Mobile GC-MS and Hand-held Air Sampling in Environmental Analysis;** Garth Patterson; Cynthia Liu; John Grossenbacher; Donna Powell; Jane Likens; Mitch Wells; Dennis Barket, Jr.; *Griffin Analytical Technologies LLC, West Lafayette, IN*
- MP 163 **Simple and Rapid Quantitative LC-MS-MS Method to Determine Exposure to Tetranitromethane;** Huijuan Zhang; Patrick Dhooze; *New Mexico Department of Health SLD, Albuquerque, NM*
- MP 164 **Characterization of the Distributed Plasma Ionization Source (DPIS) for the Analysis of Explosives;** Alex C. Wu; Marilyn Prieto; Leonard Rorrer; Richard A. Yost; *University of Florida, Gainesville, FL*
- MP 165 **Atmospheric Pressure Thermal Desorption-Extractive-ESI-MS Detection of Dipicolinic Acid in Bacterial Spores and Dimethyl Methylphosphonate in Water;** Shaofeng Zhang; Yong-seung Shin; Franco Basile; *University of Wyoming, Laramie, WY*
- MP 166 **Attribution of Explosive Origin from Natural Isobaric Ion Profiles Determined by FT/MS Analysis;** Sigrid Baumgarten<sup>1</sup>; Denis Lesage<sup>1</sup>; Martine Barbe-Le-Borgne<sup>2</sup>; Olivier Vigneau<sup>3</sup>; Xavier Machuron-Mandard<sup>3</sup>;

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- MP 167 **Detection of Improvised Explosive Devices using a Wire-Type Linear Ion Trap;** Masuyuki Sugiyama<sup>1</sup>; Yuichiro Hashimoto<sup>2</sup>; Hisashi Nagano<sup>2</sup>; Yasuaki Takada<sup>2</sup>; Hideki Hasegawa<sup>2</sup>; <sup>1</sup>Hitachi, Tokyo, Japan; <sup>2</sup>Hitachi, Ltd, Central Research Lab, Kokubunji, Tokyo, Japan
- MP 168 **Studies on Botulinum Neurotoxins C and C/D using Endopep-MS, Epitope Mapping by Mass Spectrometry, and Proteomics;** Hercules Moura<sup>1</sup>; Suzanne R. Kalb<sup>1</sup>; Adrian R. Woolfitt<sup>1</sup>; Vince L. Maggio<sup>2</sup>; John R. Barr<sup>1</sup>; <sup>1</sup>Centers For Disease Control And Prevention, Atlanta, GA; <sup>2</sup>Battelle under contract at the CDC, Atlanta, GA
- MP 169 **Rapid Screening and Identification of Chemical Warfare Agents in Environmental Samples using LC-MS and an MS-MS-Library;** Martin M. Schaefer; Spiez Laboratory, Spiez, Switzerland
- MP 170 **Development of a Light-Weight Integrated Direct Analysis Mass Spectrometer;** Adam Keil; Garth Patterson; Tri Le; Jane Likens; Mitch Wells; Brent Rardin; Jeff Corpstein; Jason Springston; Dennis Barket, Jr.; Griffin Analytical Technologies LLC, West Lafayette, IN
- MP 171 **Identification and Protein Fingerprinting of Legionella using Whole Cell MALDI-TOF Mass Spectrometry;** Michal Drevinek<sup>1</sup>; Vladimir Drasar<sup>2</sup>; <sup>1</sup>Natl Inst for NBC Protection, Milin, Czech Republic; <sup>2</sup>Public Health Inst., Natl Legionella Reference Lab, Vyskov, Czech Republic
- MP 172 **Rapid and Sensitive Detection and Identification of Orthopoxvirus by PCR and Mass Spectrometry (PCR/ESI-MS);** Mark Eshoo<sup>1</sup>; David J. Ecker<sup>1</sup>; Aysegul Nalca<sup>2</sup>; Scott Zoll<sup>1</sup>; Carson Baldwin<sup>2</sup>; Ranga Sampath<sup>1</sup>; Lawrence Blyn<sup>1</sup>; Thomas Hall<sup>1</sup>; Chris A. Whitehouse<sup>2</sup>; Steven A. Hofstadler<sup>1</sup>; <sup>1</sup>Ibis Biosciences, Inc., Carlsbad, CA; <sup>2</sup>U.S. Army Med. Res. Inst. of Infectious Dis., Fort Detrick, MD
- MP 173 **Characterization of Inorganic Nitrate and Perchlorate Compounds by Negative MALDI-TOF and TOF/TOF Mass Spectrometry;** Bing Guan; Richard B. Cole; University of New Orleans, New Orleans, LA
- MP 174 **Processing of Microbial Samples using Protein Ultrafiltration Devices for Identification of Bacteria by Mass Spectrometry;** Rabih Jabbour<sup>1</sup>; Jacek P. Dworzanski<sup>1</sup>; Samir Deshpande<sup>2</sup>; Mary Wade<sup>3</sup>; Michael F. Stanford<sup>3</sup>; Charles H. Wick<sup>3</sup>; Alan W. Zulich<sup>3</sup>; <sup>1</sup>SAIC, Gunpowder, MD; <sup>2</sup>STC, Edgewood, MD; <sup>3</sup>U.S. Army Edgewood Chemical Biological Center, APG, MD
- MP 175 **Ion Mobility Separation of Organophosphates using a Quadrupole Time-Of-Flight Mass Spectrometer;** Paul D'agostino<sup>1</sup>; Claude Chenier<sup>1</sup>; Andrew Baker<sup>2</sup>; <sup>1</sup>DRDC Suffield, Medicine Hat, AB, Canada; <sup>2</sup>Waters, Inc., Dublin, CA
- MP 176 **Rapid Detection of Explosives on Human Skin by Neutral Desorption Extractive Electrospray Ionization (ND-EESI) Mass Spectrometry;** Bin Hu<sup>1</sup>; Zhanfeng Zhao<sup>2</sup>; Yan Hu<sup>1</sup>; Zhiqian Zhou<sup>2</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Technology, Fuzhou, China; <sup>2</sup>Harbin Institute of Technology Weihai, Weihai, China
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- MP 177 **UPLC-MS Approaches to Examining the Degradation Pathway of a Sympathomimetic Amine Vasopressor;** Samantha A Leidner; Zhaohai J Zhu; Christopher M McGinley; Zvetlana Zelechonok; Esther Hwang; Lala Szmyt; Paul M. Bigwarfe Jr.; Hospira, Inc., Lake Forest, IL
- MP 178 **The Use of 'Semi' UPLC-MS-MS to Enhance LLOQ and Cycle Time for Perphenazine and BL 1020;** Kean Woodmansey<sup>1</sup>; Stephen Brookes<sup>1</sup>; Tair Lapidot<sup>2</sup>; <sup>1</sup>Charles River Laboratories, Edinburgh, Scotland; <sup>2</sup>Bioline RX, Jerusalem, Israel
- MP 179 **Validation of a Sensitive LC-MS-MS Bioanalytical Assay for CVT-6883 in Human Urine using SDBS Additive to Eliminate Adsorptive Losses;** Chungwen (William) Chen; Lakshmikanth Bajpai; Nevena Mollova; Kwan Leung; CV Therapeutics, Palo Alto, CA
- MP 180 **High pH Mobile Phase Sensitivity Gain in LC-ESI+/MS-MS: Choice of Modifiers to Improve Signal Intensity and Applications in Bioanalysis;** Jean-Nicholas Mess; Mathieu Lahaie; Milton Furtado; Troy Bradley; Fabio Garofolo; Algorithm Pharma Inc., Laval (Montreal), QC, Canada
- MP 181 **SPE Automated Method Development for Three Antibiotics in Plasma using Phenomenex Polymeric Sorbent Plates on a Hamilton Microlab Star;** Shawn F. Charles; Shawn F. Charles; Schering-Plough, Lafayette, NJ
- MP 182 **Managing Ionization Effect in LC-MS-MS Assay -- Case Study with Varenicline;** Beijing Tan; Qun Gu; Bret Hurshman; Olga Kavetskaia; Pfizer, Inc., Groton, CT
- MP 183 **Analysis of Coccidiostats by Liquid Chromatography/Tandem Mass Spectrometry;** Encarnacion Moyano; Anna Martinez-Villalba; Maria Teresa Galceran; University of Barcelona, Barcelona, Spain
- MP 184 **Application of Laser Diode Thermal Desorption APCI-MS-MS in Early Stage Pharmaceutical Product Development;** Louis-Philippe Labranche<sup>1</sup>; Audrey Tousignant<sup>1</sup>; Yves G. Leblanc<sup>1</sup>; Daniel Abran<sup>1</sup>; Pierre Picard<sup>2</sup>; Patrice Tremblay<sup>2</sup>; Alain Carrier<sup>1</sup>; <sup>1</sup>Sandoz Canada, Boucherville, Canada; <sup>2</sup>Phytonix Technologies, Inc., Quebec, QC
- MP 185 **Rapid Determination of the "Chemical Zip Codes" of Diacylglycerol-Lactone Combinatorial Library Components using Mass Spectrometry;** James A. Kelley<sup>1</sup>; Christopher C. Lai<sup>1</sup>; Said El Kazzouli<sup>1</sup>; Lawrence R. Phillips<sup>2</sup>; Lyndsay L. Smith<sup>2</sup>; Victor E. Marquez<sup>1</sup>; <sup>1</sup>CCR, NCI-Frederick, Frederick, MD; <sup>2</sup>DCTD, NCI-Frederick, Frederick, MD
- MP 186 **Method Development and Validation of a Bioanalytical LC-MS-MS Method for Bortezomib in Human Plasma;** Wenyi Hua; John Eddy; Brian Hoffman; Sara Jones; Daniel E Mulvana; Advion BioServices, Ithaca, NY
- MP 187 **A Highly Automated Workflow for Fast and Comprehensive Identification of Impurities and Degradation Products in Pharmaceutical Products using LC-MS-MS;** John Gibbons<sup>1</sup>; David Ducan<sup>2</sup>; Nicolas Rupcich<sup>2</sup>; <sup>1</sup>MDS Sciex, Concord, Ontario, Canada; <sup>2</sup>Genpharm Pharmaceuticals, Etobicoke, Ontario, Canada

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- MP 188 **Investigation of an Effective Strategy for ESI Source Stabilization to Increase Sample Throughput for Macrolide Compounds in Bioanalysis;** Marie-Pierre Taillon; Jean-Nicholas Mess; Milton Furtado; Troy Bradley; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, Canada*
- MP 189 **Structure Elucidation Utilizing a Unique, Complementary Product Ion Series Resulting from Collision Induced Dissociation of Silver Adduct Ions by LC/CIS/MS;** Byron S. Johnson; David J. Burinsky; *GlaxoSmithKline, Raleigh, NC*
- MP 190 **A Rapid Quantitative Method for Multiple Anabolic Steroids in Equine Serum by Turbulent Flow Chromatography Tandem MS-MS;** Benjamin C Moeller; Scott D Stanley; *University of California at Davis, Davis, CA*
- MP 191 **A Comparison of the Fragmentation of Acetoxy-Substituted Rapalogs;** Barry D. Davis; Michael I. Carr; Joseph T. Snodgrass; Leonard W. Rozamus; Stephan G. Zech; Christopher K. Murray; *ARIAD Pharmaceuticals, Cambridge, MA*
- MP 192 **Application of LC-MS to Stability Screening of Pre-Clinical Drug Candidates;** Xuezhi (James) Qin; Yang Yuan; *Merck & Co., Lansdale, PA*
- MP 193 **Surface-Ionization Mass Spectrometry of Butyrophenone Derivatives;** Utkur Rasulev; Dilshodbek Usmanov; Usman Khasanov; *Arifov Institute of Electronics, Tashkent, Uzbekistan*
- MP 194 **API-MS Fragmentation Pathways of Methylphenidate and Related Compounds Revealed by Ion Trap MS<sup>n</sup> and H/D Exchange;** R. Randy Wilhelm; John E. Johnson; *Covidien, Ltd / Mallinckrodt Pharmaceutical R&D, St. Louis, MO*
- MP 195 **LC-MS<sup>n</sup> Analysis of New Erectile Dysfunction Drug Analogues in Regulatory Samples;** Teresa C. Cain<sup>1</sup>; Samuel Gratz<sup>2</sup>; <sup>1</sup>*Food & Drug Admin. PLRSW, Irvine, CA*; <sup>2</sup>*Fda Forensic Chemistry Center, Cincinnati, OH*
- MP 196 **Development and Characterization of Uniform Steroid Isotopic Standards for Gas Chromatography Combustion Isotope Ratio Mass Spectrometry (GCC-IRMS);** Ying Zhang; Herbert Tobias; J Thomas Brenna; *Cornell University, Ithaca, NY*
- MP 197 **Effect of pH on the Quantification and Ion Suppression of Basic Drugs in Samples of Biological Origin by RP LC-ESI<sup>+</sup>-MS-MS;** Tivadar Farkas; Liming Peng; *Phenomenex, Inc., Torrance, CA*
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- QUANTITATION OF SMALL MOLECULES: PHARMACEUTICAL FOCUS, 198 - 208**
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- MP 198 **Simultaneous Quantitation of BILR 355 and Its Metabolite in Mouse Plasma by Automated 96-well SPE and LC-MS-MS;** Yan Mao; David L. Dube; Jeffrey X. Duggan; *Boehringer-Ingelheim Pharmaceuticals, Ridgefield, CT*
- MP 199 **Determination of Antineoplastic Drugs by High Resolution MS-MS to Monitor Occupational Exposure;** Claudio Baiocchi<sup>1</sup>; Claudio Medana<sup>1</sup>; Francesco Carbone<sup>1</sup>; Valeria Giancotti<sup>1</sup>; Alberta Chiappa<sup>2</sup>; Enrico Davoli<sup>3</sup>; <sup>1</sup>*University of Turin, Torino, Italy*; <sup>2</sup>*RQA srl, Rodano, Italy*; <sup>3</sup>*Mario Negri Institute, Milano, Italy*
- MP 200 **A Novel Derivatization-LC-MS Approach for Determination of Trace Level Alkyl Esters of Sulfonates and Sulfates Genotoxic Impurities in Drug Substances;** Jianguo An<sup>2</sup>; lin bai<sup>1</sup>; Mingjiang Sun<sup>1</sup>; ted chen<sup>1</sup>; Dr. David Q. Liu<sup>1</sup>; alireza kord<sup>1</sup>; <sup>1</sup>*GlaxoSmithKline, King of Prussia, PA*; <sup>2</sup>*Glaxosmithkline Pharmaceuticals, King of Prussia, PA*
- MP 201 **Quantitation of a Low-Level Impurity with a Weak UV Chromophore in an Active Pharmaceutical Ingredient using the LC-MS Approach;** Hongfei Yue; Xin Bu; *Bristol-Myers Squibb, New Brunswick, NJ*
- MP 202 **Quantification of Small Pharmaceutical Drugs by MALDI-TOF;** Markus Persike; Michael Karas; *Johann Wolfgang Goethe University, Frankfurt/Main, Germany*
- MP 203 **Practical Automated Algorithm Design for High Throughput Method Optimization in ADME/PK Environments;** Xavier Misonne<sup>1</sup>; Anthony Romanelli<sup>1</sup>; John Janiszewski<sup>3</sup>; Kevin Shirey<sup>2</sup>; Ghobarah Hesham<sup>1</sup>; Christopher Borton<sup>1</sup>; Loren Olson<sup>1</sup>; <sup>1</sup>*Applied Biosystems, San Jose, CA*; <sup>2</sup>*Sounds Analytics, East Lyme, CT*; <sup>3</sup>*Pfizer, Groton, CT*
- MP 204 **Enhanced LC-ESI-MS-MS Detection of the Benzoxaborole AN2718 by Derivatization with (+)-Pinanediol;** Dale Schoener<sup>1</sup>; Liang Liu<sup>2</sup>; Conrad Wheeler<sup>2</sup>; Stephen Baker<sup>2</sup>; Michael Buonarati<sup>1</sup>; <sup>1</sup>*Alta Analytical Laboratory, El Dorado Hills, CA*; <sup>2</sup>*Anacor Pharmaceuticals, Palo Alto, CA*
- MP 205 **Overcoming Challenges in Development of LC-MS-MS Methods for Highly Polar, Low Molecular Weight, Zwitterionic Compounds: A Quantitative Assay for Pregabalin;** Ryan S. Adler; Spencer Carter; Troy Voelker; *Tandem Labs, Salt Lake City, UT*
- MP 206 **Evaluation of a Surface Sampling Probe for Quantitative Analysis of Drug Transporter Samples;** Richard King<sup>1</sup>; Gary J. Van Berkel<sup>2</sup>; Vilmos Kertesz<sup>3</sup>; <sup>1</sup>*Merck & Company, Inc., West Point, PA*; <sup>2</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>3</sup>*Oak Ridge National Lab, Oak Ridge, TN*
- MP 207 **A Rapid and Simple Liquid Chromatography-Tandem Mass Spectrometry Method for Simultaneous Quantification of Multiple Antiepileptic Drugs in Human Serum;** Heng Shi; Dean Carlow; *Children's Hospital of Philadelphia, Philadelphia, PA*
- MP 208 **Determination of the Antifungal Posaconazole in Human Fingernails and Toenails using Liquefaction, Liquid-Liquid Extraction, Liquid Chromatography and Mass Spectrometric Detection;** Mark Leahy<sup>1</sup>; Janet Nelson<sup>1</sup>; Michelle J. Cannon<sup>1</sup>; Monika Martinho<sup>2</sup>; Robert P. Clement<sup>2</sup>; Bhavna S. Kantesaria<sup>2</sup>; <sup>1</sup>*Covance, Madison, WI*; <sup>2</sup>*Schering-Plough Research Institute, Summit, New Jersey*
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- TOXICOLOGY, 209 - 230**
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- MP 209 **A Quantitative General Unknown Screening Method for Drugs and Toxic Compounds in Urine using Liquid Chromatography-Mass Spectrometry;** Taha Rezaei; Marta Kozak; Alan E. Schoen; *Thermo Fisher Scientific, San Jose, CA*
- MP 210 **Structure Elucidation of Formaldehyde-Induced DNA-protein Cross-Links by Mass Spectrometry and NMR;** Kun Lu; Wenjie Ye; Li Zhou; Leonard Collins; Xian Chen; James Swenberg; *University of North Carolina, Chapel Hill, NC*
- MP 211 **Mass Spectrometric Analysis of the Nucleotide Pool as a Target for Nitrosative Deamination during Inflammation;** Vasileios Dendroulakis<sup>1</sup>; William M. Deen<sup>1</sup>; Peter C. Dedon<sup>2</sup>; <sup>1</sup>*MIT, Chemical Engineering Dept, Cambridge, MA*; <sup>2</sup>*MIT, Biological Engineering Dept, Cambridge, MA*

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- MP 212 **4-Aminobiphenyl DNA Adducts as Biomarkers in Human Bladder Cell Samples and the Role of Isothiocyanates as a Chemopreventive Phytochemical;** Dayana Argoti<sup>1</sup>; Kristen Randall<sup>1</sup>; Yuesheng Zhang<sup>2</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Roswell Park Cancer Institute, Buffalo, NY
- MP 213 **Evaluation of the Toxicokinetics of Sub-Lethal Inhalation Exposures of Cyclosarin in Guinea Pigs via Large-Volume Injection GC-MS;** Jeffrey M. McGuire<sup>1</sup>; Christopher E. Whalley<sup>1</sup>; Ronald A. Evans<sup>1</sup>; Julie A. Renner<sup>2</sup>; Allison L. Totura<sup>3</sup>; E. Michael Jakubowski, Jr.<sup>1</sup>; Sandra A. Thomson<sup>1</sup>; <sup>1</sup>US Army ECBC, APG, MD; <sup>2</sup>SAIC, APG, MD; <sup>3</sup>UNC School of Medicine, Chapel Hill, NC
- MP 214 **Mass Spectrometric Analysis of Protein Adducts Formed by Acrylates *in vitro*;** Christian Lindh; Marina Jeppsson; Bo AG Jönsson; *Occupational and Environmental Medicine, Lund, Sweden*
- MP 215 **Rapid LC-MS-MS Analysis of Biomarkers of Drug-Induced Phospholipidosis in Rats Treated with Amiodarone and Gentamicin;** David A. Peake<sup>1</sup>; Bradley L. Ackermann<sup>2</sup>; David G. Hall<sup>2</sup>; Bartley W. Halstead<sup>2</sup>; Ming-Shang Kuo<sup>1</sup>; Barry S. Lutzke<sup>2</sup>; Craig E. Thomas<sup>2</sup>; <sup>1</sup>Eli Lilly & Company, Lilly Corporate Center, Indianapolis, IN; <sup>2</sup>Eli Lilly & Company, Greenfield Laboratories, Greenfield, IN
- MP 216 **Development of a LC-MS-MS Method for Determining Ethyl Methylphosphonic Acid (EMPA) Concentration in Plasma following VX Exposure;** Ronald A. Evans<sup>1</sup>; Julie A. Renner<sup>2</sup>; E. Michael Jakubowski, Jr.<sup>1</sup>; Sandra A. Thomson<sup>1</sup>; <sup>1</sup>U.S. Army ECBC, Aberdeen Proving Ground, MD; <sup>2</sup>SAIC, Aberdeen Proving Ground, MD
- MP 217 **Detection of Cytochrome P450 Adducts after Oxidative Desulfuration of Methyl Parathion;** Patrick B. Kyle; Rodney C. Baker; Robert E. Kramer; *University of Mississippi Medical Center, Jackson, MS*
- MP 218 **Identification of New Biomarkers of Organophosphates Intoxication in Peptide Fraction of Rat Plasma;** Ekaterina Podolskaya<sup>1</sup>; Nikolay Goncharov<sup>2</sup>; Lidia Glashkina<sup>2</sup>; Nikita Polyakov<sup>3</sup>; Vladimir Babakov<sup>2</sup>; Ilya Krasnov<sup>1</sup>; Andrey Radilov<sup>2</sup>; Nikolay Krasnov<sup>1</sup>; <sup>1</sup>Institute for Analytical Instrumentation, RAS, St. Petersburg, Russia; <sup>2</sup>Res Inst of Hygiene, Occup Pathol, Hum Ecology, St. Petersburg, Russia; <sup>3</sup>Institute of Bioorganic Chemistry, Moscow, Russia
- MP 219 **Performance Evaluation of three Liquid Chromatography Mass Spectrometry Techniques for Broad Spectrum Drug Testing in the Clinical Laboratory;** Kara L. Lynch<sup>1</sup>; Judy A. Stone<sup>2</sup>; Autumn Breaud<sup>3</sup>; Katherine Chen<sup>2</sup>; Eva Wong<sup>2</sup>; Marilyn Weeks<sup>2</sup>; Houssain El Aribi<sup>4</sup>; Alan H. B. Wu<sup>1</sup>; William Clarke<sup>3</sup>; <sup>1</sup>University of California-San Francisco, San Francisco, CA; <sup>2</sup>San Francisco General Hospital, San Francisco, CA; <sup>3</sup>The Johns Hopkins Medical Institutes, Baltimore, MD; <sup>4</sup>Applied Biosystems/MDS SCIEX, Concord, ON, Canada
- MP 220 **Ciguatoxin Analogues in Ciguatera Outbreak Samples;** Ann Abraham; Edward L.E. Jester; Hudson R. Granade; Steven M. Plakas; Robert W. Dickey; *FDA, Dauphin Island, AL*
- MP 221 **Targeted Quantitative Proteomic Analysis in Human Hepatoma HepG2 Cells Exposed by Cadmium;** Jun Adachi; Keishi Kihara; Tomonari Matsuda; *Kyoto University, Kyoto, JAPAN*
- MP 222 **An Automated SPE/LC-MS Method for the Analysis of THC and Metabolites in Biological Fluids;** Eshwar Jagerdeo<sup>1</sup>; Martin Sibum<sup>2</sup>; Madeline Montgomery<sup>1</sup>; Marc LeBeau<sup>1</sup>; John Crutchfield<sup>2</sup>; <sup>1</sup>FBI, Springfield, VA; <sup>2</sup>Spark Holland Inc., Emmen, Netherlands
- MP 223 **Reactivity Testing Strategies: Covalent Modification of Single Nucleophile Peptides;** Maja Aleksic; Delphine Roger; Emma Thain; Sandrine Jacquilleot; Raniero Zazzeroni; *Unilever, Bedford, UK*
- MP 224 **Damage Products in Cellular RNA and Blood-Borne Nucleic Acids as Biomarkers of Inflammation;** Erin G. Prestwich; Jose L. McFaline; Bo Pang; Matthew R. Sullivan; Koli Taghizadeh; Debra Dederich; Peter C. Dedon; *Massachusetts Institute of Technology, Cambridge, MA*
- MP 225 **Analysis of Rat Urine, Plasma and Tissues for Fluoride and Fluorosulfate via Ion Chromatography with Suppressed Conductivity and Mass Spectrometry;** Adam W Perala; Dan A Markham; Kathy A Brzak; *The Dow Chemical Company, Midland, MI*
- MP 226 **Gas Chromatography-Tandem Mass Spectrometry (GC-MS-MS) Analysis of Gottingen® Minipig Dermis following Percutaneous Exposure to the Chemical Warfare Agent VX;** Christopher Byers<sup>1</sup>; Jeffrey M. McGuire<sup>1</sup>; Benjamin Wright<sup>2</sup>; Stanley Hulet<sup>1</sup>; E. Michael Jakubowski, Jr.<sup>1</sup>; Sandra Thomson<sup>1</sup>; <sup>1</sup>US Army ECBC, APG, MD, MD; <sup>2</sup>SAIC, Abingdon, MD
- MP 227 **Rapid Method for Analysis of Dialkylphosphate Metabolites of Organophosphorus Insecticides in Human Urine using Weak Anion Exchange SPE and GC-MS-MS;** Martins Odetokun<sup>1</sup>; Maribel Gallegos<sup>1</sup>; Samuel Baker<sup>1</sup>; Dana Barr<sup>1</sup>; Larry Needham<sup>1</sup>; Gayanga Weerasekera<sup>2</sup>; <sup>1</sup>CDC, Atlanta, GA; <sup>2</sup>Nektar Therapeutics, San Carlos, CA
- MP 228 **Measurements of Estrogen-Modified DNA Adduct: Potential Biomarker for Breast Cancer;** Qiang Zhang; Michael L. Gross; Rebecca L. Aft; *Washington University, St Louis, MO*
- MP 229 **Does Genistein Help Prevent or Promote Breast Cancer? An *in vitro* Study of DNA Depurination by Genistein Quinone;** Ingting Tu; Qiang Zhang; Andre' D. d' Avignon; Michael L. Gross; *Washington University in St. Louis, Saint Louis, MO*
- MP 230 **Gas Chromatography Tandem Mass Spectrometry for Biomarkers of Alcohol Abuse in Human Hair;** Carolyn M. Zimmermann; Glen P. Jackson; *Ohio University, Athens, OH*
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- MP 231 **Facilitating CYP Inhibition Assays with the Use of Automated Open Access Software;** Jenny Moshin<sup>1</sup>; Pengdeth Lim<sup>2</sup>; Alexandre Wang<sup>1</sup>; Jane Huang<sup>2</sup>; Huafen Liu<sup>1</sup>; Loren Olson<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Roche Palo Alto, Palo Alto, CA
- MP 232 **Development of a High Throughput Cocktail Drug-Drug Interaction Screen using MALDI Tandem Mass Spectrometry;** Hui Zhang; Kevin Whalen; Mark Cole; Michael West; *Pfizer Inc., Groton, CT*
- MP 233 **Multiplexed LC-MS-MS for Rapid Method Development and Sample Analysis in Drug Discovery Bioanalysis;** Jian Wang; Christian Caporuscio; Georgia Cornelius; Bogdan Slecza; Asoka Ranasinghe; Mohammed Jemal; Timothy Olah; *Bristol-Myers Squibb, Princeton, NJ*

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- MP 234 **Analysis of Drug Metabolites in Biological Fluids using Mixed-Mode Solid Phase Extraction and UltraPerformance Liquid Chromatography-Tandem Mass Spectrometry;** Kenneth J Fountain; Jane Xu; Erin E Chambers; Diane M Diehl; *Waters Corporation, Milford, MA*
- MP 235 **A Simple Metabolite Screening Method Requiring No Knowledge of Metabolism;** Jenny E. Moshin<sup>1</sup>; James A. Ferguson<sup>1</sup>; Sai Y. Chang<sup>2</sup>; Jeffrey D. Miller<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*; <sup>2</sup>*MSMS Science LLC, Sedona, AZ*
- MP 236 **Development of an LC-MS-MS Assay for Simultaneously Determining Metabolic Stability of 2-Arylthiazolidine-4-Carboxylic Acid Amide Derivatives;** Chien-Ming Li<sup>1</sup>; Yan Lu<sup>2</sup>; Mitch A Phelps<sup>1</sup>; Duane D Miller<sup>2</sup>; James T Dalton<sup>1</sup>; <sup>1</sup>*College of Pharmacy, Ohio State University, Columbus, OH*; <sup>2</sup>*College of Pharmacy, University of Tennessee, Memphis, TN*
- MP 237 **Is MALDI-TOF MS Ready for Bioanalytical Analysis?** Patrick Bennett<sup>2</sup>; Qing Zhu<sup>3</sup>; Kc Van Horne<sup>2</sup>; Ming-chih D. Ho<sup>3</sup>; Lily Li<sup>1</sup>; <sup>1</sup>*TandemLabs, Woburn, MA*; <sup>2</sup>*Tandem Labs, Salt Lake City, UT*; <sup>3</sup>*Tandem Labs New England, Woburn, MA*
- MP 238 **A Heuristic Automated Software Workflow for Triple Quadrupole Linear Ion Trap Analysis of High Throughput *in vitro* Metabolite Screens;** Shaokun Pang<sup>1</sup>; Elliott Jones<sup>2</sup>; Rongda Xu<sup>3</sup>; Daniel B. Kassel<sup>4</sup>; <sup>1</sup>*Takeda San Diego, San Diego, CA*; <sup>2</sup>*Applied Biosystems, Foster City, CA*; <sup>3</sup>*Takeda San Diego, Inc., San Diego, CA*; <sup>4</sup>*Takeda San Diego, Inc, San Diego, CA*
- MP 239 **Screening for Protease Inhibitors using Liquid Chromatography/Electrospray-Mass Spectrometry (LC/ESI-MS) with a Post-Column Continuous-Flow Enzyme Assay;** Nils Helge Schebb<sup>1</sup>; Ferry Heus<sup>2</sup>; Jeroen Kool<sup>2</sup>; Martin Vogel<sup>1</sup>; Hubertus Irth<sup>2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>*University of Münster, Inst. of Inorg.&Anal. Chem, Münster, Germany*; <sup>2</sup>*Vrije Universiteit Amsterdam, Analytical Chemistry, Amsterdam, The Netherlands*
- MP 240 **Approaches towards Rapid Drug Metabolite Identification using Ion Trap Mass Spectrometry;** Stephen Holman<sup>1</sup>; Patricia Wright<sup>2</sup>; G. John Langley<sup>1</sup>; <sup>1</sup>*University of Southampton, Southampton, UK*; <sup>2</sup>*Pfizer Global Research and Development, Sandwich, UK*
- MP 241 **Detection and Characterization of Metabolites in Complex Biological Samples using Perfusion 2-D Chromatography Linear Ion Trap- Triple Quadrupole MS;** Robert Ellis<sup>1</sup>; Takeo Sakuma<sup>2</sup>; Tom Biesenthal<sup>1</sup>; Carmai Seto<sup>1</sup>; Doina Caraiman<sup>1</sup>; Curtis Campbell<sup>3</sup>; Masatoshi Takahashi<sup>3</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>*Mds Sciex, Concord, ON*; <sup>3</sup>*Shimadzu, Columbia, MD*
- MP 242 **Analysis of Metabolites by UHPLC-MALDI/MS-MS on a Triple Quadrupole Linear Ion Trap;** Gerard Hopfgartner<sup>1</sup>; Guenter Boehm<sup>2</sup>; Emmanuel Varesio<sup>1</sup>; <sup>1</sup>*University of Geneva, Geneva, Switzerland*; <sup>2</sup>*Thermo Fisher Scientific (Flux Instrument), Basel, Switzerland*
- MP 243 **PIF: Precursor Ion Fingerprinting – Searching for Genesis Fragments using LC-ddMSn;** Julie A. Horner<sup>1</sup>; Mark Sanders<sup>1</sup>; Robert Mistrik<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Highchem, Ltd., Bratislava, Slovakia*
- MP 244 **Midazolam and 1-Hydroxymidazolam Determination in Human EDTA Plasma by LDTD/MS-MS in 8 Seconds;** Jean Lacoursière<sup>1</sup>; Pierre Picard<sup>2</sup>; Patrice Tremblay<sup>1</sup>; <sup>1</sup>*Phytronix Technologies, Québec, CANADA*; <sup>2</sup>*Phytronix Technologies, Inc., Québec, QC*
- MP 245 **Development of a High-quality Automated Bioanalytical Platform in Support of a High-Throughput *in-vitro* Metabolic Stability Assay;** Shu Li; Kasia Kiełtyka; Marianne Vath; Andrew Wagner; Jun Zhang; Chris Baglieri; Cheryl Ferraro; Tatyana Zvyaga; Harold Weller; Wilson Shou; *Bristol-Myers Squibb Company, Wallingford, CT*
- MP 246 **Integration of Hardware and Software Systems for High-Throughput Sample Processing in ADME-Screening Bioanalysis;** James Federico<sup>1</sup>; John Janiszewski<sup>1</sup>; Peter Kovarik<sup>2</sup>; Wayne Lootsma<sup>3</sup>; Kevin Shirey<sup>3</sup>; Thomas Covey<sup>2</sup>; Mark Cole<sup>4</sup>; <sup>1</sup>*Pfizer Inc., Westerly, RI*; <sup>2</sup>*Mds Sciex, Concord, ON*; <sup>3</sup>*Sound Analytics, Llc, Niantic, CT*; <sup>4</sup>*Pfizer, Inc., Groton, CT*
- MP 247 **Simultaneous Analysis of 19 Non-Steroidal Anti-Inflammatory Drugs in Equine Plasma by LC-ESI-MS-MS;** Yowen You<sup>1</sup>; Cornelius Uboh<sup>2</sup>; Lawrence Soma<sup>1</sup>; Fuyu Guan<sup>1</sup>; Xiaoqing Li<sup>1</sup>; Yin Liu<sup>1</sup>; Jinwen Chen<sup>1</sup>; Jeffrey Rudy<sup>2</sup>; <sup>1</sup>*University of Pennsylvania, West Chester, PA*; <sup>2</sup>*West Chester University, West Chester, PA*
- MP 248 **Screening Chinese Botanicals for COX-2 Inhibitors using Ultrafiltration LC-MS;** Hongmei Cao<sup>1</sup>; Yongsoo Choi<sup>1</sup>; Dejan Nikolic<sup>1</sup>; Hongjie Zhang<sup>1</sup>; Wei Xiang<sup>1</sup>; Zhongze Ma<sup>2</sup>; David Y-W Lee<sup>2</sup>; Brian Berman<sup>3</sup>; Harry S. Fong<sup>1</sup>; Richard B. Van Breemen<sup>1</sup>; <sup>1</sup>*University of Illinois College of Pharmacy, Chicago, IL*; <sup>2</sup>*McLean Hospital/Harvard Medical School, Belmont, MA*; <sup>3</sup>*University of Maryland School of Medicine, Baltimore, MD*
- MP 249 **A Parallel Three-Column System and Direct Pooling of Samples in one Minute: Especially Suitable for *in vitro* Screens;** Annelie Lindqvist<sup>1</sup>; Jenny Johansson<sup>2</sup>; <sup>1</sup>*Medivir AB, Huddinge, Sweden*; <sup>2</sup>*AstraZeneca R&D Sodertalje, Sodertalje, Sweden*
- MP 250 **A High Sensitive and High Throughput LC-MS-MS Method for Determination of Fluticasone Propionate Various Rat Matrices;** Xiaodong Zhu<sup>2</sup>; Tom Addison<sup>2</sup>; Lisa Magis<sup>1</sup>; Dennis Alton<sup>1</sup>; Xiang-yu Jiang<sup>2</sup>; Qin Ji<sup>2</sup>; <sup>1</sup>*Covance Laboratories, Madison, WI*; <sup>2</sup>*Covance, Bioanalytical Chemistry, Madison, WI*
- MP 251 **Development of a 384-Well, Single Time-Point, Microsome Stability Assay;** Christopher Wegerski; Sam Sperry; Tuan Do; *SGX Pharmaceuticals, Inc., San Diego, CA*
- MP 252 **A Sub One Minute Assay for Determining P450 Inhibition and Drug Interaction Utilizing sub 2 micron particles and Mass Spectrometry;** Paul Rainville; Peter Alden; Joanne Mather; Rob Plumb; *Waters Corporation, Milford, MA*
- MP 253 **A New Approach for Screening and Identification of Radioactively Labeled Metabolites for *in vitro* and *in vivo* Metabolism Studies;** Timothy Snow; Shawn Gannon; *DuPont Haskell Laboratory, Newark, DE*
- MP 254 **Ideal Sample Preparation and HPLC Column Choice for the Analysis of Drug Compounds in Biomatrices;** Liming Peng; Tivadar Farkas; *Phenomenex, Inc., Torrance, CA*
- MP 255 **Cross-Validation of a High-Throughput Metabolic Stability Screening Assay using Laser Diode Thermal Desorption (LDTD) - Atmospheric Pressure Chemical Ionization;** Nicholas Duczak, Jr.<sup>1</sup>; James Kapron<sup>2</sup>; <sup>1</sup>*Thermo Electron Corporation, Somerset, NJ*; <sup>2</sup>*Thermo Fisher, Ottawa, ON*

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- MP 256 **Development of LC-MS-MS Methods for P450 Inhibition Studies in Human Liver Microsomes and Optimization of Incubation Conditions;** Ganesh S. Moorthy; Xinhe D. Jiang; Richard J. Grater; Charles F. Mchugh; Charles B. Davis; Ramesh B. Bambal; *GlaxoSmithKline, Collegeville, PA*
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- DRUG METABOLISM: XENOBIOTIC METABOLITE PROFILING, 257 - 284**
- MP 257 **Biosynthesis of Oxidative and conjugated Metabolites of VRX-480773, and Identification of their Structures by LC-MS-MS and NMR;** Hong Ki Kim; Virginia M. Borges; Dongmei Zhou; Li-tain Yeh; *Ardea Biosciences, Costa Mesa, CA*
- MP 258 **Characterization of *in vivo* Metabolites of the Potent 5-HT1D Receptor Antagonist, CP-448,187 in Sprague-Dawley Rats by HPLC/RAM/ESI/MS-MS;** Kevin Colizza<sup>2</sup>; Wendy Wang<sup>1</sup>; John Davis<sup>1</sup>; Amin M. Kamel<sup>1</sup>; <sup>1</sup>*Pfizer, Inc., Groton, CT*; <sup>2</sup>*Pfizer, Groton, CT*
- MP 259 **Plant Hormone Analysis by HPLC and Multiple Reaction Monitoring with Polarity Switching: SPE Fractionation of Plant Extracts and Trapped Injections;** Stephen J. Ambrose; *Nat'l Research Council, Saskatoon, Canada*
- MP 260 **Utilizing High Resolution Accurate Mass Spectrometry for Metabolite Identification of Small Interfering RNA Duplexes;** Yan Zou; Philip Tiller; I-Wu Chen; Michael B. Beverly; Jerome Hochman; *Merck & Co., West Point, PA*
- MP 261 **Structural Evaluation of Glucuronides of Morphine and Formoterol using Chemical Derivatization with 1,2-Dimethylimidazole-4-Sulfonyl Chloride and LC-MS<sup>n</sup>;** Matilda L. Salomonsson<sup>1</sup>; Ulf Bondesson<sup>2</sup>; Mikael Hedeland<sup>2</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*; <sup>2</sup>*National Veterinary Institute, Uppsala, Sweden*
- MP 262 **Metabolite Profiling of Development Compounds using Accurate Mass UPLC-MS-MS;** Richard Clayton; John Kendrick; *Covance Laboratories, Ltd, Harrogate, North Yorkshire, UK*
- MP 263 **Utility of High Accurate Mass (MSn) in the *in vitro* Disposition of Model CYP P450 Substrates-Novel and Known Metabolites;** Scott W. Womble<sup>1</sup>; Ron Aoyama<sup>1</sup>; Atul Ramaiya<sup>1</sup>; Yan Chen<sup>2</sup>; Laurance Lee<sup>2</sup>; Sanjeev Thohan<sup>1</sup>; <sup>1</sup>*Exelixis Inc, So. San. Francisco, CA*; <sup>2</sup>*Thermo Fisher Scientific, Inc., San Jose, CA*
- MP 264 ***In vitro* Metabolism of CRx-137, an Orally Synergistic Combination Drug Candidate, Detected by Liquid Chromatography-Tandem Mass Spectrometry LC-MS-MS;** Jennifer Chen<sup>1</sup>; Granvil Camille<sup>2</sup>; Mei Chen<sup>1</sup>; Mahesh V Padval<sup>1</sup>; Vikram Kansra<sup>1</sup>; <sup>1</sup>*CombinatoRx, Inc, Cambridge, MA*; <sup>2</sup>*Bausch & Lomb, Rochester, NY*
- MP 265 **<sup>13</sup>C Isotope Labeling in Combination with UPLC-FT-ICR MS and Fraction Collection for Accurate Metabolite Analysis;** Bettina Seiwert; Jan Hummel; Lothar Willmitzer; Patrick Giavalisco; *MP for molecular plant physiology, Potsdam, Germany*
- MP 266 **Metabolism and Metabolic Stability of a Novel Anti-Tuberculosis Compound Investigated using LC-MS-MS;** Yang Song; Jialin Mao; Richard B. Van Breemen; Scott Franzblau; *University of Illinois, Chicago, IL*
- MP 267 ***In vitro* Metabolism of Zapotin from Casimiroa edulis in Human Liver Microsomes and Cryopreserved Human Hepatocytes;** Jinghu Li<sup>1</sup>; Mark Cushman<sup>2</sup>; John M. Pezzuto<sup>3</sup>; Richard B. Van Breemen<sup>1</sup>; <sup>1</sup>*University of Illinois, Chicago, IL*; <sup>2</sup>*Purdue University, West Lafayette, IN*; <sup>3</sup>*University of Hawaii at Hilo, Hilo, HI*
- MP 268 **A Study of *in vitro* Metabolism of Minor Alkaloids in Tobacco using HILIC UPLC-MS-MS;** Gary D. Byrd; Michael Ogden; *R.J. Reynolds Tobacco Co., Winston-Salem, NC*
- MP 269 **Metabolite Identification of IPI-609, a Novel and Potent Inhibitor of the Hedgehog Pathway in Different Species;** Teresa M. Alvarez-Diez; Joseph Manna; Martin Tremblay; Michael J. Grogan; James R. Porter; Alfredo C. Castro; Jens R. Sydor; *Infinity Pharmaceuticals Inc., Cambridge, MA*
- MP 270 **Mass Spectrometric Analysis of Laccase-Mediated Transformation of Triclosan;** Kumarasamy Murugesan; Young-Mo Kim; Jong-Rok Joen; Eun-Ju Kim; Yoon-Seok Chang; *Pohang University of Science and Technology, Pohang, South Korea*
- MP 271 **Elucidation of a Novel Metabolic Pathway for 20-epi Analogs of Vitamin D<sub>3</sub>: C-1 Esterification with Stearic and Oleic Acids;** Caroline Ceailles<sup>1</sup>; Andrew Weiskopf<sup>1</sup>; Paul Vouros<sup>1</sup>; Gino J. Sasso<sup>2</sup>; Milan R. Uskokovic<sup>3</sup>; G. atyanarayana Reddy<sup>4</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Hoffmann-La Roche Inc., Nutley, NJ*; <sup>3</sup>*Bioxell Inc., Nutley, NJ*; <sup>4</sup>*Epimer LLC, Providence, RI*
- MP 272 **Distinguishing Hepatic N-oxidation from Hydroxylation using High Mass Accuracy - Application in Elucidating the Role of Flavin-Containing Monooxygenase Enzyme;** Atul Ramaiya; Scott Womble; Ron Aoyama; Lester Bornheim; Sanjeev Thohan; *Exelixis Inc, So. San. Francisco, CA*
- MP 273 **Elucidation of the Impact of Met30 on the Phospholipid Profile of *Saccharomyces cerevisiae* using Matrix-Assisted Laser Desorption Mass Spectrometry;** S. Mariccor Andresa Batoy<sup>1</sup>; Sabine Borgmann<sup>4</sup>; Peter Kaiser<sup>2,3</sup>; Charles L. Wilkins<sup>1</sup>; Jeffrey J. Jones<sup>2,3</sup>; <sup>1</sup>*University of Arkansas, Fayetteville, AR*; <sup>2</sup>*University of California, Irvine, Irvine, CA*; <sup>3</sup>*University of California, Irvine, Irvine, CA*; <sup>4</sup>*ISAS -Institute for Analytical Sciences, Dortmund, Germany*
- MP 274 **The Influence of Higher Mass Resolution and Larger Dynamic Range on the Identification of Relevant Metabolites of Pharmaceuticals by LC-MS;** Edgar Naegel; *Agilent Technologies, Waldbronn, Germany*
- MP 275 **Comprehensive Investigation of Injection Time and Auto Gain Control on Ion Trap Instruments for the LC-MS Application of Metabolite Identification;** Zhe-ming Gu<sup>2</sup>; Dan Bachalis<sup>2</sup>; Ming Gu<sup>1</sup>; <sup>1</sup>*Cerno Bioscience, Yardley, PA*; <sup>2</sup>*XenoBiotic Laboratories, Inc., Plainsboro, NJ*
- MP 276 **Metabolism and excretion of CP-448,187 in Humans: Structural Characterization of Novel Cyclized Products by 1H LC-NMR and Chemical Approaches;** Amin M. Kamel<sup>1</sup>; Kevin Colizza<sup>2</sup>; Wendy Wang<sup>1</sup>; Tom O'Connell<sup>1</sup>; <sup>1</sup>*Pfizer, Inc., Groton, CT*; <sup>2</sup>*Pfizer, Groton, CT*
- MP 277 **Characterization of Alkyl Hydroxylated Plasma Metabolites of Fentanyl, Verapamil, Amitriptyline, Doxepin and Pylarimine by Accurate Mass Ion Tree Mass Spectrometry;** Jeffrey Rudy<sup>1</sup>; Fran Xu<sup>2</sup>; Heidi M Snapp<sup>4</sup>; Cornelius Uboh<sup>3</sup>; Lawrence Soma<sup>4</sup>; <sup>1</sup>*PA Equine Toxicology, West Chester, PA*; <sup>2</sup>*Jnj, Raritan, NJ*; <sup>3</sup>*West Chester University, West Chester, PA*; <sup>4</sup>*University of Pennsylvania, Kennett Square, PA*



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- MP 278 **Induction of Oxidative Stress in Human Lung Cells after Exposure to a Benzo[A]Pyrene Metabolite;** Dipti Mangal<sup>1</sup>; Jong-Heum Park<sup>1</sup>; Seon Hwa Lee<sup>2</sup>; Clementina Mesaros<sup>1</sup>; Trevor M. Penning<sup>3</sup>; Ian A. Blair<sup>3</sup>; <sup>1</sup>*Ctr for Cancer Pharmacology, UPenn, Philadelphia, PA;* <sup>2</sup>*Tohoku Univ., Dept. Pharm, Sendai, Japan;* <sup>3</sup>*Ctr for Excellence in Environ Tox, UPenn, Philadelphia, PA*
- MP 279 **Small Molecule Profiling of Saccharomyces Cerevisiae Secretions and the Related Effects of ABC Transporter Mutations;** Matthew R. Lewis; Elie G. El Kassis; Corey D. Broekling; Dayakar V. Badri; Jessica Prenni; Jorge M. Vivanco; *Colorado State University, Fort Collins, CO*
- MP 280 **Electrospray, APCI and MALDI MS of tert-Butyldimethylsilyl (TBDMS) Derivatives of Compounds of Biological Interest;** John M. Halket; Anna M. Przyborowska; Mark C. Parkin; Norman W. Smith; Andrew T. Kicman; David A. Cowan; Sukhvinder Bansal; *King's College London, London, UK*
- MP 281 **In vitro Identification of Intermediates from the Biodegradation of Chlorobenzenes by Pseudonocardia benzenovorans;** Eun-Ju Kim; Young-Mo Kim; Jong-Rok Jeon; Kumarasamy Murugesan; Yoon-Seok Chang; *Postech, Pohang, South Korea*
- MP 282 **Use of Q-Trap Mass Spectrometry in Cytochrome P450 (CYP450) Reaction Phenotyping of Bupropion;** Yuan Chen<sup>1</sup>; Khanh Nguyen<sup>1</sup>; Liling Liu<sup>1</sup>; Adrian Fretland<sup>1</sup>; Elliott Jones<sup>2</sup>; Huaifen Liu<sup>2</sup>; <sup>1</sup>*Roche Palo Alto LLC, Palo Alto, CA;* <sup>2</sup>*Applied Biosystems, Foster city, CA*
- MP 283 **Metabolite Identification of Astilpin in Biological Specimen by ESI-IT-TOF Tandem Mass Spectrometry;** Yan Liang<sup>1</sup>; Lin Xie<sup>1</sup>; An Kang<sup>1</sup>; Longsheng Sheng<sup>1</sup>; Leren Wan<sup>2</sup>; Guang-Ji Wang<sup>1</sup>; <sup>1</sup>*China Pharmaceutical University, Nan Jing, China;* <sup>2</sup>*Shimadzu Beijing Office, Beijing, China*
- MP 284 **Identification of Intermediates from the Bacterial Transformation of Triclosan using Mass Spectrometry;** Young-Mo Kim; Kumarasamy Murugesan; Jong-Rok Jeon; Eun-Ju Kim; Yoon-Seok Chang; *Postech, Pohang, South Korea*
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- METABOLOMICS 1, 285 - 307**
- MP 285 **High Throughput Metabolomics using Sample Fractionation and Direct Infusion Nanospray in Combination with High Resolution MSn;** Elwin Verheij; Leon Coulier; Ivana Bobeldijk-Pastorova; *TNO Quality of Life, Zeist, Netherlands*
- MP 286 **High-Throughput Screening of Plant Metabolic Phenotypes Based upon Fused-Core HPLC Coupled with Multiplexed CID TOF/MS;** Feng Shi; Anthony L. Schillmiller; Jeongwoon Kim; Robert L. Last; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 287 **Metabolic Profiling to Determine Phenotypes of Chronic Obstructive Pulmonary Disease (COPD);** Nichole Reisdorph<sup>1</sup>; Michael Armstrong<sup>1</sup>; Talia Muram<sup>2</sup>; Michael Burson<sup>2</sup>; Richard Reisdorph<sup>1</sup>; Russell Bowler<sup>1</sup>; <sup>1</sup>*National Jewish Medical and Research Center, Denver, CO;* <sup>2</sup>*UCHSC, Denver, CO*
- MP 288 **Use of ICR-FT/MS to Study the Metabolic Evidence for Biogeographic Isolation of the Extremophilic Bacterium Salinibacter Ruber;** Marianna Lucio<sup>2</sup>; Ramon Rosselló-Mora<sup>1</sup>; Josefa Antón<sup>3</sup>; Philippe Schmitt-Kopplin<sup>2</sup>; <sup>1</sup>*Institut Mediterrani d'Estudis Avançats, Esporles, Spain;* <sup>2</sup>*Helmholtz Zentrum München, Neuherberg, Germany;* <sup>3</sup>*Instituto Multidisciplinar de Estudios del Medio, Alicante, Spain*
- MP 289 **High-Throughput Non-Targeted Metabolic Profiling with Hybrid Stationary Phase LC Column Coupled to Q-TOF-MS in Cancer Research;** Hyun-Jin Jung<sup>1</sup>; Man-Ho Choi<sup>1</sup>; Kyung Mi Kim<sup>1</sup>; Won-Yong Lee<sup>2</sup>; Bong Chul Chung<sup>1</sup>; <sup>1</sup>*Life Sciences Division / KIST, Seoul, Korea;* <sup>2</sup>*Dept. of Chemistry / Yonsei Univ., Seoul, Korea*
- MP 290 **Metabolic Analysis of Cancer and Normal Cells;** Munehiro Teshima; Norma Pawley; Steven Brumby; James Freyer; Clifford Unkefer; Pat Unkefer; *Los Alamos National Laboratory, Los Alamos, NM*
- MP 291 **Global Metabolite Profiling of Carbon Metabolism in Mycobacterium Tuberculosis: An LC-MS TOF-Based Approach;** Kyu Rhee<sup>1</sup>; Steven M. Fischer<sup>2</sup>; Theodore Sana<sup>2</sup>; Steven Gross<sup>3</sup>; <sup>1</sup>*Weill Cornell Medical Colleg, NY, NY;* <sup>2</sup>*Agilent Technologies, Santa Clara, CA;* <sup>3</sup>*Weill Medical College of Cornell University, New York, NY*
- MP 292 **A Metabolomic Investigation of Novel Uremic Biomarkers by Two-Dimensional Liquid Chromatography Mass Spectrometry;** Ruth Godfrey<sup>1</sup>; Gareth Brenton<sup>1</sup>; Russell Newton<sup>1</sup>; Edward Dudley<sup>1</sup>; Peter Willshaw<sup>1</sup>; Ashraf Mikhail<sup>2</sup>; Lisa Bastin<sup>2</sup>; Gary Woffendin<sup>3</sup>; Helen Welchman<sup>3</sup>; <sup>1</sup>*Swansea University, Swansea, UK;* <sup>2</sup>*Morrison Hospital, Swansea NHS Trust, Swansea, UK;* <sup>3</sup>*Thermo Fisher Scientific, Hemel Hempstead, UK*
- MP 293 **Large-Scale Screening for Specialized Metabolites using Multiplexed Collision Induced Dissociation and Time-of-Flight Mass Spectrometry;** A. Daniel Jones<sup>1</sup>; Feng Shi<sup>1</sup>; Xiaoli Gao<sup>2</sup>; <sup>1</sup>*Michigan State University, East Lansing, MI;* <sup>2</sup>*Michigan State University, East Lansing, MI*
- MP 294 **Lipidomics Based Diagnostics for Ovarian Cancer;** Aaron Z Fernandis; Narasimhan Kothandaraman; Gek Huey Chua; Xue Li Guan; Guanghou Shui; Mahesh Choolani; Markus Wenk; *National University of Singapore, Singapore*
- MP 295 **Application of Nano-Electrospray Tandem Mass Spectrometry for Direct Fingerprinting of Rat Urine in Metabolomics;** Haiwei Gu; Hongling Han; Yanping Sun; Zhengzheng Pan; Jian Zhang; Scott A. McLuckey; Daniel Raftery; *Purdue University, West Lafayette, IN*
- MP 296 **Phytochemical Prospecting for Anti-Insect Molecules from Alfalfa (Medicago sativa) Trichomes;** Wensheng Li; Richard A Dixon; Lloyd W. Sumner; *The Noble Foundation, Ardmore, OK*
- MP 297 **Comprehensive Metabolomics Study of CHO Cell Line Cultivation;** Olaf Boernsen; Guido Wahl; Nadege Villemin; Joerg Schmidt; Stephan Gatzek; *Novartis Pharma AG, Basel, Switzerland*
- MP 298 **Searching Biomarkers for the Complex Regional Pain Syndrome by Metabolic Profiling of Urine using CE/MS;** Rawi Ramautar<sup>1</sup>; Anne v.d. Plas<sup>3</sup>; Karsten Michelmann<sup>4</sup>; Rico J.E. Derks<sup>2</sup>; Gabriela Zurek<sup>4</sup>; Govert W. Somsen<sup>1</sup>; Gerhardus J. de Jong<sup>1</sup>; J.J. van Hilten<sup>3</sup>; Andre M. Deelder<sup>2</sup>; Oleg A. Mayboroda<sup>2</sup>; <sup>1</sup>*Biomedical Analysis, Utrecht University, Utrecht, Netherlands;* <sup>2</sup>*Biomolecular MS, LUMC, Leiden, Netherlands;* <sup>3</sup>*Neurology, LUMC, Leiden, Netherlands;* <sup>4</sup>*Bruker Daltonik, Bremen, Germany*



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- MP 299 **Metabolomic Approach to the Identification of Robust Markers for the Detection of Mechanically Recovered Meat in Food Products;** Izabella Surowiec; Paul D. Fraser; John Halket; Raj Patel; Peter M. Bramley; *Royal Holloway University of London, Egham, UK*
- MP 300 **Integrated Plant Metabolomics by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Jun Han<sup>1</sup>; Ryan M. Danell<sup>2</sup>; Dustin Lippert<sup>3</sup>; Monica H. Elliott<sup>1</sup>; Joerg Bohlmann<sup>3</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Center, Victoria, BC, Canada*; <sup>2</sup>*Danell Consulting, Greenville, NC*; <sup>3</sup>*University of British Columbia, Vancouver, BC*
- MP 301 **Differential Metabolomics Analysis of Serum from Metabolic Syndrome Ossabaw Swine by Stable Isotope Labeling and Pattern Recognition;** Xiaodong Huang<sup>1</sup>; Cheolhwan Oh<sup>1</sup>; Zhidong Xu<sup>2</sup>; Ashraf Madian<sup>1</sup>; Mouhamad Alloosh<sup>3</sup>; Michael Sturek<sup>3</sup>; Charles Buck<sup>1</sup>; Fred Regnier<sup>1</sup>; Xiang Zhang<sup>4</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Methodist Research Institute, Indianapolis, IN*; <sup>3</sup>*Indiana University School of Medicine, Indianapolis, IN*; <sup>4</sup>*University of Louisville, Louisville, KY*
- MP 302 **A Conservation Study to Investigate Mycobacterium Avium Lipid Metabolites in the Endangered White-Winged Wood Duck;** Heather Lucas; Razeq Jennifer; Jody M. Modarelli; *Hiram College, Hiram, Ohio*
- MP 303 **Liquid Chromatography Time-of-Flight Mass Spectrometry-Based Metabolic Fingerprinting of Human Sera for Ovarian Cancer Biomarker Discovery;** Manshui Zhou; John McDonald; Facundo Fernandez; *Georgia Institute of Technology, Atlanta, GA*
- MP 304 **The Use of MS Based Metabonomics for the Discovery of a Potential Biomarker Associated Acute Kidney Injury;** Ricky D. Holland<sup>1</sup>; Jinchun Sun<sup>1</sup>; Laura K. Schnackenberg<sup>1</sup>; Page Moore<sup>2</sup>; Catherine L. Dent<sup>3</sup>; Prasad Devarajan<sup>3</sup>; Didier Portilla<sup>2</sup>; Richard D. Beger<sup>1</sup>; <sup>1</sup>*USFDA/NCTR, Jefferson, AR*; <sup>2</sup>*UAMS, Little Rock, AR*; <sup>3</sup>*University of Cincinnati School of Medicine, Cincinnati, OH*
- MP 305 **Probing the Plasmodium Metabolome;** Kellen L Olszewski<sup>1</sup>; Joshua D. Rabinowitz<sup>1</sup>; JoAnne Morrissey<sup>2</sup>; James M Burns<sup>2</sup>; Akhil Vaidya<sup>2</sup>; Manuel Llinas<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ*; <sup>2</sup>*Drexel University, Philadelphia, PA*
- MP 306 **HPLC-MS Metabolic Profiling for the Detection of Bladder Cancer;** Haleem J. Issaq<sup>1</sup>; Timothy Waybright<sup>1</sup>; Brian Luke<sup>1</sup>; Ofer Nativ<sup>2</sup>; Elias J Issaq<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>*SAIC-Frederick, Inc., Frederick, MD*; <sup>2</sup>*Bnai-Zion Medical Center, Haifa, Israel*
- MP 307 **Application of Mass Spectrometry Based Metabolic Profiling to Bronchial Lavage Fluids from Cystic Fibrosis Subjects;** Gunnar Boysen<sup>1</sup>; Thomas M. O'Connell<sup>1</sup>; Justyna E. Wolak<sup>1</sup>; Marianne S. Muhlebach<sup>1</sup>; Julie Wingate<sup>2</sup>; Xu Guo<sup>2</sup>; Alina Dindyal-Popescu<sup>2</sup>; James A Swenberg<sup>1</sup>; Charles R Esther Jr<sup>1</sup>; <sup>1</sup>*UNC at Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*Applied Biosystems, Concord, ON*
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- PEPTIDES: QUANTITATION, 308 - 333**
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- MP 308 **Quantitative Analysis of a Therapeutic Protein in Human Plasma by LC-MS-MS using Accelerated Digestion;** Antoine Lesur<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Nathalie Oudry<sup>1</sup>; Olivier Heudi<sup>2</sup>; Dieter Zimmer<sup>2</sup>; Stephan Beck<sup>2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>*Life Sciences Mass Spectrometry, Geneva University, Geneva, Switzerland*; <sup>2</sup>*Novartis, Basel, Switzerland*
- MP 309 **Tandem Mass Tags and MRM Mass Spectrometry for the Evaluation of Candidate Markers of Alzheimer's Disease;** Darragh O'Brien<sup>1</sup>; Simon Lovestone<sup>3</sup>; Karsten Kuhn<sup>2</sup>; Peter Schulz-Knappe<sup>2</sup>; Malcolm Ward<sup>1</sup>; Helen Byers<sup>1</sup>; Ian Pike<sup>1</sup>; <sup>1</sup>*Proteome Sciences PLC, London, UK*; <sup>2</sup>*Proteome Sciences R&D GmbH, Frankfurt, Germany*; <sup>3</sup>*MRC Centre for Neurodegeneration Research, London, UK*
- MP 310 **Quantification and Normalization of Complex Label-Free Mass Spectrometry Data for Proteomic Analysis;** Noelle M Griffin<sup>1</sup>; Jingyi Yu<sup>1</sup>; Phil Oh<sup>1</sup>; Sabrina Shore<sup>1</sup>; Fred Long<sup>1</sup>; Yan Li<sup>1</sup>; Jim Koziol<sup>2</sup>; Jan E Schnitzer<sup>1</sup>; <sup>1</sup>*Sidney Kimmel Cancer Cent, San Diego, CA*; <sup>2</sup>*Scripps Research Institute, La Jolla, CA*
- MP 311 **Quantitating Dynamic Changes in Phosphorylation of the Vasopressin-Sensitive Water Channel Aquaporin-2 using Targeted MRM Methods;** Brigitte Simons<sup>1</sup>; Jason Hoffert<sup>2</sup>; Mark Knepper<sup>2</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, CANADA*; <sup>2</sup>*National Heart Lung and Blood Institute, NIH, Bethesda, MD*
- MP 312 **Quantitative Analysis of Oxytocin and Vasopressin by Nano-LC-MS-MS;** Theresa McLaughlin; Karolina M. Krasinska; Allis S. Chien; *Stanford University, Stanford, CA*
- MP 313 **Acid-Catalyzed 18O-Labeling of Peptides - a New, Versatile Tool for Proteomics;** Richard Niles<sup>1</sup>; H. Ewa Witkowska<sup>2</sup>; Steven C. Hall<sup>2</sup>; Susan J. Fisher<sup>1</sup>; Markus Hardt<sup>1</sup>; <sup>1</sup>*University of California at San Francisco, San Francisco, CA*; <sup>2</sup>*UCSF Core Mass Spectrometry Facility, San Francisco, CA*
- MP 314 **MS Approaches to Investigate the Role of an Amyloid-β Peptide Isoform in Alzheimer's Plaque Formation Onset;** Igor A. Popov<sup>2</sup>; Sergey A. Kozin<sup>1</sup>; Alexey S. Kononikhin<sup>3</sup>; Elena V. Kugaevskaya<sup>1</sup>; Philipp O. Tsvetkov<sup>4</sup>; Alexander A. Makarov<sup>4</sup>; Alexander I. Archakov<sup>1</sup>; Eugene N. Nikolaev<sup>3</sup>; <sup>1</sup>*Orekhovich Institute of Biomedical Chemistry RAMS, Moscow, Russia*; <sup>2</sup>*Emanuel Institute of Biochemical Physics, Moscow, Russia*; <sup>3</sup>*The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation*; <sup>4</sup>*Engelhardt Institute of Molecular Biology, Moscow, Russia*
- MP 315 **LC-FAIMS-MS-MS Quantitation of 1-Methyl and 3-Methylhistidine in the Assessment of Skeletal Muscle Degradation;** Gabriela A. Kulp<sup>1</sup>; Calin G. Znamirovski<sup>2</sup>; <sup>1</sup>*Shriners Hospital for Children, Galveston, TX*; <sup>2</sup>*Thermo Fisher Scientific, West Palm Beach, FL*
- MP 316 **Towards Comparative Peptidome Analysis of Unicellular Signaling Molecules using Isobaric Mass Tagging;** Martijn W.H. Pinkse<sup>1</sup>; Inez M.O. Finoulst<sup>1</sup>; Peter Schulze-Knappe<sup>2</sup>; Peter D.E.M. Verhaert<sup>1</sup>; <sup>1</sup>*Delft University of Technology, Delft, The Netherlands*; <sup>2</sup>*Proteome Sciences, Frankfurt, Germany*
- MP 317 **FAIMS: GLP-Validated Quantitation Method for a Peptide in Biological Matrix;** Axel Roemer; Tobias Klaassen; *A&M Labor fuer Analytik und Metabolismusforschung, Bergheim, Germany*
- MP 318 **High Throughput Plasma Stability Screening of Peptide Drug Candidates by LC-MS in a Parallel Mode;** Isabelle Tcholakov; Chris Bellows; Yan Wang; Chao-Xuan Zhang; *Amylin Pharmaceuticals, Inc., San Diego, CA*

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- MP 319 **Absolute Quantitation of Peptide/Protein Biomarkers by Means of Immuno-MALDI-TOF MS**; Katrin Sparbier<sup>1</sup>; Hassan Dihazi<sup>2</sup>; Sabine Blaschke<sup>2</sup>; Gongyi Shi<sup>3</sup>; Gerd-Anton Mueller<sup>2</sup>; Thomas Flad<sup>4</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Leipzig, Germany*; <sup>2</sup>*University Hospital Goettingen, Goettingen, Germany*; <sup>3</sup>*Bruker Daltonics Inc., Fremont, CA*; <sup>4</sup>*Panatecs GmbH, Tuebingen, Germany*
- MP 320 **Quantification of ANGI-7 and ANGI-5 in Rat Plasma by SPE-HPLC-MS-MS**; Sebastien Gagne; Marc Ouellet; Rene St-Jacques; Sylvie Toulmond; Jean-Francois Levesque; *Merck Frosst Canada & Co, Kirkland, CANADA*
- MP 321 **N, N-Dimethyl Amino Acids as iTRAQ Reagent for Improved Peptidomics and Proteomics**; Feng Xiang<sup>1</sup>; Qiang Fu<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Schering Plough, Westfield, NJ*
- MP 322 **Proteomic Profiling of Glioblastoma Cells following miR-21 Knockdown**; MARJORIE MINKOFF<sup>1</sup>; Thales Papagiannakopoulos<sup>2</sup>; Philip Ross<sup>1</sup>; Matthew Willetts<sup>1</sup>; Kenneth Kosik<sup>2</sup>; Darryl J Pappin<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*; <sup>2</sup>*University of Santa Barbara, Santa Barbara, CA*
- MP 323 **Investigation on the Use of MALDI MS-MS for Absolute Quantification of Peptides**; Carmen L. Fernandez-Metzler<sup>1</sup>; Elizabeth A. Mahan<sup>2</sup>; Kristin Geddes<sup>2</sup>; Richard King<sup>3</sup>; <sup>1</sup>*Merck Research Labs, West Point, PA*; <sup>2</sup>*Merck & Co., West Point, PA*; <sup>3</sup>*Merck & Company, Inc., West Point, PA*
- MP 324 **Quantitative Analysis of Single Amino Acid Changes using a 4000 QTRAP® system**; Bruno Manadas<sup>1</sup>; Vera Mendes<sup>1</sup>; Raquel Silva<sup>2</sup>; Manuel Santos<sup>2</sup>; Euclides Pires<sup>1</sup>; <sup>1</sup>*Center for Neuroscience and Cell Biology, Coimbra, Portugal*; <sup>2</sup>*Department of Biology and CESAM, Un. of Aveiro, Aveiro, Portugal*
- MP 325 **Pandemic Influenza Preparedness: The New Role for Mass Spectrometry**; Tracie Williams; Jessica Norrgran; Leah Luna; James L Pirkle; John Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- MP 326 **MRM Based, Multiplexed, Absolution Quantitation of 31 High Abundance Proteins in Human Plasma**; Derek Smith<sup>1</sup>; Michael A Kuzyk<sup>1</sup>; Tyra Cross<sup>1</sup>; Juncong Yang<sup>1</sup>; Angela Jackson<sup>1</sup>; Darryl Hardie<sup>1</sup>; Leigh Anderson<sup>2</sup>; Christoph H Borchers<sup>1</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*Plasma Proteome Institute, Washington, DC*
- MP 327 **Quantification of a Polypeptide Drug, Desirudin, in Human Plasma using Electrospray LC-MS-MS with an Analog Polypeptide as Internal Standard**; Wenzhong Liang<sup>1</sup>; Xinping Fang<sup>1</sup>; Jinn Wu<sup>1</sup>; Tony Yu<sup>2</sup>; <sup>1</sup>*XenoBiotic, Plainsboro, NJ*; <sup>2</sup>*Canyon Pharmaceuticals, Hunt Valley, MD*
- MP 328 **Model-Based Protein Quantification for Label-Free LC-MS Proteomics Profiling Experiments**; Melissa Key<sup>1</sup>; Susanne Ragg<sup>2</sup>; Gunther Schadow<sup>2</sup>; Olga Vitek<sup>1</sup>; ilka Ott<sup>3</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Indiana University, Indianapolis, IN*; <sup>3</sup>*Deutsches Herzzentrum Munchendes, Munich, Germany*
- MP 329 **Quantification of Endogenous  $\alpha$ - and  $\beta$ -Endorphins in Rat Brain by LC-MS-MS**; Hari Kosanam<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Chhabil Dass<sup>1</sup>; <sup>1</sup>*The University of Memphis, Memphis, TN*; <sup>2</sup>*University of Tennessee Health Science Center, Memphis, TN*
- MP 330 **Rapid and Accurate Analysis of Peptides Used as Standards for Quantitative Proteomics**; Narisa K. Bordeerat<sup>1</sup>; Nadia I. Georgieva<sup>1</sup>; Leonard B. Collins<sup>1</sup>; Christoph H. Borchers<sup>2</sup>; James A. Swenberg<sup>1</sup>; Gunnar Boysen<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*Uvic-gbc Proteomics Centre, Victoria, BC*
- MP 331 **Development and Validation of a Quantitative Assay for the Measurement of Desmopressin in Rat Plasma by Liquid Chromatography-Tandem Mass Spectrometry**; Yun Chen; Toni Jean Thompson; *Charles River Laboratories, Shrewsbury, MA*
- MP 332 **HPLC-MS-MS Analysis of A $\beta$  Peptides in Biological Matrices**; Mark Dreyer; Donald Walker; *Elan Pharmaceuticals, South San Francisco, CA*
- MP 333 **Peptide Quantitation by Triple Quadrupole Mass Spectrometry using Selectively Sequence-Modified Internal Standards**; Steven K. Drake; Tracey A. Sutton; Glen L. Hortin; *NIH Clinical Center, Bethesda, MD*
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- Peptides: Fragmentation, 334 - 355**
- MP 334 **Fragment Structures in Collision-Induced Dissociation of Peptides Investigated by H/D Exchange**; Xian Chen; David H. Powell; Nicolas Polfer; *University of Florida, Gainesville, FL*
- MP 335 **Study of Fragmentation Pattern of Intramolecular Cross-Linked Peptides by ESI and MALDI-MS-MS**; Luiz Fernando A Santos; Amadeu H Iglesias; Fabio C Gozzo; *Brazilian Synchrotron Light Source, Campinas, Brazil*
- MP 336 **Manipulating the Dissociation Chemistry of Transition-Metal-Peptide Complexes by Controlling their Oxidation States**; Warren K. Mino<sup>1</sup>; Nick C. Polfer<sup>1</sup>; Craig M. Whitehouse<sup>2</sup>; Randall E. Pedder<sup>3</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*; <sup>2</sup>*Analytica of Branford, inc., Branford, CT*; <sup>3</sup>*Ardara Technologies L.P., Monroeville, PA*
- MP 337 **Improved Sequencing of Peptides by CID Spectra Interpretation with Focus on Redundant Peptide End Information**; Wolf D. Lehmann; Joerg Seidler; Dominic Winter; *German Cancer Research Center, Heidelberg, Germany*
- MP 338 **Formation of x-Type Ions from Collision Induced Dissociation of Metal Cationized Peptides**; Kevin Kmiec; Shane Tichy; David H. Russell; *Texas A&M University, College Station, TX*
- MP 339 **Structural Characterisation of a- and b- Ions Obtained by CID of Peptides using Ion Mobility and Tandem Mass Spectrometry**; Isabel Riba<sup>1</sup>; Kevin Giles<sup>2</sup>; Robert Bateman<sup>2</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- MP 340 **Selecting Fixed-Charge Groups for Electron-Based Peptide Dissociations: A Computational Study of Substituted Pyridinium Charge Tags**; Thomas W. Chung; Frantisek Turecek; *University of Washington, Seattle, WA*
- MP 341 **Characterization of Formaldehyde Modified Peptides**; Maria Ospina; Adrienne Barry; Hubert Vesper; *Center/Disease Control & Prevention, Atlanta, GA*
- MP 342 **Fragmentation Pathways of Doubly Protonated Tryptic Peptides**; Christian Bleiholder<sup>1</sup>; Arpad Somogyi<sup>2</sup>; Sandor Suhai<sup>1</sup>; Bela Paizs<sup>1</sup>; <sup>1</sup>*German Cancer Research Center, Heidelberg, Germany*; <sup>2</sup>*University of Arizona, Tucson, AZ*
- MP 343 **Use of Reporter Ion for the Identification of Cross-Linked Peptides**; Fabio C Gozzo; Amadeu H Iglesias; Luiz Fernando A Santos; *Brazilian Synchrotron Light Source, Campinas, Brazil*

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- MP 344 **N-Cα Backbone Cleavage without Loss of a Phosphate Group in a Charge Reduced Phosphopeptide using an Alkali Metal Target;** Hirofumi Nagao<sup>1</sup>; Shigeo Hayakawa<sup>2</sup>; Michisato Toyoda<sup>1</sup>; Mami Hashimoto<sup>2</sup>; Kunio Awazu<sup>1</sup>; <sup>1</sup>Osaka University, Osaka, Japan; <sup>2</sup>Osaka Prefecture University, Sakai, Japan
- MP 345 **The Utilization of Orbitrap Higher Collision Decomposition Device for PTM Analysis and iTRAQ-based Quantitation;** Katalin F. Medzihradskyy<sup>1</sup>; Robert Chalkley<sup>1</sup>; Jonathan Trinidad<sup>1</sup>; Izhak Michaelovski<sup>2</sup>; David A. Maltby<sup>1</sup>; Mike Fainzilber<sup>2</sup>; A.I. Burlingame<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>Weizmann Institute, Rehovot, Israel
- MP 346 **The Effects of Peptide End Group (Acid versus Amide) on CID, ETD, and PSD Mass Spectra;** Samantha Bokatzian-Johnson; Carolyn J. Cassidy; University of Alabama, Tuscaloosa, AL
- MP 347 **The Use of Transition Metal Complex Cations for Electron Transfer and Metal Transfer Ion/Ion Reactions with Negatively Charged Peptides;** David Crizer; Yu Xia; Scott A. McLuckey; Purdue University, West Lafayette, IN
- MP 348 **ECD vs. ETD: Observations from an O-Glycosylated Peptide;** Matthew B. Renfrow<sup>1</sup>; Stephanie B. Wall<sup>1</sup>; Anthony High<sup>2</sup>; Raghu K Chitta<sup>2</sup>; James Mobley<sup>1</sup>; Jan Novak<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>St Jude Children's Research Hospital, Memphis, TN
- MP 349 **The Formation and Structures of Histidine-Containing b2 Ions: A Time-Resolved Tandem Mass Spectrometric and Theoretical Study;** Pui Yee Lau; Jackie M K Cheng; Carrie H S Wong; Ida N. Ma; Chun Wai Tsang; The Hong Kong Polytechnic University, Hong Kong, Hong Kong
- MP 350 **Gas Phase Fragmentation of Peptides by MALDI in-Source Decay Occurs with Limited Amide Hydrogen (1H/2H) Scrambling;** Thomas J.D. Jorgensen; Nicolai H Bache; Kasper Rand; Peter Roepstorff; University of Southern Denmark, Odense M, Denmark
- MP 351 **Investigation of Acetylation Specific Neutral Loss in Collision Induced Dissociation of O-Acetylated Peptides;** Jiang Zhang; Qiang Fu; Lingjun Li; Univ Wisconsin, Madison, WI
- MP 352 **Radical Directed Dissociation at Aromatic Residues in Peptides Initiated by Noncovalently Attached Radical Precursors;** Qingyu Sun; Ryan R. Julian; University of California, Riverside, Riverside, CA
- MP 353 **Fragmentation Pattern of Intermolecular Cross-Linked Tryptic Peptides;** Amadeu H Iglesias; Luiz Fernando A Santos; Fabio C Gozzo; Brazilian Synchrotron Light Source, Campinas, Brazil
- MP 354 **Collision-Induced Dissociation and Electron Capture Dissociation in a Radio Frequency Ion Trap;** Hiroyuki Satake; Naomi Manri; Takashi Baba; Central Research Laboratory, Hitachi Ltd., Tokyo, Japan
- MP 355 **Preferential Fragmentation of Singly Charged Phosphopeptides Adjacent to Phosphorylated Serines and Threonines;** Peter M. Gehrig; Dorothea Rutishauser; Bernd Roschitzki; Ralph Schlapbach; Functional Genomics Center Zurich, Zurich, Switzerland
- MP 357 **On-line Capillary Weak-Cation Exchange Method for Removal of Non-Ionic Detergent from Monoclonal Antibody Samples;** Jakub Baudys; Ola M. Saad; Valerie Quarmby; Surinder Kaur; Genentech, Inc., South San Francisco, CA
- MP 358 **Novel Tandem IgY12-SuperMix Immunoaffinity Separation Strategy for Enhanced Detection of Low-Abundant Human Plasma Proteins;** Weijun Qian<sup>1</sup>; David T. Kaleta<sup>1</sup>; Brianne O. Petritis<sup>1</sup>; Hongliang Jiang<sup>2</sup>; Tao Liu<sup>1</sup>; Xu Zhang<sup>1</sup>; Heather M. Mottaz<sup>1</sup>; Susan M. Varnum<sup>1</sup>; David G. Camp II<sup>1</sup>; Lei Huang<sup>3</sup>; Xiangming Fang<sup>3</sup>; Wei-Wei Zhang<sup>3</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Covance Laboratories Inc., Madison, WI; <sup>3</sup>GenWay Biotech, Inc., San Diego, CA
- MP 359 **The Optimization for Enhanced Proteome Coverage of Complex Protein Mixture;** Sunil Hwang<sup>1</sup>; Kimberly, Q. McKinney<sup>1</sup>; Sung-Hee Park<sup>2</sup>; Deborah, H. Lundgren<sup>2</sup>; David, K. Han<sup>2</sup>; <sup>1</sup>Carolinas Healthcare System, Charlotte, NC; <sup>2</sup>University of Connecticut Health Center, Farmington, CT
- MP 360 **Alternatives to SCX for the Separation of ITRAQ Labeled Plasma Proteins;** Monica H. Elliott; Michael Kuzyk; Derek Smith; Darryl Hardie; Christoph H. Borchers; University of Victoria-Genome BC Proteomics Centre, Victoria, Canada
- MP 361 **Comparison of Sample Preparation and Solubilization Techniques for Shotgun Proteomic Analysis of Laser Capture Microdissected Cells from Breast Tumors;** Lisa Zimmerman<sup>2</sup>; Eduardo C. Dias<sup>1</sup>; Julie A. Coleman<sup>1</sup>; Amy-joan L. Ham<sup>2</sup>; Carlos L. Arteaga<sup>2</sup>; Daniel C. Liebler<sup>2</sup>; Melinda E. Sanders<sup>2</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt University School of Medicine, Nashville, TN
- MP 362 **Extensive Fractionation and Identification of Proteins within Nasal Lavage Fluids from Allergic Rhinitis and Asthmatic Chronic Rhinosinusitis Patients;** Linda M Benson; Christopher J Mason; Oren Friedman; Hirohito Kita; H. Robert Bergen III; Douglas A Plager; Mayo Clinic, Rochester, MN
- MP 363 **Rapid Digestion Protocol for Membrane Proteome using Phase Transfer Surfactants;** Takeshi Masuda; Tomita Masaru; Yasushi Ishihama; Institute for Advanced Biosciences Keio University, Tsuruoka, JAPAN
- MP 364 **New Application of Agarose Gel Electrophoresis in Proteomics;** Emiko Yamauchi-Kamakura; Yoshiya Oda; Tsuyoshi Tabata; Junro Kuromitsu; Eisai Co. Ltd., Tsukuba, JAPAN
- MP 365 **Multiple Protease Digestion using Immobilized Enzymes: An Effective Sample Preparation Method for the Protein Structural Analysis by Mass Spectrometry;** Yukie Sasakura; Ayumi Suzuki; Kimiyoshi Koda; Katsuhiko Kanda; Izumi Waki; Hitachi High-technologies, Hitachinaka, Japan
- MP 366 **Systematic Identification of Artificial in vitro Protein Modifications Introduced during Sample Preparation;** Yue Chen; Gang Xing; Junmei Zhang; Yingming Zhao; University of Texas Southwestern Medical Center, Dallas, TX
- MP 367 **Elimination of Polymer Contamination prior to Mass Spectrometric Analysis;** Tine E. Thingholm<sup>1</sup>; Valentina A. Valova<sup>2</sup>; Martin R. Larsen<sup>1</sup>; Phillip J. Robinson<sup>2</sup>; <sup>1</sup>Univ. Southern Denmark, Odense, Denmark; <sup>2</sup>Children's Medical Research Institute, Westmead, NSW, Australia
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- LC-MS SAMPLE PREP: PROTEIN ANALYSIS, 356 - 367**
- MP 356 **NanoLC-QTOF MS-MS Analysis of Micro- and Nano-scale Proteomic Samples;** Mingguo Xu; Nan Wang; Peng Wang; Sandra Marcus; Liang Li; University of Alberta, Edmonton, AB

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**PHOSPHOPROTEINS: CHARACTERIZATIONS, 368 - 382**

- MP 368 **Identification of New Cytochrome P450 Phosphorylation Sites and Quantification by Relative MRM; Gorden Redlich<sup>1</sup>; Ulrich M. Zanger<sup>2</sup>; Frederic Brosseron<sup>1</sup>; Stephan Riedmaier<sup>2</sup>; Nicolai H Bache<sup>3</sup>; Anders B.M. Giessing<sup>3</sup>; Martin Eisenacher<sup>1</sup>; Christian Stephan<sup>1</sup>; Helmut E. Meyer<sup>1</sup>; Ole N. Jensen<sup>3</sup>; Katrin Marcus<sup>1</sup>; <sup>1</sup>Ruhr-Universitaet Bochum, Bochum, Germany; <sup>2</sup>Dr. M. Fischer-Bosch Inst. of Clin. Pharmacology, Stuttgart, Germany; <sup>3</sup>University of Southern Denmark, Odense, Denmark**
- MP 369 **Mass Spectrometry Determination of the Phosphorylation Sites of the Four Serine/Threonine Protein Kinases and the Substrate MurC from Corynebacterium Glutamicum; Isabelle Zanella-Cleon; Maria Fiuza-Perez; Aurelie Cornut; Jean-Philippe Robin; Virginie Molle; Michel Becchi; CNRS, Lyon Cedex 07, France**
- MP 370 **Characterization of Endogenous Phosphorylation Level in p130Cas, an anti-Estrogen Resistance Generating Protein in Human Breast Cancer; Giuseppe Infusini; Anthony Makkinje; David H. Perlman; Adam Lerner; Catherine E. Costello; Boston University School of Medicine, Boston, MA**
- MP 371 **Characterization of Heat Shock Protein 27 in Human Umbilical Vein Endothelial Cells (HUVEC) with the Microbial Dithiole Thiolutin Stimulation; Shujia Dai<sup>1</sup>; Shiao-Lin Wu<sup>1</sup>; yifeng Jia<sup>2</sup>; David D. Roberts<sup>2</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>National Cancer Institute, Bethesda, MD**
- MP 372 **Identification of Phosphorylation Sites in Soluble Guanylyl Cyclase by Proteomic Analysis using Stable Isotope Labeling and LC-nESI Q-ToF Tandem MS; Fotini Bazoti<sup>1</sup>; Spiros D. Garbis<sup>2</sup>; Andreas papapetropoulos<sup>2</sup>; Anthony Tsarbopoulos<sup>3</sup>; <sup>1</sup>GALA Research Center, Kifissia, Greece; <sup>2</sup>Foundation for Biomedical Research of the Athens, Athens, Greece; <sup>3</sup>University of Patras, Patras, Greece**
- MP 373 **Serine 395, Is Important for Transcriptional Activity in Mouse Aryl Hydrocarbon Receptor (AhR), is Phosphorylated by Protein Kinase A; Alan Friedman<sup>2</sup>; Michael Easterling<sup>1</sup>; Brent R. Kobielush<sup>2</sup>; Daria Vorobjekina<sup>2</sup>; Gary D. Minsavage<sup>2</sup>; Thomas A. Gasiewicz<sup>2</sup>; <sup>1</sup>Bruker Daltonics, Inc., Billerica, MA; <sup>2</sup>University of Rochester Medical Center, Palmyra, NY**
- MP 374 **Specific Phosphorylation Sites on Epidermal Growth Factor Receptor (EGFR) Dictate Recruitment of Downstream Signaling Proteins; Amanuel Y Kehasse; David H. Perlman; Giuseppe Infusini; Ilene Boucher; Mark E. McComb; Vickery Trinkaus-Randall; Catherine E. Costello; Boston Univ School of Medicine, Boston, MA**
- MP 375 **Mass spectrometry using ETD/CID Fragmentation and Neutral Loss Scanning Allows for Identification of Phosphorylation Sites on Centaurin-Alpha 1; BobbiJo Littrell-Miller<sup>2</sup>; Roger Powell<sup>1</sup>; Nichole Reisdorph<sup>1</sup>; Rick Reisdorph<sup>1</sup>; <sup>1</sup>National Jewish Medical and Research Center, Denver, CO; <sup>2</sup>CU Denver, Denver, CO**
- MP 376 **Identification of Novel Phosphorylation Sites in Poly (ADP-ribose) Polymerase-1 and Poly (ADP-ribose) Glycohydrolase using Mass Spectrometry; Sylvie Bourassa<sup>1</sup>; Isabelle Kelly<sup>1</sup>; Jean-Philippe Gagné<sup>2</sup>; Yves Labelle<sup>2</sup>; Arnaud Droit<sup>2</sup>; Mélissa Chevalier-Paré<sup>2</sup>; Guy Poirier<sup>2</sup>; <sup>1</sup>Proteomics, Quebec Genomics Center, Québec, Québec, Canada; <sup>2</sup>Laval University Medical Research Center, Quebec, Québec, Canada**
- MP 377 **Phosphohydroxyproline – a Proteinogenic Amino Acid: Identification and Characterization in Proteins by Mass Spectrometry; Sabine Metzger; Axel Kuehlberg; University of Duesseldorf, Duesseldorf, Germany**
- MP 378 **A Human Gene Polymorphism Reprograms Hormonal Signaling by Altering Kinase Recognition Sites: Identification of an SNP Generated Site of Phosphorylation; Saverio Gentile; Negin Martin; Erica Scappini; Peter Smutko; Jason Williams; Katina Johnson; Christian Erxleben; David Armstrong; NIEHS/NIH/DHHS, Research Triangle Park, NC**
- MP 379 **Differential Phosphoproteomics of Multiple Adhesion Proteins using Reversed-Phase C18 LC-MS-MS and TiO<sub>2</sub> Phospho-Enrichment; Erin D Jeffery; Pablo R. Grigera; J. Thomas Parsons; Donald F. Hunt; University of Virginia, Charlottesville, VA**
- MP 380 **Identification of Phosphorylation Sites on Heterochromatin Protein 1 by Electron Transfer Dissociation; Hillary Montgomery<sup>1</sup>; Holger Dormann<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; C. David Allis<sup>2</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>The Rockefeller University, New York, NY**
- MP 381 **Identification of Phosphorylation Sites in DNA/RNA Binding Proteins in Arabidopsis Thaliana by Mass Spectrometry; Kangling Zhang; Loma Linda University, Loma Linda, CA**
- MP 382 **Targeted On-Line Liquid Chromatography Electron Capture Dissociation Mass Spectrometry for Localization of Sites of *in vivo* Phosphorylation in Human Sprouty2; Helen Cooper; Steve Sweet; Faraz K Mardakkeh; Amy J Langton; Kevin J.P. Ryan; John K. Heath; University of Birmingham, Birmingham, UK**

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- MP 383 **Identification of Nitrosyl Iron Complexes by Nanospray Mass Spectrometry; Ya-Chen Cheng; Kuo-Kuo Ku; National Chiayi University, Chiayi City, Taiwan**
- MP 384 **Post-Translational Modifications of Histone H1 in Lung Cancer Cell Lines; Pang-Hung Hsu; Chi-Shuen Chu; Ming-Daw Tsai; Li-Jung Juan; The Genomics Research Center, Academia Sinica, Taipei, Taiwan**
- MP 385 **Characterization of Phosphorylation Sites on Histone H1t using Electron Transfer Dissociation Mass Spectrometry; Kristie Lindsey Rose<sup>1</sup>; Andra Li<sup>2</sup>; Juan Ausio<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>University of Victoria, Victoria, BC**
- MP 386 **Phosphoamino Acid Analysis and Identification of the Site of Histidine Phosphorylation of Histone H4 by a Variant of Transglutaminase 2; Paul V. Attwood<sup>1</sup>; Aygul Abzalov<sup>1</sup>; XinLin Zu<sup>2</sup>; Paul G. Besant<sup>1</sup>; <sup>1</sup>The University of Western Australia, Crawley, Australia; <sup>2</sup>Adolf Butenandt Institute, Munich, Germany**
- MP 387 **Histone H2b from Neurospora Crassa Is Extensively Methylated and some Post-Translational Modifications Are Sensitive to Histone Deacetylase 1 Inactivation; D. C. Anderson; Univ. of Oregon, Eugene, OR**

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- MP 388 **Utility of ETD for Quantitative Readout of Histone Acetyltransferase Activity**; Samuel Mackintosh; Lauren P. Blair; Rick Edmondson; Alan Tackett; *University of Arkansas For Medical Sciences, Little Rock, AR*
- MP 389 **Lysine Acetylation in Huntingtin and its Role in the Pathogenesis of Huntington's Disease**; Xin Cong; Birgit Schilling; Lisa Ellerby; Bradford W. Gibson; *Buck Institute For Age Research, Novato, CA*
- MP 390 **A Large Scale Screening Method for Analyzing Proteins with Heavy Post-Translational Modifications by Bioinformatics and Tandem FTICR/ECD Mass Spectrometry**; Frank Li; Raya Talroze; Feixia Chu; Shenheng Guan; Al Burlingame; *University of California, San Francisco, San Francisco, CA*
- MP 391 **Sensitive, Specific and Quantitative FT-ICR Mass Spectrometry of Combinatorial Post-Translational Modifications in Intact Histone**; C. Logan Mackay<sup>1</sup>; Nick Gilbert<sup>2</sup>; R. Larry Hayward<sup>2</sup>; Ted Hupp<sup>2</sup>; Pat Langridge-Smith<sup>1</sup>; Bernard Ramsahoye<sup>2</sup>; <sup>1</sup>*SIRCAMS, Edinburgh, UK*; <sup>2</sup>*Institute of Genetics and Molecular Medicine Divis, Edinburgh, UK*
- MP 392 **A Correlative Proteomics Study of Histone Methylation and Acetylation in *Saccharomyces Cerevisiae***; Lanhao Yang; Shengjiang Tu; Ming-Daw Tsai; Michael A. Freitas; *Ohio State University, Columbus, OH*
- MP 393 **Identification of Post Translational Modifications of the Avian Linker Histones H1 and H5 using Tandem Mass Spectrometry**; Ambrosius Snijders<sup>1</sup>; Sayampong Pongdam<sup>2</sup>; Christopher Wood<sup>3</sup>; John Baldwin<sup>2</sup>; Mark Dickman<sup>1</sup>; <sup>1</sup>*University of Sheffield, Sheffield, UK*; <sup>2</sup>*Liverpool John Moores University, Liverpool, UK*; <sup>3</sup>*CCLRC Daresbury Laboratory, Warrington, UK*
- MP 394 **Determination of Post-Translational Modifications of Histone H3 using Chromatography, Ion Mobility Tandem Mass Spectrometry and Customized Bioinformatics Tools**; Hye R Jung; Wei Liu; Ole N. Jensen; *University of Southern Denmark, Odense, Denmark*
- MP 395 **Evaluation of Human Histone H3 Lysine 99 Methylation and Acetylation Status using MRM**; Lynn Spruce; Jessica Y. Lee; Christopher R. Vakoc; Gerd Blobel; Steven H. Seeholzer; *Children's Hospital of Philadelphia, Philadelphia, PA*
- MP 396 **Analysis of Post Translational Modifications of *S. Cerevisiae* Histones using LTQ-Orbitrap**; ANITA SARAF<sup>1</sup>; Joshua Gilmore<sup>2</sup>; Zhihui Wen<sup>2</sup>; Michael Coleman<sup>2</sup>; Laurence Florens<sup>2</sup>; Michael Washburn<sup>2</sup>; <sup>1</sup>*Stowers Institute, Kansas City, MO*; <sup>2</sup>*Stowers Institute For Medical Research, Kansas City, MO*
- MP 397 **Lifespan Analysis of the Modification States of Histone H4 in *Xenopus laevis***; Joshua J. Nicklay<sup>1</sup>; David Shechter<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; C. David Allis<sup>2</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, VA*; <sup>2</sup>*The Rockefeller University, New York, NY*
- MP 398 **Mapping Novel Post-Translational Modifications in Yeast Histones by PTMap Algorithm**; Kai Zhang; Yue Chen; Zhihong Zhang; Yingming Zhao; *UT Southwestern Medical Center, Dallas, TX*
- MP 399 **Unbiased Post-Translational Modification Discovery through a Novel Spectral Matching Algorithm**; Corey E Bakalarski; Joshua E Elias; Jan Seebacher; Steven Gygi; *Harvard Medical School, Boston, MA*
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- PROTEINS CROSS LINKING, 400 - 422**
- MP 400 **A Collection of Novel Isotopically-Coded Crosslinkers for Structural Proteomics**; Evgeniy Petrotchenko; Jamie M. Thomas; Christoph Borchers; *UVic-GBC Proteomics Centre, Victoria, Canada*
- MP 401 **Exploring CYP2B4-Cytochrome b5 Interaction by Crosslinking Reaction and Mass Spectrometry**; Miroslav Sulc<sup>1</sup>; Katerina Peslova<sup>1</sup>; Tomas Jecmen<sup>2</sup>; Petr Hodek<sup>2</sup>; Petr Novak<sup>1</sup>; <sup>1</sup>*Institute of Microbiology, Prague, Prague 4, Czech Republic*; <sup>2</sup>*Charles University, Faculty of Science, Prague 2, Czech Republic*
- MP 402 **Multiplexed MS-MS Methods and Protein Interaction Identification**; Hye In Nam; Gerhard R. Munske; Li Yang; Haizhen Zhang; James E. Bruce; *Washington State University, Pullman, WA*
- MP 403 **Chemical Crosslinking and Chemical Modification Studies of LaSSB and Ro52, Autoantigens Associated with Sjogren's Syndrome**; Leesa Deterding; Rachele Bienstock; Kenneth B. Tomer; *NIEHS, RTP, NC*
- MP 404 **Analysis of Protein Cross-Linking by LC-MS-MS and a Simple Database Search Method**; Caifeng Zhao<sup>1</sup>; Daniel Henriquez<sup>2</sup>; Monica Roth<sup>3</sup>; Oscar Leon<sup>2</sup>; Haiyan Zheng<sup>1</sup>; <sup>1</sup>*CABM, UMDNJ-RWJMS, Piscataway, NJ*; <sup>2</sup>*Programa de Virologia, ICBM, University of Chile, Santiago, Chile*; <sup>3</sup>*Department of Biochemistry, UMDNJ-RWJMS, Piscataway, NJ*
- MP 405 **Design and Evaluation of a Novel Homobifunctional Cross-Linker with Selective Metal Dioxide-Based Enrichment Potential**; Bo Wang; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- MP 406 **Mining Protein-Protein Interactions of Proteins in *Synechocystis* sp. PCC 6803: Novel Chemical Cross-Linking and Mass Spectrometry**; Chunxiang Zheng; Haizhen Zhang; Gerhard R. Munske; Xiaoting Tang; James E. Bruce; *Washington State University, Pullman, WA*
- MP 407 **Proteomics Analysis of Mammalian Cell Cultures for Biopharmaceutical Manufacturing**; Tyler Carlage<sup>1</sup>; Li Zang<sup>1</sup>; Yelena Lyubarskaya<sup>1</sup>; Marina Hincapie<sup>2</sup>; Rohin Mhatre<sup>1</sup>; William Hancock<sup>2</sup>; <sup>1</sup>*Biogen Idec, Cambridge, MA*; <sup>2</sup>*Northeastern University, Boston, MA*
- MP 408 **Specific, Quantitative Enrichment of Cross-Linked Peptides from Complex Mixtures**; Lau Sennels<sup>1</sup>; Adam Belsom<sup>2</sup>; Mark Bradley<sup>2</sup>; Juri Rappsilber<sup>1</sup>; <sup>1</sup>*Wellcome Trust Centre for Cell Biology, Edinburgh, UK*; <sup>2</sup>*School of Chemistry, University of Edinburgh, Edinburgh, UK*
- MP 409 **A New Cross-Linking Strategy for Exploring Protein-Protein Interactions**; Christian Tagwerker; Danielle Vellucci; Ryan Benz; Pierre Baldi; Scott Rychnovsky; Lan Huang; *University of California, Irvine, CA*
- MP 410 **Studying the Stepwise Progression of Formaldehyde Mediated Protein Crosslinking with Mass Spectrometry**; Judy Toews<sup>3</sup>; Jason Rogalski<sup>1</sup>; Juergen Kast<sup>2</sup>; <sup>1</sup>*Biomedical Research Centr, Vancouver, Canada*; <sup>2</sup>*University of British Columb, Vancouver, BC*; <sup>3</sup>*Biomedical Research Centre, Vancouver, BC*
- MP 411 **Annexin A2/P11 Interaction: New Insights into Annexin A2 Tetramer Structure by Chemical Crosslinking, High-Resolution Mass Spectrometry, and Computational Modeling**; Daniela M. Schulz<sup>1</sup>; Stefan Kalkhof<sup>2</sup>; Andreas Schmidt<sup>3</sup>; Christian H. Ihling<sup>2</sup>; Christoph Stingl<sup>3</sup>; Karl Mechtler<sup>3</sup>; Olaf Zschörnig<sup>4</sup>; Andrea Sinz<sup>2</sup>; <sup>1</sup>*Biotechnological-Biomedical Center, Leipzig, Germany*; <sup>2</sup>*Institute of Pharmacy, Halle,*

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- Germany; <sup>3</sup>Imp Research Institute of Mo, Vienna, Austria; <sup>4</sup>Institute for Medical Physics & Biophysics, Leipzig, Germany; <sup>5</sup>Cd Laboratory / Vienna, Vienna, Austria; <sup>6</sup>Institute of Moleculare Biotechnology, Vienna, Austria
- MP 412 **Characterizing the 26S Proteasome Network in Yeast using a Quantitative *in-vivo* Crosslinking Strategy and PPI Network Analysis;** Cortnie Guerrero<sup>1</sup>; Tijana Milenkovic<sup>1</sup>; Jeffrey J. Jones<sup>2</sup>; Natasa Przulj<sup>1</sup>; Peter Kaiser<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>UC Irvine, Santa Ana, CA; <sup>2</sup>Applied Proteomics, Glendale, CA
- MP 413 **Cross-Linking Analysis of Affinity-Purified Multi-Protein Complexes;** Zhuo Chen; Morten Rasmussen; Salman Tahir; Sjaak van der Sar; Kevin G. Hardwick; Juri Rappsilber; Wellcome Trust Centre for Cell Biology, Edinburgh, UK
- MP 414 **Novel Techniques for Affinity Enrichment of Crosslinked Peptides for Studying Multi-Component Protein Complex Structures by Crosslinking Combined with Mass Spectrometry;** Evgeniy Petrotchenko; Christoph Borchers; UVic-GBC Proteomics Centre, Victoria, Canada
- MP 415 **Application of Reductive Amination to Protein Crosslinking;** Nagarajan Chandramouli; Joseph P Fernandez; Haiteng Deng; Proteomics Resource Center, Rockefeller University, New York, NY
- MP 416 **Identification of a Helicase/Single-Stranded DNA Binding Protein Interaction Site by Mass Spectrometric Analysis;** Lauren P. Blair; Kevin D. Raney; Alan J. Tackett; UAMS Biochemistry & Molecular Biology, Little Rock, AR
- MP 417 **Exploring Conformational Changes of Akt Altered by Inhibitors using Chemical Cross-Linking and Mass Spectrometry;** Bill Huang; Hee-Yong Kim; NIAAA/NIH, Rockville, MD
- MP 418 **Identifying Interactions between Small Heat Shock Proteins and Substrate by Site Directed Incorporation of a Photoactivatable Cross-Linker and Mass Spectrometry;** Nomalie N Java; Victor Garcia; Elizabeth Vierling; University of Arizona, Tucson, AZ
- MP 419 **A Novel Photo-Cleavable Protein Interaction Reporter (pcPIR) Cross-Linking Strategy to Study Protein-Protein Interactions;** Li Yang; Nathan K. Kaiser; Hye In Nam; Haizhen Zhang; Gerhard R. Munske; James E. Bruce; Washington State University, Pullman, WA
- MP 420 **Investigating the Detailed Chemistry of Chemical Cross-linking: Reactivities of Different Amino Acids;** Stefanie Mädler; Claudia Bich; David Touboul; Renato Zenobi; Eth Zurich, Zurich, Switzerland
- MP 421 **Laser Induced Selective Retrieval of Cross-linked Peptides for Mass Spectrometric Analysis of Protein Complexes;** Funing Yan; Fa-yun Che; Dmitry Rykunov; Edward Nieves; Andras Fiser; Louis M. Weiss; Ruth Hogue Angeletti; Albert Einstein College of Medicine, Bronx, NY
- MP 422 **Interactions of the Peroxisome Proliferator-Activated Receptor alpha (PPARα) with Ligands Analyzed by Chemical Cross-Linking and Nano-HPLC/MALDI-TOF/TOF-MS and HPLC/ESI-FTICR-MS;** Mathias Mueller<sup>1</sup>; Christian Ihling<sup>1</sup>; Leo J. de Koning<sup>2</sup>; Ronald Aardema<sup>2</sup>; Henk L. Dekker<sup>2</sup>; Yvonne Syha<sup>3</sup>; Manfred Schubert-Zsilavecz<sup>3</sup>; Chris G. de Koster<sup>2</sup>; Andrea Sinz<sup>1</sup>; <sup>1</sup>Martin Luther University Halle-Wittenberg, Halle, Germany; <sup>2</sup>Universiteit van Amsterdam, Amsterdam, The Netherlands; <sup>3</sup>Johann-Wolfgang-Goethe University Frankfurt, Frankfurt, Germany
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- PROTEINS: MEMBRANES, 423 - 450**
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- MP 423 **Thermodynamic Analysis of Membrane Bound Receptor-Ligand Interactions;** Patrick D. DeArmond<sup>1</sup>; Michael J. Campa<sup>2</sup>; Edward F. Patz, Jr.<sup>2</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>Duke University Medical Center, Durham, NC
- MP 424 **Identification of the Mitochondrial ND3 Subunit as a Structural Component Involved in the Active/Deactive Enzyme Transition of Respiratory Complex I;** Bjoern Meyer<sup>1</sup>; Alexander Galkin<sup>1</sup>; Ilka Wittig<sup>1</sup>; Hermann Schaegeger<sup>1</sup>; Andrei Vinogradov<sup>2</sup>; Ulrich Brandt<sup>1</sup>; Michael Karas<sup>1</sup>; <sup>1</sup>Johann Wolfgang Goethe-University, Frankfurt/Main, Germany; <sup>2</sup>Moscow State University, Moscow, Russia
- MP 425 **An Efficient In-Gel Extraction and Fractionation Strategy for the Comprehensive Membrane Proteomic Profiling;** Yi-Chung Chen; Yet-Ran Chen; Academia Sinica, Taipei, Taiwan
- MP 426 **New Methodology for Membrane Protein Identification;** Caroline Tokarski<sup>1</sup>; Marianne Fillet<sup>2</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Univ. des Science/Tech de Lille, Villeneuve d'Ascq, France; <sup>2</sup>Universite de Liège, Liège, Belgium
- MP 427 **Ligand Based Structural Biology: Cannabinoid Receptor Investigation by Covalent Probes;** Martha Malvina Papanastasiou<sup>1</sup>; Dennis Szymanski<sup>1</sup>; Nikolai Zvonok<sup>2</sup>; Alex Makriyannis<sup>2</sup>; <sup>1</sup>northeastern Univer/Sity, Boston, MA; <sup>2</sup>Center for Drug Discovery, Boston, MA
- MP 428 **Enhancing Identifications of Lipid-Embedded Proteins by Mass Spectrometry for Improved Mapping of Endothelial Plasma Membranes *in vivo*;** Yan Li; Jingyi Yu; Yipeng Wang; Fred Long; Sabrina Shore; Phil Oh; Jan Schnitzer; Sidney Kimmel Cancer Center, San Diego, CA
- MP 429 **Toward the Development of a "Tagless" Method for the Isolation and Identification of Membrane Complexes in *Desulfovibrio vulgaris* Hildenborough;** Simon Allen<sup>1</sup>; Peter J. Walian<sup>2</sup>; Evelin Szakal<sup>1</sup>; Haichuan Liu<sup>1</sup>; Ming Dong<sup>2</sup>; Eric Johansen<sup>1</sup>; Lee L. Yang<sup>2</sup>; Steven C. Hall<sup>1</sup>; Susan J. Fisher<sup>1</sup>; Terry C. Hazen<sup>2</sup>; Jil T. Geller<sup>2</sup>; Mary E. Singer<sup>2</sup>; Jian Jin<sup>2</sup>; Mark D. Biggin<sup>2</sup>; Bing Jap<sup>2</sup>; H. Ewa Witkowska<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley, CA
- MP 430 **Cell Wall (Surface) Proteome of Pathogenic Yeast *Candida albicans* Profiled by Chemical Labeling and LC-MS;** Jiang Qian<sup>1</sup>; Jim E. Cutler<sup>1</sup>; Richard B. Cole<sup>2</sup>; Yang Cai<sup>1</sup>; <sup>1</sup>The Research Institute for Children, New Orleans, New Orleans, LA; <sup>2</sup>Department of Chemistry, University of New Orleans, New Orleans, LA
- MP 431 **Mass Spectrometric Analysis of Thiocitrulline Bound Proteins Extracted from Human Keratinocyte Cells;** Mulu Gebremedhin<sup>1</sup>; Dave Mah<sup>1</sup>; Peggy Nelson<sup>2</sup>; Thomas Sawyer<sup>2</sup>; Nora Chan<sup>2</sup>; <sup>1</sup>canada west biosciences Inc, Medicine hat, AB, CANADA; <sup>2</sup>Defense R & D Suffield, Medicine hat, AB, canada
- MP 432 **Shotgun Proteomic Analysis of the Human Monocyte Membrane Subproteome using Alternative Solubilization Techniques;** Xiaoying Ye<sup>1</sup>; Ramin M. Hakami<sup>2</sup>; Bradley Hollinger<sup>1</sup>; Robert G. Ulrich<sup>2</sup>; Haleem J. Issaq<sup>1</sup>; Timothy D. Veenstra<sup>1</sup>; Josip Blonder<sup>1</sup>; <sup>1</sup>SAIC-Frederick Inc., Frederick, MD; <sup>2</sup>US Army Medical Research, Frederick, MD

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- MP 433 **Stable Isotope -Based Quantitative Organelle Proteomics: Improving Resolution and Protein Coverage;** Pawel Grzegorz Sadowski; Kathryn S Lilley; *University of Cambridge, Cambridge, UK*
- MP 434 **The Mechanism and Target of Aliphatic Azides as Novel Protein Photo-Labeling Reagents;** Dennis Szymanski<sup>1</sup>; Lakshmiathi Pandarinathan<sup>2</sup>; Alexander Makriyannis<sup>2</sup>; <sup>1</sup>, *Boston, MA*; <sup>2</sup>*Center for Drug Discovery, Boston, MA*
- MP 435 **Proteomic Analysis of Photosynthetic Membranes Isolated From Rhodobacter Sphaeroides;** Hilary Lewis; Jaimey Tucker; Mark Dickman; C. Neil Hunter; *University of Sheffield, Sheffield, UK*
- MP 436 **Blue Native Electrophoresis combined with Stable Isotope Labeling Shows that Saccharomyces Cerevisiae Mitochondrial Respiratory Supercomplexes Are Still Present under Anaerobiosis;** Andreas Helbig<sup>2</sup>; Marco J.L. de Groot<sup>1</sup>; Renske A. van Gestel<sup>2</sup>; Shabaz Mohammed<sup>2</sup>; Jack Pronk<sup>1</sup>; Jack T. Pronk<sup>1</sup>; Pascalle Daran Lapujade<sup>1</sup>; Albert J.r. Heck<sup>2</sup>; Slijper Monique<sup>2</sup>; <sup>1</sup>*Delft University of Technology, Delft, Netherlands*; <sup>2</sup>*Utrecht University, Utrecht, Netherlands*
- MP 437 **Optimizing uLC-MS-MS Analysis of Hydrophobic Peptides;** Anna Speers; Christine Wu; *Univ of CO School of Med, Aurora, CO*
- MP 438 **Shaving off the Biological Membranes with a Protease and Mass Spectrometry Identification of Membrane Interacting Peptides;** Natalia Mast<sup>1</sup>; Wei-Li Liao<sup>2</sup>; Irina A. Pikuleva<sup>1</sup>; Illarion V. Turko<sup>2</sup>; <sup>1</sup>*University of Texas Medical Branch, Galveston, TX*; <sup>2</sup>*Center for Advanced Research in Biotechnology/NIST, Rockville, MD*
- MP 439 **Analysis of the Membrane Protein Fraction of Halobacterium salinarum by Comparative CID and ETD Fragmentation of Highly Enriched Hydrophobic Peptides;** Christian Klein<sup>1</sup>; Frank Siedler<sup>2</sup>; Beatrix Scheffer<sup>2</sup>; Andrea Schneider<sup>3</sup>; Friedhelm Pfeiffer<sup>2</sup>; Marcus Macht<sup>3</sup>; Ali Kettani<sup>1</sup>; Dieter Oesterhelt<sup>2</sup>; <sup>1</sup>*Bruker Daltonics Inc., Fremont, CA*; <sup>2</sup>*Max-Planck Institute for Biochemistry, Martinsried, Germany*; <sup>3</sup>*Bruker Daltonics GmbH, Bremen, Germany*
- MP 440 **Microfluidic Electrocapture Assisted Mass Spectrometry of Membrane-Associated Polypeptides;** Mohammadreza Shariatgorji<sup>1</sup>; Juan Astorga-wells<sup>2</sup>; Hans Jornvall<sup>2</sup>; Leopold L. Ilag<sup>1</sup>; <sup>1</sup>*stockholm university, stockholm, Sweden*; <sup>2</sup>*Karolinska Institutet, Stockholm, Sweden*
- MP 441 **Functional Genomic Approaches to Study Adenovirus Species B Receptors;** Hung Viet Trinh<sup>1</sup>; Markus Eisenhut<sup>2</sup>; Urs Greber<sup>2</sup>; Silvio Hemmil<sup>1</sup>; <sup>1</sup>*University of Zurich, Zurich, Switzerland*; <sup>2</sup>*Institute of Zoology, Univ of Zurich, Zurich, Switzerland*
- MP 442 **Comprehensive Proteomic Analysis of Membrane Proteins in Toxoplasma.gondii;** Fa-yun Che; Berta Burd; Hongshan Zhang; Carlos Madrid-Aliste; Edward Nieves; Kami Kim; Andras Fiser; Louis M. Weiss; Ruth Hogue Angeletti; *Albert Einstein College of Medicine, Bronx, NY*
- MP 443 **Intact Analysis of Membrane Proteins from Acetylcholine Receptor and Bovine Mitochondria;** Mahbod R. Hajivandi; Xiquan Liang; R. Marshall Pope; *Invitrogen, Carlsbad, CA*
- MP 444 **Identification of Surface Membrane Immunogenic Proteins of Actinobacillus Pleuropneumoniae as Potential Candidates for Vaccine Therapy;** Jacqueline W. Chung; Chris Ng-Thow-Hing; Lorne I. Budman; James W. Coulton; Bernard Gibbs; *McGill University, Montreal, Canada*
- MP 445 **An Alternative Method for Investigation of Whole Membrane Samples using Elastase as Digestive Protease;** Benjamin Rietschel<sup>1</sup>; Tabiwang Ndipanquang Arrey<sup>1</sup>; Bjoern Meyer<sup>1</sup>; Michael Karas<sup>1</sup>; Ansgar Poetsch<sup>2</sup>; <sup>1</sup>*Johann Wolfgang Goethe-University, Frankfurt/Main, Germany*; <sup>2</sup>*Ruhr University, Bochum, Germany*
- MP 446 **Deciphering the Plasma Membrane Proteome of the Mouse Olfactory Epithelium;** Bettina Warscheid<sup>2</sup>; Jenny Adler<sup>2</sup>; Silke Oeljeklaus<sup>2</sup>; Jon Barbour<sup>1</sup>; Hanns Hatt<sup>1</sup>; Eva M. Neuhaus<sup>1</sup>; Helmut E. Meyer<sup>2</sup>; <sup>1</sup>*Ruhr-University Bochum, Bochum, Germany*; <sup>2</sup>*Medical Proteom Center, Bochum, Germany*
- MP 447 **Membrane Proteomic Analysis of the Protozoan Parasite Trypanosoma cruzi;** Xiang Zhu; James A Atwood III; Brent Weatherly; Todd A Minning; Rick L Tarleton; Ron Orlando; *University of Georgia, Athens, GA*
- MP 448 **Overcoming Hurdles in Membrane Proteomics by the Implementation of Complementary Approaches;** Dörte Becher; Susanne Wolff; Hannes Hahne; Michael Hecker; *University Greifswald, Greifswald, Germany*
- MP 449 **Identifying Induced Non-Gal Antibody Response Proteins following Pig-to-Primate Cardiac Xenotransplantation;** Carrie J. Heppelmann<sup>1</sup>; Paul G. Stalboerger<sup>1</sup>; Guerard W. Byrne<sup>3</sup>; Christopher G. A. McGregor<sup>3</sup>; H. Robert Bergen, III<sup>2</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*; <sup>2</sup>*Mayo Clinic College of Medicine, Rochester, MN*; <sup>3</sup>*Mayo Clinic Department of Surgery, Rochester, MN*
- MP 450 **Characterization of the Liver Membrane Proteome using Peptide Immobilized pH Gradient Isoelectric Focusing (IPG IEF);** Joel M Chick<sup>1</sup>; Paul A Haynes<sup>1</sup>; Bengt Bjellqvist<sup>2</sup>; Mark S Baker<sup>1</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*GE Healthcare, Uppsala, Sweden*
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- PROTEIN CONFORMATION, 451 - 462**
- MP 451 **Using Charge State Distributions ESI MS to Investigate Conformational Integrity of PEGylated Proteins;** Agva Frimpong<sup>1</sup>; Igor A. Kaltashov<sup>2</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*University of Massachuset, Amherst, MA*
- MP 452 **Microwave-Assisted Acid and Base Hydrolysis Combined with MALDI-MS for Structural Studies of the Prion Protein;** Bela Reiz; David Wishart; Adina Bujold; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 453 **Analysis of Disulfide Bond Folding in Recombinant Human Resistin Protein;** Eric Beil; Thomas Malia; Tatiana Ort; Jill Carton; Ashok Mathur; Jennifer Nemeth; *Centocor R&D, Radnor, PA*
- MP 454 **Mass Spectrometry Driven Characterication of Early Aggresome-Like Structures;** Anders Dahl Knudsen<sup>1</sup>; Poul H Jensen<sup>2</sup>; Allan Stensballe<sup>1</sup>; <sup>1</sup>*Aalborg University, Aalborg, Denmark*; <sup>2</sup>*Aarhus University, Aarhus, Denmark*
- MP 455 **Quadrupole Ion Trap Bath Gas Pressure and Protein Conformation;** Brittany Butler; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- MP 456 **Probing Conformational Changes in Peptide Hormones Complexed with Transition Metal Cations using Electron Capture Dissociation;** Yuri E.M. Van Der Burgt; Magnus Palmblad; Hans C. Dalebout; André



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- M. Deelder; *Leiden University Medical Center, Leiden, Netherlands*
- MP 457 **Travelling Wave Ion Mobility Mass Spectrometry-Based Conformational Studies of Prion Protein – Effects of Metal Cation Binding and Buffer Gas;** Susan E. Slade<sup>1</sup>; Konstantinos Thalassinos<sup>1</sup>; Gillian R. Hilton<sup>1</sup>; Teresa Pinheiro<sup>1</sup>; Claudia A Blindauer<sup>1</sup>; Michael T. Bowers<sup>2</sup>; James Scrivens<sup>3</sup>; <sup>1</sup>*University of Warwick, Coventry, UK*; <sup>2</sup>*University of California, Santa Barbara, CA*; <sup>3</sup>*Univ of Warwick, Coventry, UK*
- MP 458 **Irreversible Thermal Unfolding of Cytochrome c Studied by ESI-MS;** Jenna-Jiangjiang Liu; Lars Konermann; *University of Western Ontario, London, Canada*
- MP 459 **Conformational Effects of Small Molecule Binding to Parkinson's Protein  $\alpha$ -Synuclein and its Disease-Related A30P and A53T Mutants;** Megan Grabenauer<sup>1</sup>; Thomas Wyttenbach<sup>1</sup>; Nicholas F. Dupuis<sup>1</sup>; Jay R. Winkler<sup>2</sup>; Harry B. Gray<sup>2</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>*University of California, Santa Barbara, CA*; <sup>2</sup>*California Institute of Technology, Pasadena, CA*
- MP 460 **Structural Characterization and Antibody- Epitope Identification of Parkinson's Disease Target Protein  $\alpha$ -Synuclein using Epitope- Mass Spectrometry;** Camelia Vlad<sup>1</sup>; Karin Danzer<sup>2</sup>; Bastian Hengerer<sup>2</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*Laboratory of Analytical Chemistry and Biopolymer, Konstanz, Germany*; <sup>2</sup>*Boehringer Ingelheim Pharma GmbH & Co. KG, ZNS Res, Biberach, Germany*
- MP 461 **What Is the Smallest Protein whose Native Fold Can Be Preserved in a Mass Spectrometer?;** Jason Kalapothakis; Andrew Stopford; Perdita Barran; *The University of Edinburgh, Edinburgh, UK*
- MP 462 **Optical Characteristics of the Enhanced Green Fluorescent Protein (EGFP) in the Gas Phase;** Matthew W. Forbes; Abbas Kassam; Qunzhou Bian; Francis Talbot; Rebecca A. Jockusch; *University of Toronto, Toronto, Canada*
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- MP 463 **Absolute Quantification of Protein Phosphorylation by Liquid Chromatography Mass Spectrometry;** Michael J. Previs; Peter Van Buren; Kelly J. Begin; Jim O. Vigoreaux; Martin M. Lewinter; Dwight E. Matthews; *University of Vermont, Burlington, VT*
- MP 464 **Differentiation of Specific and Non-Specific Protein Interactions in Bacteria by Isotopic Labeling and Mass Spectrometry;** W. Judson Hervey, IV<sup>1</sup>; Gurusahai Khalasa-Moyers<sup>1</sup>; Patricia K. Lankford<sup>2</sup>; Linda J. Foote<sup>2</sup>; Elizabeth T. Owens<sup>2</sup>; Tse-Yuan Lu<sup>2</sup>; Jennifer L. Morrell-Falvey<sup>2</sup>; W. Hayes McDonald<sup>2</sup>; Dale A. Pelletier<sup>2</sup>; Greg Hurst<sup>2</sup>; <sup>1</sup>*UT-ORNL Graduate School of Genome Science, Oak Ridge, TN*; <sup>2</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*
- MP 465 **Protein Identification of Desalted iTRAQ-Labeled Nasal Lavage Samples using On-Line 2-D LC-MS-MS;** Marina C Jeppsson; Monica H Kristiansson; Christian Lindh; *Lund University, Lund, Sweden*
- MP 466 **Targeted Detection and Quantification of Adenylyl Cyclase 7 Protein in Mouse Whole Brain using MRM;** Kathleen Grant; Christine Wu; *Univ. of Colorado at Denver, Denver, CO*
- MP 467 **Robust and Sensitive iTRAQ Quantification on an LTQ-Orbitrap Mass Spectrometer using PQD and HCD Fragmentation;** Marcus Bantscheff; Markus Hermann Boesche; Dirk Eberhard; Gavain Sweetman; Bernhard Kuster; *Cellzome AG, Heidelberg, Germany*
- MP 468 **Identification of Proteins Essential for Muscle Development using SILAC;** Michael Rosenblatt<sup>1,2,4,5</sup>; Yair Argon<sup>3</sup>; David Sarracino<sup>1,2,4,5</sup>; Mary F Lopez<sup>1,2,4,5</sup>; John C. Rogers<sup>1,2,4,5</sup>; <sup>1</sup>*Thermo Scientific, Rockford, IL*; <sup>2</sup>*Thermo Scientific, Rockford, IL*; <sup>3</sup>*Children's Hospital of Philadelphia, Philadelphia, PA*; <sup>4</sup>*Thermo Scientific, Cambridge, MA*; <sup>5</sup>*Thermo Scientific, Cambridge, MA*
- MP 469 **Characterization and Absolute Quantification of Intact Proteins by Liquid Chromatography Time-of-Flight or Ion-Trap Mass Spectrometry;** Manuela Huegel<sup>1</sup>; Christian G. Huber<sup>2</sup>; <sup>1</sup>*Saarland University, Instr. Analysis and Bioanalysis, Saarbruecken, Germany*; <sup>2</sup>*Paris-Lodron-University, Dept of Molecular Biology, Salzburg, Austria*
- MP 470 **Targeted Quantitative Mass Spectrometric Identification of Differentially Expressed Proteins between Bax Positive and Bax Deficient Colorectal Cancer Clones;** Andy Lo<sup>1</sup>; Peng Wang<sup>1</sup>; J. Bryce Young<sup>1</sup>; Charlie Hao<sup>2</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, CANADA*; <sup>2</sup>*Emory University, Atlanta, GA*
- MP 471 **Identification of Novel  $\alpha$ -Synuclein Post-Translational Modifications Isolated from MAO-B Over-Expressing Models of Parkinson's Disease;** Steven R. Danielson; Jason Held; Jyothi Kumar; Bradford W. Gibson; Julie K. Andersen; *Buck Institute For Age Research, Novato, CA*
- MP 472 **Quantitative Proteomics using Stable Isotope Labeling of Primary Neurons Reveals Diverse Changes in Synaptic Protein Content in *fmr1* Knockout Mice;** Lujian Liao; Sung Kyu Park; Peter Vanderklish; John Yates; *The Scripps Research Institute, La Jolla, CA*
- MP 473 **Accurate Quantitative Determination of Plasma Membrane Protein Concentrations in Intact Arabidopsis thaliana Plants using Metabolic Labeling and Mass Spectrometry;** Katja Bernfur; Olaf Larsson; Christer Larsson; Niklas Gustavsson; *Department of Biochemistry, Lund, Sweden*
- MP 474 **Delineation of a Carcinogenic *Helicobacter pylori* Proteome using Difference Gel Electrophoresis and Mass Spectrometry (DIGE/MS);** David B. Friedman; Aime T. Franco; Corbin W. Whitwell; Dawn A. Israel; Richard M. Peek, Jr; *Vanderbilt University School of Medicine, Nashville, TN*
- MP 475 **Utility and Limitations of Measuring Protein Expression Levels in Complex Mixtures using iTRAQ;** Sara P. Gaucher; Michele Fleck; Kirsten Benjamin; Tahera Iqbal; Michael Leavell; *Amryris Biotechnologies, Emeryville, CA*
- MP 476 **Label-Free LC-MS Quantification of Modified Peptides by Pseudo-MRM Analysis using Ion-trap Mass Spectrometers;** Amy-Joan L. Ham; Jeremy S Myers; Ying Xiong; Daniel C. Liebler; *Vanderbilt University School of Medicine, Nashville, TN*
- MP 477 **Absolute Protein Quantification for Pre-Clinical Drug Safety Evaluation;** Ben Collins<sup>1</sup>; Ning Tang<sup>2</sup>; Peter Stone<sup>3</sup>; Thomas Lau<sup>1</sup>; Albrecht Gruhler<sup>4</sup>; Jean-Charles Gautier<sup>5</sup>; William Gallagher<sup>1</sup>; Stephen Pennington<sup>1</sup>; <sup>1</sup>*UCD Conway Institute, University College Dublin, Dublin, Ireland*; <sup>2</sup>*Agilent Technologies US, Santa Clara, CA*; <sup>3</sup>*Agilent Technologies Uk Ltd, Manchester, UK*; <sup>4</sup>*Novonordisk, Maaloev, Denmark*; <sup>5</sup>*Sanofi-Aventis, Vitry sur Seine, France*
- MP 478 **DIGE Analysis Reveals that Bicyclomycin Evokes a Distinct Fingerprint of Protein Expression in *E. coli*;** Lewis M. Brown<sup>1</sup>; Christopher J. Cardinale<sup>2</sup>; Robert S.



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- Washburn<sup>3</sup>; Vasisht R. Tadigotla<sup>4</sup>; Max E. Gottesman<sup>3</sup>; Evgeny Nudler<sup>2</sup>; <sup>1</sup>*Columbia University, New York, NY*; <sup>2</sup>*New York University School of Medicine, New York, NY*; <sup>3</sup>*Columbia University Medical Center, New York, NY*; <sup>4</sup>*Rutgers, The State University of New Jersey, Piscataway, NJ*
- MP 479 **Data Quality Assurance of Label-Free LC-MS Differential Proteome Analysis**; Daniel C. Chamrad<sup>1</sup>; Wolfgang Jabs<sup>2</sup>; Klaus Marquart<sup>1</sup>; Barbara Sitek<sup>3</sup>; Kai Stühler<sup>3</sup>; Helmut E. Meyer<sup>3</sup>; Carsten Baessmann<sup>2</sup>; Martin Blueggel<sup>1</sup>; <sup>1</sup>*Protagen AG, Dortmund, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Medizinisches Proteom-Center, Bochum, Germany*
- MP 480 **Protein Profiling of *Escherichia coli* Wild-Type Strain and Reduced-Genome Strain by Label-Free Quantitative Proteomics**; Hanako Ataku<sup>1</sup>; Miyako Mise<sup>1</sup>; Keiko Nishijima<sup>1</sup>; Jun Yamazaki<sup>1</sup>; Kazumi Sasaki<sup>1</sup>; Syuji Yamazaki<sup>1</sup>; Hideo Mori<sup>2</sup>; Hiroshi Mizoguchi<sup>2</sup>; Nobuyuki Fujita<sup>1</sup>; <sup>1</sup>*National Institute of Technology and Evaluation, Tokyo, Japan*; <sup>2</sup>*Kyowa Hakko Kogyo Co., Ltd., Tokyo, Japan*
- MP 481 **Analysis of Activity-Dependent Changes in the Post Synaptic Density by Primary Neuronal SILAC and Mass Spectrometry**; Helene Cardasis<sup>1</sup>; Bryen Jordan<sup>2</sup>; Daniel Spellman<sup>1</sup>; Edward Ziff<sup>2</sup>; Thomas Neubert<sup>1</sup>; <sup>1</sup>*Skirball Institute, NYU SoM, New York, NY*; <sup>2</sup>*Department of Biochemistry, NYU SoM, New York, NY*
- MP 482 **Quantitation of Reversible Cysteine Oxidation Levels in Endogenous Proteins using MRM on a Hybrid Linear Ion Trap/Triple Quadrupole Mass Spectrometer**; Jason M. Held; Steven R. Danielson; Christian Atsriku; David J Britton; Judy Campisi; Julie Andersen; Chris Benz; Bradford W. Gibson; *Buck Institute for Age Research, Novato, CA*
- MP 483 **A Nano LC-MALD-Based Shotgun Quantitative Proteomic Approach to Investigate Virulence Factors of *Pseudomonas syringae* and its Proteome**; Yong Yang; Dave Schneider; Philip Bronstein; Sam Cartinhour; Theodore Thannhauser; *US R.W.H Center for Agriculture and Health, Ithaca, NY*
- MP 484 **Quantitative Analysis of Redox-Sensitive Proteome with DIGE and ICAT**; Cexiong Fu; Hong Li; *UMDNJ, Newark, NJ*
- MP 485 **Analysis of iTRAQ Data using Mascot and Peaks Quantification Algorithms**; Carla M R Lacerda; Kenneth Reardon; *Colorado State University, Fort Collins, CO*
- MP 486 **Investigation of Iron-Limitation Inducible Proteins of *Neisseria Meningitidis* using the Isobaric Labelling Approach Tandem Mass Tags (TMT)**; Thorsten Prinz<sup>1</sup>; Karsten Kuhn<sup>1</sup>; Harald Legner<sup>1</sup>; Peter Schmid<sup>1</sup>; Christian Baumann<sup>1</sup>; Peter van Ulsen<sup>2</sup>; Jan Tommassen<sup>2</sup>; <sup>1</sup>*Proteome Sciences, Frankfurt am Main, Germany*; <sup>2</sup>*Utrecht University, Utrecht, The Netherlands*
- MP 487 **Absolute Quantification of C-Reactive Protein in Plasma Utilizing Isotope Dilution Mass Spectrometry**; Dennis Keith Williams, Jr.; Robert Dixon; Adam Hawkridge; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- MP 488 **Comparative Analysis of Surface Plasma Membrane Proteins of Primary and Metastatic Melanoma Cells**; Haibo Qiu; Yinsheng Wang; *Dept. of Chem, UC Riverside, Riverside, CA*
- MP 489 **Expediting the Development of Targeted SRM Assays: Combining *in silico* Modeling with Data from Shotgun Proteomics to Automate Method**
- Development**; Michael J. Maccoss<sup>1</sup>; Daniela Tomazela<sup>1</sup>; Barbara Frewen<sup>2</sup>; Gennifer Merrihew<sup>1</sup>; Amol Prakash<sup>3</sup>; Scott Peterman<sup>4</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Univ of Washington, Genome Sciences, Seattle, WA*; <sup>3</sup>*ThermoFisher Scientific, Cambridge, MA*; <sup>4</sup>*Thermo Electron, Somerset, NJ*
- MP 490 **Proteome-Scale Measurement of Protein Turnover by Quantitative Mass Spectrometry**; Joshua E. Elias<sup>1</sup>; Corey E Bakalarski<sup>2</sup>; Steven Gygi<sup>2</sup>; <sup>1</sup>*Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- MP 491 **Application of a New Q-TOF Mass Spectrometer to Monitor Differential Expression of histone Modifications in Response to HDACi Treatment**; Paul Drogaris<sup>1</sup>; Anda Vintiloiu<sup>1</sup>; Christelle Pomies<sup>1</sup>; Eric Bonneil<sup>1</sup>; Christine Miller<sup>2</sup>; Georges Gauthier<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montréal, Canada*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- MP 492 **Label-Free Quantification of Hormone-Induced Membrane Protein Abundance Changes in *Arabidopsis thaliana***; Uma Kota; Kevin Blackburn; Srijeet Mitra; Benjamin T. Walters; Steven D. Clouse; Michael B. Goshe; *NC State University, Raleigh, NC*
- MP 493 **Strategies for Stringent Cataloguing of Methylophaga Thiooxidans using an Alternative Scanning LC-MS Approach**; Joanne B. Connolly<sup>1</sup>; Nick Tomczyk<sup>1</sup>; Susan E. Slade<sup>2</sup>; Vibhuti Patel<sup>1</sup>; Rich Boden<sup>2</sup>; Konstantinos Thalassinou<sup>2</sup>; Hendrik Shaefer<sup>2</sup>; James Scrivens<sup>2</sup>; <sup>1</sup>*Waters, Manchester, UK*; <sup>2</sup>*University of Warwick, Coventry, UK*
- MP 494 **Global Analysis of Pathogen-Induced Plant Protein Secretion Responses using Label-Free Quantification**; Fang-yi Cheng; Kevin Blackburn; John Williamson; Michael B. Goshe; *NC State University, Raleigh, NC*
- MP 495 **Optimized Platform for iTRAQ-Based Quantitative Proteomics**; Scott Ficarro<sup>1</sup>; Feng Zhou<sup>1</sup>; Guillaume Adelmant<sup>1</sup>; Job Cardoza<sup>1</sup>; Rositsa Koleva<sup>1</sup>; Manor Askenazi<sup>2</sup>; Yi Zhang<sup>1</sup>; Jarrod Marto<sup>1</sup>; <sup>1</sup>*Dana-Farber Cancer Institute, Boston, MA*; <sup>2</sup>*Dana-farber Cancer Institute And Hebrew University, Boston, MA*
- MP 496 **Absolute Quantification of Potential Cancer Markers using Targeted Mass Spectrometric Analysis of Isotope Labeled Clinical Samples**; Leroi V. DeSouza<sup>1</sup>; Adrian M. Taylor<sup>2</sup>; Marjorie Minkoff<sup>3</sup>; Christie L Hunter<sup>3</sup>; Mark M. Garner<sup>3</sup>; K W Michael Siu<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*; <sup>2</sup>*Mds Analytical Technologies, Concord, ON*; <sup>3</sup>*Applied Biosystems, Framingham, MA*
- MP 497 **Identification and Quantification of Intact Proteins from *A. flavus* using SILAC and Nano-Flow LC-LTQ-FT-ICR-MS**; Timothy S Collier; Adam M. Hawkridge; David R. Georgianna; Gary A Payne; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- MP 498 **Impact of Na<sup>+</sup>/K<sup>+</sup> Transporting ATPase Silencing on the Mitochondrial Proteome of SY5Y Neuroblastoma Cells: A Study Combining siRNA and SILAC**; Youn Jun Fu; Shu-Ling Xiong; Mark A Lovell; Bert C Lynn; *University of Kentucky, Lexington, KY*
- MP 499 **Stable Isotopic Labeling Studies to Determine the Protein Turnover within the Nuclear Pore Nup107-160 Subcomplex**; Joseph Glavy<sup>1</sup>; Ileana M. Cristea<sup>2</sup>; David Fenyo<sup>3</sup>; Brian Chait<sup>3</sup>; <sup>1</sup>*Stevens Institute of Tech., Hoboken, NJ*; <sup>2</sup>*Rockefeller University, New York, NY*; <sup>3</sup>*The Rockefeller University, New York, NY*
- MP 500 **Comparative Analysis of Different Peptide and Protein Fractionation Approaches for Use in Label-**

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- MP 501 **Free Quantitative Shotgun Proteomics;** Paul A. Haynes; Joel Chick; Gayani Gammulla; Thi Huynh; Karlie A. Neilson; *Macquarie University, North Ryde, Sydney, Australia*
- MP 502 **Investigation of the Antibiotic Detoxification Response of Escherichia coli cells Toward Fosmidomycin via Differential Proteomics;** Suraj Dhungana<sup>2</sup>; Charles A. Testa<sup>3</sup>; David T. Fox<sup>1</sup>; Timothy Sanchez<sup>1</sup>; Kenneth B. Tomer<sup>2</sup>; Srinivas Iyer<sup>1</sup>; Andy Koppisch<sup>1</sup>; <sup>1</sup>*Los Alamos National Laboratory, Los Alamos, NM*; <sup>2</sup>*Niehs, Durham, NC*; <sup>3</sup>*Echelon Biosciences, Salt Lake City, UT*
- MP 503 **The APEX Quantitative Proteomics Tool: A Free Analysis Tool for Deriving Large Scale Protein Expression Estimates using the APEX Technology;** John C. Braisted<sup>1</sup>; Srilatha Kuntumalla<sup>1</sup>; Alan R. Rodrigues<sup>1</sup>; Rong Wang<sup>1</sup>; Shih-Ting Huang<sup>1</sup>; Christine Vogel<sup>2</sup>; Edward M. Marcotte<sup>2</sup>; Erik S. Ferlanti<sup>1</sup>; Alexander I. Saeed<sup>1</sup>; Robert D. Fleischmann<sup>1</sup>; Scott N. Peterson<sup>1</sup>; Rembert Pieper<sup>1</sup>; <sup>1</sup>*J. Craig Venter Institute, Rockville, MD*; <sup>2</sup>*University of Texas, Austin, TX*
- MP 504 **APEX-Based Differential Protein Abundance Analysis of Shigella Dysenteriae Type I Comparing in vitro and in vivo Proteomes;** Srilatha Kuntumalla<sup>1</sup>; David J. Clark<sup>1</sup>; Alan R. Rodrigues<sup>1</sup>; John C. Braisted<sup>1</sup>; Shih-Ting Huang<sup>1</sup>; Quanshun Zhang<sup>2</sup>; Arthur Donohue-Rolfe<sup>2</sup>; Saul Tzipori<sup>2</sup>; Scott N. Peterson<sup>1</sup>; Rembert Pieper<sup>1</sup>; <sup>1</sup>*J Craig Venter Institute, Rockville, MD*; <sup>2</sup>*Tufts University, North Grafton, MA*
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- PROTEIN SEQUENCING, 504 - 521**
- MP 504 **De novo Sequencing of TBD-1, the First Beta-Defensin Isolated from Reptiles;** Christin Stegemann<sup>1</sup>; Alexander Kolobov<sup>2</sup>; Olga Shamova<sup>3</sup>; Vladimir Kokryakov<sup>2</sup>; Ralf Hoffmann<sup>1</sup>; <sup>1</sup>*University of Leipzig, Leipzig, Germany*; <sup>2</sup>*St. Petersburg State University, St. Petersburg, Russia*; <sup>3</sup>*Institute for Experimental Medicine RAMS, St. Petersburg, Russia*
- MP 505 **Top-Down Study of Major Urinary Proteins by in-Source Decay;** Stephen C.C. Wong<sup>1</sup>; Duncan H.L. Robertson<sup>2</sup>; Sarah R Hart<sup>1</sup>; Marcus Macht<sup>3</sup>; Jane L. Hurst<sup>2</sup>; Robert L. Beynon<sup>2</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>*The University of Manchester, Manchester, UK*; <sup>2</sup>*University of Liverpool, Liverpool, UK*; <sup>3</sup>*Bruker Daltonics GmbH, Bremen, Germany*
- MP 506 **A Combination of Mass Spectrometry Techniques to Prove the Formation of a Covalent Thiosulfinate Intermediate between Peroxiredoxin and Sulfiredoxin;** Guillaume Béchade<sup>1</sup>; Xavier Roussel<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Sarah Sanglier<sup>1</sup>; Guy Branlant<sup>2</sup>; Sophie Rahuel-Clermont<sup>2</sup>; <sup>1</sup>*Université Louis Pasteur, IPHC-DSA, ULP-CNRS, Strasbourg, France*; <sup>2</sup>*Nancy Université, MAEM, UHP-CNRS, Vandoeuvre-lès-Nancy, France*
- MP 507 **Combining the Features of ETD and CID: Increased Peptide Identification;** Chris Adams; Allis S. Chien; *Stanford University, Stanford, CA*
- MP 508 **Identification of Sequencing Errors in the Genome of B. subtilis;** Matthew Lauber; James P. Reilly; *Indiana University, Bloomington, IN*
- MP 509 **Common Types of False-Positives Identified in Shotgun Proteomics;** Gang Xing; Yue Chen; Yingming Zhao; *UT Southwestern Medical Center at Dallas, Dallas, TX*
- MP 510 **Large-Scale de novo Sequencing of Ion Channel Modulators from Predatory Venomous Species;** Beatrix Ueberheide<sup>1</sup>; David Fenyo<sup>1</sup>; Paul F Alewood<sup>2</sup>; Brian Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*The University of Queensland, Brisbane, Australia*
- MP 511 **A Use of HPLC Data for Filtering and Validation of MS Based Peptide Identifications;** Irina A. Tarasova<sup>1</sup>; Anton A. Goloborodko<sup>2</sup>; Roman A. Zubarev<sup>3</sup>; Mikhail V. Gorshkov<sup>1</sup>; <sup>1</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation*; <sup>2</sup>*Moscow Institute of Physics and Technology, Dolgoprudny, Russia*; <sup>3</sup>*Uppsala University, Uppsala, Sweden*
- MP 512 **Dynamic Study of Tryptic Digestion Processes of Proteins by Ambient Liquid Mass Spectrometry (ALMS);** Cheng-Hui Yuan; Chih-Yuan Cheng; Li-Hua Lo; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 513 **Improved Prediction of Peptide Fragmentation Spectra using a Machine Learning Approach;** Arunima Ram; Randy J. Arnold; Haixu Tang; Predrag Radivojac; *Indiana University, Bloomington, IN*
- MP 514 **De novo Sequencing of an Antibody using an Ion-Trap Mass Spectrometer;** Jane Nagel; Rita Steeves; Mark Mellman; Kathryn Underwood; Jas Seehra; *Accelaron Pharma, Cambridge, MA*
- MP 515 **Comparative Analysis of Cysteine Alkylation and the Effects on Tandem Mass Spectra and Protein Identification;** Mark J. Raftery; *Bioanalytical Mass Spect, Kensington, Australia*
- MP 516 **Isolation and Identification of Low Molecular Weight Proteins from the American Alligator (Alligator mississippiensis) using Gel Separation with Nano ESI-Q-TOF;** Lancia N.F. Darville<sup>1</sup>; Mark E. Merchant<sup>2</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>*Louisiana State University, Baton Rouge, LA*; <sup>2</sup>*McNesse State University, Lake Charles, LA*
- MP 517 **Improved Coverage in Global Proteomics Survey Experiments by Decreasing Cycle Time on a Linear Ion Trap Mass Spectrometer;** Barbora Brazdova; Julie A. Horner; Julian J Phillips; *Thermo Fisher Scientific, San Jose, CA*
- MP 518 **Hidden Gems in Unassigned MS-MS Spectra Reveal a Higher Order Code for Translating mRNA into Protein;** Rachel O. Loo<sup>1</sup>; Yanan Yang<sup>3</sup>; Juni Samos<sup>1</sup>; Housna Mouttaki<sup>2</sup>; Michael McInerney<sup>2</sup>; Robert P. Gunsalus<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>*UCLA, Los Angeles, CA*; <sup>2</sup>*University of Oklahoma, Norman, OK*; <sup>3</sup>*Agilent Technologies, Inc, Santa Clara, CA*
- MP 519 **Large-Scale Sequencing of Charge-Enhanced Peptide Ions using Electron Transfer Dissociation and Collision-Activated Dissociation;** Frank Kjeldsen; Anders B. M. Giessing; Christian Ravnsborg; Thomas A. Hansen; Ole N. Jensen; *Univ. of Southern Denmark, Odense, Denmark*
- MP 520 **Large Peptide Sequencing - Experimental Strategies using Electron Transfer Dissociation;** Zhiqi Hao; Terry Zhang; Andreas Huhmer; *Thermo Fisher Scientific, San Jose, CA*
- MP 521 **Isolation of C-Terminal Peptides of Proteins by Exhaustive Amidation Followed by Proteolytic Digestion for Mass Spectrometric Sequencing;** Mariko Nakagawa<sup>1</sup>; Minoru Yamaguchi<sup>2</sup>; Hiroki Kuyama<sup>3</sup>; Eiji Ando<sup>2</sup>; Osamu Nishimura<sup>3</sup>; Susumu Tsunasawa<sup>3</sup>; Takashi Nakazawa<sup>1</sup>; <sup>1</sup>*Nara Women's University, Nara, JAPAN*; <sup>2</sup>*Shimadzu Corp, Kyoto, Japan*; <sup>3</sup>*Institute for Protein Research, Osaka, Japan*

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MP 523	<b>A quantitatively Optimized and Improved Digestion Protocol for Human Plasma;</b> <u>Michael A Kuzyk</u> <sup>1</sup> ; Roarke Copeland <sup>1</sup> ; Juncong Yang <sup>1</sup> ; Monica H Elliott <sup>1</sup> ; Leigh Anderson <sup>2</sup> ; Christoph H Borchers <sup>1</sup> ; <sup>1</sup> <i>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada</i> ; <sup>2</sup> <i>Plasma Proteome Institute, Washington, DC</i>
MP 524	<b>Biodiversity Exploration using MS-Based Proteomics for the Improved Understanding of extreme Physiopathological Situation Adaptations;</b> <u>Laetitia Fouillen</u> <sup>1</sup> ; Thierry Raclot <sup>2</sup> ; Alain Van Dorselaer <sup>1</sup> ; Fabrice Bertile <sup>1</sup> ; <sup>1</sup> <i>IPHC-DSA, ULP, CNRS, Strasbourg, France</i> ; <sup>2</sup> <i>IPHC-DEPE, ULP, CNRS, Strasbourg, France</i>
MP 525	<b>Plasma Proteome Analysis of The Effect of NO Synthase Inhibition on SJL Mice Bearing RcsX Lymphoma;</b> <u>I. Ramesh Babu</u> <sup>1</sup> ; Yingwu Wang <sup>2</sup> ; John S. Wishnok <sup>1</sup> ; Steven R. Tannenbaum <sup>1</sup> ; <sup>1</sup> <i>Massachusetts Institute of Technology, Cambridge, MA</i> ; <sup>2</sup> <i>Jilin University, Changchun, P.R. China</i>
MP 526	<b>Proteomic Analysis of Rat and Human Plasma in search of Potential Biomarkers for Type 2 Diabetes;</b> <u>Mike Galligan</u> <sup>1</sup> ; Mike Kimzey <sup>1</sup> ; Timothy R. Radabaugh <sup>1</sup> ; George Tsapraillis <sup>1</sup> ; Daniel C Link <sup>1</sup> ; Chad R. Borges <sup>2</sup> ; Hussein Yassine <sup>1</sup> ; Erik J Henriksen <sup>1</sup> ; Randall Nelson <sup>2</sup> ; Craig S Stump <sup>1</sup> ; Serrine S Lau <sup>1</sup> ; <sup>1</sup> <i>University of Arizona, Tucson, AZ</i> ; <sup>2</sup> <i>Arizona State University, Tempe, AZ</i>
MP 527	<b>Comparison of Approaches for Enrichment of Low Abundant Serum Proteins;</b> <u>Ravi Chandra Dwivedi</u> <sup>1</sup> ; Oleg V. Krokhin <sup>2</sup> ; John A. Wilkins <sup>2</sup> ; <sup>1</sup> <i>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, Canada</i> ; <sup>2</sup> <i>University of Manitoba, Winnipeg, Canada</i>
MP 528	<b>Extension of the Human Plasma Proteome using Electron Transfer Dissociation and Proton Transfer Reaction;</b> <u>Sarah R Hart</u> <sup>1</sup> ; Carsten Baessmann <sup>2</sup> ; Laura Main <sup>3</sup> ; Simon J. Gaskell <sup>1</sup> ; <sup>1</sup> <i>University of Manchester, Manchester, UK</i> ; <sup>2</sup> <i>Bruker Daltonik GmbH, 28359 Bremen, Germany</i> ; <sup>3</sup> <i>Bruker Daltonics, Coventry, UK</i>
MP 529	<b>Optimisation of On-Line NanoLC, FT-ICR ECD-MS-MS Hyphenation for Top Down Oxidized Protein Identification;</b> <u>Pauline Le Faouder</u> <sup>1</sup> ; Iman Emami <sup>2</sup> ; Christian Rolando <sup>1</sup> ; Caroline Tokarski <sup>1</sup> ; <sup>1</sup> <i>Univ. des Science/Tech de Lille, Villeneuve d'Ascq, France</i> ; <sup>2</sup> <i>Biosyntheac, Paris, France</i>
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MP 531	<b>Optimization of Nanoelectrospray with Plasma Derived Samples for Qualitative and Quantitative Biomarker Analysis;</b> <u>Jeff Wynn</u> <sup>1</sup> ; Amanda Berg <sup>2</sup> ; Gary Valaskovic <sup>2</sup> ; <sup>1</sup> <i>New Objective Inc, Woburn, MA</i> ; <sup>2</sup> <i>New Objective, Inc., Woburn, MA</i>
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MP 550	<b>A Novel Proteolytic Treatment Capable of Digesting Transmembrane Proteins in Presence of Strong Anionic Detergent;</b> <u>Malte Schürken</u> ; Michael Karas; <i>Jw Goethe Univ. of Frankf, Frankfurt Am Main, Germany</i>
MP 551	<b>Microwave-Assisted Enzymatic Digestion of Proteins as a Rapid and Efficient Digestion Approach in Proteomics;</b> <u>Iveta Klouckova</u> <sup>1</sup> ; Yuening Zhang <sup>1</sup> ; Milan Madera <sup>2</sup> ; Yehia Mechref <sup>2</sup> ; Milos Novotny <sup>2</sup> ; <sup>1</sup> <i>Indiana University, Bloomington, IN</i> ; <sup>2</sup> <i>National Center of Glycomics and Glycoproteomics, Bloomington, IN</i>
MP 552	<b>Application of Iodoacetamide Derivatives Utilized to Increase Ion Abundance through the ALiPHAT Strategy;</b> <u>David C. Muddiman</u> <sup>1</sup> ; Dennis Keith Williams, Jr. <sup>3</sup> ; Corey W Meadows <sup>2</sup> ; Daniel L Comins <sup>1</sup> ; Adam Hawkridge <sup>4</sup> ; <sup>1</sup> <i>North Carolina State University, Raleigh, NC</i> ; <sup>2</sup> <i>Concord University, Concord, WV</i> ; <sup>3</sup> <i>North Carolina State Univ, Raleigh, NC</i> ; <sup>4</sup> <i>Nc State University, Raleigh, NC</i>
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MP 554	<b>Integrating Mass Spectrometry with Sucrose Gradient Ultracentrifugation and Blue-Native PAGE for the Isolation of Intact Endogenous Protein Complexes;</b> Jianhong Zhou; <u>Yu-Chun Du</u> ; <i>University of Arkansas, Fayetteville, AR</i>
MP 555	<b>An IPG MudPit Workflow for MS Analysis of Protein Complexes Purified by Blue Native Gels;</b> Mahbod R. Hajivandi <sup>1</sup> ; Thomas Beardslee <sup>2</sup> ; Xiquan Liang <sup>1</sup> ; Paul Predki <sup>1</sup> ; <u>R. Marshall Pope</u> <sup>1</sup> ; <sup>1</sup> <i>Invitrogen, Carlsbad, CA</i> ; <sup>2</sup> <i>Invitrogen Corporation, Carlsbad, CA</i>
MP 556	<b>Reduction of Dynamic Concentration Range Allows Detecting Low-Abundance Proteins: RBC Lysate and CSF Cases;</b> Egisto Boschetti; <i>Bio-Rad Laboratories, Gif-sur-Yvette, France</i>
MP 557	<b>A Novel and Versatile Chemo-Proteomics Technique for Drug Target Deconvolution;</b> <u>Chaitanya Saxena</u> <sup>1</sup> ; Yuejun Zhen <sup>1</sup> ; John Hale <sup>2</sup> ; <sup>1</sup> <i>Eli Lilly &amp; Company, Greenfield, IN</i> ; <sup>2</sup> <i>Lilly Research Labs, Greenfield, IN</i>
MP 558	<b>Quantitation of Serum and Plasma Proteins after Depletion of Abundant Proteins with a Combinatorial Bead Library;</b> <u>Vanitha Thulasiraman</u> ; Katrina Academia; Steve Freeby; Steve Roth; Hongmin Zhang; Steven Gu; Mariana Rusa; Tim Wehr; Ning Liu; Kate Smith; Aran Paulus; Fiona Plows; <i>Bio-rad Laboratories, Inc., Fremont, CA</i>
MP 559	<b>iTRAQ<sup>®</sup> Reagent-Based "Tagless" Strategy of Identification and Purification of Soluble Protein Complexes in Bacteria: Development of High-Throughput Protocols;</b> Haichuan Liu <sup>1</sup> ; Ming Dong <sup>2</sup> ; Lee L. Yang <sup>2</sup> ; Simon Allen <sup>1</sup> ; Eric Johansen <sup>1</sup> ; Steven C. Hall <sup>1</sup> ; Susan J. Fisher <sup>1</sup> ; Terry C. Hazen <sup>2</sup> ; Jil T. Geller <sup>2</sup> ; Mary E. Singer <sup>2</sup> ; Jian Jin <sup>2</sup> ; Mark D. Biggin <sup>1</sup> ; <u>H. Ewa Witkowska</u> <sup>1</sup> ; <sup>1</sup> <i>UCSF Core Mass Spectrometry Facility, San Francisco, CA</i> ; <sup>2</sup> <i>Lawrence Berkeley National Laboratory, Berkeley, CA</i>

## MONDAY POSTERS

- MP 560 **Performance Evaluation of Endoproteinase Lys-C Spin-Column Rapid Digestion Compared to Traditional in-Solution Endoproteinase Lys-C Digestion;** Aaron Aslanian<sup>1</sup>; Xuemei Han<sup>2</sup>; John Yates<sup>2</sup>; <sup>1</sup>Salk Institute, La Jolla, CA; <sup>2</sup>The Scripps Research Institute, La Jolla, CA
- MP 561 **Online Microwave Digestion LC-MS-MS of Proteins;** Nicolas Hauser<sup>1</sup>; Hongling Han<sup>2</sup>; Scott A. McLuckey<sup>2</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY; <sup>2</sup>Purdue University, West Lafayette, IN
- MP 562 **Selective Affinity Purification of RNA and DNA Binding Proteins using Immobilised Anilide Compounds;** Chris Sutton<sup>1</sup>; Martyn W. Inman<sup>2</sup>; Jason Gill<sup>1</sup>; Colin W. G. Fishwick<sup>2</sup>; Ron Grigg<sup>2</sup>; <sup>1</sup>Institute of Cancer Therapeutics, Bradford, UK; <sup>2</sup>University of Leeds, Leeds, UK
- MP 563 **Protein Immobilization via Cysteine Residues for Enzymatic Digestion of Samples Containing Detergent;** Jennifer J. Hill; Cody J. Dey; Maria J. Moreno; John F. Kelly; *National Research Council Canada, Ottawa, Canada*
- MP 564 **On-Probe Fractionation and High Confidence Protein Identification of Complex Protein Mixtures using RF Plasma Modified MALDI Targets;** Ganga Fernando; Rebecca Hopkins; Gary R Kinsel; *Southern Illinois University at Carbondale, Carbondale, IL*
- MP 565 **Assessing the Binding Selectivity of Molecularly Imprinted Polymer Artificial Antibodies by Mass Spectrometry-Based Profiling System;** Yu-Chang Tyan<sup>1</sup>; Chung-Yao Wang<sup>2</sup>; Tse-Chuan Chou<sup>2</sup>; Jing-Fang Hsu<sup>2</sup>; Pao-Chi Liao<sup>2</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>National Cheng Kung University, Tainan, Taiwan
- MP 566 **Metalloenes as Selective Labeling Reagents in Bioanalysis;** Susanne Bomke<sup>1</sup>; Andy Scheffer<sup>1</sup>; Björn Meermann<sup>1</sup>; Bettina Seiwert<sup>2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>2</sup>MP Golm, Potsdam, Germany
- MP 567 **Microwave Enhanced Proteolysis: Mechanism and Optimization for Difficult Proteins;** Brian Imai<sup>1</sup>; Peter Yau<sup>1</sup>; Grace S Vanier<sup>2</sup>; Mike Collins, Jr<sup>2</sup>; Jonathan Collins<sup>2</sup>; <sup>1</sup>University of Illinois, Urbana Champaign, IL; <sup>2</sup>CEM Corporation, Matthews, NC
- MP 568 **A Proteomics Approach for Identifying Phosphoinositides (PtdInsPn) Interacting Proteins;** Steve Nguyen; Michel Vermeulen; Michael Lund Nielsen; Matthias Mann; *Max Planck Institute, Martinsried, Germany*
- MP 569 **Use of Off-Gel Electrophoresis as the First Dimension Separation in Shotgun Proteomic Analysis;** Lashanda Waller<sup>1</sup>; Kevin S. Shores<sup>2</sup>; Daniel R. Knapp<sup>1</sup>; <sup>1</sup>Medical University of SC, Charleston, SC; <sup>2</sup>University of Texas, Austin, TX
- MP 570 **Application of Pressurized Solvents for Ultra Fast Proteolysis: Proteomics on the fly;** Daniel Lopez Ferrer; Konstantinos Petritis; Natacha M Lourette; Brian H. Clowers; Kim K. Hixson; Tyler H Heibeck; Eric A. Livesay; Ryan Kelly; David Prior; Ljiljana Pasa-tolic; David G. Camp; Mikhail Belov; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- MP 571 **Characterizing Chemical Ligands by Heat Map Analysis of Binding Proteins and Enrichment of Kinases by Selected Chemical Ligands;** Yoshiya Oda; Yasutaka Takase; Ken Aoshima; Hiroyuki Katayama; Tsuyoshi Tabata; Takashi Owa; Junro Kuromitsu; *Eisai, Tsukuba, Japan*
- MP 572 **Magnetic Nanoparticle-Based Microwave-Assisted Phosphoproteomic Analysis;** Wei-Yu Chen; Yu-Chie Chen; *National Chiao Tung Univ., Hsinchu, Taiwan*
- MP 573 **Equalisation of Protein Amounts for Overcoming the High Dynamic Protein Expression Range in the Analysis of Plant Proteomes;** Laurence V. Bindschedler; Rainer Cramer; *The University of Reading, Reading, UK*
- MP 574 **A High-Throughput Method for Phosphopeptide Enrichment of Spliceosomal Proteins;** He-Hsuan Hsiao<sup>1</sup>; Mads Gronborg<sup>2</sup>; Reinhard Luehrmann<sup>3</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>Bioanalytical Mass Spectrometry Group, MPIIbpc, Goettingen, Germany; <sup>2</sup>Department of Neurobiology, MPIIbpc, Goettingen, Germany; <sup>3</sup>Department of Cellular Biochemistry, MPIIbpc, Goettingen, Germany
- MP 575 **Identification of Sulfenated Proteome using a Biotin-Tagged Sulfenic Acid Specific Reagent (DCP-bio1);** Revati Wani; Allen W. Tsang; Chananat Klomsiri; Bruce S. King; Leslie Poole; Cristina M. Furdui; *Wake Forest University School of Medicine, Winston Salem, NC*
- MP 576 **Application of Carrier-Free Enzyme Immobilization to Proteomics: On-plate Proteolysis using Cross-linked Trypsin Aggregate;** Chenxi Jia<sup>1</sup>; Zhimin He<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Tianjin University, Tianjin, China
- MP 577 **Effect of pH on Immobilized Trypsin Microreactors for Protein Digestion and Identification;** Ying Long<sup>1</sup>; Cheng Zhao<sup>3</sup>; Troy D. Wood<sup>2</sup>; <sup>1</sup>Univeristy at Buffalo, Buffalo, NY; <sup>2</sup>University at Buffalo/nanogenesys. Inc., Buffalo, NY; <sup>3</sup>Abbott Laboratories, Abbott Park, IL
- MP 578 **A Comparison of Poly Co-(N-Isopropylacrylamide-Methacrylic Acid) (NIPAAAM-MAA) Polymer Brush Surfaces and Plasma Polymer Surfaces for On-Target Peptide Fractionation;** Venney Wong; Gary R. Kinsel; Daniel Dyer; Ganga Fernando; Zaneer Segu; *Southern Illinois University Carbondale, Carbondale, IL*
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- PROTEOMICS: BIOMARKER DISCOVERY 1, 579 - 604**
- MP 579 **Determination of Potential Amyotrophic Lateral Sclerosis Biomarkers in Cortex Samples by MALDI-TOF MS, MALDI Imaging MS, and MALDI-Q-FT-ICR MS;** Kristin J. Boggio<sup>1</sup>; Long Li<sup>1</sup>; Michael L. Easterling<sup>2</sup>; Christopher J. Thompson<sup>2</sup>; Nathalie YR Agar<sup>3</sup>; Jeffrey N. Agar<sup>1</sup>; <sup>1</sup>Brandeis University, Waltham, MA; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA; <sup>3</sup>Harvard Medical School, Neurosurgery, Boston, MA
- MP 580 **Phosphoproteomics as a Platform for Biomarker Discovery in Lung Cancer;** Rui Xi Xie<sup>1</sup>; Haochen Li<sup>1</sup>; Arminja Kettenbach<sup>1</sup>; Brendan Faherty<sup>2,3</sup>; Scott A. Gerber<sup>1</sup>; <sup>1</sup>Dartmouth Medical School, Lebanon, NH; <sup>2</sup>Dartmouth College, Lebanon, NH; <sup>3</sup>Dartmouth College, Lebanon, NH
- MP 581 **Improvement of Subcellular Fractionation and Novel 2-D Separation Method for the Identification of Phospho-Biomarkers for Cancer;** Karin Grosstessner-Hain<sup>1</sup>; Björn Hegemann<sup>1</sup>; Jan-Michael Peters<sup>1</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>Research Institute of Molecular Pathology (IMP), Vienna, Austria; <sup>2</sup>Institute of Molecular Biotechnology (IMBA), Vienna, Austria
- MP 582 **Can Quantitative, Label-Free Methods Be Extended to Top-Down Strategies? A Proof of Principle Experiment for Analyzing Human HDL;** Matthew T. Mazur; Kai Zhou; Nathan A. Yates; Ronald C. Hendrickson; *Merck Research Laboratories, Rahway, NJ*

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- MP 583 **Identification of Differentially Expressed Proteins in Neurotensin Receptor Wild Type vs Knockout Mice using PF 2D and Mass Spectrometry**; Katrina Williams; Mona Boules; Bernadette Cusack; Elliott Richelson; *Mayo Clinic, Jacksonville, FL*
- MP 584 **Orbitrap and FTICR: Figures of Merit and Methodology for Comparing Unbiased Biomarker Discovery Platforms**; YI DU; Matthew Mazur; Fanyu Meng; Ronald Hendrickson; Nathan Yates; *Merck Research Laboratories, Rahway, NJ*
- MP 585 **Proteomic Progression of Human Prostate Cancer using Urogenital Mesenchyme (UGM)/BPH-1 Recombinants, Stimulated by Testosterone (T) and Estradiol 17b (E2)**; John D. Lapek; Lauren Jensen; William A. Ricke; Alan E. Friedman; *University of Rochester Medical Center, Palmyra, NY*
- MP 586 **Comparative Investigation of the Chicken and Human Plasma Proteome: Implications for Biomarker Discovery in Epithelial Ovarian Cancer**; Adam Hawkridge<sup>1</sup>; Becca Wysocky<sup>1</sup>; James N. Petitte<sup>1</sup>; Paul E. Mozdziak<sup>1</sup>; Kenneth E. Anderson<sup>1</sup>; William A. Cliby<sup>2</sup>; Jonathan M. Horowitz<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*Mayo Clinic College of Medicine, Rochester, MN*
- MP 587 **Strategies for Measuring Protein Markers for Pancreatic Cancer from Salivary Fluid**; Pinmanee Boonthueung; Prasanna Ramachandran; James J. Farrell; David T. Wong; Joseph A. Loo; *UCLA, Los Angeles, CA*
- MP 588 **Discovery of Brain Damage-Related Biomarkers in Human Ante-mortem and Post-mortem Cerebrospinal Fluids with Sixplex Isobaric Tandem Mass Tags**; Loïc Dayon<sup>1</sup>; Alexandre Hainard<sup>1</sup>; Virginie Licker<sup>1</sup>; Natacha Turck<sup>1</sup>; Karsten Kuhn<sup>2</sup>; Denis F. Hochstrasser<sup>3</sup>; Pierre R. Burkhard<sup>4</sup>; Jean-Charles Sanchez<sup>1</sup>; <sup>1</sup>*Biomedical Proteomics Group, University of Geneva, Geneva, Switzerland*; <sup>2</sup>*Proteome Sciences R&D GmbH & Co. KG, Frankfurt am Main, Germany*; <sup>3</sup>*Clinical Proteomics Group, Geneva Uni. Hospital, Geneva, Switzerland*; <sup>4</sup>*Department of Neurology, Geneva Uni. Hospital, Geneva, Switzerland*
- MP 589 **Stercobilin Depletion in Autistics' Urine: Testing Hypotheses to Explain Metabolism using Electrospray Ionization Mass Spectrometry**; Nhu Quynh, Thi Nguyen<sup>1</sup>; Troy D. Wood<sup>2</sup>; <sup>1</sup>*Chemistry Department, SUNY Buffalo, Buffalo, NY 14, Buffalo, NY*; <sup>2</sup>*University At Buffalo/nanogenesys. Inc., Buffalo, NY*
- MP 590 **Identification of Candidate Plasma Biomarkers for Pancreatic Cancer with and without Diabetes: A Case Control Study**; Vikram Palamalai<sup>2</sup>; David A Ahlquist<sup>1</sup>; Olson E Janet<sup>2</sup>; Jeanette Eckel-passow<sup>1</sup>; Ann L Oberg<sup>1</sup>; Kenneth L. Johnson<sup>1</sup>; Michael W. Holmes<sup>2</sup>; H. Robert Bergen, Iii<sup>2</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*; <sup>2</sup>*Mayo Clinic College of Medicine, Rochester, MN*
- MP 591 **Correlation of miRNA and SILAC Protein Expression in a Primary Cancer Cell Line**; Lisa Wenrich; Xiquan Liang; Mahbod R. Hajivandi; Brad Love; Christopher Adams; Paul Predki; R. Marshall Pope; *Invitrogen, Carlsbad, CA*
- MP 592 **High Throughput Analysis of FFPE Tissue Samples Combined with Microelectrophoresis and MALDI MS**; Hans-Rudolf Aerni; M. Reid Groseclose; M. Lisa Manier; Dale S. Cornett; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- MP 593 **MALDI TOF Profiling of Low Molecular Weight Serum Protein Fraction from Breast Cancer sera for Pattern Analysis**; V.S. Kumar Kolli<sup>1</sup>; Bernard Seth<sup>1</sup>; Brian. J Leech<sup>1</sup>; Tapan Maity<sup>4</sup>; David Malehorn<sup>2</sup>; William Bigbee<sup>2</sup>; Sun Mai<sup>2</sup>; Richard Mural<sup>1</sup>; Michael Liebman<sup>1</sup>; Craig Shriver<sup>3</sup>; <sup>1</sup>*Windber Research Institute, Windber, PA*; <sup>2</sup>*CPF, University of Pittsburgh, Pittsburgh, PA*; <sup>3</sup>*Walter Reed Army Medical Center, Washington DC*; <sup>4</sup>*University of Maryland, Baltimore, MD*
- MP 594 **Mass Spectrometry Can Show Potential Cancer Biomarkers in Urine**; Maria A Hamilton<sup>1</sup>; Clare Kenny Carney<sup>1</sup>; Guangyu Zhang<sup>1</sup>; Madhuri Mulekar<sup>2</sup>; Rodney Rocconi<sup>1</sup>; Raymond Wynn<sup>1</sup>; Rajeev S. Samant<sup>1</sup>; Lalita A. Shevde<sup>1</sup>; Lewis K. Pannell<sup>1</sup>; <sup>1</sup>*Mitchell Cancer Institute, Mobile, AL*; <sup>2</sup>*University of South Alabama, Mobile, AL*
- MP 595 **Multiple-Reaction-Monitoring of Putative Biomarkers of Hepatocellular Carcinoma Identified by Tissue-to-Plasma Strategy**; Sheeno Thyparambil<sup>1</sup>; Richard C Jones<sup>2</sup>; Ricky D Edmondson<sup>3</sup>; <sup>1</sup>*National Center for Toxicological Research, Jefferson, AR*; <sup>2</sup>*Nextgen Sciences, Ann Arbor, MI*; <sup>3</sup>*Uams, Little Rock, AR*
- MP 596 **Proteomic Characterization of Human Cervical Mucous Proteins**; Yiming Ye; Gitika Panicker; Dongxia Wang; Elizabeth Unger; *Centers of Disease Control And Prevention (cdc), Atlanta, GA*
- MP 597 **Characterization of Peptides from Elastin Degradation**; Jiangtao He; Shuren Ma; Gerard M Turino; Yong Lin; *St.Luke/Roosevelt Hospital Center, New York, NY*
- MP 598 **A Quantitative Proteomic Approach for Identification Of Potential Biomarkers in Hepatocellular Carcinoma using 8-Plex iTRAQ Reagents**; Raghothama Chaerkady<sup>1</sup>; Paul J Thuluvath<sup>2</sup>; Marjan Gucek<sup>2</sup>; Genaro Pimienta<sup>2</sup>; Anuradha Nalli<sup>1</sup>; Perumal Vivekanandan<sup>2</sup>; Robert N Cole<sup>2</sup>; Michael A Choti<sup>2</sup>; Michael Torbenson<sup>2</sup>; Akhilesh Pandey<sup>2</sup>; <sup>1</sup>*Institute of Bioinformatics, Bangalore , Karnataka, IN*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*
- MP 599 **Proteomic Analysis of Chronic Methamphetamine Treatment in Rat Cortex**; William K. Russell<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Issa Issac<sup>3</sup>; Kevin S. Wang<sup>2</sup>; David H. Russell<sup>1</sup>; Mark S. Gold<sup>2</sup>; <sup>1</sup>*Texas A&M University, College Station, TX*; <sup>2</sup>*University of Florida, Gainesville, FL*; <sup>3</sup>*Genomic Solutions, Ann Arbor, MI*
- MP 600 **Investigation into Biomarkers of Antidepressant Response in a Mouse Model of Depression using Isobaric Labels (Tandem Mass Tags) and 2DE**; Helen L Byers<sup>1</sup>; James Campbell<sup>1</sup>; Karsten Kuhn<sup>3</sup>; Richard Joubert<sup>3</sup>; Elke Binder<sup>2</sup>; Jose L Paya-Cano<sup>2</sup>; Malcolm A Ward<sup>1</sup>; Peter McGuffin<sup>2</sup>; Peter Schulz-Knappe<sup>3</sup>; Katherine J Aitchison<sup>2</sup>; Leonard C Schalkwyk<sup>2</sup>; <sup>1</sup>*Proteome Sciences plc, London, UK*; <sup>2</sup>*MRC SGDP Centre, Institute of Psychiatry's at KCL, London, UK*; <sup>3</sup>*Proteome Sciences R&D GmbH & Co KG, Frankfurt Am Main, Germany*
- MP 601 **Diagnosis of Gastric Cancer by Peptidomic Analysis of Gastric Juice**; Wei-Chao Chang<sup>1</sup>; Ping-I Hsu<sup>2</sup>; Yuan-Yan Chen<sup>1</sup>; Michael Hsiao<sup>1</sup>; Pei-Jung Lu<sup>2</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>*The Genomics Research Center, Academia Sinica., Taipei, TAIWAN*; <sup>2</sup>*Kaohsiung Veterans General Hospital, Kaohsiung, Taiwan*
- MP 602 **Novel Sensitive and Specific Method for Search for Serum Biomarkers of Cancer**; Rustam Ziganshin<sup>1</sup>; Dmitry Alexeev<sup>1</sup>; Georgii Arapidi<sup>1</sup>; Vadim Govorun<sup>2</sup>; <sup>1</sup>*Shemyakin and Ovchinnikov Institute of Bioorganic,*

## MONDAY POSTERS

- Moscow, Russian Federation; <sup>2</sup>Ripcm, Moscow, Russian Federation
- MP 603 **Combining Exploratory and Targeted Analysis for Identification and Quantitation of Biomarker Candidates in a Single NanoLC-MS Run; Reinaldo Almeida<sup>1</sup>; Leonie F. Waanders<sup>2</sup>; Peter Bandilla<sup>2</sup>; Gary A. Schultz<sup>3</sup>; Mark Allen<sup>1</sup>; Matthias Mann<sup>2</sup>; <sup>1</sup>Advion Biosciences Ltd, Norwich, Norfolk, UK; <sup>2</sup>Mpi For Biochemistry, Martinsried, Germany; <sup>3</sup>Advion Biosystems, Ithaca, NY**
- MP 604 **Quantitative Proteomic Analysis Reveals Redirection of Karyopherin-Mediated Nuclear Transport in Primary CD4 Cells Infected with HIV-1; Eric Y Chan<sup>1</sup>; Jon M Jacobs<sup>3</sup>; Jennifer N Sutton<sup>2</sup>; Matthew E Monroe<sup>3</sup>; Andrew Keller<sup>4</sup>; David C Camp II<sup>3</sup>; Richard D Smith<sup>3</sup>; Michael G Katze<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Thermo Fisher Scientific, Cambridge, MA; <sup>3</sup>Pacific Northwest National Lab, Richland, WA; <sup>4</sup>Rosetta Biosoftware, Seattle, WA**
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- PROTEOMICS: CLINICAL APPLICATIONS, 605 - 631**
- MP 605 **Differential Proteomic Characterization of Multiple Sclerosis-Associated Proteins as Potential Biomarkers in Human Cerebrospinal Fluid (CSF); Dawn Chen; WenXue Li; Noline Schiess; Yan Huang; Benjamin Greenberg; Robert Cotter; Avindra Nath; Johns Hopkins University, Baltimore, MD**
- MP 606 **Proteome Changes Induced by Knock-Out of the Prostaglandin-Degrading Enzyme, 15-PGDH; Chao Yuan; Min Yan; Sanford D. Markowitz; Mark Chance; Jinsook Chang; Case Western Reserve University, Cleveland, OH**
- MP 607 **Quantitative Mass Spectrometry for Analysis of Membrane Expression of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR); Alexis A. Ramos<sup>1</sup>; Bonita A. Coutermarsh<sup>2</sup>; Pamela C. Diego<sup>1</sup>; Bruce A. Stanton<sup>2</sup>; Xudong Yao<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Connecticut, Storrs, CT; <sup>2</sup>Department of Physiology, Dartmouth Medical School, Hanover, NH**
- MP 608 **Proteomic Comparison of Ascites from Ovarian Cancer Patients and Ovarian Cancer Cell Lines using HPLC-Orbitrap Mass Spectrometry; Guangyu Zhang<sup>1</sup>; Rodney Rocconi<sup>1</sup>; Madhuri Mulekar<sup>2</sup>; Lalita A Shevde<sup>1</sup>; Rajeev S Samant<sup>1</sup>; Lewis K. Pannell<sup>1</sup>; <sup>1</sup>Mitchell Cancer Institute, Mobile, AL; <sup>2</sup>University of South Alabama, Mobile, AL**
- MP 609 **Deep Protein Identification Analysis of the Plasma Glycoproteome for Clinical Proteomics; Majlinda Kullolli; William S. Hancock; Marina Hincapie; Northeastern University, Boston, MA**
- MP 610 **Targeted Proteomic Analysis of the Beta-Adrenergic Receptor Signaling Pathway in Human Cardiac Biopsies Collected over the Course of Beta-Blocker Treatment; Kelli Kline; Wayne Minobe; Brian Lowes; J. David Port; Michael Bristow; Christine Wu; University of Colorado, Aurora, CO**
- MP 611 **Proteomics of Neoplastic Stem Cells in Children's Germ Cell Tumors; Sruthi Eedala<sup>1</sup>; Elizabeth Perlman<sup>2</sup>; William Haskins<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, TX; <sup>2</sup>Chicago Memorial Hospital, Chicago, IL**
- MP 612 **Investigating the Reproducibility of Proteomic Data across Different Instrument Configurations and Platforms; Keith Fadgen; Martha D. Stapels; Waters Corporation, Milford, MA**
- MP 613 **Absolute Quantification of Targeted Endogenous Salivary Peptides using Heavy Isotope-Labeled Internal Standards and High Resolution Selected Reaction Monitoring Mass Spectrometry; Reiko Kiyonami<sup>1</sup>; Markus Hardt<sup>1</sup>; Rosa Viner<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; H. Ewa Witkowska<sup>1</sup>; Steven C. Hall<sup>1</sup>; Susan Fisher<sup>1</sup>; <sup>1</sup>University of California At San Francisco, San Francisco, CA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA**
- MP 614 **Examining the Correlation of Modified Serum Albumin and Disease using Intact Mass Measurements and Multiple Reaction Monitoring; Rebekah L. Gundry<sup>1</sup>; Christie L Hunter<sup>2</sup>; Irina Chernysheva<sup>1</sup>; Jennifer E Van Eyk<sup>1</sup>; <sup>1</sup>The Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Applied Biosystems, Foster City, CA**
- MP 615 **Phosphoproteome of Human Skeletal Muscle Cells – Insights into Improved Insulin Action Due to Nutritional Intervention; Nagireddy Putluri; Liana Coleman; Ginger Ku; Zhong Wang; Xian Zhang; William Cefalu; Indu Khetarpal; Pennington Biomedical Research Center, Baton Rouge, LA**
- MP 616 **Proteomic Analysis of Oral/Head and Neck Cancer; Shen Hu; Lifeng Zhang; Jiang Jiang; Martha Arellano; David T Wong; UCLA School of Dentistry, Los Angeles, CA**
- MP 617 **Analysis of the Innate Inflammatory Response to Injury by Quantitative Blood Leukocyte Proteomics for Severe Trauma Patients; Weijun Qian<sup>1</sup>; Brianne O. Petritis<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Lyle L. Moldawer<sup>2</sup>; Ronald V. Maier<sup>3</sup>; Ronald G. Tompkins<sup>4</sup>; David G. Camp<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Florida, Gainesville, FL; <sup>3</sup>University of Washington, Seattle, WA; <sup>4</sup>Massachusetts General Hospital, Boston, MA**
- MP 618 **Profiling Multiple Myeloma: Correlation of Protein and Gene Expression Data; Rick Edmondson; John Shaughnessy Jr; Bart Barlogie; UAMS, Little Rock, AR**
- MP 619 **Identification of F-Box/LLR-Repeated Protein 17 as Potential Useful Biomarker for Breast Cancer Therapy; Gary Guishan Xiao<sup>1</sup>; Bing-sen Zhou<sup>2</sup>; Yun Yen<sup>2</sup>; <sup>1</sup>Creighton University Medical Center, Omaha, NE; <sup>2</sup>City of Hope National Medical Center, Los Angeles, CA**
- MP 620 **Reference Materials for Measurement Quality Assurance in MS-based Clinical Proteomics; David Bunk; Stephen Stein; NIST, Gaithersburg, MD**
- MP 621 **Tandem Affinity Purification and Proteome-Wide Identification of Oncoprotein NPM/ALK Interacting Proteins by Mass Spectrometry; Fang Wu; Peng Wang; Leah C. Young; Raymond Lai; Liang Li; University of Alberta, Edmonton, Alberta, Canada**
- MP 622 **Diagnostics for Clinical Proteomics: Immuno Matrix Assisted Laser/Desorption Ionization (iMALDI) for the Detection of Epidermal Growth Factor Receptor (EGFR); Brinda Shah<sup>1</sup>; Jian Jiang<sup>2</sup>; Carol E. Parker<sup>2</sup>; Jennifer Reid<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, BC; <sup>2</sup>University of North Carolina, Chapel Hill, NC**
- MP 623 **Clinical Proteomic Technologies for Cancer; Christopher R. Kinsinger; Mehdi Mesri; Henry Rodriguez; NIH/NCI, Bethesda, MD**
- MP 624 **A Robust and Sensitive Automated Method for MS-Based Serum Pattern Diagnostics using Well-Established ZipTip Technology and Ultrafiltration; Ali Tiss<sup>1</sup>; Celia Smith<sup>1</sup>; John Timms<sup>2</sup>; Zhiyuan Luo<sup>3</sup>;**

## MONDAY POSTERS

- Alex Gammerman<sup>3</sup>; Mike Waterfield<sup>2</sup>; Usha Menon<sup>2</sup>; Ian Jacobs<sup>2</sup>; Rainer Cramer<sup>1</sup>; <sup>1</sup>University of Reading, Reading, UK; <sup>2</sup>University College of London, London, UK; <sup>3</sup>Royal Holloway University of London, London, UK
- MP 625 **A Multiplexed Quantitative Strategy for Membrane Proteomics: Opportunities for Mining Therapeutic Targets in Human Colorectal Cancer;** Chia-Li Han; Chih-Wei Chien; Chien-Peng Wu; Yu-Ju Chen; *Institute of Chemistry, Academia Sinica, Taipei, TAIWAN*
- MP 626 **Computational Detection and Experimental Verification of Ionization Noise versus Molecular Signals in MALDI-TOF of Protein Mixtures;** Dariya Malyarenko<sup>1</sup>; Christine Bunai<sup>1</sup>; Maureen Tracy<sup>1</sup>; Julius Nyalwidhe<sup>2</sup>; Lisa Cazares<sup>2</sup>; Dennis Manos<sup>1</sup>; Karl Kuschner<sup>1</sup>; Eugene Tracy<sup>1</sup>; William Cooke<sup>1</sup>; <sup>1</sup>College of William and Mary, Williamsburg, VA; <sup>2</sup>Eastern Virginia Medical School, Norfolk, VA
- MP 627 **Proteomic Analysis of the Cytoskeleton Regulation in Chronic Myelogenous Leukemia Cells JURL-MK1: Effect of Imatinib Mesylate Treatment;** Petr Halada<sup>1</sup>; Katerina Peslova<sup>1</sup>; Dana Grebenova<sup>2</sup>; Zbynek Hrkal<sup>2</sup>; <sup>1</sup>Institute of Microbiology v.v.i., Prague 4, Czech Republic; <sup>2</sup>Institute of Hematology and Blood Transfusion, Prague 2, Czech Republic
- MP 628 **SELDI Array-Based Amyloid B Assays;** Quan Gu; Fiona Plows; Steve Roth; Vanitha T; Hongmin zhang; Mariana Rusa; *bio-rad laboratories, fremont, CA*
- MP 629 **An Online Nano LC Tandem Mass Spectrometric Approach for Identification of Specific MS-MS Signature Ions from Peptides Related to Glycation Pathologies;** Jessica Z. Bereszczak<sup>1</sup>; Roberta Seraglia<sup>2</sup>; Annunziata Lapolla<sup>3</sup>; Pietro Traldi<sup>2</sup>; Francesco L. Brancia<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory, Manchester, UK; <sup>2</sup>CNR-ISTM, Padova, Italy; <sup>3</sup>University of Padova, Padova, Italy
- MP 630 **Myocardial Proteomic Profiling Helps Identify Different Forms of Heart Disease;** Gökhan Baykut<sup>1</sup>; Matthias Witt<sup>1</sup>; Maria Bergquist<sup>2</sup>; Franz Mayer-Posner<sup>1</sup>; Per Hakansson<sup>4</sup>; Hans-Reinhard Zerkowski<sup>3</sup>; Doan Baykut<sup>3</sup>; Jonas Bergquist<sup>2</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Biomedical Centre, Uppsala University, Uppsala, Sweden; <sup>3</sup>University Hospital Basel, Basel, Switzerland; <sup>4</sup>Uppsala University, Uppsala, Sweden
- MP 631 **Back to the Future...Direct MALDI MS of a 109 Year Old Formaldehyde Preserved Biopsy;** Erin H. Seeley<sup>1</sup>; Mark R. Groseclose<sup>1</sup>; Charles L. Murphy<sup>2</sup>; Per Westermark<sup>3</sup>; Knut Sletten<sup>4</sup>; Alan Solomon<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>2</sup>Univ. of Tennessee Graduate School of Medicine, Knoxville, TN; <sup>3</sup>Uppsala University, Uppsala, Sweden; <sup>4</sup>University of Oslo, Oslo, Norway
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- BIOINFORMATICS 1, 632 - 658**
- MP 632 **Increasing True Positive Rates in MS-MS Sequence Searching Algorithms by Incorporating Corrections to Precursor Mass Calculations;** Viswanadham Sridhara<sup>1</sup>; Lewis Y. Geer<sup>1</sup>; Dina L. Bai<sup>2</sup>; An Chi<sup>3</sup>; Jeffrey Shabanowitz<sup>2</sup>; Donald F. Hunt<sup>2</sup>; Stephen Bryant<sup>1</sup>; <sup>1</sup>NCBI/NLM/NIH, Bethesda, MD; <sup>2</sup>University of Virginia, Charlottesville, VA; <sup>3</sup>Merck Research Laboratories, Boston, MA
- MP 633 **MassSieve v1.0: A Tool for Parsimony Analysis and Multiple Search Engine Comparisons of LC-MS-MS Proteomics Data;** Melinda A. McFarland<sup>1</sup>; Douglas J. Slotta<sup>2</sup>; Sanford P. Markey<sup>1</sup>; <sup>1</sup>NIMH, NIH, Bethesda, MD; <sup>2</sup>NCBI, NIH, Bethesda, MD
- MP 634 **Comparative Study of Data Imputation Methods for Metabolomics Data from Two Dimensional Gas Chromatography Time-of-Flight Mass Spectrometry;** Hyeoung Cho<sup>1</sup>; Cheolhwan Oh<sup>2</sup>; Xiaodong Huang<sup>2</sup>; Charles Buck<sup>2</sup>; Xiang Zhang<sup>3</sup>; <sup>1</sup>Korea Advanced Institute of Science and Technology, Daejeon, South Korea; <sup>2</sup>Purdue University, West Lafayette, IN; <sup>3</sup>University of Louisville, Louisville, KY
- MP 635 **High Confident Protein Identification of ETD and ECD Spectra with a New Mass List Preprocessor;** Martin Zeller; Torsten Ueckert; Bernard Delanghe; *Thermo Fisher Scientific, Bremen, Germany*
- MP 636 **Design and Implementation of a Complete Data Storage, Processing and Management Solution for a Core-Based Mass Spectrometry Laboratory;** James West<sup>1</sup>; Weiwei Tong<sup>1</sup>; Kip L Bodi<sup>2</sup>; Mark E. McComb<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Amyloid Treatment and Research Program, Boston, MA
- MP 637 **Refining the Spectrum Mill Peptide MS-MS Fragmentation Model for Improved Confidence in Sequence/Spectrum Matching;** Karl R. Clauser; Steven A. Carr; *Broad Institute of MIT and Harvard, Cambridge, MA*
- MP 638 **Identification of Peptide Sequences using Characteristics of MALDI\_QIT Mass Spectral Data;** Matthew J Kelly; Jingwen Yao; *Shimadzu Research Laboratory (Europe) Ltd, Manchester, UK*
- MP 639 **Bioinformatic Strategies for More Complete and Accurate Identification of Neuropeptides;** Timothy A. Richmond<sup>1</sup>; Geert Baggerman<sup>1</sup>; Tom T. M. Vandekerkhove<sup>2</sup>; Gerben Menschaert<sup>2</sup>; Steven J. Husson<sup>1</sup>; Peter Verleyen<sup>1</sup>; Liliane Schoofs<sup>1</sup>; Wim Van Criekinge<sup>2</sup>; <sup>1</sup>K.U.Leuven, Leuven, Belgium; <sup>2</sup>U.Gent, Gent, Belgium
- MP 640 **Comprehensive Analysis of a Standard Dataset using Protein Prospector;** Peter R Baker; Robert J Chalkley; Katalin F Medzihradzsky; Alma L Burlingame; *UCSF, San Francisco, CA*
- MP 641 **HeXicon: Fully Automated HX-MS Data Analysis with Complete Deuteration Distribution Estimation;** Xinghua Lou<sup>1</sup>; Marc Kirchner<sup>1</sup>; Bernhard Y. Renard<sup>1</sup>; Ullrich Koethe<sup>1</sup>; Bjoern M. Voss<sup>1</sup>; Christian Graf<sup>1</sup>; Judith A. J. Steen<sup>2</sup>; Hanno Steen<sup>2</sup>; Matthias P. Mayer<sup>1</sup>; Fred A. Hamprecht<sup>1</sup>; <sup>1</sup>University of Heidelberg, Heidelberg, Germany; <sup>2</sup>Harvard Medical School/Children's Hospital Boston, Boston, MA
- MP 642 **Peptide Retention Prediction in 2D-HPLC as a Tool for Comparison of MS-MS Search Engines;** Oleg V. Krokhin<sup>1</sup>; Ravi Chandra Dwivedi<sup>2</sup>; Mike Harder<sup>1</sup>; Vic Spicer<sup>1</sup>; Ron Beavis<sup>3</sup>; John A. Wilkins<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, Canada; <sup>3</sup>University of British Columbia, Vancouver, Canada
- MP 643 **The Effect of Peaklist Generation Software on Database Search Results;** Aenoch Lynn; Robert J Chalkley; Peter R Baker; Katalin F. Medzihradzsky; Shenheng Guan; A.L. Burlingame; *University of California San Francisco, San Francisco, CA*
- MP 644 **Interpreting Top-Down Mass Spectra using Spectral Alignment;** Ari Frank<sup>1</sup>; Jim Pesavento<sup>2</sup>; Craig A. Mizzen<sup>3</sup>; Neil L. Kelleher<sup>3</sup>; Pavel Pevzner<sup>1</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Uc Berkeley, Berkeley, CA; <sup>3</sup>University of Illinois, Urbana, IL



## MONDAY POSTERS

- MP 645 **SysPTM – A Systematic Resource for Proteomics Research of Post-Translational Modifications**; Hong Li<sup>1</sup>; Xiaobing Xing<sup>1</sup>; Guohui Ding<sup>1</sup>; Qingrun Li<sup>1</sup>; Chuan Wang<sup>1</sup>; Rong Zeng<sup>1</sup>; Lu Xie<sup>2</sup>; Yixue Li<sup>1</sup>; <sup>1</sup>*Shanghai Institutes For Biological Sciences, Shanghai, China*; <sup>2</sup>*Shanghai Center for Bioinformation Technology, Shanghai, China*
- MP 646 **Improved Identification of Phospho Peptide Spectra from MSn Data**; Flavio Monigatti; Ozlu Nurhan; Judith Steen; Hanno Steen; *Children's Hospital Boston/Harvard Medical School, Boston, MA*
- MP 647 **Evaluation of Normalization Approaches for Label-Free Quantification of Endogenous Peptides**; Kim Kultima; Anna Nilsson; Maria Fálth; Birger Scholz; Per E. Andren; *Uppsala University, Uppsala, Sweden*
- MP 648 **Automation of Extracted Ion Chromatographic Peak Quality Validation to Improve Accuracy of Protein Abundance Calculations in High Throughput Proteomics**; William Nelson; Kert Viele; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- MP 649 **Optimizing and Adding Advanced Features to the DASER-MMF Processing and Search Scheme to Improve Protein Identification within Mixtures**; Ryan Danell<sup>1</sup>; Jun Han<sup>2</sup>; Derek Smith<sup>2</sup>; Christoph Borchers<sup>2</sup>; <sup>1</sup>*Danell Consulting, Greenville, NC*; <sup>2</sup>*University of Victoria-Genome BC Proteomics Center, Victoria, BC, Canada*
- MP 650 **MaXIC-Q: A Fully Automated Generic Tool using Statistical and Computational Methods for Protein Quantitation Based on Isotope Labeling and LC-MS**; Ethan Y. H. Tsui<sup>1</sup>; Yi-Hwa Yian<sup>1</sup>; Chih-Chiang Tsou<sup>1</sup>; Paul C. Y. Yu<sup>1</sup>; Ke-Shiuan Lynn<sup>1</sup>; Wen-Chi Chou<sup>1</sup>; Yi-Ju Chen<sup>2</sup>; Yu-Ju Chen<sup>2</sup>; Ting-Yi Sung<sup>1</sup>; Wen-Lian Hsu<sup>1</sup>; <sup>1</sup>*Institute of Information Science, Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*
- MP 651 **Protein Biomarker Discovery: Added Value of using 3 Different Search Engines on Proteomic MS-MS Datasets Containing Heavily Modified Peptides**; Dominique Vlieghe; Filip D'hondt; Roos Colman; Katleen Verleysen; Koen Kas; Koen De Cremer; *Pronota nv, Zwijnaarde-Ghent, Belgium*
- MP 652 **Sum Formula Generation of Chemical Compounds using Isotope Distribution Abundances and Exact Masses- A comparison of Two Instruments**; Matthias C. Letzel<sup>1</sup>; Zsuzsanna Lipták<sup>1</sup>; Anton Pervukhin<sup>2</sup>; Sebastian Böcker<sup>2</sup>; <sup>1</sup>*University of Bielfeld, Bielefeld, NRW, Germany*; <sup>2</sup>*Universität Jena, Jena, Germany*
- MP 653 **STRAP-Pro: Sparse Profile Reconstruction for LC-MS Peak Identification**; Sebastian Boppel<sup>1</sup>; Bernhard Y. Renard<sup>1</sup>; Marc Kirchner<sup>1</sup>; Judith A.J. Steen<sup>2</sup>; Hanno Steen<sup>2</sup>; Ullrich Koethe<sup>1</sup>; Fred A. Hamprecht<sup>1</sup>; <sup>1</sup>*University of Heidelberg, Heidelberg, Germany*; <sup>2</sup>*Harvard Medical School/Children's Hospital Boston, Boston, MA*
- MP 654 **Further Improving Elemental Composition Determination with FT ICR MS**; Scott Pennino<sup>1</sup>; Fenghe Qiu<sup>1</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>*Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT*; <sup>2</sup>*Cerno Bioscience, Danbury, CT*
- MP 655 **Application of Charge Manipulation Reactions to Improve Deconvolution Algorithm Output**; David E. Erickson; Jian Liu; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- MP 656 **Standard Retention Time Scale for Collaborative Generation of Accurate Mass And Time Tag (AMT) Databases**; Marina L. Pridatchenko<sup>1</sup>; Irina A. Tarasova<sup>1</sup>; Alexey S. Kononikhin<sup>1</sup>; Vilem Guryca<sup>2</sup>; Dmitry A. Tolmachev<sup>1</sup>; Alexander Yu. Agapov<sup>1</sup>; Christopher Adams<sup>3</sup>; Igor A. Popov<sup>5</sup>; Alexander V. Gorshkov<sup>4</sup>; Christophe D. Masselon<sup>2</sup>; Roman A. Zubarev<sup>3</sup>; Eugene N. Nikolaev<sup>5</sup>; Mikhail V. Gorshkov<sup>1</sup>; <sup>1</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russia*; <sup>2</sup>*CEA, Université Joseph Fourier, Grenoble, France*; <sup>3</sup>*Uppsala University, Uppsala, Sweden*; <sup>4</sup>*Institute of Chemical Physics, Moscow, Russia*; <sup>5</sup>*Institute of Biochemical Physics, Moscow, Russia*
- MP 657 **A Statistical Machine Learning Model of Peptide Fragmentation in Tandem Mass Spectrometry Data**; Matthew J Sniatynski; Jason C Rogalski; Juergen Kast; *The Biomedical Research Centre (UBC), Vancouver, Canada*
- MP 658 **Protein Identification and Validation by using Data Independent Scanning and a Protein Identification Repository**; Johannes P.C. Vissers<sup>15</sup>; Lennart Martens<sup>2</sup>; Arthur Moseley<sup>3</sup>; Will Thompson<sup>3</sup>; Stefan Tenzer<sup>4</sup>; James I. Langridge<sup>15</sup>; Scott J. Geromanos<sup>15</sup>; <sup>1</sup>*Waters Corporation, Manchester, UK*; <sup>2</sup>*EMBL-European Bioinformatics Institute, Hinxton, UK*; <sup>3</sup>*Duke University, Raleigh, NC*; <sup>4</sup>*University of Mainz, Mainz, Germany*; <sup>5</sup>*Waters Corporation, Milford, MA*
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- SYSTEMS BIOLOGY: QUANTITATIVE, 659 - 372**
- MP 659 **Global Proteome and Phosphoproteome Profiling of Human Embryonic Stem Cells**; Zhouxin Shen; Pei-Jen Lee; Steven P. Briggs; *UCSD, La Jolla, CA*
- MP 660 **Development of a Malignancy-Specific Proteome for Non-Hodgkin's Lymphoma**; Paul Romesser; David H. Perlman; Mark E. McComb; Douglas V Faller; Catherine E. Costello; Gerald V Denis; *Boston University School of Medicine, Boston, MA*
- MP 661 **Nitrite Systems Biology: Transient Metabonomic Changes and Long-Lasting Cardiac Proteomic, Redox, and Functional Alterations after a Single Spike in Nitrite**; David H. Perlman; Selena Bauer; Giuseppe Infusini; Maria F. Garcia-Saura; Chee C. Lim; Bernadette O. Fernandez; Mark E. McComb; Catherine E. Costello; Martin Feelisch; *Boston University School of Medicine, Boston, MA*
- MP 662 **Ex vivo Pharmacoproteomic and Toxicoproteomic Study of  $\gamma$ -tocopherol in DU-145 Prostate Cancer Cells using iTRAQ Labeling with 2DLC-nESI-MS-MS**; Theodoros I. Roumeliotis<sup>1</sup>; Anastasios Keramidas<sup>2</sup>; Eugenia G. Giannopoulou<sup>3</sup>; Sophia Kossida<sup>1</sup>; Andreas Constantinou<sup>2</sup>; Spiros D. Garbis<sup>1</sup>; <sup>1</sup>*Academy of Athens - Biomedical Foundation, Athens, Greece*; <sup>2</sup>*University of Cyprus, Leukosia, Cyprus*; <sup>3</sup>*University of Peloponnese, Tripoli, Greece*
- MP 663 **Brain Injury Proteome Dynamics**; Daniel E. Hillman; Shankar Sadasivan; Andrew K. Ottens; *McKnight Brain Institute of the University of Flor, Gainesville, FL*
- MP 664 **Quantitative Proteomic Analysis of Bean Plants Infected with Virulent and Avirulent Strains of an Obligate Rust Fungus**; Bret Cooper<sup>1</sup>; Joohyun Lee<sup>1</sup>; Wesley M. Garrett<sup>1</sup>; Jian Feng<sup>2</sup>; Brian Scheffler<sup>1</sup>; Talo Pastor-Corrales<sup>1</sup>; Gary Stacey<sup>3</sup>; Daniel Q. Naiman<sup>2</sup>; <sup>1</sup>*USDA-ARS, Beltsville, MD*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*; <sup>3</sup>*University of Missouri, Columbia, MO*
- MP 665 **Application of Non-Tagged, Global Systems-Based Proteomic Analysis to the Affects of Branched-Chain Fatty Acid Metabolism in Human Prostate Cancer Models**; Colleen Martin<sup>1</sup>; Erik Busby<sup>1</sup>; Gregory J Bowersock<sup>1</sup>; Hector Ramos<sup>2</sup>; James Mobley<sup>1</sup>;



## MONDAY POSTERS

- <sup>1</sup>*University of Alabama At Birmingham, Birmingham, AL;* <sup>2</sup>*Institute for Systems Biology, Seattle, WA*
- MP 666 **Deciphering Deregulated cdc42 Activity by Combining Mass Spectrometry with Enhanced Formaldehyde-Based Affinity-Enrichment and SILAC-Based Proteomic Strategies;** Brent W Sutherland<sup>1</sup>; Juergen Kast<sup>2</sup>; <sup>1</sup>*BioMedical Research Centre, University of British, Vancouver, Canada;* <sup>2</sup>*University of British Columb, Vancouver, BC*
- MP 667 **Examination of Cadmium Tolerance in the Heavy-Metal Accumulator Brassica Juncea using Two Quantitative Proteomic Methods: DIGE and iTRAQ;** Bertram M. Berla; Sophie Alvarez; Jeanne Sheffield; Rebecca E. Cahoon; Joseph M. Jez; Leslie M. Hicks; *Donald Danforth Plant Science Center, St Louis, MO*
- MP 668 **A Quantitative Proteomic Investigation of the Cold Adaptation of the Marine Bacterium *Sphingopyxis alaskensis*;** Lily Ting<sup>1</sup>; Mark Cowley<sup>1</sup>; Mark J. Raftery<sup>2</sup>; Rick Cavichhioli<sup>1</sup>; <sup>1</sup>*University of New South Wales, Randwick, Australia;* <sup>2</sup>*Bioanalytical Mass Spectrometry Facility, Randwick, Australia*
- MP 669 **Characterization of Stress Hormone-Mediated Drug Resistance to Paclitaxel In Breast Cancer using SILAC Combined with High Resolution Mass Spectrometry;** Melanie Flint<sup>1</sup>; Grace Kim<sup>1</sup>; Brian Hood<sup>1</sup>; Jennifer Sutton<sup>2</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>*The University of Pittsburgh Cancer Institute, Pittsburgh, PA;* <sup>2</sup>*ThermoFisher, Cambridge, MA*
- MP 670 **Complete, Mass Spectrometry-Based Proteome Quantitation of Haploid versus Diploid Yeast;** Jesper V. Olsen; Lyris MF De Godoy; Jürgen Cox; Michael L. Nielsen; Nina C. Hubner; Florian Froehlich; Tobias C. Walther; Matthias Mann; *Max-Planck-Institute for Biochemistry, Martinsried, Germany*
- MP 671 **QconCAT Technology Yielding Molecules per Cell; Accurate Quantification of Absolute Enzyme Concentrations in Yeast by LC-MS;** Kathleen M Carroll<sup>1</sup>; Deborah M Simpson<sup>2</sup>; Claire E Eyers<sup>1</sup>; Chris Knight<sup>1</sup>; Douglas B Kell<sup>1</sup>; Robert Beynon<sup>2</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK;* <sup>2</sup>*University of Liverpool, Liverpool, UK*
- MP 672 **A Time-Course Analysis of 3T3-L1 Adipocyte Differentiation using LC-MS<sup>E</sup> Protein Profiling;** Paula Davidson; Sok Kean Khoo; Pam Swiatek; Eric Xu; Gregory Cavey; *Van Andel Research Institute, Grand Rapids, MI*

## TUESDAY POSTERS

INSTRUMENTATION: FTMS, 004 - 020	
TP 004	<b>Ion Accumulation and Storage in a Radiofrequency Octopole Ion Trap;</b> <u>Maria Van Agthoven</u> <sup>1</sup> ; Steve Beu <sup>2</sup> ; Greg T. Blakney <sup>1</sup> ; John Paul Quinn <sup>1</sup> ; Chris Hendrickson <sup>1</sup> ; Alan G. Marshall <sup>1</sup> ; <sup>1</sup> National High Magnetic Fields Laboratory, Tallahassee, FL; <sup>2</sup> S C Beu Consulting, Austin, TX
TP 005	<b>A Compact FT-ICR Mass Spectrometer with a Field-Emission Cathode for Metabolomics and Proteomics Applications;</b> <u>Andrey N. Vilkov</u> ; Chaminda M. Gamage; Vladimir M. Doroshenko; <i>MassTech Inc., Columbia, MD</i>
TP 006	<b>Performance Enhancement for a Hybrid 1 T Permanent Magnet ESI-FTICR Mass Spectrometer using Multiple Frequency Detection;</b> Pavel N. Sagulenko <sup>1</sup> ; Dmitry A. Tolmachev <sup>1</sup> ; Andrey Vilkov <sup>2</sup> ; Vladimir M. Doroshenko <sup>2</sup> ; <u>Mikhail V. Gorshkov</u> <sup>1</sup> ; <sup>1</sup> Institute of Energy Problems of Chemical Physics R, Moscow, Russian Federation; <sup>2</sup> Masstech, Inc., Columbia, MD
TP 007	<b>Simulation Study on Stacked Ring Ion Guide for FT-ICR MS to Reduce Time of Flight Discrimination;</b> <u>Sunghwan Kim</u> ; Myoung-choul Choi; Seungyong Kim; Hyun Sik Kim; Young Hwan Kim; Jong Shin Yoo; <i>Korea Basic Science Institute, Ochang-myun, Korea</i>
TP 008	<b>Broadband Phase Correction of Complex FT-ICR Mass Spectra;</b> <u>Feng Xian</u> <sup>5</sup> ; Chris Hendrickson <sup>1</sup> ; Greg T. Blakney <sup>2</sup> ; Steve Beu <sup>3</sup> ; Alan G. Marshall <sup>4</sup> ; <sup>1</sup> National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup> National Ft-icr Program At Nhmfl, Tallahassee, FL; <sup>3</sup> S C Beu Consulting, Austin, TX; <sup>4</sup> Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>5</sup> Florida State University, Tallahassee, FL
TP 009	<b>Subtle Behaviors in an Electrically Compensated Cylindrical ICR Cell;</b> <u>Adam Brustkern</u> ; Don L. Rempel; Michael L. Gross; <i>Washington University, St. Louis, MO</i>
TP 010	<b>Changes in Ion Kinetic Energy Distribution during Transfer through a Multipole Ion Guide in a Strong Magnetic Field Gradient;</b> <u>Steve Beu</u> <sup>1</sup> ; Chris Hendrickson <sup>2</sup> ; Alan G. Marshall <sup>2</sup> ; <sup>1</sup> S C Beu Consulting, Austin, TX; <sup>2</sup> National High Magnetic Field Laboratory, Tallahassee, FL
TP 011	<b>Application of a "Lock Mass" on an LTQ Orbitrap to Maintain Accurate Mass Assignments throughout Large Biomarker Discovery Studies;</b> <u>Ekaterina G. Devanova</u> <sup>1</sup> ; Wolfgang Metelmann-strupat <sup>2</sup> ; Emile Deleeuw <sup>2</sup> ; Matthew Mazur <sup>1</sup> ; Nathan Yates <sup>1</sup> ; Kai Zhou <sup>1</sup> ; Robert Settlege <sup>1</sup> ; Ronald Hendrickson <sup>1</sup> ; <sup>1</sup> Merck Research Laboratories, Rahway, NJ; <sup>2</sup> Thermo Electron (Bremen) GmbH, Bremen, Germany
TP 012	<b>Improving the Performance of a GC-FT-ICR MS using an External EI/CI Ion Source;</b> <u>Jan E. Szulejko</u> ; Behrooz Zekavat; Touradj Solouki; <i>University of Maine, Orono, ME</i>
TP 013	<b>Trapping Ring Electrode Cell (TREC): A Novel ICR Cell for Ultra-High Sensitivity, Resolution, and Mass Measurement Accuracy;</b> <u>Chad R. Weisbrod</u> ; Nathan K. Kaiser; Gunnar E. Skulason; James E. Bruce; <i>Washington State University, Pullman, WA</i>
TP 014	<b>Synchronization of Ion Activation and Electron Capture Dissociation with Ion Magnetron Motion in an FT-ICR Mass Spectrometer;</b> <u>Victor A. Mikhailov</u> ; Helen Cooper; <i>University of Birmingham, Birmingham, UK</i>
TP 015	<b>Experimental Evidence of Ion Cyclotron Resonance Frequency Modulations Induced by Inhomogeneities of the Trapping Electric Field;</b> <u>Konstantin Aizikov</u> <sup>1</sup> ; Nadezda P. Sargaeva <sup>2</sup> ; Jason J. Cournoyer <sup>3</sup> ; Cheng Lin <sup>2</sup> ; Peter B. O'connor <sup>2</sup> ; <sup>1</sup> BUSM Mass Spectrometry, Boston, MA; <sup>2</sup> Boston University, Boston, MA; <sup>3</sup> Boston University Medical School, Boston, MA
TP 016	<b>Performance of a High-Field Orbitrap Mass Analyzer;</b> <u>Alexander Makarov</u> ; Eduard Denisov; Oliver Lange; Wilko Balschun; Jens Griep-raming; <i>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany</i>
TP 017	<b>A Wire-Ion-Guide ICR Cell for Low-Magnetic-Field FT-ICR MS;</b> <u>Chaminda M. Gamage</u> <sup>1</sup> ; Andrey N. Vilkov <sup>1</sup> ; Kent J. Gillig <sup>2</sup> ; David H. Russell <sup>2</sup> ; Vladimir M. Doroshenko <sup>1</sup> ; <sup>1</sup> MassTech, Inc., Columbia, MD; <sup>2</sup> Texas A&M University, College Station, TX
TP 018	<b>New Hardware for Ultrahigh Resolution and/or Data-Dependent SWIFT Ion Isolation in an FT-ICR Mass Spectrometer;</b> <u>Greg T. Blakney</u> ; Chris Hendrickson; John Paul Quinn; Alan G. Marshall; <i>National ICR Program at NHMFL, Tallahassee, FL</i>
TP 019	<b>A Representation of the Possible Frequency Surfaces for an FTMS Cylindrical Compensable Trap that Facilitates Investigation of Trap Operation;</b> <u>Don L. Rempel</u> ; Adam Brustkern; Michael L. Gross; <i>Washington University, St. Louis, MO</i>
TP 020	<b>External Calibration Strategies for High Magnetic Field FT-ICR MS Coupled with Automatic Gain Control;</b> <u>Tanner M. Schaub</u> <sup>1</sup> ; Chris Hendrickson <sup>2</sup> ; Alan G. Marshall <sup>3</sup> ; <sup>1</sup> National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup> Ion Cyclotron Resonance Prog, Tallahassee, FL; <sup>3</sup> Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL
DIRECT IONIZATION 2, 021 - 036	
TP 021	<b>A Comparative Study of DESI and DART on a Mobile Lab Atmospheric Pressure Ionization Ion Trap MS;</b> <u>Michael Roth</u> ; Mitch Wells; <i>Griffin Analytical Technologies, West Lafayette, IN</i>
TP 022	<b>Profiling Intact Untreated Bacteria <i>in vivo</i> using Desorption Electrospray Ionization (DESI);</b> <u>Isabella Zhang</u> ; Nari Talaty; Anthony Costa; W. Andy Tao; R. Graham Cooks; <i>Purdue University, West Lafayette, IN</i>
TP 023	<b>Heat Transfer and Fluid Dynamic Simulations of a DART-type Ambient Mass Spectrometry Ion Source;</b> <u>Facundo Fernandez</u> ; Glenn A. Harris; <i>Georgia Institute of Technology, Atlanta, GA</i>
TP 024	<b>Development of Automated Protein Identification by nLC EWOD DESI FT-ICR ECD MS-MS;</b> <u>Adam A. Stokes</u> <sup>1</sup> ; Chris Galloway <sup>2</sup> ; Yifan Li <sup>1</sup> ; William Parkes <sup>1</sup> ; Dryden David <sup>1</sup> ; Anthony J. Walton <sup>1</sup> ; Pat Langridge-Smith <sup>1</sup> ; C. Logan Mackay <sup>1</sup> ; <sup>1</sup> The University of Edinburgh, Edinburgh, UK; <sup>2</sup> Bruker Daltonics, Coventry, UK
TP 025	<b>Second Generation DESI Ion Source for FTICR;</b> <u>Vladimir Havlicek</u> <sup>1</sup> ; Gary Kruppa <sup>2</sup> ; Karel Lemr <sup>3</sup> ; Petr Novak <sup>1</sup> ; Marian Hajduch <sup>1</sup> ; Vaclav Kobilha <sup>1</sup> ; Karel Sefcik <sup>1</sup> ; Zoltan Takats <sup>4</sup> ; <sup>1</sup> Institute of Microbiology, Prague 4, Czech Republic; <sup>2</sup> Bruker Daltonics Inc., New York, NY; <sup>3</sup> Palacky University, Olomouc, Czech Republic; <sup>4</sup> Semmelweis University, Budapest, Hungary
TP 026	<b>Enabling More Efficient Ion Collection in Surface Ionization Experiments;</b> <u>Elizabeth A. Crawford</u> ; Brian D. Musselman; Joseph Tice; <i>IonSense, Inc., Saugus, MA</i>

## TUESDAY POSTERS

- TP 027 **HPTLC/DESI-MS Imaging of Tryptic Protein Digests Separated in Two Dimensions**; Sofie P. Pasilis<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; Gary J. Van Berkel<sup>1</sup>; Michael Schulz<sup>2</sup>; Susanne Schorch<sup>2</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*Merck KGaA, Darmstadt, Germany*
- TP 028 **Enhanced Performance of a Liquid Microjunction Surface Sampling Probe using ESI and APCI**; Gary J. Van Berkel<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; Bradley Schneider<sup>2</sup>; Thomas Covey<sup>2</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*Mds Sciex, Concord, ON*
- TP 029 **Laser-Induced Acoustic Desorption/Electrospray Ionization Mass Spectrometry for Directly Characterizing the Biological Compounds in Liquids under Ambient Conditions**; Sy-Chyi Cheng; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, TAIWAN*
- TP 030 **Utility of Reactions in the Source of a Helium Metastable-Beam Open-Air-Ion-Source Mass Spectrometer**; Matthew Curtis; Patrick R. Jones; O. David Sparkman; *University of the Pacific, Stockton, CA*
- TP 031 **Developing reliable measurements in DESI**; Felicia Green<sup>1</sup>; Peter Stokes<sup>2</sup>; Gavin O'Connor<sup>2</sup>; Ian Gilmore<sup>1</sup>; <sup>1</sup>*National Physical Laboratory, Teddington, UK*; <sup>2</sup>*Lgc Limited, Teddington, UK*
- TP 032 **DESI-MS Direct Analysis of Anabolic Steroids Separated with Pressurized Planar Electrochromatography (PPEC)**; Dariusz J. Jannecki<sup>1</sup>; Scott D. Woodward<sup>2</sup>; Justin M. Wiseman<sup>1</sup>; David Nurok<sup>2</sup>; <sup>1</sup>*Prosolia Inc., Indianapolis, IN*; <sup>2</sup>*Department of Chemistry and Chemical Biology IUPUI, Indianapolis, IN*
- TP 033 **Analysis of Continuous-Flow Liquid Samples by Desorption Electrospray Ionization-Mass Spectrometry (DESI-MS)**; Zhixin Jessie Miao; Hao Chen; *Ohio University, Athens, OH*
- TP 034 **Factors Affecting Signal Levels in HPTLC/DESI-MS of Dipeptides and Tryptic Peptides**; Arnon B. Wolk<sup>1</sup>; Sofie P. Pasilis<sup>2</sup>; Vilmos Kertesz<sup>2</sup>; Gary J. Van Berkel<sup>2</sup>; <sup>1</sup>*Colorado College, Colorado Springs, CO*; <sup>2</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 035 **Comparison of Drug Distribution Images from Thin Tissue Sections Obtained using Desorption Electrospray Ionization Tandem Mass Spectrometry and Whole-Body Autoradiography**; Vilmos Kertesz<sup>1</sup>; Gary J. Van Berkel<sup>1</sup>; Marissa Vavrek<sup>2</sup>; Kenneth A. Koeplinger<sup>2</sup>; Bradley B. Schneider<sup>3</sup>; Thomas R. Covey<sup>3</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*Merck Research Laboratories, West Point, PA*; <sup>3</sup>*MDS Sciex, Concord, ON*
- TP 036 **Transmission Mode Sample Introduction for High Throughput Desorption Electrospray Ionization**; Joe Chipuk; Jennifer Brodbelt; *University of Texas, Austin, TX*
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- MALDI SAMPLE PREPARATION, 037 - 066**
- TP 037 **Solvent-Free MALDI TOF/TOF Analysis of Metal Complexes**; John F. Berry<sup>1</sup>; Shu Yao<sup>1</sup>; Michael Nippe<sup>1</sup>; Sergei Dikler<sup>2</sup>; Martha M. Vestling<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Bruker Daltonics, Inc., Billerica, MA*
- TP 038 **Development of Copolymer Planar Microarray Chips (pMALDI) for Mass Spectrometry Based Proteomic and Genomic Analysis**; Alexandr Muck; Alfredo J. Ibanez; Vincentius A. Halim; Ales Svatos; *Max Planck Institute for Chemical Ecology, Jena, Germany*
- TP 039 **Protein Identification by Rapid Acid Hydrolysis using MALDI Matrices: Comparison to Formic Acid Proteolysis**; Elizabeth R. Remily; Hayley Dirscherl; Nupam Mahajan; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- TP 040 **DNA Isolation and Desalting Directly on Stainless Steel MALDI Plate for MS Analysis**; Igor P. Smirnov; Galina E. Pozmogova; Vadim M. Govorun; *Institute of Physico-Chemical Medicine, Moscow, Russian Federation*
- TP 041 **Isolation and Identification of Sulfated Oligosaccharides by MALDI-MS**; Ming Lei; *Indiana University, Bloomington, IN*
- TP 042 **CHCA or DHB? Matrix Selection and Optimization from a Facility Point of View**; Cunjie Zhang; Haixia Zhang; David W. Litchfield; Ken Yeung; Kristina Jurcic; *University of Western Ontario, London, ON, Canada*
- TP 043 **Accurate Mass Measurement of Negative Radical Ions by MALDI-TOFMS: Application to Functionalized Fullerenes**; Shao Zhecheng; Mark F Wyatt; Bridget Stein; Gareth Brenton; *Swansea University, Swansea, UK*
- TP 044 **Surface-Assisted Laser Desorption/Ionization Mass Spectrometry (SALDI-MS) of Low Molecular Weight Organic Compounds using ZnO Nanoparticles**; Ryuichi Arakawa<sup>1</sup>; Hideya Kawasaki<sup>1</sup>; Takehiro Watanabe<sup>1</sup>; Tetsu Yonezawa<sup>2</sup>; <sup>1</sup>*Kansai University, Osaka, Japan*; <sup>2</sup>*The University of Tokyo, Tokyo, Japan*
- TP 045 **Comparison of Solvent-Free and Solvent-Based Sample Preparations for the Analysis of Polyethylene Glycols using Dihydroxybenzoic Acid Isomers in MALDI-MS**; Aera Lee<sup>1</sup>; Hyo-Jik Yang<sup>1</sup>; Jeongkwon Kim<sup>1</sup>; Yongsun Kim<sup>2</sup>; <sup>1</sup>*Chungnam National University, Daejeon, South Korea*; <sup>2</sup>*Hudson Surface Technology, Newark, NJ*
- TP 046 **Atmospheric Pressure Laser Desorption Ionization using Colloidal Graphite and Silver Colloid for the Determination of Plant Metabolites**; David Perdian; Gregg Schieffer; R. Sam Houk; *Iowa State University, Ames, IA*
- TP 047 **High-Sensitivity Liquid UV-MALDI-MS Analysis**; Mark W Towers; Rainer Cramer; *The University of Reading, Reading, UK*
- TP 048 **The Comparison of Pencil Assisted Laser Desorption/Ionisation (PALDI) and MALDI for Quantitative Analysis**; Julie Herniman; G. John Langley; *University of Southampton, Southampton, UK*
- TP 049 **Increased Sensitivity for Neuropeptide Analysis by Atmospheric Pressure Matrix-Assisted Laser Desorption/Ionization with Dynamic On-Chip Purification and Preconcentration/Focusing Targets**; Arti Navare<sup>1</sup>; Marcela Nouzova<sup>3</sup>; Salvador Hernandez<sup>4</sup>; Fernando Noriega<sup>3</sup>; Facundo Fernandez<sup>2</sup>; <sup>1</sup>*Georgia Tech, Atlanta, GA*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>3</sup>*Florida International University, Miami, FL*; <sup>4</sup>*Instituto Nacional de Salud Publica, CISEI, Cuernavaca, Mexico*
- TP 050 **Site-directed Nanoprobe-Based Affinity Mass Spectrometry for Multiple Biomarkers Identification and Quantitation**; Po-Chiao Lin<sup>3</sup>; Shu-Hua Chen<sup>1</sup>; Avijit Kumar Adak<sup>2</sup>; Mu-Lin Chen<sup>2</sup>; Yu-Ju Chen<sup>1</sup>; Chun-Cheng Lin<sup>2</sup>; <sup>1</sup>*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan*; <sup>3</sup>*Taiwan International Graduate Program, Taipei, Taiwan*

## TUESDAY POSTERS

- TP 051 **MALDI-TOF Interrogation of Protein Arrays Facilitated by Patterned Porous Gold Substrates;** Kenyon EVANS-Nguyen; Dwella M Nelson; Sheng-Ce Tao; Heng Zhu; Robert J. Cotter; *Johns Hopkins University, Baltimore, MD*
- TP 052 **Functionalized Magnetic Nanoparticle for Rapid Screening and Structure Determination of Small Molecules by MALDI MS;** Mei-Chun Tseng<sup>1</sup>; Rofe-Amor Obena<sup>1</sup>; Ying-Wei Lu<sup>3</sup>; Po-Chiao Lin<sup>4</sup>; Chia-Chun Chen<sup>2</sup>; Chun-Cheng Lin<sup>3</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>*Institute of Chemistry, Academia Sinica, Taipei, Taiwan;* <sup>2</sup>*Department of Chemistry, Taiwan Normal University, Taipei, Taiwan;* <sup>3</sup>*Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan;* <sup>4</sup>*Taiwan International Graduate Program, Taipei, Taiwan*
- TP 053 **Surface-Assisted Laser Desorption/Ionization on Titania Nanotube Arrays;** Chun-Yuan Lo; Wei-Yu Chen; Yu-Chie Chen; *National Chiao Tung University, Hsinchu, Taiwan*
- TP 054 **Biochips with Antibodies Immobilized via Traceless Cleavable Linkers for Immunoaffinity Mass Spectrometry by MALDI-TOF-MS;** Mark Stolowitz; *Stratos Biosystems LLC, San Jose, CA*
- TP 055 **Sample Preparation and Concentration for MALDI Mass Spectrometry on a Perforated Film or Plate Containing Chromatographic Media;** Mukta M. Shukla<sup>1</sup>; Deepak K. Butani<sup>1</sup>; Ashok K. Shukla<sup>1</sup>; Vladimir M. Doroshenko<sup>2</sup>; Appavu K. Sundaram<sup>2</sup>; <sup>1</sup>*Glygen Corp., Columbia, MD;* <sup>2</sup>*MassTech, Inc., Columbia, MD*
- TP 056 **Combining Tissue Extraction and Off-Line Capillary Electrophoresis-MALDI FTMS for Neuropeptide Analysis using 2,5-Dihydroxybenzoic Acid;** Junhua Wang; Ruibing Chen; Xiaoyue Jiang; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*
- TP 057 **MALDI Sample Preparation - The Use of Biomap MS Imaging to Study Electrospray Sample Deposition;** Andy Mahan; Kevin G. Owens; *Drexel University, Philadelphia, PA*
- TP 058 **Single-Use Composite MALDI Targets for the Analysis of Synthetic Technical Polymers and Natural Polysaccharides;** Wolfgang Winkler<sup>1</sup>; Werner Balika<sup>2</sup>; Peter Hausberger<sup>2</sup>; Harald Kraushaar<sup>2</sup>; Guenter Allmaier<sup>1</sup>; <sup>1</sup>*Vienna Univ. of Technology, Vienna, Austria;* <sup>2</sup>*Sony DADC, Anif, Austria*
- TP 059 **Negative-Mode MALDI Mass Spectrometry for the Analysis of Pigments using Tetrathiafulvalene as a Matrix;** Daiki Asakawa; Lee Chuin Chen; Kenzo Hiraoka; *University of Yamanashi, Kofu, Japan*
- TP 060 **Novel 3-D Sample Plate using Monolithic Capture Media in Collimated-Hole Structures for Interfacing High Capacity Separations with MALDI-TOF;** Stephen J. Hattan; Marvin Vestal; *Virgin Instruments Corporation, Sudbury, MA*
- TP 061 **Vacuum MALDI Linear TOF Mass Spectrometry of High Molecular Mass Nanoparticles and Proteins;** Martina Marchetti<sup>1</sup>; Christian Laschober<sup>1</sup>; Ryan Wenzel<sup>2</sup>; Emmanuel Raptakis<sup>3</sup>; Guenter Allmaier<sup>1</sup>; <sup>1</sup>*Vienna University of Technol, Vienna, Austria;* <sup>2</sup>*CovalX, Zuerich, Switzerland;* <sup>3</sup>*Shimadzu Biotech, Manchester, UK*
- TP 062 **Titania Micropowder and Nanoparticles for In-Vitro Analysis and In-Situ Imaging of Phospholipids by MALDI-MS;** Pawel Lorkiewicz; Marta C. Yappert; *University of Louisville, Louisville, KY*
- TP 063 **Comparison of Deposition Methods for MALDI Mass Analysis of Intact Proteins and Tryptic Digests;** Brent Hilker<sup>3</sup>; Kevin Clifford<sup>3</sup>; Drew Sauter<sup>2</sup>; Julie Harmon<sup>3</sup>; John Koomen<sup>1</sup>; <sup>1</sup>*H. Lee Moffitt Cancer Center, Tampa, FL;* <sup>2</sup>*Nanoliter, Llc, Henderson, NV;* <sup>3</sup>*University of South Florida, Tampa, FL*
- TP 064 **Electrochromatographic Separation of a Model Naturally Occurring Peptide from Multiple Complex Biological Samples for Analysis and Quantification by MALDI-TOF;** Benjamin Katz; *Protein Discovery, Inc., Knoxville, TN*
- TP 065 **The Role of Hydrated Water in MALDI with Serine-Doped CHCA;** Mitsuo Takayama; Takashi Nishikaze; *Yokohama City University, Yokohama, Japan*
- TP 066 **Comparison of Approaches in Improving MALDI MS Sensitivity;** Lijuan Peng; Zaneer Segu; Joseph Mathai; Gary R. Kinsel; *Southern Illinois University Carbondale, Carbondale, IL*
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- MALDI / TANDEM MS, 067 - 076**
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- TP 067 **NanoLC-MALDI Orbitrap Coupling Evaluation: An Attempt to Optimize the Acquisition Strategy;** Joelle Vinh; Iman Haddad; Sega Ndiaye; Anne-Marie Hesse; Jean Rossier; *CNRS UMR7637/ESPCI ParisTech, Paris, France*
- TP 068 **MALDI-Tandem Mass Spectrometric Analysis of Painted Works of Art;** Michael P. Napolitano<sup>1</sup>; Julie Arslanoglu<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL;* <sup>2</sup>*The Metropolitan Museum of Art, New York, NY*
- TP 069 **MALDI-Produced Ions Analyzed by Higher Energy Collisional Dissociation (HCD) using an Linear Ion Trap - Orbitrap Mass Analyzer;** Thomas Moehring<sup>1,2</sup>; Rosa Viner<sup>1,2</sup>; Viatcheslav V. Kovtoun<sup>1,2</sup>; Huy Bui<sup>1,2</sup>; George Stafford<sup>1,2</sup>; Julian J Phillips<sup>1,2</sup>; Stevan R. Horning<sup>1,2</sup>; Kerstin Strupat<sup>1,2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 070 **Improving the Efficiency of LC-MS-MS Peptide Sequencing using a vMALDI-LTQ Linear Ion Trap Mass Spectrometer;** Mark Wall; Alan A. Doucette; *Dalhousie University, Halifax, Canada*
- TP 071 **Analysis of Mitotic Phosphorylation Sites in the Nuclear Pore Complex using a MALDI-LTQ Orbitrap Mass Spectrometer;** Justin Blehrow<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Rosa Viner<sup>2</sup>; Joseph Glavy<sup>1</sup>; <sup>1</sup>*Stevens Institute of Tech., Hoboken, NJ;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 072 **Rapid Detection and Identification of Pathogenic Neisseria by Atmospheric Pressure MALDI MS-MS;** Seshu Gudlavalleti<sup>1</sup>; Appavu Sundaram<sup>2</sup>; Jane Razumovski<sup>1</sup>; Vladimir M. Doroshenko<sup>2</sup>; <sup>1</sup>*Science and Engineering Serv, Columbia, MD;* <sup>2</sup>*Masstech, Inc., Columbia, MD*
- TP 073 **Modified Silver Nanoparticle as a Hydrophobic Affinity Probe for Analysis of Peptides and Proteins by using MALDI Mass Spectrometry;** Hui-Fen Wu; Kamlesh Shrivastava; *Chemistry department, National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TP 074 **Direct Analyses of UV Absorbents in Polymer Film by MALDI-TOF MS-MS in Comparison with ESI and APPI MS-MS Analyses;** Shouxun Zhao; Bogdan Piatek; Huayi Tong; *Ciba Corp, Tarrytown, NY*
- TP 075 **Formation of Gas Phase Silver Anions and Silver-Iodide Radical Anions by Laser Ablation;** Timothy Dunne; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*

## TUESDAY POSTERS

- TP 076 **A Comparison of LC-MALDI and LC-ESI for the Analysis of a Highly Complex Mixture of Peptides;** Keith Ashman; Mitchell Isaacs; Xiaomin Song; Chris Clark; Lewis Adler; *APAF, Sydney, Australia*
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- ECD/ETD/EDD, 077 - 090**
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- TP 077 **Data-Dependent Supplemental Activation to Enhance ETD Efficiency for High M/Z Precursors Regardless of Charge;** Aaron Ledvina; Graeme McAlister; Joshua J. Coon; *The University of Wisconsin, Madison, WI*
- TP 078 **High-Energy Electron Transfer Dissociation (ETD) on Collision with Alkali Metal Targets;** Shigeo Hayakawa<sup>1</sup>; Mami Hashimoto<sup>1</sup>; Hirofumi Nagao<sup>2</sup>; Michisato Toyoda<sup>2</sup>; <sup>1</sup>*Osaka Prefecture Univ., Sakai, Osaka, Japan*; <sup>2</sup>*Osaka University, Toyonaka, Japan*
- TP 079 **Effect of Ion Activation on Radical Driven Reactions in Electron Capture Dissociation;** Cheng Lin; Jason J Cournoyer; Xiaojuan Li; Peter B. O'Connor; *Boston University School of Medicine, Boston, MA*
- TP 080 **Electron Detachment Dissociation in a Hybrid Radio Frequency Linear Ion Trap/Time of Flight Mass Spectrometer;** Travis F. Greene<sup>1</sup>; Jared M. Bushey<sup>1</sup>; Takashi Baba<sup>2</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*University of North Carolina and Hitachi, Ltd., Tokyo, Japan*
- TP 081 **Modeling of Metastable Atoms and Protonated Peptide Ions Interaction;** Vadym Berkout<sup>2</sup>; Sergey Kryuchkov<sup>1</sup>; Vladimir M. Doroshenko<sup>2</sup>; <sup>1</sup>*University of Calgary, Calgary, Canada*; <sup>2</sup>*MassTech, Inc., Columbia, MD*
- TP 082 **Electron Transfer Dissociation Facilitates the Measurement of Deuterium-Incorporation into Selectively Labeled Peptides with Single Residue Resolution;** Martin Zehl; Kasper D. Rand; Ole N. Jensen; Thomas J. D. Jørgensen; *University of Southern Denmark, Odense, Denmark*
- TP 083 **ECD within a Linear Magnetic (no-RF) Cell;** Valery G. Voinov; Max L. Deinzer; Douglas F. Barofsky; *Oregon State University, Corvallis, OR*
- TP 084 **Multistage Electron Capture Dissociation for the Investigation of Charge Reduced Peptide Ions;** Takashi Baba<sup>1</sup>; Jared Bushey<sup>2</sup>; Gary L. Glish<sup>2</sup>; <sup>1</sup>*University of North Carolina and Hitachi, Ltd., Tokyo, Japan*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*
- TP 085 **Electron Capture/Transfer Dissociation of Alpha-Helical Peptides: Characteristic Features and Interpretation;** Yury O. Tsybin<sup>1</sup>; Hisham Ben Hamidane<sup>1</sup>; Aleksey Vorobyev<sup>1</sup>; Adrien Schmid<sup>1</sup>; Oleg Yu. Tsybin<sup>2</sup>; Clemence Corminbeuf<sup>1</sup>; Vincent Pouthier<sup>3</sup>; <sup>1</sup>*EPFL (Ecole Polytechnique Federale de Lausanne), Lausanne, Switzerland*; <sup>2</sup>*State Polytechnical University, Saint-Petersburg, Russian Federation*; <sup>3</sup>*Universite de Franche-Comte, Besancon, France*
- TP 086 **Hot Electron Capture Dissociation in a Linear Radio Frequency Quadrupole Ion Trap;** Naomi Manri<sup>1</sup>; Hiroyuki Satake<sup>1</sup>; Takashi Baba<sup>1</sup>; Kuriko Yamada<sup>2</sup>; Hiroaki Nakagawa<sup>2</sup>; Kisaburo Deguchi<sup>2</sup>; <sup>1</sup>*Hitachi, Ltd., Kokubunji, Japan*; <sup>2</sup>*Univ, Hokkaido, Sapporo, Japan*
- TP 087 **ECD, EDD and CID of Polyamidoamine (PAMAM) Dendrimer Ions with Amino, Amidoethanol and Sodium Carboxylate Surface Groups;** Malgorzata A Kaczorowska; Helen Cooper; *University of Birmingham, Birmingham, UK*
- TP 088 **Electron Current and Kinetic Energy Effects on the Electron Detachment Dissociation of Glycosaminoglycan Carbohydrates;** Franklin E. Leach III<sup>1</sup>; Jeremy Wolff<sup>1</sup>; Tatiana Laremore<sup>2</sup>; Robert J. Linhardt<sup>2</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*Rensselaer Polytechnic Institute, Guilderland, NY*
- TP 089 **Evaluation of Electron Transfer Dissociation in a Hybrid Quadrupole-Hexapole Fourier Transform Ion Cyclotron Resonance Mass Spectrometer;** Desmond A. Kaplan<sup>1</sup>; Ralf Hartmer<sup>2</sup>; Michael L. Easterling<sup>1</sup>; Jiong Yang<sup>1</sup>; Melvin A. Park<sup>1</sup>; <sup>1</sup>*Bruker Daltonics, Inc., Billerica, MA*; <sup>2</sup>*Bruker Daltronik, Bremen, Germany*
- TP 090 **Electron Transfer Dissociation of iTRAQ Labeled Peptide Ions;** Hongling Han<sup>1</sup>; Darryl J. Pappin<sup>2</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Applied Biosystems, Foster City, CA*
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- EMERGING CONTAMINANTS 1, 091 - 109**
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- TP 091 **Characterization of Dissolved Protein in Seawater using LTQ-FT MS;** Yuchen Lu; Brent, Reschke; Kathleen Kelly; Aaron Timperman; *West Virginia University, Morgantown, WV*
- TP 092 **MALDI-ToF MS Used for Fast Detection of Legionella Species in Water Supplies: A New Rapid Response to Legionellosis;** Xaviera Pennanec; *Laboratoire CGI, Ploemeur, France*
- TP 093 **Quantitation of Perchlorate, Nitrate, Thiocyanate and Iodide in Infant Urine from Disposable Diapers;** Samaret Otero; Liza Valentin-Blasini; Benjamin Blount; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 094 **Integrated Disinfection By-Products Mixtures Research: Results from the Four Lab Study;** Jane Ellen Simmons<sup>1</sup>; Susan Richardson<sup>2</sup>; Michael G. Narotsky<sup>1</sup>; Larry D. Claxton<sup>1</sup>; E. Sidney Hunter III<sup>1</sup>; Richard J. Miltner<sup>1</sup>; Jonathan Pressman<sup>1</sup>; Thomas F. Speth<sup>1</sup>; Glenn Rice<sup>1</sup>; Linda K. Teuschler<sup>1</sup>; Stuart W. Krasner<sup>4</sup>; Howard S. Weinberg<sup>3</sup>; <sup>1</sup>*U.S. EPA, RTP, NC, NC*; <sup>2</sup>*Us Epa, Athens, GA*; <sup>3</sup>*University of North Carolina, Chapel Hill, NC*; <sup>4</sup>*Metropolitan Water District of Southern California, LaVerne, CA*
- TP 095 **Multidimensional Analysis of Environmental Samples: Gas Chromatography/Fourier Transform Ion Cyclotron Resonance Mass Spectrometry and Ab-Initio Calculations;** Indira Silwal; Jayendran C. Rasaiah; Touradj Solouki; *University of Maine, Orono, ME*
- TP 096 **Evidences of the Existence of Multiple Charged Constituents in Suwannee River Dissolved Organic Matter;** Andras Gaspar<sup>15</sup>; Erast Kunenkov<sup>3</sup>; Richard Lock<sup>2</sup>; Michael Desor<sup>4</sup>; Irina Perminova<sup>3</sup>; Philippe Schmitt-kopplin<sup>15</sup>; <sup>1</sup>*Helmholtz Zentrum münchen, Neuherberg, Germany*; <sup>2</sup>*Waters Corporation, Manchester, England*; <sup>3</sup>*Lomonosov Moscow State University, Moscow, Russia*; <sup>4</sup>*Waters, Eschborn, Germany*; <sup>5</sup>*Helmholtz Zentrum München, Neuherberg, Germany*
- TP 097 **Characterization of Natural Organic Matter in Raw Water with QTOF Mass Spectrometry;** Douglas B. Mawhinney; Fernando L. Rosario-Ortiz; Seungyun Baik; Brett J. Vanderford; Shane A. Snyder; *Southern Nevada Water Authority, Las Vegas, NV*
- TP 098 **Illicit Drugs and their Metabolites as Environmental Contaminants;** Roberto Fanelli; Sara Castiglioni; Chiara Chiabrando; Renzo Bagnati; Ettore Zuccato; *Mario Negri Institute, Milano, Italy*
- TP 099 **The Silica Speciation by FAB-MS for the Uptake to the Diatom: Photic Layer of Tokyo Bay;** Miho Tanaka<sup>1</sup>; Kazuya Takahashi<sup>2</sup>; Masao Nemoto<sup>1</sup>; Hideki Nagashima<sup>1</sup>; <sup>1</sup>*Tokyo University of Marine Science and*

## TUESDAY POSTERS

- Technology, Minato-ku, Tokyo, Japan; <sup>2</sup>Riken, Wako-shi, Saitama, Japan*
- TP 100 **Characterization of Organic Matter in a Waste Landfill Leachate;** Laurent Badoil<sup>1</sup>; David Benanou<sup>1</sup>; Jean-claude Tabet<sup>2</sup>; Denis Lesage<sup>2</sup>; <sup>1</sup>Anjou Recherche, Maisons-Laffitte, France; <sup>2</sup>University Paris Vi (upmc), Paris, France
- TP 101 **Detection of Cyanobacterial Peptide Toxins Microcystins in Exposed Animal Tissues by the MMPB Method and LC-MS-MS;** Milla-Riina Neffling<sup>1</sup>; Emilie Lance<sup>2</sup>; Jussi AO Meriluoto<sup>1</sup>; <sup>1</sup>Abo Akademi University, Turku, Finland; <sup>2</sup>University of Rennes, Rennes, France
- TP 102 **Quantitative Analysis of Perchlorate by Ion Chromatography MS-MS;** Mathew Johnson<sup>3</sup>; Jay Gandhi<sup>2</sup>; Sheher Mohsin<sup>1</sup>; <sup>1</sup>Agilent Technologies, Schaumburg, IL; <sup>2</sup>Metrohm-peak Llc, Houston, TX; <sup>3</sup>USEPA Region 6, Houston, TX
- TP 103 **Determination of Haloacetic Acids in Drinking Water using Liquid Chromatography / Tandem Mass Spectrometry;** Shueh-Ni Chang; Chia-Yang Chen; National Taiwan University, Taipei City, Taiwan
- TP 104 **Determination of Macrocytic Trichothecenes in a Water Damaged House by LC-MS;** Masahiko Takino<sup>1</sup>; Yoshiko Sugita-Konishi<sup>2</sup>; James J Pestka<sup>3</sup>; <sup>1</sup>Agilent Technologies, Hachioji-shi, JAPAN; <sup>2</sup>National Institute of Health Sciences, Tokyo, Japan; <sup>3</sup>Michigan State University, East Lansing, MI
- TP 105 **Characterization of Dissolved Organic Matter in Marine Pore Waters by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Frauke Schmidt<sup>3</sup>; Boris Koch<sup>2</sup>; Marcus Elvert<sup>3</sup>; Matthias Witt<sup>1</sup>; Kurt Haag<sup>4</sup>; Kai-Uwe Hinrichs<sup>3</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Alfred-Wegener Institute, Bremerhaven, Germany; <sup>3</sup>Bremen University, Bremen, Germany; <sup>4</sup>Bruker Daltonics, Shoreline, WA
- TP 106 **HPLC-MS-MS Determination of Nine N-Nitrosamines in Thirty-Nine North American Drinking Water Systems;** Jessica M. Boyd<sup>1</sup>; Yuan-yuan Zhao<sup>1</sup>; Feng Qin<sup>1</sup>; Patrick Levallois<sup>3</sup>; Susan Richardson<sup>2</sup>; Xing-fang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada; <sup>2</sup>US EPA, Athens, GA; <sup>3</sup>Institut National de Sante Publique du Quebec, Quebec, Canada
- TP 107 **Determination of Perchlorate in River by Electrospray Ionization Tandem Mass Spectrometry Following Ion-Pair Hollow-Fiber Liquid-Phase Microextraction;** Wen-Tsen Chen; Hsin-Chang Chen; Wang-Hsien Ding; National Central University, Chung-li, Taiwan
- TP 108 **The Influence of Substrate Levels, Temperature, pH, Inorganic Salts on the Yield of Disinfection By-Products in Aquatic Chlorination of Anisole;** Olga Polyakova; Alina Bobrel; Albert T. Lebedev; Moscow State University, Moscow, Russian Federation
- TP 109 **Simultaneous Analysis of Iodoacetic Acids, Bromoacetic Acids and Other Halogenated Compounds in Water using Ion Chromatography/Inductively Coupled Plasma/Mass Spectrometry (IC/ICP/MS);** Honglan Shi<sup>1</sup>; Craig D. Adams<sup>2</sup>; <sup>1</sup>Missouri S&T/ERC, Rolla, MO; <sup>2</sup>Missouri University of Science and Technology, Rolla, MO
- Borum; Timothy Garrett; Richard A. Yost; *University of Florida, Gainesville, FL*
- TP 111 **Laser Desorption 7.87 eV Postionization Mass Spectrometry of Cysteine-Containing Peptides by Pyrenyl Tagging;** Luke Hanley<sup>2</sup>; Artem Akhmetov<sup>2</sup>; Gerald Gasper<sup>2</sup>; Jerry F. Moore<sup>1</sup>; <sup>1</sup>Massthink LLC, Naperville, IL; <sup>2</sup>University of Illinois at Chicago, Chicago, IL
- TP 112 **Concise Representation of MS Images by Probabilistic Latent Semantic Analysis;** Michael Hanselmann<sup>1</sup>; Bernhard Y. Renard<sup>1</sup>; Marc Kirchner<sup>1</sup>; Andriy Kharchenko<sup>2</sup>; Lennaert Klerk<sup>2</sup>; Ullrich Koethe<sup>1</sup>; Ron M.a. Heeren<sup>2</sup>; Fred Hamprecht<sup>1</sup>; <sup>1</sup>University of Heidelberg, Heidelberg, Germany; <sup>2</sup>Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands
- TP 113 **Enhanced Interpretation of Imaging Mass Spectrometry Data using Non-negative Matrix Factorization;** Raf Van de Plas; Bart Vanluyten; Bart De Moor; Etienne Waelkens; *K.U.Leuven, Leuven, Belgium*
- TP 114 **Improvement on Sensitivity of High-Spatial-Resolution Mass Imaging Based on MALDI-QIT-TOF-Type Mass Spectrometer;** Osamu Furuhashi; Hideaki Izumi; Takahiro Harada; Kengo Takeshita; Kiyoshi Ogawa; Yoshikazu Yoshida; *Shimadzu Corporation, Soraku-gun, Japan*
- TP 115 **Laser Desorption 7.87 eV Postionization Mass Spectrometry of Antibiotics in *S. epidermidis* Bacterial Biofilms;** Gerald Gasper<sup>3</sup>; Ross Carlson<sup>2</sup>; Artem Akhmetov<sup>3</sup>; Jerry F. Moore<sup>1</sup>; Luke Hanley<sup>3</sup>; <sup>1</sup>MassThink LLC, Naperville, IL; <sup>2</sup>Montana State University, Bozeman, MT; <sup>3</sup>University of Illinois at Chicago, Chicago, IL
- TP 116 **Enabling Multivariate Exploration of Large Imaging Mass Spectrometry Data Sets using Discrete Wavelet Transform;** Raf Van de Plas; Bart De Moor; Etienne Waelkens; *K.U.Leuven, Leuven, Belgium*
- TP 117 **Hierarchical Clustering: A New Approach using Unsupervised Classification of MALDI Imaging Data for Cancer Biomarker Detection in Tissue;** Axel Walch<sup>3</sup>; Sören-Oliver Deininger<sup>1</sup>; Shi Gongyi<sup>2</sup>; Michael Becker<sup>1</sup>; Martin Schürenberg<sup>1</sup>; Arne Fütterer<sup>1</sup>; Marc Gerhard<sup>1</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Freemont, CA; <sup>3</sup>GSF-Institut für Pathologie, Munich, Germany
- TP 118 **Peak Intensity Weighted PCA for the Multivariate Exploration of Tissue via Imaging Mass Spectrometry;** Raf Van de Plas; Bart De Moor; Etienne Waelkens; *K.U.Leuven, Leuven, Belgium*
- TP 119 **Enhancements in Analysis and Imaging of Small Molecules in Tissue by MALDI-MS Afforded by Prolonged Sample Storage at Reduced Pressure;** Hazel R Dickson; Josephine Bunch; Cameron W. Mcleod; *University of Sheffield, Sheffield, UK*
- TP 120 **Automatic Spotting Solution for MALDI Imaging: Process Optimization and New Developments;** Julien Franck<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Mohamed El-Ayed<sup>1</sup>; David Bonne<sup>1</sup>; Alan Barnes<sup>2</sup>; Isabelle Fournier<sup>1</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>University of Lille 1, Fre-cnrs 2933, Ifr 147, Villeneuve D'ascq Cedex, France; <sup>2</sup>Shimadzu Biotech, Manchester, UK
- TP 121 **Molecular Imaging of Drug-eluting Coronary Stents (DES) by MALDI-ToF Aspects of Method Development;** Gyorgy Vas; Karin Balss; Lori Alquier; Cynthia Maryanoff; Gail Reed; *Cordis CPD, Spring House, PA*
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- IMAGING MS INSTRUMENTATION AND SAMPLE PREPARATION, 110 - 128**
- TP 110 **Localization of Endogenous Acetylcarnitine in Rat Brain Tissue using Imaging Mass Spectrometry with Porphyrins as a MALDI Matrix;** David Pirman; Peggy

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- TP 122 **A Comparison of Mass Spectrometry Imaging using Desorption Electrospray, MALDI and ToF-SIMS;** Peter Stokes<sup>1</sup>; Felicia Green<sup>2</sup>; Chris Hopley<sup>1</sup>; Ian Gilmore<sup>2</sup>; Gavin O'Connor<sup>1</sup>; <sup>1</sup>LGC Limited, Teddington, UK; <sup>2</sup>National Physical Laboratory, Teddington, UK
- TP 123 **New System for Efficient and Rapid Encoding of Mass Spectral Data for Interactive Visualization of 2D and 3D Hyperspectral Images;** Alex Henderson<sup>1</sup>; Stephen E. Reichenbach<sup>3</sup>; Qingping Tao<sup>2</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>GC Image, LLC, Lincoln, NE; <sup>3</sup>University of Nebraska – Lincoln, Lincoln, NE
- TP 124 **ToF Instrumentation for High Speed MALDI Imaging;** Mark D. Mills; Vic Parr; David Evason; Alexis Polley; Steve Thompson; *Scientific Analysis Instrument, Manchester, UK*
- TP 125 **Adapting the Stretch Sample Method from Tissue Profiling to Imaging;** Tyler A Zimmerman; Eric Monroe; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 126 **Improving Analysis Time in MALDI-MS Imaging by Rastering Acquisition;** Douglas A. Simmons; Adam Lau; *MDS Analytical Technologies, Concord, Canada*
- TP 127 **Femtosecond Laser Imaging Mass Spectrometry;** Yves Coello; Tissa C Gunaratne; Marcos Dantus; *Michigan State University, East Lansing, MI*
- TP 128 **High Mass, Low Saturation Detectors in Imaging Mass Spectrometry;** Liam McDonnell; Alexandra van Remoortere; André M. Deelder; René J.M. van Zeijl; *LUMC, Leiden, Netherlands*
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- HIGH THROUGHPUT ANALYSIS / ROBOTICS, 129 - 155**
- TP 129 **Adulteration of Soybean Biodiesel and Petrodiesel with Soybean Oil and Quantification of Their Mixtures by ESI(+)-MS Fingerprinting;** Rodrigo Ramos Catharino<sup>1</sup>; Patricia Verardi Abdelnur<sup>1</sup>; Camila M. Garcia<sup>2</sup>; Sérgio A. Saraiva<sup>1</sup>; Ulf Schuchardt<sup>2</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>Thomson Mass Spectrometry Laboratory - Unicamp, Campinas, Brazil; <sup>2</sup>Phoenix Laboratory - Unicamp, Campinas, Brazil
- TP 130 **What's New with the 5 Pump, 4 Detector LC-MS Based Purification Systems at Lundbeck;** Xu Zhang; David P Budac; Mark J. Hayward; *Lundbeck Research USA, Stockton, NJ*
- TP 131 **Solid Phase Extraction - Liquid Chromatography (SPE-LC) Interface for Automated Peptide Separation and Identification by Tandem Mass Spectrometry;** O.B. Hoerning; M.B. Andersen; O. Vorm; *Proxeon A/S, Odense, Denmark*
- TP 132 **Fingerprint Analysis of Intact Cells using a Microfluidic Chip Coupled with MALDI-TOF MS;** Jeonghoon Lee; Steven A. Soper; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- TP 133 **Poster : Affinity Selection Mass Spectrometry (ASMS) in Oncology Drug Discovery to Identify Small Molecule Inhibitors of Novel Target Proteins;** Andrew Cooke; Andrew Cooke; *OSI Pharmaceuticals, Boulder, CO*
- TP 134 **Walk Up UPLC-MS for Rapid High Quality Sample Analysis in Support of Discovery Chemistry;** Bethanne Warrack<sup>1</sup>; Dieter Drexler<sup>2</sup>; Chiuwa Emily Luk<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb Co, Princeton, NJ; <sup>3</sup>Bristol Myers Squibb, Wallingford, CT
- TP 135 **An Integrated Approach for an Ultra-High Throughput On-Line SPE-MS-MS System and its Applications to ADME Assays;** Rongda Xu; Marianne T. Quintos; Melinda Manuel; Joshua E. Cramlett; Kheng B. Lim; Daniel B. Kassel; *Takeda San Diego, Inc., San Diego, CA*
- TP 136 **Understanding the Use of Temperature Regulation to Optimize Mass Transfer in Fast Gradient Reversed Phase Liquid Chromatography;** Mark J. Hayward; *Lundbeck Research USA, Stockton, NJ*
- TP 137 **Two Dimensional Achiral/Chiral LC/LC-MS System with Multiple Mass-trigger Functions for Streamlined Purification of Enantiomeric Compounds;** Yinong Zhang; Lu Zeng; Rongda Xu; Daniel B. Kassel; *Takeda San Diego, Inc., San Diego, CA*
- TP 138 **Direct Coupling of Ion-Exchange High-Performance Liquid Chromatography (HPLC) with Mass Spectrometry (MS) Utilizing BioTrove's RapidFire™ Technology (RF);** Maxine Jonas<sup>1</sup>; Nikunj Parikh<sup>1</sup>; Peter T. Rye<sup>1</sup>; Michael Frank<sup>2</sup>; Kelly M. Schermerhorn<sup>1</sup>; Lauren Frick<sup>1</sup>; William A. LaMarr<sup>1</sup>; Can "Jon" Ozbal<sup>1</sup>; <sup>1</sup>BioTrove, Inc., Woburn, MA; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- TP 139 **Automated Purification and Sample Preparation Robot for Lab and Portable Mass Spec Analysis;** David P Fries; Brian P Gregson; Stan Ivanov; Matthew Smith; James Wilson; *U South Florida, St Petersburg, FL*
- TP 140 **Enhancing Open Access MS -- Accurate Mass Measurement and Rapid Resolution;** Timothy J. Blake; *AstraZeneca, Wilmington, DE*
- TP 141 **Evaluation of Molecular Isotope Patterns for Elemental Composition Identification on a Unit Resolution Quadrupole Mass Spectrometer;** Maria Cristina A. Dancel<sup>1</sup>; David H. Powell<sup>1</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Cerno Bioscience, Danbury, CT
- TP 142 **Chemical ID: Automated High-Throughput Formula Determination and Confirmation;** Catherine Stacey<sup>2</sup>; Sebastian Goetz<sup>1</sup>; Thomas Zey<sup>1</sup>; Jens Vagts<sup>1</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA
- TP 143 **Optimizing LC-MS-MS System Performance for High Throughput Analysis of Affinity Isolated Protein Complexes;** Keiji G. Asano; Patricia K. Lankford; Gregory B. Hurst; W. Hayes McDonald; *Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 144 **Determination of Fast Enzyme Kinetics using RapidFire Mass High-Throughput Spectrometry (RF-MS);** Can "Jon" Ozbal<sup>1</sup>; Maxine Jonas<sup>1</sup>; Michael Frank<sup>2</sup>; Nikunj Parikh<sup>1</sup>; Peter T. Rye<sup>1</sup>; Kelly M. Schermerhorn<sup>1</sup>; Lauren Frick<sup>1</sup>; William A. LaMarr<sup>1</sup>; <sup>1</sup>BioTrove, Inc., Woburn, MA; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- TP 145 **Cassette Analysis of in vivo Pharmacokinetic Studies in Rat using UPLC-MS-MS;** Jessie Dahlström<sup>1</sup>; Tjerk Bueters<sup>1</sup>; Kristine Kvalvågnaes<sup>1</sup>; Sveinn Briem<sup>1</sup>; Ingvar Betnér<sup>2</sup>; <sup>1</sup>Astrazeneca, Stockholm, Sweden; <sup>2</sup>Waters Corporation, Sollenlunda, Sweden
- TP 146 **Fast Drug-Protein Binding Screening using Affinity Chromatography-Tandem Mass Spectrometry;** Yunsheng Hsieh; Fangbiao Li; Walter Korfmacher; *Schering-Plough, Kenilworth, NJ*
- TP 147 **Increasing Sample Throughput of NanoLC-MS through Hadamard Transform;** Sau Lan Tang Staats; Andris Suna; Art Fogiel, Jr.; *Phoenix S and T, Inc, Elkton, MD*

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- TP 148 **Analysis of Impurities and Degradants using a New Open-Access LC-MS-MS Software System in a Pharmaceutical Development Environment;** Larry M. Mallis<sup>1</sup>; Byron Kieser<sup>2</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Applied Biosystems, Concord, ON
- TP 149 **Fully Automated Bioanalytical Sample Preparation for LC-MS-MS Assays with Tecan - from Tecan Programming to Sample Extraction;** Huidong Gu; Yuzhong Deng; Wenying Jian; Yunlin Fu; Duxi Zhang; Steve E. Unger; Mark E. Arnold; *Bristol-Myers Squibb, Princeton, NJ*
- TP 150 **Development of a High Throughput Screening Method for the Detection of Glycosylated Flavonoids by DESI;** Ayanna U. Jackson<sup>1</sup>; Marcela Neffiu<sup>1</sup>; Sean R. Werner<sup>2</sup>; Sheran Oradu<sup>1</sup>; John A. Morgan<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>2</sup>School of Chemical Engineering, Purdue University, West Lafayette, IN
- TP 151 **Rapid Proteomic Sample Preparation for Sensitive, Reproducible, High-throughput MALDI-MS Analyses;** Vivek N. Bhatia; David H. Perlman; Mark E. McComb; Catherine E. Costello; *Boston Univ. School of Medicine, Boston, MA*
- TP 152 **A Turbulent-Flow LC-MS Method to Measure Nicotine and Cotinine in Plasma and Urine Samples;** Joseph Di Bussolo<sup>1</sup>; Hidehiko Azumaya<sup>2</sup>; Felix Boakye-Agyeman<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, West Chester, PA; <sup>2</sup>Pennsylvania Equine Toxicology & Research Lab, West Chester, PA; <sup>3</sup>Mayo Clinic Dept. of Laboratory Medicine, Rochester, PA
- TP 153 **High Throughput LC-MS-MS Assay to Support Cassette Dosing PK Screening from Automated Method Development to Electronic Data Archiving;** Louis Lo; Jinsong Ni; Fang He; Gaurang Patel; Andrew Acheampong; *Allergan, Irvine, CA*
- TP 154 **Automatic MS-MS Methods Development Utilizing an IDA-Logic Approach to Enhance the Specificity and Range of Optimized Parameters;** John Janiszewski<sup>1</sup>; Richard Schneider<sup>2</sup>; Kevin Shirey<sup>3</sup>; Loren Olson<sup>4</sup>; Anthony Romanelli<sup>4</sup>; Steven Ainley<sup>5</sup>; Elliott Jones<sup>4</sup>; Eva Duchoslav<sup>6</sup>; Lyle Burton<sup>7</sup>; <sup>1</sup>Pfizer Inc., Westbury, RI; <sup>2</sup>Pfizer Global R&D, Groton, CT; <sup>3</sup>Sound Analytics, East Lyme, CT; <sup>4</sup>Applied Biosystems, San Jose, CA; <sup>5</sup>Sound Analytics, Llc, Niantic, CT; <sup>6</sup>Mds Analytical Technologies, Concord, ON; <sup>7</sup>Mds Sciex, Concord, ON
- TP 155 **Multiplex Enzyme Inhibition Screening via MALDI-3Q-MS;** Kenneth D. Greis<sup>1</sup>; Rakesh Rathore<sup>1</sup>; George Scott<sup>2</sup>; Pauline J. Vollmerhaus<sup>2</sup>; Jay Corr<sup>2</sup>; <sup>1</sup>University of Cincinnati, Genome Research Inst., Cincinnati, OH; <sup>2</sup>MDS Sciex, Concord, ON
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- CARBOHYDRATES/OLIGOSACCHARIDES – GENERAL,  
156 - 178**
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- TP 156 **A Tissue Extraction Procedure Compatible with LC-MS for Profiling of Heparan Sulfate and Chondroitin Sulfate in Rat Tissues;** Xiaofeng Shi; Joseph Zaia; *Boston University, Boston, MA*
- TP 157 **A Glycomics Approach for Characterizing Mutations in N - and O -glycosylation Pathways of the Nematode *Caenorhabditis elegans*;** Elizabeth Palaima<sup>1</sup>; Maria Gravato-Nobre<sup>2</sup>; Jonathan Hodgkin<sup>2</sup>; Catherine E. Costello<sup>1</sup>; John F. Cipollo<sup>3</sup>; <sup>1</sup>Boston University Medical School, Boston, MA; <sup>2</sup>University of Oxford, Oxford, UK; <sup>3</sup>FDA, CBER, Bethesda, MD
- TP 158 **Old Standard, New Structures: The Differentiation and Detailed Characterization of Previously Unreported High Mannose Isomers in Ribonuclease B;** Justin M Prien; David Ashline; Anthony Lapadula; Vernon N. Reinhold; *University of New Hampshire, Durham, NH*
- TP 159 **Enrichment and Mass Detection of Glycans using Fluorous Affinity Tags;** Hui Zhou; Vernon N. Reinhold; *University of New Hampshire, Durham, NH*
- TP 160 **A Computational and Experimental Study of the Binding of Lithium to Methyl N-acetylglucosamine;** Cesar Contreras<sup>1</sup>; Nicolas Polfer<sup>1</sup>; Jos Oomens<sup>2</sup>; John R. Eyley<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Fom Rijnhuizen, Nieuwegein, Netherlands
- TP 161 **Exact Time and Mass Tags for the Rapid Identification of Oligosaccharides;** Nannan Tao<sup>2</sup>; Ed DePeters<sup>2</sup>; Samara Freeman<sup>2</sup>; J. Bruce German<sup>2</sup>; Rudolf Grimmand<sup>1</sup>; Carlito Lebrilla<sup>2</sup>; <sup>1</sup>Agilent Technologies Inc, Santa Clara, CA; <sup>2</sup>University of California, Davis, CA
- TP 162 **An Integrated Profiling and Quantification Method for Glycan Expression: Application in Screening Bacterial Collections for Probiotics Properties;** Milady R. Ninonuevo; Riccardo G. LoCascio; Scott Kronewitter; Samara L. Freeman; J. Bruce German; David A. Mills; Carlito B. Lebrilla; *University of California, Davis, CA*
- TP 163 **Mass Spectrometric Quantification of Complex Bacterial Glycolipids;** Buko Lindner<sup>1</sup>; Sven Müller-Loennies<sup>1</sup>; Satoshi Fukuoka<sup>2</sup>; Helmut Brade<sup>1</sup>; <sup>1</sup>Research Center Borstel, Borstel, Germany; <sup>2</sup>Health Technology Research Center, AIST Shikoku, Takamatsu, Japan
- TP 164 **Analysis of Permethylated Glycans Derived from Biological Samples by Reversed-phase LC-MS;** William R. Alley, Jr.; Yehia Mechref; Milos V. Novotny; *Dept of Chemistry, Indiana University, Bloomington, IN*
- TP 165 **Glycan Phenotype Analysis of Organ-Specific Heparan Sulfate;** Gregory O Staples; Michael J. Bowman; Nancy Leymarie; Catherine E. Costello; Joseph Zaia; *Boston University School of Medicine, Boston, MA*
- TP 166 **Characterization of Acidic Carbohydrates through Peptide Complexation;** John J. Thomas; Paul Salinas; Philip J. Savickas; *Shire HGT, Cambridge, MA*
- TP 167 **A Study for Quantitative Analysis of Glycans by MALDI-TOF MS without using Stable Isotopes;** Akihiko Kameyama<sup>1</sup>; Osamu Tani<sup>2</sup>; Hisashi Narimatsu<sup>1</sup>; <sup>1</sup>Research Center for Medical Glycoscience, AIST, Tsukuba, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- TP 168 **Qualitative and Quantitative Analysis of Non-Human Carbohydrate Epitopes from Specific Pathogen-Free Miniature Pig Kidney;** Yun-Gon Kim<sup>1</sup>; Geun-Cheol Gil<sup>1</sup>; Kyoung-Soon Jang<sup>1</sup>; David J. Harvey<sup>2</sup>; Byung-Gee Kim<sup>1</sup>; <sup>1</sup>Seoul National University, Seoul, South Korea; <sup>2</sup>University of Oxford, Oxford, UK
- TP 169 **O-linked Glycan Site Identification by  $\beta$ -Elimination and MALDI-TOF/TOF Mass Spectrometry;** Alison Wallace; Sanaz Jankhah; John Valliere-Douglass; Alain Ballard; *Amgen, Seattle, WA*
- TP 170 **Isolation and Chemical Characterization of the Extracellular Polysaccharide Required for Biofilm Formation in *Bacillus Subtilis*;** Ahmed Hussein<sup>1</sup>; Daniel Kearns<sup>2</sup>; Yehia Mechref<sup>1</sup>; Milos Novotny<sup>1</sup>; <sup>1</sup>National Center for Glycomics and Glycoproteomics, Bloomington, IN; <sup>2</sup>Biology Department Indiana University, Bloomington, IN
- TP 171 **Investigating the Occurrence of Phosphorylated N-linked Oligosaccharides in Human Gonadotropins by**



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- MALDI-TOF Mass Spectrometry;** Sergei I. Snovida<sup>1</sup>; Helene Perreault<sup>1</sup>; George R. Bousfield<sup>2</sup>; <sup>1</sup>University of Manitoba, Winnipeg, , Canada; <sup>2</sup>Wichita State University, Wichita, KS
- TP 172 **Glycomics using LC-MS after Fractional Enrichment of Neutral, Sialylated and Sulphated Oligosaccharides;** Brendan Harhen; Niclas Karlsson; NCBES NUIG, Galway, Ireland
- TP 173 **The False Positive Rates Associated with the Methods Currently Used to Identify Sites of N-linked Glycosylation;** Lei Cheng<sup>1</sup>; Art Nuccio<sup>1</sup>; James A Atwood III<sup>2</sup>; D. Brent Weatherly<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>BioInquire, Athens, GA
- TP 174 **Glycomic Profiling of Drosophila Melanogaster from Embryo to Larva;** John A. Goetz<sup>1</sup>; Lei Gong<sup>2</sup>; Thomas Kaufman<sup>2</sup>; Milos V. Novotny<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Indiana University Dept. of Chemistry, Bloomington, IN; <sup>2</sup>Department of Biology, Indiana University, Bloomington, IN
- TP 175 **A New Approach to Analyze Fluorescent APTS-Labeled Glycans by MALDI-TOF-MS;** Xiaorong (Sharon) Wei; Steven L. Cohen; Melissa Hamm; Richard R. Rustandi; Merck Research Laboratory, West Point, PA
- TP 176 **A Facile Strategy for Characterization of Mucins using a Novel Membrane Electrophoresis and MALDI-TOF MS;** Yu-Ki Matsuno; Kahori Tachibana; Hisashi Narimatsu; Akihiko Kameyama; Research Center for Medical Glycoscience, AIST, Tsukuba, Japan
- TP 177 **An Improved ESI-MS Analysis of Unprotected, Partially and Fully Protected Sugars by using Post-Column Injection of Potassium Chloride;** Tatiana N. Laremore; Dmitri Zagorevski; Robert J. Linhardt; Rensselaer Polytechnic Institute, Troy, NY
- TP 178 **Investigation of Endoglucanase Selectivity on Carboxymethyl Cellulose by Mass Spectrometric Techniques;** Jonas Enebro; Dane Momcilovic; Sigbritt Karlsson; KTH Royal Institute of Technology, Stockholm, Sweden
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- LIPIDS: BIOCHEMISTRY & STEROIDS 1, 179 - 195**
- TP 179 **Nanomanipulation Coupled to Mass Spectrometry: Single Cotton seed Lipid Body Extraction from a Cell;** Kameron Jorgensen; Kent Chapman; Nicole Ledbetter; Guido F. Verbeck; University of North Texas, Denton, TX
- TP 180 **Lipid Biomarker Discovery of Clear Cell Renal Cell Carcinoma by Direct-Tissue MALDI MS Profiling and Imaging;** Satu Puolitaival<sup>1</sup>; Deming Mi<sup>1</sup>; Stephen Milne<sup>2</sup>; H. Alex Brown<sup>2</sup>; Richard M. Caprioli<sup>3</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>3</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- TP 181 **Analysis of Triradyl Neutral Lipids Isolated from Cells by LC-MS;** Patrick M. Hutchins; Thomas J. Leiker; Robert M. Barkley; Robert C. Murphy; Univ. of Colorado Denver, Aurora, CO
- TP 182 **Study of Unbranched Long Chain Fatty Acid  $\alpha$  Oxidation in 3T3-L1 Adipocytes by Stable Isotope Labeling and GC-MS;** Adewole L. Okunade; Yingqiu Liu; Xiong Su; Washington University, St. Louis, MO
- TP 183 **Shotgun Lipidomics Identifies Alterations in the Phospholipid Content of the Rat Lens Associated with Diet;** Jessica R Nealon<sup>1</sup>; Stephen J Blanksby<sup>1</sup>; Roger JW Truscott<sup>2</sup>; Todd W Mitchell<sup>1</sup>; <sup>1</sup>University of Wollongong, Wollongong, Australia; <sup>2</sup>Save Sight Institute, University of Sydney, Sydney, Australia
- TP 184 **Identification of Eoxins: Novel Proinflammatory Arachidonic Acid Metabolites Formed in Human Eosinophils and Mast Cells;** Åsa Brunström<sup>1</sup>; Stina Feltenmark<sup>1</sup>; Gautam Narinder<sup>2</sup>; William Griffiths<sup>3</sup>; Charlott Edenius<sup>1</sup>; Linda Backman<sup>1</sup>; Lennart Lindbom<sup>2</sup>; Magnus Björkholm<sup>4</sup>; Hans-Erik Claesson<sup>1</sup>; <sup>1</sup>Orexo AB, Stockholm, Sweden; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>Swansea University, Swansea, UK; <sup>4</sup>Karolinska University Hospital, Stockholm, Sweden
- TP 185 **Progress Towards Comprehensive 2D Gas Chromatography Combustion Isotope Ratio Mass Spectrometry (GCxGC-C-IRMS);** Herbert Tobias; Gavin Sacks; Ying Zhang; J Thomas Brenna; Cornell University, Ithaca, NY
- TP 186 **Sphingolipidomic Profiling of the Stratum Corneum of Mice with Keratinocyte-Specific Deletion of Aryl Hydrocarbon Receptor Nuclear Translocator Gene;** Hiromasa Tojo; Osaka University Graduate School of Medicine, Suita, Japan
- TP 187 **Probing Neuronal Specific Phosphatidylserine Synthesis by Mass Spectrometry;** Kei Hamazaki; Mohammed Akbar; Bill Huang; Hee-Yong Kim; National Institutes of Health, Bethesda, MD
- TP 188 **Determining LTA<sub>4</sub> Stabilization in Human Neutrophils by the S100A8/A9 Complex using LC-MS-MS;** Christopher Rector; Miguel A. Gijon; Simona Zarini; Robert C. Murphy; Univ. Colorado Denver, Denver, CO
- TP 189 **Characterization of Bile Components Associated with Gallbladder Infection by *Listeria monocytogenes*;** Karolina M. Krasinska<sup>1</sup>; Jonathan W. Hardy<sup>2</sup>; Theresa M. McLaughlin<sup>1</sup>; Christopher H. Contag<sup>2</sup>; Allis S. Chien<sup>1</sup>; <sup>1</sup>SUMS, Stanford University, Stanford, CA; <sup>2</sup>Dept. of Pediatrics, Stanford School of Medicine, Stanford, CA
- TP 190 **The Relative Quantitation of Cell Membrane Aminophospholipids Lipids using Isotope-Tagged Derivatives;** Karin A. Zemski-Berry<sup>1</sup>; John Hevko<sup>2</sup>; Robert C. Murphy<sup>1</sup>; <sup>1</sup>UCHSC/UCH at Fitzsimons, Aurora, CO; <sup>2</sup>Applied Biosystems, Philadelphia, PA
- TP 191 **Cytoplasmic Lipid Droplet Analysis by Microcapillary Liquid Chromatography-Tandem Mass Spectrometry ( $\mu$ LC-MS-MS);** Brittany Hodges; Julie Weisz; Christine Wu; University of Colorado, Aurora, CO
- TP 192 **Analysis of Intracellular Lipid Hydroperoxide-Mediated Oxidative Stress by Stable Isotope Dilution LC-MS;** Ian A. Blair<sup>1</sup>; Peijuan Zhu<sup>2</sup>; <sup>1</sup>Univ. of Penn/Center for Can, Philadelphia, PA; <sup>2</sup>Schering Plough, Clark, NJ
- TP 193 **Ceramides: Distribution and Quantitation in Mitochondrial Membranes of the Aging Heart;** Alan W. Taylor; Jeffrey S. Monette; Tory M. Hagen; Oregon State University, Corvallis, OR
- TP 194 **Measurement of Eicosanoids and Docosanoids in Rat Brain Following Decapitation-Induced Ischemia using LC-MS-MS;** Santiago Farias<sup>1</sup>; Mireille Basselin<sup>2</sup>; Stanley Rapoport<sup>2</sup>; Robert Murphy<sup>1</sup>; <sup>1</sup>University of Colorado, Denver, CO; <sup>2</sup>NIH, Bethesda, MA
- TP 195 **Profiling of Yeast Sphingolipids by LC-MS-MS to Study the Regulation of Ceramide Synthesis in Cells Impaired for TORC2 Activity;** Sofya Aronova; Karen Wedaman; Pavel Aronov; Karmela Ramos; Bruce D Hammock; Ted Powers; UC Davis, Davis, CA

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- LIPID STRUCTURAL ANALYSIS, 196 - 223**
- TP 196 **Quantitative Shotgun Profiling of the Mammalian Glycosphingolipidome**; Julio Lopes Sampaio; Christer Ejsing; Mathias Gerl; Vineeth Surendranath; Kai Simons; Andrej Shevchenko; *MPI-CBG, Dresden, Germany*
- TP 197 **Ascorbylation of Acrolein and Lipid Derived 2-Alkenals**; Nicholas G. Kesinger; Jan F. Stevens; *Oregon State University, Corvallis, OR*
- TP 198 **Quantification of Phosphatidylcholine Molecular Species in Bile by Electrospray Ionization Tandem Mass Spectrometry**; Wujuan Zhang<sup>1</sup>; Hector Vilca-Melendez<sup>2</sup>; Kenneth Setchell<sup>1</sup>; <sup>1</sup>*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*; <sup>2</sup>*King's College Hospital, London, UK*
- TP 199 **Following the Oxidation and Thermal Decomposition of Edible Oils using MALDI-TOF Mass Spectrometry**; Jennifer Gidden; Rohana Liyanage; Jack Lay; *Univeristy of Arkansas, Fayetteville, AR*
- TP 200 **Targeted and Global Glycerophospholipid Nano ESI-MS Analysis of Liver Tissue Extracts in Patients with Non-alcoholic Steatohepatitis**; Jane Zhao<sup>1</sup>; Bianca M. Arendt<sup>2</sup>; David W. L. Ma<sup>3</sup>; Brigitte Simons<sup>1</sup>; Duchoslav Eva<sup>1</sup>; Elaheh Aghdassi<sup>2</sup>; Johane Allard<sup>2</sup>; <sup>1</sup>*Applied Biosystems/MDS Sciex, Concord, Ontario*; <sup>2</sup>*Gastroenterology and Nutrition, Univ of Toronto, Toronto, Ontario*; <sup>3</sup>*University of Guelph, College of Biological Sci, Guelph, Ontario*
- TP 201 **Direct Analysis of Lipids and Other Metabolites in Mouse Brain Tissue with Infrared Laser Ablation and Mass Spectrometry**; Bindesh Shrestha<sup>1</sup>; Peter Nemes<sup>1</sup>; Javad Nazarian<sup>2</sup>; Eric P. Hoffman<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, DC*; <sup>2</sup>*Children's National Medical Center, Washington, DC*
- TP 202 **Determination of Pyrophosphorylated Forms of Lipid A in Gram-Negative Bacteria using a Multi-Faceted Mass Spectrometric Approach**; Jace W. Jones<sup>1</sup>; Andrew G. Baker<sup>2</sup>; Scott A. Shaffer<sup>1</sup>; Robert K. Ernst<sup>1</sup>; David R. Goodlett<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Waters, Inc., Dublin, CA*
- TP 203 **Negative Ion Pencil Lead Maldi and MALDI MS-MS for the Identification and Structural Analysis of Free Fatty Acids**; Douglas J.H Olson; Mark A Smith; Melanie Dauk; Darwin W Reed; Suzanne R Abrams; *National Research Council, Saskatoon, Canada*
- TP 204 **HPLC-MS Analysis of Various Phospholipid Classes**; Miroslav Lisa; Eva Cánová; Michal Holcapek; *University of Pardubice, Pardubice, Czech Republic*
- TP 205 **Triacylglycerolomics - Characterization of Complex Triacylglycerol Mixtures in Plant Oils and Animal Fats**; Michal Holcapek; Miroslav Lisa; *University of Pardubice, Pardubice, Czech Republic*
- TP 206 **On-line Normal-Phase Chromatography LC-MS with a FTICR MS: Accurate Mass Measurement Approach for Lipid Analysis**; Yewon Lee; Han-Bin Oh; *Sogang University, Seoul, Korea*
- TP 207 **An Automated Workflow for Rapid Alignment and Identification of Lipid Biomarkers Obtained from Chip-Based Direct Infusion Nano-electrospray Tandem Mass Spectrometry**; Jens Hoefkens<sup>1</sup>; Tobias Kind<sup>2</sup>; Kent Pinkerton<sup>3</sup>; Oliver Fiehn<sup>2</sup>; <sup>1</sup>*Genedata Inc, Waltham, MA*; <sup>2</sup>*UC Davis - Metabolomics, Davis, CA*; <sup>3</sup>*UC Davis Center for Health and the Environment, Davis, CA*
- TP 208 **Lipid Analysis of Archaeological Nabatean Lamps using nanoESI-Qq-FT-ICR MS**; Caroline Tokarski<sup>1</sup>; Nicolas Garnier<sup>2</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>*Univ. des Science/Tech de Lille, Villeneuve d'Ascq, France*; <sup>2</sup>*Laboratoire Nicolas Garnier, Vic-le-Comte, France*
- TP 209 **Metabolic Profiling of Phospholipids in Rat Plasma utilizing Ultra Pressure Liquid Chromatography and oa TOF Mass Spectrometry**; Rob Plumb<sup>1</sup>; Paul Rainville<sup>1</sup>; John P Shocker<sup>2</sup>; Chris L. Stumpf<sup>2</sup>; <sup>1</sup>*Waters, Milford, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- TP 210 **Dissociation of Copper(I) and Silver(I) Cluster Ions of Fatty Acids: Ag<sub>2</sub>H<sup>+</sup> as a Marker for Double Bonds**; Voislav Blagojevic; Laura Banu; Diethard K. Bohme; *York University, Toronto, Canada*
- TP 211 **Identification and Quantification of Abundant Alkyl Ether Phospholipids in the Human Lens: A Shotgun Lipidomics Approach using Ozone Induced Dissociation**; Jane M. Deeley<sup>1</sup>; Todd W Mitchell<sup>1</sup>; Michael Thomas<sup>1</sup>; Roger J.W. Truscott<sup>2</sup>; Stephen J Blanksby<sup>1</sup>; <sup>1</sup>*University of Wollongong, Wollongong, Australia*; <sup>2</sup>*Save Sight Institute, University of Sydney, Sydney, Australia*
- TP 212 **ESI-MS of Retinal Phosphatidylcholines in a Stargardt Disease-3 Mouse Model**; Shelley N. Jackson<sup>1</sup>; Anne McMahon<sup>2</sup>; Amina S. Woods<sup>1</sup>; Wojciech Kedzierski<sup>2</sup>; <sup>1</sup>*NIDA-IRP, NIH, Baltimore, MD*; <sup>2</sup>*The University of Texas Southwestern Medical Center, Dallas, TX*
- TP 213 **The Influence of different Detergents on Spermatozoa Membrane Solubilization and the subsequent Phospholipid Analysis by MALDI-TOF Mass Spectrometry**; Beate Fuchs<sup>1</sup>; Ulrike Jakob<sup>2</sup>; Karin Müller<sup>2</sup>; Rosemarie Süß<sup>1</sup>; Jürgen Schiller<sup>1</sup>; <sup>1</sup>*University of Leipzig, Leipzig, Germany*; <sup>2</sup>*Leibniz Institute for Zoo and Wildlife Research, Berlin, Germany*
- TP 214 **CID/OzID: A New Ion Activation Approach for the Assignment of sn-Position in Phospholipids**; Michael Thomas; Todd W Mitchell; Stephen J Blanksby; *University of Wollongong, Wollongong, NSW, Australia*
- TP 215 **Identification of Significant Acylation Pattern Changes in Lipid A species from Escherichia coli lpxL- Mutants Grown at High Temperatures**; Birgit Schilling<sup>1</sup>; Michael A Apicella<sup>2</sup>; Bradford W. Gibson<sup>1</sup>; <sup>1</sup>*Buck Institute for Age Research, Novato, CA*; <sup>2</sup>*University of Iowa, Iowa City, IA*
- TP 216 **Analysis of N-Acylphosphatidylethanolamine using Electrospray Ionization Tandem Mass Spectrometry**; Giorgis Isaac<sup>1</sup>; Aruna Kilaru<sup>2</sup>; Peter Koulen<sup>3</sup>; Kent Chapman<sup>2</sup>; Ruth Welti<sup>1</sup>; <sup>1</sup>*Kansas State University, Manhattan, KS*; <sup>2</sup>*University of North Texas, Denton, TX*; <sup>3</sup>*University of North Texas Health Science Center, Fort Worth, TX*
- TP 217 **Characterization of Yeast Glycerophospholipid Composition by HPLC/ESI-FTICR-MS**; Heiko Haven; Eva-M. Hein; *ISAS - Institute for Analytical Sciences, Dortmund, Germany*
- TP 218 **Modulation of Gangliosides in U373MG Glioblastoma by ST6GalNacV Gene Transfection**; Mark R. Emmett<sup>1</sup>; Huan He<sup>2</sup>; Carol L. Nilsson<sup>3</sup>; Alan G. Marshall<sup>5</sup>; Roger A. Kroes<sup>4</sup>; Mary Schmidt<sup>4</sup>; Joseph R. Moskal<sup>4</sup>; <sup>1</sup>*Nat'l High Magnetic Field Lab, Tallahassee, FL*; <sup>2</sup>*Florida State University, Tallahassee, FL*; <sup>3</sup>*Pfizer, Inc., San Diego, CA*; <sup>4</sup>*The Falk Center for Molecular Therapeutics, Evanston, Illinois*; <sup>5</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL*

## TUESDAY POSTERS

- TP 219 **Qualitative and Quantitative Analysis of Lipid Classes from 2 Different Sources using Electrospray Ionization and High Resolution LC-MSn Mass Spectrometry;** Laurance Lee; Donna L. Wilson; Anne Ferguson; *Thermo Fisher Scientific, Inc., San Jose, CA*
- TP 220 **Identifying Lipids and Other Small Molecules from Imaging Mass Spectrometry Experiments using Tandem Mass Spectrometry and Exact Mass;** Timothy Garrett<sup>1</sup>; Ming Gu<sup>2</sup>; William W. Dawson<sup>1</sup>; David H. Powell<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL;* <sup>2</sup>*Cerno Bioscience, Yardley, PA*
- TP 221 **A Prototype for Computational Analysis of Lipid A Structural Variations using Mass Spectrometry;** Ying Ting<sup>2</sup>; Lars Malmstroem<sup>1</sup>; Scott A. Shaffer<sup>1</sup>; Wailap Ng<sup>2</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA;* <sup>2</sup>*National Yang Ming University, Taipei, Taiwan*
- TP 222 **Clustering Software for Analysis of Complex Lipid Profile Data Based on Detection of Fish Oils by MALDI Mass Spectrometry;** Helen Montgomery<sup>1</sup>; Gerald Stubiger<sup>2</sup>; Wolfgang Werther<sup>3</sup>; Emmanuel Raptakis<sup>4</sup>; Omar Belgacem<sup>4</sup>; <sup>1</sup>*Shimadzu, Koichi Tanaka MS Research laboratory, Manchester, UK;* <sup>2</sup>*Medical University of Vienna, Vienna, Austria;* <sup>3</sup>*University of Vienna, Vienna, Austria;* <sup>4</sup>*Shimadzu Biotech, Manchester, UK*
- TP 223 **Lipidomic Analysis and Comparison of Mitochondrial and Plasma Membrane Fatty Acid Profiles Isolated From Various Tissues;** Michael D. Timmons; Shuling Xiong; Mark A. Lovell; Bert C. Lynn; *University of Kentucky, Lexington, KY*
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- NON-COVALENT INTERACTIONS 1, 224 - 242**
- TP 224 **Non-Covalent Interactions between Peptides from Immunoglobulin and Selected Mono- and Oligosaccharides;** Helene Perreault<sup>1</sup>; Anna Warnet<sup>2</sup>; Jean-claude Tabet<sup>2</sup>; Sandra Alves<sup>2</sup>; <sup>1</sup>*University of Manitoba, Winnipeg, MB, Canada;* <sup>2</sup>*Université Paris VI, Paris, France*
- TP 225 **Protein-Oligonucleotide Complexes Characterization using Noncovalent Mass Spectrometry: Study of the tRNA Binding Properties of tRNA mIA58 Methyltransferase;** Cédric Atmanene<sup>1</sup>; Pierre Barraud<sup>2</sup>; Frédéric Dardel<sup>2</sup>; Carine Tisne<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Sarah Sanglier<sup>1</sup>; <sup>1</sup>*IPHC-DSA, ULP, CNRS, Strasbourg, France;* <sup>2</sup>*Laboratoire de Cristallographie et RMN biologiques, Paris, France*
- TP 226 **Comparative Thermodynamic Study of the Human ABO(H) Blood Group Glycosyltransferases using nanoES-FTICR-MS;** Naoto Soya<sup>1</sup>; Glen Shoemaker<sup>1</sup>; Monica Palcic<sup>2</sup>; John S Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada;* <sup>2</sup>*Carlsberg Laboratory, Copenhagen, Denmark*
- TP 227 **Determining a Molecular Pathway for Formation of a T=3 Capsid using ESI-MS and ESI-IMS-MS;** Victoria L. Morton; Peter G Stockley; Nicola Stonehouse; Alison E. Ashcroft; *University of Leeds, Leeds, UK*
- TP 228 **DNA-Nuclear Receptor Interaction Studied by Mass Spectrometry;** Claudia Bich<sup>1</sup>; Cédric Bovet<sup>1</sup>; Natacha Rochel<sup>2</sup>; Carole Peluso-Iltis<sup>2</sup>; Ryan Wenzel<sup>1</sup>; Dino Moras<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland;* <sup>2</sup>*Inst. Génétique et Biologie Mol. et Cell., Illkirch, France*
- TP 229 **Quantitative Determination of Metal-Protein Dissociation Constants using Metal-Catalyzed Oxidation Reactions and Mass Spectrometry;** Adam M Graichen; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TP 230 **A Comparison of Specific and Nonspecific Protein-Ligand Interactions using FTICR MS;** Michelle Sweeney; John R. Eycler; *University of Florida, Gainesville, FL*
- TP 231 **Ion Mobility Mass Spectrometry and Proton Transfer Reactions of Non-covalent Amyloid  $\beta$ -protein Oligomers;** Eric S. Pang; Rachel O. Loo; Sheng Yin; Pinmanee Boontheung; David B. Teplow; Joseph A. Loo; *UCLA, Los Angeles, CA*
- TP 232 **SUPREX Analysis of a Misfolded Disease-Related Variant of Alanine:Glyoxylate Aminotransferase;** Erin D. Hopper; Adrienne M.C. Pittman; Chandra Tucker; Michael C. Fitzgerald; *Duke University, Durham, NC*
- TP 233 **High-Mass MALDI MS: Characterization of Large Molecular Size Hemoglobin-Based Oxygen Carriers;** Tatiana Pimenova<sup>1</sup>; Claudia Pereira<sup>2</sup>; Dominik Schaefer<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland;* <sup>2</sup>*Medical Clinic Research Unit, University of Zurich, Zurich, Switzerland*
- TP 234 **The Analysis of the Interactions and Complexation of Polycyclic Aromatic Hydrocarbons and Cyclodextrin using Electrospray Ionization Mass Spectrometry;** Andrew Harron<sup>1</sup>; Catherine Bentzley<sup>1</sup>; Preston Moore<sup>1</sup>; Darryl Davis<sup>2</sup>; <sup>1</sup>*University of the Sciences in Philadelphia, Philadelphia, PA;* <sup>2</sup>*Centocor, Collegeville, PA*
- TP 235 **Development of an ESI-MS Method for DNA-Ligand Screening Applied to Recognition of T:G Mismatched Base Pairs;** Federico Riccardi Sirtori<sup>1</sup>; Roberto D'Alessio<sup>1</sup>; Giancarlo Aldini<sup>2</sup>; Maristella Colombo<sup>1</sup>; <sup>1</sup>*Nerviano Medical Sciences, Nerviano, Italy;* <sup>2</sup>*Faculty of Pharmacy, University of Milan, Milan, Italy*
- TP 236 **NanoESI-Mass Spectrometry: A Versatile Tool for a Fast Affinity Classification of Clinical Inhibitors of Human Kinases;** Matthias Jecklin<sup>1</sup>; David Touboul<sup>1</sup>; Rishi Jain<sup>2</sup>; Estee Naggat<sup>2</sup>; John Tallarico<sup>2</sup>; Paul Ramage<sup>3</sup>; Peter Drucekes<sup>3</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland;* <sup>2</sup>*Novartis Institutes for BioMedical Research, Cambridge, MA;* <sup>3</sup>*Novartis Institutes for BioMedical Research, Basel, Basel, Switzerland*
- TP 237 **Mass Spectrometry and Ion Mobility of Noncovalent Alpha-Synuclein-Ligand Complexes: Determination of Ligand Binding Sites and Protein Conformations;** Sheng Yin; Joseph A. Loo; *UCLA, Los Angeles, CA*
- TP 238 **Native and Denaturation Products of 9 MegaDalton Vault Complexes Characterized by Ion Mobility Mass Spectrometry;** Shirley H. Lomeli; Catherine S. Kaddis; Sheng Yin; Rachel R. Ogorzalek Loo; Leonard H. Rome; Joseph A. Loo; *University of California, Los Angeles, Los Angeles, CA*
- TP 239 **Anion Recognition of Glycocalix[4]arenes Studied by ESI-FTICR Mass Spectrometry;** Mika J. Torvinen<sup>1</sup>; Elina Kalenius<sup>1</sup>; Francesco Sansone<sup>2</sup>; Alessandro Casnati<sup>2</sup>; Rocco Ungaro<sup>2</sup>; Pirjo Vainiotalo<sup>1</sup>; <sup>1</sup>*University of Joensuu, Joensuu, Finland;* <sup>2</sup>*Università di Parma, Parma, Italy*
- TP 240 **Quantifying Protein-Hydrophobic Ligand Interactions by ES-MS;** Lan Liu; John S. Klassen; *University of Alberta, Edmonton, Canada*
- TP 241 **Study of Noncovalent Complexes between Siderophore-Binding Receptor Proteins from *Bacillus Cereus* and Siderophores by ESI-MS;** Rita

## TUESDAY POSTERS

- Nichiporuk; Anna M. Zawadzka; Ulla Norklit Andersen; Kenneth N. Raymond; *University of California, Berkeley, Berkeley, CA*
- TP 242 **Stereochemical Effects of Substituents in Position 11 of 17-Beta-Estradiol on Gas Phase Acidity: A Cooperative Effect**; Sandrine Voillard<sup>1</sup>; Françoise Fournier<sup>1</sup>; Yves Jacquot<sup>1</sup>; Carlos Afonso<sup>1</sup>; Guy Leclercq<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>*University Paris VI (UPMC), Paris, France*; <sup>2</sup>*Institut Jules Bordet, Brussels, Belgium*
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- MICROBIAL ANALYSIS, 243 - 265**
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- TP 243 **Global Proteomic Analysis of Psychrotrophic Bacteria, *B. psychrosaccharolyticus***; Jong Bok Seo; *Korea Basic Science Institute, Seoul, South Korea*
- TP 244 **Characterization of a Novel Cross-linkage in *Actinomyces naeslundii* Fimbriae using C-terminal Ladder Sequencing Approaches and Mass Spectrometry**; Jenny T.C. Ho<sup>1</sup>; Sonja Hess<sup>1</sup>; John O Cisar<sup>2</sup>; <sup>1</sup>*Caltech, Pasadena, CA*; <sup>2</sup>*NIDCR, National Institutes of Health, Bethesda, MD*
- TP 245 **Characterization of *Enterococcus faecium* peptidoglycan: Understanding Biosynthesis and Antibiotic Binding Sites**; Jiawei Chen; Gary Patti; Jacob Schaefer; Michael L. Gross; *Washington University in St. Louis, St. Louis, MO*
- TP 246 **Immobilization of Microorganisms with Cationic Nanoparticles for Detection by Mass Spectrometry**; Cheng-Tung Chen<sup>1</sup>; Anren Hu<sup>2</sup>; Chia-Liang Cheng<sup>1</sup>; Yen-peng Ho<sup>1</sup>; <sup>1</sup>*National Dong Hwa University, Hualien, Taiwan*; <sup>2</sup>*Tzu Chi University, Hualien, Taiwan*
- TP 247 ***Clostridium Botulinum*: Towards Strain Detection and Identification by Top-Down Mass Spectrometry of Flagellin Proteins**; Susan M. Twine<sup>1</sup>; Catherine Paul<sup>1</sup>; James Mullen<sup>1</sup>; David McMullin<sup>1</sup>; John Austin<sup>2</sup>; Susan M. Logan<sup>1</sup>; John F. Kelly<sup>1</sup>; <sup>1</sup>*National Research Council Canada, Ottawa, Canada*; <sup>2</sup>*Health Canada, Ottawa, Ontario, Canada*
- TP 248 **Analysis of Temperature-Dependent Protein Complexes from *Thermoanaerobacter tengcongensis* by Blue Native Page Electrophoresis**; Bo Meng<sup>1</sup>; Weiwei Wang<sup>1</sup>; Zhong Qian<sup>1</sup>; Chuanqi Zhou<sup>1</sup>; Quanhui Wang<sup>2</sup>; Zhuowei Wang<sup>1</sup>; Ningzhi Xu<sup>1</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>*Beijing Genomics Institute, CAS, Beijing, China*; <sup>2</sup>*Institute of Microbiology, CAS, Beijing, China*
- TP 249 **Detection and Discrimination of Extended-Spectrum  $\beta$ -lactamase (ESBL) Producing Bacteria by MALDI-TOF-MS**; Ian Edwards<sup>4</sup>; Edina Chiriseri<sup>2</sup>; Marilena Ioannou<sup>1</sup>; Ruta Furmonaviciene<sup>1</sup>; Colin Geary<sup>3</sup>; Richard O Jenkins<sup>1</sup>; <sup>1</sup>*De Montfort University, Leicester, UK*; <sup>2</sup>*Northampton General Hospital, Leicester, UK*; <sup>3</sup>*Leicester Royal Infirmary, Leicester, UK*; <sup>4</sup>*Shimadzu Biotech / Kratos Analytical Ltd, Manchester, UK*
- TP 250 **Discrimination of *Aspergillus* Isolates at the Species and Strain Level by MALDI-TOF Mass Spectrometry Fingerprinting**; Amanda D. Buskirk; Justin M. Hettick; Brett J. Green; Michael L. Kashon; James E. Slaven; Erika Janotka; Detlef Schmechel; Donald H. Beezhold; *NIOSH, Morgantown, WV*
- TP 251 **MALDI Mass Spectrometry Detection of Plant Pathogenic Bacteria**; Anja Freiwald; Magdalena Kliem; Sascha Sauer; *MPI for Molecular Genetics, Berlin, Germany*
- TP 252 **Catching the Evolution of a Killer Virus with Mass Spectrometry**; Bethny Morrissey; Alexander Schwahn; Margaret Streamer; Kevin Downard; *University of Sydney, Sydney, Australia*
- TP 253 **Discrimination of *Penicillium* isolates by MALDI-TOF Mass Spectrometry Fingerprinting**; Justin M. Hettick; Amanda D. Buskirk; Brett J. Green; Michael L. Kashon; James E. Slaven; Erika Janotka; Detlef Schmechel; Donald H. Beezhold; *NIOSH, Morgantown, WV*
- TP 254 **Rapid Method for Sensitive Screening of Oligosaccharide Epitopes in the *Campylobacter jejuni* Strains Isolated from Guillain-Barré Syndrome Patients**; Jianjun Li<sup>1</sup>; Monika Dzieciatkowska<sup>1</sup>; Xin Liu<sup>1</sup>; Astrid Heikema<sup>2</sup>; Alex van Belkum<sup>2</sup>; Elke Schweda<sup>3</sup>; Michel Gilbert<sup>1</sup>; James C. Richards<sup>1</sup>; <sup>1</sup>*National Research Council, Ottawa, Canada*; <sup>2</sup>*Erasmus University Medical Center Rotterdam, Rotterdam, The Netherlands*; <sup>3</sup>*Karolinska Institute, Huddinge, Sweden*
- TP 255 **Metaproteomics of Subsurface Microbial Communities in Metal-Contaminated Ecosystems**; Paul Abraham<sup>1</sup>; Nathan C. Verberkmoes<sup>1</sup>; Mark Lefsrud<sup>2</sup>; Karuna Chourey<sup>1</sup>; Manesh Shah<sup>1</sup>; Dawn Holmes<sup>3</sup>; Derek Lovley<sup>3</sup>; Mike Wilkins<sup>4</sup>; Ken Williams<sup>5</sup>; Jill Banfield<sup>4</sup>; Phil Long<sup>6</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge Nat'l Lab, Oak Ridge, TN*; <sup>2</sup>*McGill University, Montreal, Canada*; <sup>3</sup>*University of Massachusetts, Amherst, MA*; <sup>4</sup>*University of California, Berkeley, CA*; <sup>5</sup>*Lawrence Berkeley National Lab, Berkeley, CA*; <sup>6</sup>*Pacific Northwest National Lab, Richland, WA*
- TP 256 **Characterization of *Clostridium* Species Utilizing Liquid Chromatography/Mass Spectrometry of Intact Proteins**; Robert Everley<sup>2</sup>; Tiffany M. Mott<sup>1</sup>; Denise M. Toney<sup>1</sup>; Timothy R. Croley<sup>1</sup>; <sup>1</sup>*Commonwealth of Virginia, Richmond, VA*; <sup>2</sup>*Virginia Commonwealth University, Richmond, VA*
- TP 257 **An Automated, High-Throughput ESI-Mass Spectrometry Assay for the Identification of Enteric Bacterial Pathogens**; Sheri M. Manalili; James C. Hannis; Feng Li; Raymond Ranken; Lawrence Blyn; David J. Ecker; Steven A. Hofstadler; Ranga Sampath; *Ibis Biosciences, Inc., Carlsbad, CA*
- TP 258 **Examination of the Protein Complexes Bound on Gal Operon Promoter of *Thermoanaerobacter tengcongensis***; Zhong Qian<sup>1</sup>; Fan Wei<sup>1</sup>; Li Guo<sup>2</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>*Beijing Genomics Institute, CAS, Beijing, China*; <sup>2</sup>*Institute of Microbiology, CAS, Beijing, China*
- TP 259 **Quantitative Mass Spectrometric Characterization of Substrate-Dependent Changes in the Cellulosome of *Clostridium thermocellum***; Gregory B. Hurst<sup>1</sup>; Chongle Pan<sup>1</sup>; Patricia K. Lankford<sup>1</sup>; Babu Raman<sup>1</sup>; Miguel Rodriguez Jr.<sup>1</sup>; Catherine K. McKeown<sup>1</sup>; Steven D. Brown<sup>1</sup>; Nagiza F. Samatova<sup>2</sup>; Jonathan R. Mielenz<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*North Carolina State University, Raleigh, NC*
- TP 260 **Establishment of a Standardized Procedure for Identification of Microorganisms by MALDI TOF Mass Spectrometry**; Thomas Wenzel<sup>1</sup>; Carrie L. Seachord<sup>2</sup>; Thorsten Mieruch<sup>1</sup>; Thomas W. Fuller<sup>3</sup>; Thomas Maier<sup>1</sup>; Richard R. Drake<sup>3</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>*Brüker Daltonik GmbH, Leipzig, Germany*; <sup>2</sup>*Children's Hospital of the King's Daughter, Norfolk, VA*; <sup>3</sup>*Eastern Virginia Medical School, Norfolk, VA*
- TP 261 **Imaging MALDI of Bacteria**; David Evason<sup>1</sup>; Hesham Ganbhour<sup>2</sup>; Howard Foster<sup>2</sup>; Mark D. Mills<sup>1</sup>; Vic Parr<sup>1</sup>; <sup>1</sup>*SAI, Manchester, UK*; <sup>2</sup>*Salford University, Salford, UK*
- TP 262 **Forensic Microbial Identification Utilizing ESI-TOF Mass Spectrometry**; Raleigh W. Parrott<sup>1</sup>; Kathryn E. O'Brien<sup>1</sup>; Bruce Budowle<sup>2</sup>; James M. Robertson<sup>2</sup>; Steven

## TUESDAY POSTERS

- A. Hofstadler<sup>3</sup>; Thomas A. Hall<sup>3</sup>; Brian A. Eckenrode<sup>2</sup>;  
<sup>1</sup>*Oak Ridge Institute for Science and Education, Oak Ridge, TN*; <sup>2</sup>*Federal Bureau of Investigation, Quantico, VA*; <sup>3</sup>*Ibis Biosciences, Inc., Carlsbad, CA*
- TP 263 **High Resolution Strain Typing of Escherichia coli O157:H7 By MultiLocus PCR Based Mass Spectrometry**; James C. Hannis<sup>1</sup>; Mark W. Eshoo<sup>1</sup>; Feng Li<sup>1</sup>; Thomas A. Hall<sup>1</sup>; David M. Wagner<sup>2</sup>; Lawrence Blyn<sup>1</sup>; Ranga Sampath<sup>2</sup>; Robert E. Mandrell<sup>3</sup>; Clifton K. Fagerquist<sup>3</sup>; Amy Vogler<sup>2</sup>; Paul Keim<sup>2</sup>; Michael Cooley<sup>3</sup>; David J. Ecker<sup>1</sup>; Steven A. Hofstadler<sup>1</sup>; <sup>1</sup>*Ibis Biosciences, Inc., Carlsbad, CA*; <sup>2</sup>*Northern Arizona University, Flagstaff, AZ*; <sup>3</sup>*USDA Agricultural Research Service, Albany, CA*
- TP 264 **Rapid and Sensitive Identification of Bacterial Antigens by On-Immunoblotted Membrane Digestion**; Akira Okamoto; Keiko Yamada; Michio Ohta; *Nagoya University, Nagoya, Japan*
- TP 265 **Comparative Proteomic Analysis of Aeromonas salmonicida Grown under Conditions of Salt Stress using Methylation with Isotopically Coded Formaldehydes**; Roger Ebanks; Kenneth Chisholm; Devanand Pinto; *NRC - Institute for Marine Biosciences, Halifax, Canada*
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- SMALL MOLECULE ANALYSIS BIOLOGICAL RELEVANT COMPOUNDS, 266 - 280**
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- TP 266 **LC-MS-MS-Based Characterization of Novel Enzymatic Reaction Catalyzed by a Microbial Nitrile Hydratase**; Kayoko Taniguchi<sup>1</sup>; Takemichi Nakamura<sup>1</sup>; Shunya Takahashi<sup>1</sup>; Mizuo Maeda<sup>1</sup>; Masafumi Odaka<sup>2</sup>; <sup>1</sup>*Riken, Wako, Japan*; <sup>2</sup>*Tokyo Univ. Agric. Technol., Tokyo, Japan*
- TP 267 **Quantitative Analysis of a Acyl Coenzyme A in Plant Tissue by LC-MS-MS Electrospray Ionization Method**; Ann Perera; Suh-Yeon Choi; Wuterle Eve; Basil Nikolau; *Iowa State University, Ames, IA*
- TP 268 **Characterization of Ge(IV) and Ni(II) Complexes with Amino Acids using Ion Trap and QqTOF Electrospray Ionization Tandem Mass Spectrometry**; Robert Jirasko; Michal Holcapek; Lenka Kolarova; *University of Pardubice, Pardubice, Czech Republic*
- TP 269 **A Rapid and Sensitive Method for the Detection of Residual Biocidal Compounds in Catheter Rinse Solutions by HILIC-MS-MS**; John W. Torchia; Katrina Emilia Nizzi; Bruce Solomon; *Bioanalytical Systems, Inc., West Lafayette, IN*
- TP 270 **Analysis of Cellular Free Thiol Amino Acids and Peptides by Stable Isotope Dilution LC-MS**; Stefanie Khartulyari; Cong Wei; Alexander S. Whitehead; Ian A. Blair; *Center for Excellence in Environmental Toxicology, Philadelphia, PA*
- TP 271 **Quantitation of Gamma-Aminobutyric Acid in Cerebrospinal Fluid by LC-MS-MS Approach**; Farzin Gharahdaghi; Gennady Smagin; *AstraZeneca, Wilmington, DE*
- TP 272 **A New Approach for Highly Sensitive Quantitative LC-MS-MS Analysis of N-Nitrosornicotine**; Richard Olsen; Kirk Newland; Veni Lapko; *MDS Pharma Services, Lincoln, NE*
- TP 273 **LSIMS as a Tool to Study Metal-Complexes of Fullerenes-Porphyrins**; Thomas Mueller; Srinivas Banala; Bernhard Kraeutler; *University of Innsbruck, Innsbruck, Austria*
- TP 274 **Identification of Biomarkers to Oestrogen Exposure using MCF-7 BOS Cell Line Exposed to 17 Beta-Oestradiol**; Mike Collodoro; Pascale Lemaire; Virginie Bertrand; Rowan L. Dobson; Gabriel Mazzucchelli; Joelle Widart; Edwin De Pauw; Marie-Claire Gillet; *Liege University, Liege, Belgium*
- TP 275 **Development of a Sensitive Ultra-Performance LC-MS-MS Method for the Determination of Endogenous Corticosterone in Rat Plasma and Urine**; Yi Tao; Celia D'Arienzo; Hollie Booth; Zheng Ouyang; Timothy Olah; *Bristol Myers Squibb Co., Lawrenceville, NJ*
- TP 276 **A Robust LC-MS-MS Method for Analysis of Caffeine and its Metabolite – Paraxanthine in Human Plasma**; Zhilong Gong; Zhilong Gong; *Covance Bioanalytical Svc, Indianapolis, IN*
- TP 277 **Mercapturic Acid Conjugates of 4-Hydroxy-2-Nonenal and 4-Oxo-2-nonenal Metabolites in a Rat Model of Oxidative Stress**; Heather C. Kuiper; Cristobal L. Miranda; John Sowell; Jan F. Stevens; *Oregon State University, Corvallis, OR*
- TP 278 **Determination of Double Bond Location in Fatty Acids by Manganese Adduction and Electron Induced Dissociation**; Hyun Ju Yoo; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- TP 279 **Collision Induced Decomposition Pathways of Biliary 4,4'-Methylenedianiline Conjugates Produced in Rats**; Kan Chen<sup>1</sup>; Tammy R. Dugas<sup>2</sup>; Richard B. Cole<sup>1</sup>; <sup>1</sup>*University of New Orleans, New Orleans, LA*; <sup>2</sup>*LSU Health Sciences Center, Shreveport, LA*
- TP 280 **Serum Levels of Isoflavones in Women Receiving a Red Clover Dietary Supplement**; Linlin Dong<sup>1</sup>; Dejan Nikolic<sup>1</sup>; Wenzhong Liang<sup>1</sup>; Suzanne Banuvar<sup>2</sup>; Lee Shulman<sup>2</sup>; Stacie E. Geller<sup>3</sup>; Norman R. Farnsworth<sup>1</sup>; Richard B. Van Breemen<sup>1</sup>; <sup>1</sup>*University of Illinois College of Pharmacy, Chicago, IL*; <sup>2</sup>*Northwestern University Feinberg School of Medicine, Chicago, IL*; <sup>3</sup>*University of Illinois College of Medicine, Chicago, IL*
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- QUANTITATION OF SMALL MOLECULES/PLASMA MATRIX, 281 - 314**
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- TP 281 **A Rapid LC-MS-MS Method for the Simultaneous Determination of Vildagliptin and Two Metabolites in Monkey, Human and Rat Plasma**; Wei Zhou; Sagar Kawle; Shaoyong Li; John Doherty; Harold T Smith; Francis Tse; *Novartis Pharmaceuticals Corporation, East Hanover, NJ*
- TP 282 **Development and Validation of an Inductively Coupled Plasma Mass Spectrometric Method for the Quantitation of Total Platinum from Oxaliplatin**; Amy Lapaglia; Paula Lee; *ABC Laboratories, Inc., Columbia, MO*
- TP 283 **Development of a Highly Sensitive UPLC-MS-MS Method for Quantitative Analysis of CAPE and FCAPE in Rat Plasma**; Jihai Pang; *M.D. Anderson Cancer Center, Houston, TX*
- TP 284 **Rapid Method for the Quantitative Determination of Tricin in Human and Rat Plasma using LC-MS-MS**; Gregory Gorman<sup>1</sup>; Lori Coward<sup>1</sup>; Corenna Kerstner-Wood<sup>1</sup>; Lea Freeman<sup>1</sup>; Charles Hebert<sup>1</sup>; Izet Kapetanovic<sup>2</sup>; <sup>1</sup>*Southern Research Institute, Birmingham, AL*; <sup>2</sup>*National Cancer Institute, Bethesda, MD*
- TP 285 **Monitoring of Endogenous Interferences by LC-MS-MS and UV/Vis Spectroscopy: Application to the Determination of Albuterol in Human Plasma**; BRYAN VINING; James Havel; David A Kuntz; Billy G. Hudson; *CRL, Lenexa, KS*
- TP 286 **A Sensitive, High-Throughput Method for the Quantitation of Theophylline in Human Plasma via**

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- TP 287 **Solid Phase Purification and LC-MS-MS Detection;** Sarah K. Roby; Yousef J. Basir; Kirk E. Newland; *MDS Pharma Services, Lincoln, NE*
- TP 288 **High-Throughput Analysis of Mifepristone and Two Mifepristone Analogues in Mouse Heparin Plasma by LDTD-MS-MS in 9 seconds;** Philippe Nobert<sup>2</sup>; Patrice Tremblay<sup>2</sup>; Sylvain Letarte<sup>1</sup>; Pierre Picard<sup>2</sup>; <sup>1</sup>*Phytronix Technologies, Blainville, Canada*; <sup>2</sup>*Phytronix Technologies, Inc., Quebec, QC*
- TP 289 **A Highly Sensitive LC-MS-MS Method for Quantification of a Pan-erbB kinase Inhibitor-Pd168393 in Plasma;** Jeevan Prasain; Alireza Arabshahi; Ray Moore; Stephen Barnes; Steve Carroll; *University of Alabama at Birmingham, Birmingham, AL*
- TP 290 **Determination of Endocannabinoid Antagonist Rimonabant (SR141716) in Plasma by LC-ESI-MS-MS;** Melissa A Mcculloch<sup>1</sup>; Xiang Zhou<sup>1</sup>; Yan Xu<sup>1</sup>; Steve Brunell<sup>2</sup>; Linda Spear<sup>2</sup>; <sup>1</sup>*Cleveland State University, Cleveland, OH*; <sup>2</sup>*Binghamton University, Binghamton, NY*
- TP 291 **Chiral Chromatographic Method Development and Validation for the Quantitation of Eszopiclone in Human Plasma using LC-MS-MS;** Min Meng<sup>1</sup>; Lisa Rohde<sup>1</sup>; Vladimir Capka<sup>2</sup>; Patrick Bennett<sup>1</sup>; <sup>1</sup>*Tandem Labs, Salt Lake City, UT*; <sup>2</sup>*Astra Zeneca Pharmaceuticals LP, Waltham, MA*
- TP 292 **Stable-Isotope Dilution Liquid Chromatography-Tandem Mass Spectrometry Assay for the Quantification of Testosterone in Human Plasma in Diagnosis of Androgen-Mediated Diseases;** Xueheng Zhao; Kenneth D. R. Setchell; *Cincinnati Children's Hospital Medical Center, Cincinnati, OH*
- TP 293 **Difficulties in Developing a Sensitive Assay for the Quantification of Rifampin in Multiple Biological Matrices by LC-MS-MS;** Keith Zientek; Michael Nelson; Lori Payne; *BASi, McMinnville, OR*
- TP 294 **Stable Isotope Dilution LC-MS Analysis and Biological Relevance of 15-oxo-EETE, A Novel 15-lipoxygenase-Derived Arachidonic Acid Metabolite;** Cong Wei<sup>1</sup>; Peijuan Zhu<sup>2</sup>; Sumit Shah<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>*Center For Cancer Pharmacology, University of Penn, Philadelphia, PA*; <sup>2</sup>*Schering Plough, Clark, NJ*
- TP 295 **Simultaneous Determination of Loratadine and Betamethasone in Human Plasma using Liquid-Liquid Extraction and High-Performance Liquid Chromatography Coupled to Mass Spectrometry;** Rafael E. Barrientos-Astigarraga; Paulo A. R. Galvinas; Jane K. Finzi; Mauricio R. M. Sampaio; Washington M. Silva; Leandro S. C. Barbosa; *MAGABI Pesquisas Clinicas Farmaceuticas Ltda., Sao Paulo, Brazil*
- TP 296 **LC-MS-MS Assay Development and Validation for Determination of Total Doxorubicin (Free + Liposomal) in Human Plasma and Clinical Sample Analysis;** Chaoran Ron Huang<sup>1</sup>; Arnaldo Costa<sup>1</sup>; Dale F. Schoener<sup>2</sup>; Seema Datta<sup>2</sup>; Joseph Whitson<sup>2</sup>; Michael Buonarati<sup>2</sup>; Liyu Yang<sup>1</sup>; <sup>1</sup>*Biogen Idec, Cambridge, MA*; <sup>2</sup>*Alta Analytical Laboratory, El Dorado Hills, CA*
- TP 297 **A Rapid and Sensitive SPE-UPLC-MS-MS Method for Determination of Ropinirole in Human Plasma;** Erin E. Chambers; Diane Diehl; *Waters Corporation, Milford, MA*
- TP 298 **Effect of Lycopene on Plasma Testosterone Levels in Men as a Prostate Cancer Prevention Agent;** Ang Liu; Linlin Dong; Richard B. Van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- TP 299 **Resolving Apparent LC-MS-MS Matrix Effects in Plasma Protein Binding Analysis;** Garnet McRae; Miles Webb; Rahul Vohra; *Painceptor Pharma Corp., Ottawa, Canada*
- TP 300 **A Selective LC-MS-MS Method for Quantification of Ribavirin in Human Plasma;** Dawei Zhou; Karla Arriola; Xiping Fang; Jinn Wu; *Xenobiotic Laboratories, Inc., Plainsboro, NJ*
- TP 301 **A Highly Sensitive LC-MS-MS Method (0.4 pg/mL) for Quantitation of Formoterol in Human Plasma;** Dawei Zhou; Wenzhong Liang; Xiping Fang; Jinn Wu; *Xenobiotic Laboratories, Inc., Plainsboro, NJ*
- TP 302 **Fast Quantitation of Buprenorphine in Human Plasma by MALDI-QqQLIT using Disposable Matrix Pre-Coated MALDI Plates;** Emmanuel Varesio<sup>1</sup>; Chantal Grivet<sup>1</sup>; Christoph Menzel<sup>2</sup>; Udo Roth<sup>2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>*University of Geneva, Geneva, Switzerland*; <sup>2</sup>*Qiagen, Hilden, Germany*
- TP 303 **Evaluation of Acyl Glucuronide Metabolites during Drug Quantification in Bioanalysis by LC-MS-MS: From Sample Collection to Autosampler Stability;** Melanie Bergeron; Jean-Nicholas Mess; Milton Furtado; Troy Bradley; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, CANADA*
- TP 304 **Bioanalytical Quantitation of Roxithromycin in Human Plasma K3EDTA by LC-MS-MS;** Hassan Rashidzadeh; Yun Chen; Toni Jean Thompson; *Charles River Laboratories, Shrewsbury, MA*
- TP 305 **Strategies in Method Development and Determination of Endogenous Vitamin-D3 in Human Plasma by Atmospheric Chemical Ionization Liquid Chromatography/Tandem Mass Spectrometry;** Xuejun Peng; Rong Yi; Amara Pinnawala; Sarah Ostonal; Eliot Chung; Grace van der Gugten; David Gray; *Can Test Ltd, Burnaby, CANADA*
- TP 306 **Simultaneous Quantitation of Cytarabine and Uracil Arabinofuranoside in Human Plasma using LC-MS-MS;** Laixin Wang; Yanhui Zhang; Roger Demers; Min Meng; Patrick Bennett; *Tandem Labs, Salt Lake City, UT*
- TP 307 **High Throughput and Simultaneously Quantitative Analysis of Selegiline and Three Metabolites in Human Plasma by LC-APCI-Tandem Mass Spectrometry;** Jiongwei Pan<sup>1</sup>; Xiang-yu Jiang<sup>2</sup>; Qin Ji<sup>3</sup>; <sup>1</sup>*Covance, Madison, WI*; <sup>2</sup>*Covance - 08, Waukegan, WI*; <sup>3</sup>*Covance, Bioanalytical Chemistry, Madison, WI*
- TP 308 **Development of a High Throughput Method for the Quantification of Cholecalciferol in Human Plasma with Derivatization and LC-MS-MS Detection;** Lee Winchester; Anthony Podany; Corey Ohnmacht; Wei Sun; Chad Briscoe; *MDS Pharma Services, Lincoln, NE*
- TP 309 **A Rapid and Highly Sensitive LC-MS-MS Method (10 pg/mL) for Quantitation of Budesonide in Human Plasma;** Guangchun Zhou; Dawei Zhou; Xiping Fang; Jinn Wu; *Xenobiotic Laboratories, Inc., Plainsboro, NJ*
- TP 310 **LC-MS-MS Analysis of Aminoglycoside Drugs, Amikacin, Spectinomycin, Streptomycin and Gentamycin, the Challenges and Solutions;** Qi (Angela) Shen<sup>1</sup>; Xin Zhang<sup>1</sup>; Tuyen Nguyen<sup>2</sup>; <sup>1</sup>*Tandem Labs New England, Woburn, MA*; <sup>2</sup>*Sepracor Inc. 84 Waterford Drive, Marlborough, MA*
- TP 311 **Evaluation of Free and Protein-Bound 3-Nitrotyrosine in Human Plasma by Isotope Dilution LC-QqQ with an Artifacts-Free Nitrification-Free Proteolysis;** Thierry Delatour; Aurélien Desmarchelier;

## TUESDAY POSTERS

- Janique Richoz; Christophe Cavin; *Nestle Research Center, Lausanne, Switzerland*
- TP 311 **Challenges in Quantitating Low Picogram/mL Levels of Endogenous Compounds;** Kathy Jo Champion<sup>1</sup>; Matthew W. Chapple<sup>1</sup>; Ted Green<sup>1</sup>; George Hade<sup>1</sup>; John R. Perkins<sup>1</sup>; Margret Thorsteinsdottir<sup>2</sup>; <sup>1</sup>*Advion Biosciences, Ithaca, NY*; <sup>2</sup>*Decode, Reykjavik, Iceland*
- TP 312 **Simple and Rapid LC-MS-MS Method to Analyze Anti-Tuberculosis Drugs Ethambutol and Pyrazinamide in Human Plasma;** Yousef Basir; Zhilong Gong; *Covance Bioanalytical, Indianapolis, IN*
- TP 313 **Method Development for Measuring 5-Hydroxyindole-3-Acetic Acid in Human Plasma using Liquid Chromatography Tandem Mass Spectrometry;** Changyu Quang; Theodore Brus; Melanie McCort-Tipton; Qin Ji; *Covance, Indianapolis, IN*
- TP 314 **Development and Validation of an Improved LC-MS Method to Quantitate Vitamins A, D, and K in a Complex Mixture;** Esther Hwang; Svetlana Zhechonok; Samantha Leidner; Paul M. Bigwarfe Jr.; *Hospira, Inc., Lake Forest, IL*
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- DRUG METABOLISM PHARMACOKINETICS, 315 - 328**
- TP 315 ***In vitro* Metabolism of LY-320135, a Novel Inverse Agonist for Cannabinoid Receptor (CB1);** Qiang Zhang; Peng Ma; Guangdi Wang; *Xavier University of Louisiana, New Orleans, LA*
- TP 316 **Small Molecules and Metabolites Analysis by LC-MS in Plasma using Polymer-Based Internal Surface Reversed Phase Column;** Junji Sasuga<sup>1</sup>; Kei Oide<sup>1</sup>; Eiji Kagawa<sup>1</sup>; Hideyuki Kondo<sup>1</sup>; Yuichi Fusho<sup>2</sup>; Ken Tseng<sup>2</sup>; <sup>1</sup>*Showa Denko, KK, Kawasaki, Japan*; <sup>2</sup>*Shodex, New York, NY*
- TP 317 **Metabolite Identification of Precision-Deuterated Linezolid;** Changfu Cheng; Gary Bridson; Art Morales; David Wells; *Concert Pharmaceuticals, Lexington, MA*
- TP 318 **GC-MS Analysis of Human Breath as a Method for Determining Chemical Exposure and Monitoring Human Uptake and Clearance Rates;** Audrey N. Martin<sup>1</sup>; George R. Farquar<sup>1</sup>; A. Daniel Jones<sup>2</sup>; Matthias Frank<sup>1</sup>; <sup>1</sup>*Lawrence Livermore National Laboratory, Livermore, CA*; <sup>2</sup>*Michigan State University, East Lansing, MI*
- TP 319 **LC-MS Detection of Bisphosphonates in Equine Urine and Plasma and Application to an Administration Study of Tiludronic Acid in Horse;** April S Y Wong<sup>1</sup>; Emmie N M Ho<sup>1</sup>; Terence S M Wan<sup>1</sup>; Colton H F Wong<sup>1</sup>; Kenneth K H Lam<sup>2</sup>; Brian D Stewart<sup>2</sup>; <sup>1</sup>*Racing Laboratory, The Hong Kong Jockey Club, Shatin Racecourse, Shatin, N.T., Hong Kong*; <sup>2</sup>*Veterinary Regulation & International Liaison, Shatin Racecourse, Shatin, N.T., Hong Kong*
- TP 320 **Hardware and Software Design Strategies for the Rapid Determination of Optimal Quantitative MS-MS Conditions;** April Smith<sup>1</sup>; Anthony Romanelli<sup>1</sup>; Elliott Jones<sup>1</sup>; John Janiszewski<sup>2</sup>; Hua-fen Liu<sup>1</sup>; Steve Ainley<sup>3</sup>; Richard Schneider<sup>2</sup>; Kevin Shirey<sup>3</sup>; Eva Duchoslav<sup>1</sup>; Loren Olson<sup>1</sup>; <sup>1</sup>*Applied Biosystems, San Jose, CA*; <sup>2</sup>*Pfizer Inc., Westerly, RI*; <sup>3</sup>*Sound Analytics, East Lyme, CT*
- TP 321 **Study of RNA and Aminoglycoside Complex Binding Properties by ESI-MS-MS;** Keling Dong; Jeffrey Miller; Matthew Willetts; Christie L Hunter; *Applied Biosystems, Framingham, MA*
- TP 322 **Evaluation of Immobilized Liquid Extraction to Minimize Ion Suppression for LC-MS Analysis of**
- Drugs in Physiological Fluids;** Kerry Nugent<sup>1</sup>; Yixin Zhu<sup>1</sup>; Robert Woleb<sup>2</sup>; <sup>1</sup>*Michrom Bioresources, Inc., Auburn, CA*; <sup>2</sup>*ILE, Inc., Ferndale, CA*
- TP 323 **Investigation of Ultra-High Clearance in Rat for an Inhaled Drug;** Bruce R Heyde; Yiding Hu; Faith Hartsfield; Steve P Wene; Lesley A Albin; *Pfizer, Chesterfield, MO*
- TP 324 **Advanced HPLC-MS-MS Methods for Quantitation of Nucleotide and Nucleoside HIV Reverse Transcriptase Inhibitor Metabolites;** Zsuzsanna Kuklennyik; Amy Martin; Chou-Pong Pau; Gerardo Garcia-Lerma; Walid Heneine; John Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 325 **Application of ESI-LC-MS-MS to Mouse Pharmacokinetic Studies using Serial and Parallel Sampling Techniques;** Kevin Kennedy; Jun Tang; Jill Olson; Yun Xiao; Polina Kazavchinskaya; Kim Stringham; Cheryl Wu; *Cerep, Redmond, WA*
- TP 326 **Practical Bioanalytical Approach for Analyzing Dose-Formulations Used in PK Studies;** Andrei Stefanescu; Lucy Hetsco; *Seventh Wave Labs, Chesterfield, MO*
- TP 327 **Application of UPLC/Dynamic-Flow RAD/MS for Metabolite Identification and Profiling;** Jie Chen; Jie Chen; *JNJPRD, Raritan, NJ*
- TP 328 **Plasma Pharmacokinetics and Metabolism of NSC 644221 (A Small Molecule Inhibitor of the Hypoxic Signaling Pathway) in Mice;** Lawrence R. Phillips<sup>2</sup>; Christine Bramhall<sup>1</sup>; Mark Creighton-Gutteridge<sup>2</sup>; Kimberly D. Hill<sup>1</sup>; Giovanni Melillo<sup>2</sup>; Sherman Stinson<sup>2</sup>; Melinda G. Hollingshead<sup>2</sup>; <sup>1</sup>*SAIC, Frederick, MD*; <sup>2</sup>*NCI/NIH, Frederick, MD*
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- DRUG METABOLISM QUANTITATION 1, 329 - 342**
- TP 329 **Quantitative Determination of A Novel CC-Chemokine Receptor 2 (CCR2) Antagonist in Human Plasma using Liquid Chromatography-Tandem Mass Spectrometry;** Hengchang Song; Xiaohui Xu; *Merck & Co, West Point, PA*
- TP 330 **The Quantitative Analysis of Clodronate in Human Plasma by Liquid Chromatography/Tandem Mass Spectrometry;** Wen-Ying Huang; Chin-Hsiung Wang; Yi-Fan Shieh; Shu-Hui Yang; Cheng-Chin Chang; Wen-Lin Wu; *Protech Pharmaservices Corporation, Taipei, Taiwan*
- TP 331 **Method Development and Validation for the HPLC-MS-MS Bioanalysis of Vancomycin Extracted from Rat Plasma;** Matthew Pollard; Shane Needham; Chad Christianson; *Alturas Analytics, Inc., Moscow, ID*
- TP 332 **Bioanalytical Cross Validation: A Best Practice;** William Bullen<sup>1</sup>; David Muirhead<sup>2</sup>; Trevor Smart<sup>2</sup>; <sup>1</sup>*Pfizer, New London, CT*; <sup>2</sup>*Pfizer, Sandwich, UK*
- TP 333 **Determination of AMP, ADP and ATP using Capillary Ion-Pairing LC-MS-MS;** Jin Ren; Zaichuan Mi; EK Jackson; *University of Pittsburgh, Pittsburgh, PA*
- TP 334 **Development of a Bioanalytical LC-MS-MS Assay for the Quantitative Analysis of Amikacin, Neomycin and Gentamicin in Plasma and Tissue;** Jennifer Zimmer<sup>1</sup>; Shane Needham<sup>1</sup>; Jenny McKinnell<sup>2</sup>; Robert Cass<sup>2</sup>; Dane Kart<sup>2</sup>; <sup>1</sup>*Alturas Analytics, Inc., Moscow, ID*; <sup>2</sup>*Achaogen, South San Francisco, CA*
- TP 335 **An Ultrasensitive LC-MS-MS Method for the Quantitation of 6-β-Naltrexol in Human Plasma using Peak Summing;** Erica Nachi; Ginny B. James; Chris Kafonek; Curtis Sheldon; Chad Briscoe; *MDS Pharma Services, Lincoln, NE*



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- TP 336 **Validated LC-MS-MS Method for the Quantitative Analysis of the Endocannabinoid Anandamide and Other Ethanolamides in Human Plasma;** Joe Palandra; Jenny Zhang; Jeff Prusakiewicz; Timothy G Heath; *Pfizer, Chesterfield, MO*
- TP 337 **Quantitative Analysis of Taurocholate using Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry;** Amy Q Wang; Hong Cao; Erin D Hugger; Charles B Davis; Charles F McHugh; *DMPK, Oncology CEDD, GlaxoSmithKline, Collegeville, PA*
- TP 338 **Simultaneous Determination of Oxymorphone and 6 $\beta$ -Hydroxyoxymorphone with d3-IS in Human Plasma Despite Isotopic Distribution Overlap by Adjusting Transitions in HILIC-MS-MS;** Jing Ke; Michael Xinzhang Zhang; Siriporn Garritt; Qian Liu; Guiyan Chen; Allan Xu; *Keystone Analytical, Inc., North Wales, PA*
- TP 339 **Analysis of Tamoxifen and Midazolam in Plasma: Application of a Non-Linear Weighted Least-Squares Regression Model;** Larry Sallans; Ganesh M. Mugundu; Stephen F. Macha; Pankaj B. Desai; *University of Cincinnati, Cincinnati, OH*
- TP 340 **LC-MS-MS Quantitative Analysis of Hydrocortisone in Mouse Serum: Comparison of Liquid-Liquid Extraction (LLE) with Supported Liquid Extraction (SLE);** Shari Wu; Wenkui Li; Tapan Majumdar; Harold T Smith; Francis LS Tse; *Novartis, East Hanover, NJ*
- TP 341 **A Sensitive Semi-Automated Method for the Quantification of Dexamethasone in Human Plasma by LC-MS-MS;** Jonathan Rathe; Karl Linderholm; Chris Kafonek; Dale Raines; Curtis Sheldon; Chad Briscoe; *MDS Pharma Services, Lincoln, NE*
- TP 342 **Quantitation of Corticosteroid in Equine Joint Fluid using the 4000 QTRAP<sup>TM</sup> System;** Lorraine B Anderson<sup>1</sup>; Mary K Boyce<sup>1</sup>; Seijin Park<sup>2</sup>; Erin D Malone<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Seoul National University, Seoul, South Korea
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- DRUG METABOLISM ACCELERATING METABOLITE IDENTIFICATION, 343 - 364**
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- TP 343 **Differentiating Regional Variations in Red Wine with Accurate Mass LC-MS Authors:** Ravikanth Veluri, Jonathan Wilson, Ray Sanchez, Ali Kettani, Catherine Stacey; Ravikanth Veluri; *Bruker Daltonics, Burlington, MA*
- TP 344 **Phase I and Phase II Metabolite Identification on a Triple-Quadrupole Mass Spectrometer using 2 millisecond Dwell Times;** Allen Zhang<sup>123</sup>; Laurance Lee<sup>123</sup>; Patrick Jeanville<sup>123</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, West Palm Beach, FL
- TP 345 **Identification of Metabolites by Ultra High-Pressure Liquid Chromatography and Data-Dependent Accurate Mass Analysis using LTQ/Orbitrap in Internal Mass Calibration Mode;** Heng-keang Lim; Jose Silva; *Johnson and Johnson PRD, Raritan, NJ*
- TP 346 **Automated Software Analysis of Isotope Cluster Mass Differences for Components in LC-MS Datasets;** Graham A. McGibbon<sup>1</sup>; Mark A. Bayliss<sup>1</sup>; Margaret Antler<sup>1</sup>; Vitaly Lashin<sup>2</sup>; <sup>1</sup>Advanced Chemistry Development Inc., Toronto, ON; <sup>2</sup>ACD, Moscow, Russia
- TP 347 **Metabolic Interspecies Comparison by LC-MS and Principle Component;** Tania A. Sasaki<sup>1</sup>; Robert Cho<sup>2</sup>; Claire Bramwell-german<sup>1</sup>; Elliott Jones<sup>1</sup>; Ji Ma<sup>2</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Amgen Inc., South San Francisco, CA
- TP 348 **An Integrated Approach to Metabolite ID through Combination of Experimental LC-MS Data and In Silico Metabolite and Fragmentation Prediction;** Kim A. Johnson<sup>1</sup>; Vinod K. Arora<sup>1</sup>; W. Griffith Humphreys<sup>2</sup>; Yue-Zhong Shu<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Wallingford, CT; <sup>2</sup>Bristol-Myers Squibb, Princeton, NJ
- TP 349 **The Benefits of Small Particle Columns with Conventional HPLC Systems for Metabolite Profiling of Radioactive and Non-Radioactive Samples by LC-MS;** Natalia Penner; Zhiling Li; Swapan Chowdhury; *Schering-Plough Res. Inst., Kenilworth, NJ*
- TP 350 **Correlation and Convolution Analysis of Accurate Mass Spectrometry Data for Detection of Metabolites;** Eva Duchoslav<sup>2</sup>; Yves G. Leblanc<sup>1</sup>; <sup>1</sup>MDS Analytical Technologies, Concord, ON; <sup>2</sup>MDS Sciex, Concord, ON
- TP 351 **Metabolite Identification using a Unit Mass Resolution Liquid Chromatography/Mass Spectrometry with Accurate Formula Identification and Mass Defect Filtering;** Mei-yi Zhang<sup>1</sup>; Ming Gu<sup>2</sup>; Natasha Kagan<sup>1</sup>; Anokha Ratnayake<sup>1</sup>; <sup>1</sup>Wyeth Research, Princeton, NJ; <sup>2</sup>Cerno Bioscience, Danbury, CT
- TP 352 **Identification of Drug Metabolites by UPLC-MS with Isotope Pattern Directed Mass Chromatograms and UPLC with Radioactivity Flow Detection;** William de Maio; Matthew Hoffmann; Michael Carbonaro; Robin Moore; Abdul Mutlib; Rasmy E. Talaat; *Wyeth Research, Philadelphia, PA*
- TP 353 **Structural Characterization of in vitro Rat Liver Microsomal Metabolites of a Selective Muscarinic M<sub>2</sub> Receptor Antagonist using LTQ-Orbitrap Mass Spectrometer;** Guodong Chen; Ibrahim Daaro; Joseph Kozlowski; Birendra N. Pramanik; *Schering-Plough Research Inst., Kenilworth, NJ*
- TP 354 **High Resolution Metabolite Identification for Lafutidine in Rat Urine by UPLC/oa-TOF MS;** Kate Yu<sup>1</sup>; Jose Castro-perez<sup>1</sup>; John P. Shockcor<sup>1</sup>; Yuya Wang<sup>2</sup>; Xiaoyan Chen<sup>2</sup>; Dafang Zhong<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Chinese Academy of Science, Shanghai, China
- TP 355 **Rapid Metabolic Stability Screening with Simultaneous Metabolite Profiling Studies of Clozapine in Rat Hepatocytes;** Yingbo Yang; Ru Qiu (Sophie) Pan; Concettina Catalano; Julia Izhakova; Douglas J. Turk; *NoAb BioDiscoveries Inc., Mississauga, ON*
- TP 356 **Extracting Relevant Data Out of the MS Background;** Filip Cuyckens; Rob Hurkmans; Laurent Leclercq; Russell Mortishire-smith; *Johnson & Johnson Pharma R&D, Beerse, Belgium*
- TP 357 **Gender Specific In-Vitro Metabolism Analysis from Tri-Cyclic Antidepressant Drugs by Hybrid Quadrupole Time-of-Flight Mass Spectrometry and Principle Component Software;** Susan Leonard; Johnnie Brown; Jeffrey Miller; Elliott Jones; *Applied Biosystems, Framingham, MA*
- TP 358 **New Approach for Identification of Metabolites of a Model Drug; Partial Isotope-Enrichment Combined with Novel Mass Spectral Modelling Software;** Richard T. Gallagher<sup>1</sup>; Ian D. Wilson<sup>1</sup>; Kirsten Hobby<sup>2</sup>; <sup>1</sup>AstraZeneca, Macclesfield, UK; <sup>2</sup>Kisotopic Solutions, Manchester, UK
- TP 359 **Isoscore: Automated Localization of Biotransformations by Mass Spectrometry using Product Ion Scoring of Virtual Regioisomers;** Laurent Leclercq<sup>1</sup>; Russell Mortishire-smith<sup>1</sup>; Maarten



## TUESDAY POSTERS

- Huisman<sup>1</sup>; Filip Cuyckens<sup>1</sup>; Alastair Hill<sup>2</sup>; Michael Hartshorn<sup>2</sup>; <sup>1</sup>*Johnson & Johnson, Beerse, Belgium*; <sup>2</sup>*Dotmatics, Bishop Stortford, UK*
- TP 360 **Characterization of C- and N-oxidized Clemastine Metabolites using LC-MS<sup>n</sup>**; Annica Tevell Åberg<sup>1</sup>; Ulf Bondesson<sup>2</sup>; Mikael Hedeland<sup>2</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*; <sup>2</sup>*National Veterinary Institute, Uppsala, Sweden*
- TP 361 **Evaluation of MS-MS Methods: CID, PQD and HCD in an LTQ-Orbitrap Mass Spectrometer for Structural Elucidation of Metabolites**; Neil Blumenkrantz; Ragu Ramanathan; Swapan Chowdhury; Kevin Alton; *Schering-Plough Research Institute, Kenilworth, NJ*
- TP 362 **An Evaluation of Different Scan Functions to Identify Nefazodone Metabolites *in vitro* Samples using a LC-QqQ/LIT Mass Spectrometry**; Daniel Lebre; Gary Impey; Julie Wingate; *Applied Biosystems/MDS Sciex, Concord, Canada*
- TP 363 **A Chemically Intelligent Metabolite Identification LC-MS-MS Workflow with a C-Heteroatom Cleavage Tool and Automatic Generation of Mass Defect Filters**; Jeff Goshawk<sup>1</sup>; Kate Yu<sup>1</sup>; Henry Shion<sup>2</sup>; John Shockcor<sup>2</sup>; Jose Castro-Perez<sup>2</sup>; Michael Hartshorn<sup>3</sup>; Alastair Hill<sup>3</sup>; Russell Mortishire-Smith<sup>4</sup>; <sup>1</sup>*Waters MS Technology, Manchester, UK*; <sup>2</sup>*Waters Corp, Milford, USA*; <sup>3</sup>*Dotmatics Ltd, Herts, UK*; <sup>4</sup>*J&J Pharmaceutical R&D, Beerse, Belgium*
- TP 364 **Frequently Reported Mass Differences and Formula for List Searching in Drug Metabolite Identification**; Peter L. Jacobs; Lars Ridder; *N.V. Organon, a part of Schering-Plough Corp., Oss, Netherlands*
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- METABOLOMICS 2, 365 - 393**
- TP 365 **Rapid Nontargeted Metabolite Profiling of Cancer Cells Treated with Potential Cancer Therapeutic Agents using Electrospray Ionization Mass Spectrometry**; Ruth N. Udey; Chrysoula Vasileiou; Babak Borhan; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- TP 366 **UPLC MS-MS Assay of Jasmonates and Related Phytohormones for Large-Scale Screening of Plant Metabolic Phenotypes**; Xiaoli Gao; Abraham J. K. Koo; Gregg A. Howe; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- TP 367 **LC-MS Multivariate Analysis of Beer for the Discovery of Commercially Important Compounds**; Masahiro Maeda<sup>1</sup>; Hideaki Uchida<sup>1</sup>; Shigeki Araki<sup>2</sup>; Toshiyuki Oshima<sup>2</sup>; Youichi Tsuchiya<sup>2</sup>; Katsuaki Maeda<sup>2</sup>; Junji Watari<sup>2</sup>; Steve Fischer<sup>3</sup>; <sup>1</sup>*Agilent technologies Japan, Tokyo, Japan*; <sup>2</sup>*Sapporo Breweries Ltd, Shizuoka, Japan*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- TP 368 **Quantitative Profiling of Metabolites of Polyunsaturated Fatty Acids Modulated by Dietary N-3 Deficiency in Rat Lung Tissues by HPLC/ESI-MS-MS**; Jeongrim Lee; Kei Hamazaki; Hee-Yong Kim; *NIH/NIAAA, Rockville, MD*
- TP 369 **Visualizing Islet Metabolism by <sup>13</sup>C Labeling and Capillary Liquid Chromatography – Nanoelectrospray Ionization Mass Spectrometry (cLC-nESI-MS)**; Qihui Ni; Robert T Kennedy; *University of Michigan, Ann Arbor, MI*
- TP 370 **High-Resolution Separation and Identification of Structural Isomers of Endogenous Acylcarnitine Metabolites in Human Urine**; Azeret Zuniga; Liang Li; *University of Alberta, Edmonton, Canada*
- TP 371 **Defining Instrument Performance and Assessing the Reproducibility of Mass Spectrometric Analyses of Complex Samples**; Paolo Lecchi; Jean Zhao; Wes Wiggins; Greg Bertenshaw; Tzong-Hao Chen; Brian Mansfield; John M. Peltier; *Correlogic Systems, Inc., Rockville, MD*
- TP 372 **Unraveling Control and Regulation in Metabolic Pathways from Quantitative Metabolomics and <sup>13</sup>C Metabolic Flux Analysis**; Nicola Zamboni; Jennifer Ewald; Stefan Jol; Anne Kuemmel; Uwe Sauer; Matthias Heinemann; *ETH Zürich, Zürich, Switzerland*
- TP 373 **Quantitative Analysis of Bile Acids in Various Biological Fluids using LC-MS-MS Isotopic Dilution Technique**; Philippe A. Guy; Mounir Meknaci; Francois-Pierre Martin; Sunil Kochhar; *Nestlé Research Center, Lausanne, Switzerland*
- TP 374 **Metabolomics for Global Assessment of Antioxidant Capacity using Capillary Electrophoresis-Mass Spectrometry**; Richard Lee; Philip Britz-McKibbin; *McMaster University, Hamilton, Canada*
- TP 375 **Metabolic Profiling of Endocannabinoids and Related Fatty Acid Amides and Glycerol Esters in Rat Tissue and Plasma Samples**; Katrin Georgi<sup>1</sup>; John W. Newman<sup>2</sup>; Bruce D. Hammock<sup>1</sup>; <sup>1</sup>*UC Davis, Davis, CA*; <sup>2</sup>*USDA, ARS, Western Human Nutrition Research Center, Davis, CA*
- TP 376 **High Resolution Mass Spectrometry: Quantitative Metabolomic Analysis of Butanol Stress Response in *E. coli***; Francesco Pingitore; Aindrila Mukhopadhyay; Jay Keasling; Marcin Joachimiak; *University of California, Berkeley/ LBNL, Berkeley, CA*
- TP 377 **Metabolic Profiling of Carnitine, Aminoacids, and Phospholipids-Based Compounds in Plasma Samples by UHPLC and Monolithic HPLC/ESI/APCI-MS**; Estela Soledad Cerutti; Timothy Garrett; Peggy Borum; Jodie V. Johnson; Richard A. Yost; David H. Powell; *University of Florida, Gainesville, FL*
- TP 378 **Characterizing Sodium Phenylbutyrate (SPB) Metabolites from Huntington's Disease (HD) Plasma using Parallel LCECA/LC-MS**; Erika N. Ebbel<sup>1</sup>; Susan Schiavo<sup>2</sup>; Lei Wang<sup>3</sup>; Wayne R. Matson<sup>4</sup>; Mikhail B. Bogdanov<sup>3</sup>; Stephen Hersch<sup>5</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston U School of Medicine, Boston, MA*; <sup>2</sup>*Northeastern University, Boston, MA*; <sup>3</sup>*Weill Medical College of Cornell University, New York, NY*; <sup>4</sup>*Bedford VA Medical Center, Bedford, MA*; <sup>5</sup>*MA General Hospital, Harvard Medical School, Boston, MA*
- TP 379 **Targeted Metabolomics Analysis of Recombinant *Saccharomyces* Strains by Capillary Electrophoresis - Electrospray Mass Spectrometry**; Joseph P.M. Hui<sup>1</sup>; Elizabeth Huenupi<sup>1</sup>; Jan-Maarten Geertman<sup>2</sup>; Theresa C. White<sup>2</sup>; Evelyn C. Soo<sup>1</sup>; <sup>1</sup>*NRC - Institute for Marine Biosciences, Halifax, Canada*; <sup>2</sup>*Iogen Corporation, Ottawa, Canada*
- TP 380 **Comparison of GC-MS and NMR Metabolite Identification in White Wines: Insights into the Chemical Basis for Wine Body**; Kirsten Skogerson<sup>1</sup>; Ron Runnebaum<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>*UC Davis Genome Center, Davis, CA*; <sup>2</sup>*UC Davis, Davis, CA*
- TP 381 **Rapid LC-MS-MS Determination of Intermediates Produced during Glycolysis**; Keri Ross; Joseph J. Dalluge; *Cargill Incorporated, Excelsior, MN*
- TP 382 **A Metabolomic Screening and Quantification of Hexose Monophosphates for Neonatal Galactosemia in Whole Blood using Electrospray Tandem Mass Spectrometry (ESI/MS-MS)**; Sung Hyun Hong; Hae-

## TUESDAY POSTERS

- Ran Moon; *Specialty Lab Solution, Suwon, Gyeonggi-Do, South Korea*
- TP 383 **Image-Based Differential Mass Spectrometry Data Analysis for the Discovery of Markers of Liver Toxicity by Metabolomics**; Peter Askovich<sup>1</sup>; Cindy Chepanoske<sup>1</sup>; Andrey Bondarenko<sup>1</sup>; Yutai Li<sup>2</sup>; Kara Pearson<sup>2</sup>; Caroline K Ferraro<sup>2</sup>; Amy F. Loughlin<sup>2</sup>; Ethan Xu<sup>2</sup>; William H. Schaefer<sup>2</sup>; <sup>1</sup>*Rosetta Biosoftware, Seattle, WA*; <sup>2</sup>*Merck & Co., Inc, West Point, PA*
- TP 384 **Validated Quantitative Metabolic Signature using Gas Chromatography-Mass Spectrometry Based Steroid Analysis**; Ju-Yeon Moon<sup>1</sup>; Man-Ho Choi<sup>1</sup>; Hyun-Jin Jung<sup>1</sup>; Myeong Hee Moon<sup>2</sup>; Bong Chul Chung<sup>1</sup>; <sup>1</sup>*Life Sciences Division / KIST, Seoul, South Korea*; <sup>2</sup>*Dept. of Chemistry / Yonsei Univ., Seoul, Korea*
- TP 385 **Identification of Novel Endogenous Metabolites of Acylglycines in Human Urine**; Avalyn Lewis; *University of Alberta, Edmonton, Canada*
- TP 386 **Identifying Biomarkers for Rheumatoid Arthritis in the Human TNF-driven Tg197 Mouse Model using High Mass Accuracy MSn Analysis**; Eleni Gika<sup>2</sup>; Georgios Theodoridis<sup>2</sup>; Neil J Loftus<sup>1</sup>; Ian Wilson<sup>1</sup>; Simon Ashton<sup>1</sup>; Lefteris Zacharia<sup>5</sup>; Yiannis Sotsios<sup>5</sup>; George Kollias<sup>3</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*Aristotle University, Thessaloniki, Greece*; <sup>3</sup>*Biomedical Sciences Research Center, Vari, Greece*; <sup>4</sup>*Astra Zeneca, Alderley Edge, UK*; <sup>5</sup>*Biomedcode Hellas SA, Vari, Greece*
- TP 387 **Metabolite Profiling of Single Secretory and Glandular Trichomes of the Genus Solanum using Laser Desorption/Ionization (LDI) Mass Spectrometry and LC-MS**; Chao Li; Feng Shi; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- TP 388 **Validated Analytical Method for Quantification and Identification of Coenzyme-A Activated Compounds in Biological Tissues by online SPE-LC-MS-MS**; Christoph Magnes<sup>1</sup>; Maria Suppan<sup>1</sup>; Thomas Pieber<sup>2</sup>; Guenter Haemmerle<sup>3</sup>; Frank Michael Sinner<sup>1</sup>; <sup>1</sup>*Joanneum Research, Inst of Med. Technologies and H, Graz, Austria*; <sup>2</sup>*Medical University of Graz, Dep. of Int. Medicine, Graz, Austria*; <sup>3</sup>*University of Graz, Inst. of Molecular Bioscience, Graz, Austria*
- TP 389 **The Capacity of the Human Endometrium to Synthesize Steroids: a Metabolomic (Mass Spectrometry) and Genomic (RT-PCR) Approach**; Angela E Taylor; John O White; Gareth Brenton; Deya Gonzalez; Edward Dudley; *Swansea University, Swansea, UK*
- TP 390 **A Simple LC-MS-MS Method for Metabolite Profiling of Mevalonate Pathway and Associated Co-Factors in Metabolically Engineered Yeast and Bacteria**; Sunil Bajaj; Nathan Moss; Tina Mahatdejl; Sunil Chandran; Michael Leavell; *Amyris Biotech, Emeryville, CA*
- TP 391 **Targeted Metabolic Profiling of Heart Failure Mouse Model by Selected-Reaction Monitoring of Fatty Acid Metabolites**; Lekha Sleno; Anthony Gramolini; Andrew Emili; *University of Toronto, Toronto, Canada*
- TP 392 **Profiling Bacterial Virulence with Quantitative Metabolomics**; Jan Crowley; John Turk; Scott Hultgren; Jeffrey Henderson; *Washington University School of Medicine, St. Louis, MO*
- TP 393 **GC-TOF-MS Based Metabolomics for the Analysis of Plant Biodiversity and Phenotypic Plasticity in a Typical Grassland Community**; Christian Scherling; Wolfram Wweckwerth; *Max-Plank-Institute, Potsdam-Golm, Germany*
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- NEUROPEPTIDES, 394 - 406**
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- TP 394 **Strategies for Sensitive Peptide Detection in Brain Homogenate using LC-MS for the Purpose of Blood-Brain-Delivery Testing**; Karin Pickl<sup>1</sup>; Christoph Magnes<sup>1</sup>; Thomas R. Pieber<sup>2</sup>; Hans-Georg Frank<sup>3</sup>; Christoph Schmitz<sup>4</sup>; Frank M. Sinner<sup>1</sup>; <sup>1</sup>*Joanneum Research, Inst.of Med.Technologies & HM, Graz, Austria*; <sup>2</sup>*Dep. Int.Med., Medical University Graz, Graz, Austria*; <sup>3</sup>*AplaGen, Baesweiler, Germany*; <sup>4</sup>*Division Neuroscience, University of Maastricht, Maastricht, Netherlands*
- TP 395 **High-Throughput Discovery of Signaling Peptides in the *Aplysia* Central Nervous System**; Fang Xie; Elena Romanova; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 396 **Novel Inactivation Technology Preserves the *in vivo* Levels of Proteins, Peptides and Phosphorylations in Tissue Samples**; Marcus Svensson<sup>1</sup>; Jonas Larsson<sup>1</sup>; Mats Borén<sup>1</sup>; Maria Fälth<sup>2</sup>; Per E. Andren<sup>2</sup>; Per Svenningsson<sup>3</sup>; Karl Sköld<sup>1</sup>; <sup>1</sup>*Denator AB, Gothenburg, Sweden*; <sup>2</sup>*Uppsala University, Uppsala, Sweden*; <sup>3</sup>*Karolinska Institutet, Stockholm, Sweden*
- TP 397 **Enrichment and Characterization of C-terminally Blocked Neuropeptides in Cancer borealis Brain Tissue**; Xin Wei; Feng Xiang; Mingming Ma; Lingjun Li; *Univ.of Wisconsin-Madison, Madison, WI*
- TP 398 **Quantitative Tandem Mass Spectrometry Based Search for Sex-Specific Neuropeptides in Insects**; Peter D. Verhaert<sup>1</sup>; Inez M. Finoulst<sup>1</sup>; Peter Schulzknappe<sup>2</sup>; Martijn Pinkse<sup>1</sup>; <sup>1</sup>*Delft University of Technology, DELFT, Netherlands*; <sup>2</sup>*Proteome Sciences R&D GmbH Co.kg, Frankfurt, Germany*
- TP 399 **Mass Spectrometry Reveals Activity Dependent Release of Protein Fragments at the Synapse**; Suresh P Annangudi; Soong Ho Kim; Ivan Jeanne Weiler; Stanislav Rubakhin; William T Greenough; Jonathan V Sweedler; *Beckman Institute, University of Illinois, Urbana, IL*
- TP 400 **Comparative Neuropeptidomic Analysis of Food Intake via a Multi-faceted MS Approach**; Ruibing Chen; Stephanie Cape; Junhua Wang; Yuzhuo Zhang; Lingjun Li; *UW, Madison, Madison, WI*
- TP 401 **Neuropeptide Characterization in Brain Tissue using Recent Advances in Mass Spectrometry**; A.F. Maarten Altelaar<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; Roger A.H. Adan<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, The Netherlands*; <sup>2</sup>*University Medical Center, Utrecht, The Netherlands*
- TP 402 **Mass Spectrometric Investigation of Individual Mammalian Cells Selected via Molecular Biology Markers**; Stanislav S. Rubakhin<sup>1</sup>; Georgina M. Aldridge<sup>2</sup>; William T. Greenough<sup>3</sup>; Jonathan V. Sweedler<sup>4</sup>; <sup>1</sup>*Beckman Institute, UIUC, Urbana, IL*; <sup>2</sup>*Neuroscience Graduate Program, UIUC, Urbana, IL*; <sup>3</sup>*Department of Cell and Structural Biology, UIUC, Urbana, IL*; <sup>4</sup>*Department of Chemistry, UIUC, Urbana, IL*
- TP 403 **Mass Spectrometric Characterization of the Crustacean Hyperglycemic Hormone (CHH) in the Sinus Gland of Cancer borealis**; MINGMING MA; Joshua J. Schmidt; Ying Ge; Lingjun Li; *University of Wisconsin---Madison, Madison, WI*
- TP 404 **Peptidomic Profiling of Secreted Products from Pancreatic Islet Culture Yields More Full Length**

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- Peptide Hormones than Cell Lysis Procedures;** Steven Taylor; Svetlana Nikoulina; Kevin Mccowen; Nancy Andon; *Amylin Pharmaceuticals, Inc., San Diego, CA*
- TP 405 **Mass Spectrometry Screening for Peptides Modulated by Psychostimulant Exposure in Defined Brain Regions;** Elena V. Romanova; Jessica J. Stanis; Joshua M. Gulley; Jonathan V. Sweedler; *University of Illinois, Urbana, IL*
- TP 406 **Peptidomic Analysis of Astrocytes using Liquid Chromatography Coupled to Mass Spectrometry (LC-MS);** Ping Yin; Ann Knolhoff; Suresh Annangudi; Larry Millett; Martha Gillette; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
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- PEPTIDES: GENERAL, 407 - 419**
- TP 407 **Structural Analysis of PEGylated Therapeutics by Acid Hydrolysis and Mass Spectrometry;** Chul Yoo; Minhui Ma; *Amgen, Inc., Thousand Oaks, CA*
- TP 408 **Time Course Studies of the Kinetics of Antigen-Antibody Interactions Employing MALDI Mass Spectrometry;** Bethny Morrissey; Kevin Downard; *University of Sydney, Sydney, Australia*
- TP 409 **Epitope- Motif Structure of an Anti-Nitrotyrosyl-Antibody in 3-Nitrotyrosine-Peptides Elucidated by Proteolytic Excision- Mass Spectrometry;** Mihaela Dragusanu; Alina Petre; Michael Przybylski; *University of Konstanz, Konstanz, Germany*
- TP 410 **Screening Zn(II)-Binding Artificial Peptides using a Simple ESI-MS Adduct Monitoring;** Soo Jin Park<sup>1</sup>; Sungsu Park<sup>2</sup>; HanBin Oh<sup>3</sup>; <sup>1</sup>*Sogang University, Interdisciplinary Program, Seoul, Korea;* <sup>2</sup>*Ewha University, Dept. of Life Science, Seoul, Korea;* <sup>3</sup>*Sogang Univ. Chemistry & Interdisciplinary Program, Seoul, Korea*
- TP 411 **Charge and Functional Group Based Extraction and Detection of Peptides using Dendrimeric Inverse Micelles and MALDI-TOF MS;** Andrea Gomez; Malar Azagarsamy; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TP 412 **Improved Mass Spectrometric Analysis of Ziconotide after Reduction and Alkylation of Disulfide Bonds;** Jhoana A. Mendoza; John R. Eyler; *University of Florida, Gainesville, FL*
- TP 413 **Ion Activation and Dissociations of the Cyclic Peptide c-(Lys-D-His-β-Ala-His) and its Cu(I), Cu(II) and Cu(III) Complexes: ECD and CID Experiments;** Gianluca Giorgi<sup>1</sup>; Mauro Ginanneschi<sup>2</sup>; Carlos Afonso<sup>3</sup>; Jean-Claude Tabet<sup>4</sup>; <sup>1</sup>*University of Siena, Siena, Italy;* <sup>2</sup>*Univ. of Florence, Florence, Italy;* <sup>3</sup>*Université Paris, Paris, France;* <sup>4</sup>*University Paris Vi (upmc), Paris, France*
- TP 414 **Generating Peptide Titration Curves using Polymeric Inverse Micelles and MALDI-MS Analysis;** Nadnudda Rodthongkum; Elamprakash N. Savariar; Ramgopal Mettu; Sankaran Thayumanavan; Richard W. Vachet; *University of Massachusetts, Amherst, MA*
- TP 415 **Detection of Helix Formation in Gas-Phase Peptides by Fluorescence Measurements of Trapped Ions;** Huihui Yao; Geng Li; Anthony Rullo; Rebecca Jockusch; *Department of Chemistry, University of Toronto, Toronto, Canada*
- TP 416 **Mechanistic Aspects of Electrochemical Oxidation of Tyrosine and Tryptophan Containing-Tripeptides by Electrochemistry-Mass Spectrometry;** Julien Roeser; Hjalmar Permentier; Andries P. Bruins; Rainer Bischoff; *University of Groningen, Groningen, Netherlands*
- TP 417 **Investigations of the Gas-Phase Binding Properties of LDV and RGD;** Xiaoning Zhao<sup>1</sup>; Jianhua Ren<sup>2</sup>; <sup>1</sup>*Stockton, CA;* <sup>2</sup>*University of The Pacific, Stockton, CA*
- TP 418 **Gas-Phase Acidities Determination of the Cysteine-Polyglycine Peptides using the Kinetic Method;** Kiran Kumar Morishetti; John Tan; Jianhua Ren; *University of The Pacific, Stockton, CA*
- TP 419 **Identification and Quantification of Malondialdehyde Oxidation of Apolipoprotein B Peptides by LC-ESI and LC-MALDI Tandem Mass Spectrometric Analysis;** Charlene X. Li<sup>1</sup>; Chris Fong<sup>1</sup>; Viswanatham Katta<sup>1</sup>; Boyan Zhang<sup>2</sup>; <sup>1</sup>*Genentech Inc., South San Francisco, CA;* <sup>2</sup>*Genentech, Inc., South San Francisco, CA*
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- PEPTIDES: SEQUENCING, 420 - 435**
- TP 420 **A Fixed-Charge Modification Strategy to Enhance ETD-MS-MS Fragmentation Efficiency;** April L. Jue; Brian L. Frey; Casey J. Krusemark; Lloyd Smith; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- TP 421 **Discovery, Sequencing and Chemical Synthesis of a Highly Selective Ligand Binding an Orphan Adrenoreceptor Subtype in the Green Mamba Venom;** Loïc Quinton<sup>1</sup>; Céline Rouget<sup>2</sup>; Gilles Mourier<sup>2</sup>; Robert Thai<sup>2</sup>; Steven Dubois<sup>2</sup>; Nicolas Gilles<sup>2</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>*University of Liege - Mass Spectrometry Laboratory, Liege, Belgium;* <sup>2</sup>*CEA Saclay, DSV/iBiTec-S/SIMOPRO, Gif-sur-Yvette, France*
- TP 422 **The Contribution of Ammonium Sulfate and In-Source Decay in Peptides Sequencing;** Alice Delvolvé; Amina S. Woods; *NIH/NIDA/IRP, Baltimore, MD*
- TP 423 **Application of Electron Transfer Dissociation in Peptidomic Analysis;** Junko Kimata<sup>1</sup>; Kazuki Sasaki<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Osaka, Japan;* <sup>2</sup>*National Cardiovascular Center, Osaka, Japan*
- TP 424 **MS Study of the Efficiency of Derivatizing Agents for the Sequencing of Disulfide Peptides of Anurans;** Tatiana Samgina; Vladimir Gorshkov; Sergey Kovalev; Konstantin Artemenko; Albert T. Lebedev; *Moscow State University, Moscow, Russian Federation*
- TP 425 **z -Type Fragment Ions are Chemically Distinct from a, b, c, and y-type Fragments;** Shane L Hubler; April Jue; Graeme Mcalister; Joshua J. Coon; Gheorghe Craciun; *UW - Madison, Madison, WI*
- TP 426 **Fragmentation of Large Peptides by Low Energy CID Fragmentation;** Heyi Yang; Rong Wang; *Mount Siani school of medicine, New York, NY*
- TP 427 **Analysis of Post-Translational Modifications using Electron-Transfer-Dissociation in Combination with a High Resolution Orbitrap Mass Analyzer;** Dirk Nolting; Martin Zeller; Jens Griep-Raming; Thomas Moehring; Eduard Denisov; Oliver Lange; Alexander Makarov; *Thermo Fisher Scientific, Bremen, Germany*
- TP 428 **Increased Sequence Coverage of Low Abundance Protein by LC-ESI LTQ FT-ICR MS and MS-MS with Gas Phase Fractionation;** Shannon M Eliuk; Matthew B. Renfrow; Stephen Barnes; Helen Kim; *University of Alabama At Birmingham, Birmingham, AL*
- TP 429 **A Physical Model for Prediction of Peptide ETD Spectra;** Zhongqi Zhang; *Amgen, Inc., Thousand Oaks, CA*
- TP 430 **Selective Derivatization of Cysteines for the Enhancement of UV Photodissociation of Peptides;** Lisa A Vasicek<sup>1</sup>; Jennifer Brodbelt<sup>2</sup>; <sup>1</sup>*University of Texas, Austin, TX;* <sup>2</sup>*The University of Texas, Austin, TX*
- TP 431 **Assessment of 'Golden Pair' Rule for Peptide Sequencing and Protein Identification using Iontrap**

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- CAD/ETD MS-MS; Thomas A. Hansen; Frank Kjeldsen; Ole N. Jensen; *Univ. of Southern Denmark, Odense, Denmark*
- TP 432 **Comparison of Infrared Multiphoton and Collisionally Activated Dissociation of Supercharged Peptides in a Quadrupole Ion Trap**; James Madsen; Jennifer Brodbelt; *University of Texas Austin, Austin, TX*
- TP 433 **Aspartocin Antibiotic Complex A, B & C: Structure Characterization by ESI-MS-MS and ESI-Nozzle-Skimmer-MS-MS**; Marshall M. Siegel; Fangming Kong; Xidong Feng; Guy Carter; *Wyeth Research, Pearl River, NY*
- TP 434 **High Sequence Coverage by Combining CID of Tryptic and ETD of Non-Tryptic Peptides**; Erik Haaf; Andreas Schlosser; *Center for Systems Biology (ZBSA), Freiburg, Germany*
- TP 435 **Enhanced de novo Sequencing of Peptides by Charge Derivatization and Photodissociation**; Yi He; James P. Reilly; *Indiana University, Bloomington, IN*
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- LC-MS SAMPLE PREPARATION, PHOSPHOLIPID REMOVAL, 436 - 443**
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- TP 436 **Evaluation of Inter-Species Phospholipid Removal, using a New Resin-based Mixed-mode SPE Sorbent and LC-MS Analysis**; Lee Williams; Scott Merriman; Matthew Cleeve; Steve Jordan; Steve Plant; Richard Calverley; Joanna Smith; *Biotage GB Limited, Hengoed, UK*
- TP 437 **Elimination of Six Human Phospholipids with Downfield Suppression Potential from Protein Precipitation Extracts using a Novel Phospholipid Scavenger Plate**; Mary Pelzer<sup>1</sup>; Hongliang Jiang<sup>2</sup>; Qin Ji<sup>3</sup>; An Trinh<sup>4</sup>; <sup>1</sup>Covance, Madison, WI; <sup>2</sup>Covance Laboratories Inc., Madison, WI; <sup>3</sup>Covance, Bioanalytical Chemistry, Madison, WI; <sup>4</sup>Sigma-Aldrich, St. Louis, MO
- TP 438 **Selective Depletion of Phospholipid Interference Utilizing Hybrid SPE Technology**; Craig Aurand<sup>1</sup>; David S. Bell<sup>2</sup>; Hillel K. Brandes<sup>2</sup>; <sup>1</sup>Supelco, Bellefonte, PA; <sup>2</sup>Supelco/Sigma Aldrich, Bellefonte, PA
- TP 439 **Eliminating Chromatography using High-Throughput Electrophoretic Sample Preparation in Quantitative Bioanalysis**; Russell P. Grant<sup>1</sup>; Patricia Holland<sup>1</sup>; Brian Rappold<sup>1</sup>; Jeremy L. Norris<sup>2</sup>; <sup>1</sup>Labcorp, Burlington, NC; <sup>2</sup>Protein Discovery, Inc., Knoxville, TN
- TP 440 **Elimination of LC-MS-MS Matrix Effect Due to Phospholipids using Specific SPE Elution Conditions**; Mathieu Lahaie; Jean-Nicholas Mess; Milton Furtado; Troy Bradley; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, Canada*
- TP 441 **Streamlining Bioanalytical Method Development using a Novel Filtration Device for Matrix Interference Removal**; David Jones; *Varian Inc., Lake Forest, CA*
- TP 442 **Balancing Sample Preparation Liquid Chromatography to Remove Phospholipid-Based Matrix Effects in Positive ESI**; Brian Rappold; Patricia Holland; Russell Grant; *Labcorp, Burlington, NC*
- TP 443 **Impact of Ion-Suppression Due to the Presence of Phospholipids on the Enantiomeric LC-MS Analysis of Clenbuterol**; Carmen T. Santasania; Craig Aurand; JT Lee; David S. Bell; Daniel Shollenberger; *Supelco/Sigma-Aldrich, Bellefonte, PA*
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- PHOSPHOPROTEINS: METHODS, 444 - 459**
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- TP 444 **Multi-Matrix Analysis of Protein Phosphorylation**; Petri Kouvonen; Eeva Rainio; Jani Ylä-Pelto; Päivi Koskinen; Garry Corthals; *Univ Turku/ Centre For Biotech, Turku, Finland*
- TP 445 **Improving Identification of Phosphorylated Peptides by Combining Affinity Purification, Dephosphorylation and Spectral Matching**; A. Jimmy Ytterberg<sup>1</sup>; Rachel O. Loo<sup>1</sup>; James Wohlschlegel<sup>2</sup>; Pinmanee Boontheung<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>Ucla - Biol Chem, Los Angeles, CA
- TP 446 **Efficient MALDI Analysis of Phosphopeptides using 2, 6-Dihydroxyacetophenone with Diammonium Hydrogen Citrate as Matrix**; Junjie Hou; Zhensheng Xie; Peng Xue; Xiulan Chen; peng wu; Linan Shi; Zhiqiang Zhao; Ziyou Cui; tanxi cai; jing li; Hongjie Zhang; Fuquan Yang; *Institute of Biophysics, CAS, Beijing, China*
- TP 447 **A Novel Approach for the Quantification of the Stoichiometry of Protein Phosphorylation**; Hannah Johnson; Claire Eyers; Patrick Eyers; Simon J. Gaskell; *The University of Manchester, Manchester, UK*
- TP 448 **ECD and CID FTICR MS Analyses of Lanthanide Metal Complexes Bound to Phosphopeptides**; Jackie Mosely; Ben S. Murray; David Parker; *Durham University, Durham, UK*
- TP 449 **CID vs. MSA vs. MS3 vs. PQD; Comparison of Different Peptide Fragmentation Modes for Phosphopeptide Analysis on an LTQ-Orbitrap**; Arjen Scholten; Gavain Sweetman; Toby Mathieson; Marcus Bantscheff; *Cellzome AG, Heidelberg, Germany*
- TP 450 **Phosphorylation Specific MS-MS Scoring for Rapid and Accurate Phospho-Proteome Analysis**; Samuel Payne; Margaret Yau; Marcus Smolka; Huilin Zhou; Vineet Bafna; *University of California San Diego, San Diego, CA*
- TP 451 **A New Approach Towards Phosphopeptide Identification in MS-MS**; Amrita Mohan; Randy J. Arnold; Predrag Radivojac; Quanhu Sheng; Haixu Tang; *Indiana University, Bloomington, IN*
- TP 452 **Comparison of MS<sup>2</sup>-only, MSA, and MS<sup>2</sup>/MS<sup>3</sup> Methodologies for Phosphopeptide Identification**; Peter Ulintz<sup>1</sup>; Anastasia K. Yocum<sup>1</sup>; Bernd Bodenmiller<sup>2</sup>; Ruedi Aebersold<sup>3</sup>; Philip Andrews<sup>1</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Eth Zürich, Zurich, Switzerland; <sup>3</sup>Swiss Federal Institute of Technology, Zurich, Switzerland
- TP 453 **Characterization of Phosphopeptides by a Combination of  $\beta$ -Elimination/Michael Addition and Gold affinity Purification**; Yi-Wen Chang; Yen-peng Ho; *National Dong Hwa University, Hualien, Taiwan*
- TP 454 **Erroneous Assignment of Protein Phosphorylation by Competing Losses of H<sub>3</sub>PO<sub>4</sub> and HPO<sub>3</sub>+H<sub>2</sub>O from Peptides Containing Multiple Potential Phosphorylation Sites**; Amanda M. Palumbo; Jetze J. Tepe; Gavin E. Reid; *Michigan State University, East Lansing, MI*
- TP 455 **Silver Staining-Induced Sulfonation: An Obstacle in the Identification of Genuine Protein Phosphorylation**; Marlene Gharib; Mathieu Courcelles; Alain Verreault; Pierre Thibault; *IRIC, Université de Montreal, Montreal, Canada*
- TP 456 **Evaluation of Nanoelectrospray Ionization Emitter Treatments for Enhancement of Phosphopeptide Ion Signal**; Troy D. Wood; Nan Li; *University at Buffalo, Buffalo, NY*
- TP 457 **Facile Identification of Phosphorylation Sites in Peptides by Site Specific Photodissociation**; Jolene K.

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- Diedrich; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- TP 458 **MALDI TOF/TOF Is a Convenient Tool for the Identification and Quantification of Multiply Phosphorylated Peptides from Low Complexity Samples**; Andreas Schmidt<sup>4</sup>; Goran Mitulovic<sup>2</sup>; Edina Csaszar<sup>3</sup>; Gustav Ammerer<sup>3</sup>; Karl Mechtler<sup>1</sup>; <sup>1</sup>IMP Research Institute of Mo, Vienna, Austria; <sup>2</sup>Imba Inst. of Mol. Biotech., Vienna, Austria; <sup>3</sup>Max F. Perutz Laboratories, Vienna, Austria; <sup>4</sup>Cd Laboratory / Vienna, Vienna, Austria
- TP 459 **Phosphoproteomics using Selective Derivatization and Structural Separations by Ion Mobility-Mass Spectrometry**; Randi L. Gant; Thomas J. Kerr; John A. McLean; *Vanderbilt University, Nashville, TN*
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- PTMs – METHYLATION, ACETYLATION, GLYCOSYLATION, UBIQUINATION, 460 - 479**
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- TP 460 **Using Targeted Proteomics to Assess the Impact of Sirtuins on Liver Metabolism in Obesity**; Mizanoor Rahman; Agnieszka Kendrick; Stephanie Thorn; Jacob E. Friedman; Karen Jonscher; *University of Colorado, Denver, CO*
- TP 461 **Investigation of Site-Specific N-Glycosylation of Glycoprotein by Reversed-Phase Capillary LC Coupled with Electrospray Linear Ion Trap Mass Spectrometry**; Pei-Jing Pai; Guor-Rong Her; *National Taiwan University, Taipei, Taiwan*
- TP 462 **Analysis of Protein Methylation using Electron Transfer Dissociation Mass Spectrometry**; Mark Dickman; Ambrosius Snijders; *University of Sheffield, Sheffield, UK*
- TP 463 **Identification of Methylglyoxal Modified Proteins in Diabetic Plasma using MudPIT**; Mike Kimzey<sup>1</sup>; Mike Galligan<sup>1</sup>; Timothy R. Radabaugh<sup>1</sup>; Chad R. Borges<sup>2</sup>; Hussein Yassine<sup>1</sup>; Randall Nelson<sup>2</sup>; Craig Stump<sup>1</sup>; George Tsapraillis<sup>1</sup>; Daniel C. Link<sup>1</sup>; Erik J. Henrikson<sup>1</sup>; Serrine Lau<sup>3</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Arizona State University, Tempe, AZ; <sup>3</sup>Univ of Arizona, Pharmacy, Tucson, AZ
- TP 464 **Global and Site-specific Perturbations of Phosphorylation in Response to Elevated O-GlcNAc Levels: the Yin-Yang Model Revisited**; Zihao Wang; Gerald W Hart; *Johns Hopkins University School of Medicine, Baltimore, MD*
- TP 465 **Mapping O-Glycosylation Sites of Secreted Proteins by Combining Lectin Chromatography, Enzymatic Deglycosylation and Multistage Mass Spectrometry**; Jakob Bunkenborg<sup>1</sup>; Martin Bennetzen<sup>1</sup>; Lasse F. Nielsen<sup>1</sup>; Per Hagglund<sup>2</sup>; Jens S Andersen<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense M, Denmark; <sup>2</sup>Biocentrum DTU, Lyngby, Denmark
- TP 466 **The Influence of Mono- and Dimethylation on Responsiveness of Peptides to MALDI and ESI**; Heike Stephanowitz<sup>1</sup>; Balamurugan Varadarajan<sup>1</sup>; Susanne Weber<sup>2</sup>; Michael Schumann<sup>1</sup>; Angelika Ehrlich<sup>1</sup>; Uta-Maria Bauer<sup>2</sup>; Eberhard Krause<sup>1</sup>; <sup>1</sup>Leibniz Institute of Molecular Pharmacology, Berlin, Germany; <sup>2</sup>Institute for Molecular Biology and Tumor Research, Marburg, Germany
- TP 467 **Study of Acetylated Lysine, Serine, Threonine, and Tri-Methylated Lysine Containing Peptides using Electrospray Collision-Induced Dissociation Tandem Mass Spectrometry**; Yan Li; Haydn Ball; *UTSW, Dallas, TX*
- TP 468 **From Top-Down to Bottom-Up: Protein Methylation in the Yeast Ribosome Large Subunit**; Kristofor Webb; Arthur Laganowsky; Tanya R. Porras-Yakushi; Julian Whitelegge; Steven G. Clarke; *UCLA, Los Angeles, CA*
- TP 469 **Multi Post-Translational Modifications Analysis for a Gel Band using MALDI-TOF MS-MS**; Yuzo Yamazaki; Masaki Yamada; *Shimadzu Corporation, Kyoto, Japan*
- TP 470 **Reciprocal Modification of Human Insulin Receptor Substrate-1 (IRS-1) by O-GlcNAc Modification and Phosphorylation**; Mary Berkaw; Lauren Ball; *Medical University of SC, Charleston, SC*
- TP 471 **A Proteomic Approach for Identification of Protein Ubiquitination in Axonal Signaling Pathways**; Guoqiang Xu; Ulrich Hengst; Alessia Deglincerti; Samie R. Jaffrey; *Weill Medical College, New York, NY*
- TP 472 **Glycopeptides Analysis using LTQ Orbitrap XL ETD and Porous Graphite Chromatography**; Terry Zhang; Rosa Viner; Zhiqi Hao; Vlad Zabrouskov; *ThermoFisher Scientific, San Jose, CA*
- TP 473 **Characterization of Posttranslational Modifications in the Cdc45-MCM-Gins (CMG) and their Role in Complex Stability and Activity**; James J Pesavento; Anthony T Iavarone; Ivar Ilves; Michael R Botchan; *UC Berkeley, Berkeley, CA*
- TP 474 **Modulation of the Phospho- and Glycoproteome of Glioma Stem Cells during Differentiation**; Xu Wang<sup>1</sup>; Mark R. Emmett<sup>2</sup>; Jeremiah D. Tipton<sup>2</sup>; Carol Nilsson<sup>3</sup>; Alan G. Marshall<sup>1</sup>; Roger A. Kroes<sup>4</sup>; Joseph R. Moskal<sup>4</sup>; Howard Colman<sup>5</sup>; Charles A. Conrad<sup>2</sup>; <sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>Nat'l High Magnetic Field Lab, Tallahassee, FL; <sup>3</sup>Pfizer, Inc., San Diego, CA; <sup>4</sup>The Falk Center for Molecular Therapeutics, Evanston, IL; <sup>5</sup>M.D. Anderson Cancer Center, Houston, TX
- TP 475 **Comparison of Higher Energy Collisional Dissociation (HCD) with Triple Quadrupoles for Identification of Constituents from Breast Milk and Substitutes**; Craig P. Dufresne; *Thermo Fisher Scientific, West Palm Beach, FL*
- TP 476 **Identification of Ubiquitination Sites on MHC-I Molecules by Mass Spectrometry**; Stephen Swatkoski<sup>1</sup>; Xiaoli Wang<sup>2</sup>; Ted Hansen<sup>2</sup>; Robert Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Washington University School of Medicine, St. Louis, MO
- TP 477 **Identification of Post Translational Modifications on SHP-1**; Jessica Chapman; Mohan Sankarshanan; Jeffrey Shabanowitz; Ulrike Lorenz; Donald F. Hunt; *University of Virginia, Charlottesville, VA*
- TP 478 **Analysis of the Functional Role of Lys-11 in Polyubiquitin Chain Formation using Quantitative Mass Spectrometry**; Jin Woo Jung<sup>1</sup>; Sung Jun Bae<sup>2</sup>; Kyun-Hwan Kim<sup>3</sup>; Jae Hong Seol<sup>2</sup>; Kwang Pyo Kim<sup>1</sup>; <sup>1</sup>Molecular Biotechnology, Konkuk University, Seoul, South Korea; <sup>2</sup>Biological Sciences, Seoul National University, Seoul, South Korea; <sup>3</sup>Pharmacology, Konkuk University, Seoul, South Korea
- TP 479 **One-Spot Detection of Oligosaccharide and Peptide using a Mixture of Two Ionic Liquid Matrixes with MALDI MS**; Kenichi Taniguchi<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Yuko Fukuyama<sup>1</sup>; Helen Montgomery<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu, Koichi Tanaka Ms Research Laboratory, Manchester, UK
- TP 468 **From Top-Down to Bottom-Up: Protein Methylation in the Yeast Ribosome Large Subunit**; Kristofor

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PROTEINS – GENERAL 1, 480 - 494	
TP 480	<b>Study of Tazobactam Inhibition of Beta-Lactamases by Electrospray Ionization Mass Spectrometry (ESI-MS) under near Physiological Conditions;</b> <u>Pui Kin So</u> ; Fung Yi Chan; Ming Shan Tsang; Yun Chung Leung; Kwok Yin Wong; Chun Wai Tsang; <i>The Hong Kong Polytechnic University, Hong Kong, China</i>
TP 481	<b>CA11, An Autocrine Protein in Gastric Epithelium, Plays a Role in Regulation of Cell Cycle;</b> <u>Rui Xing</u> <sup>1</sup> ; Jun Zhang <sup>1</sup> ; Bin Kang <sup>1</sup> ; Siqi Liu <sup>1</sup> ; Youyong Lu <sup>2</sup> ; <sup>1</sup> Beijing Genomics Institute, CAS, Beijing, China; <sup>2</sup> Peking University, School of Oncology, Beijing, China
TP 482	<b>Proteomics Approach to Identify the Components of Huntingtin Aggresome Machinery and Exploration of the Molecular Mechanisms Leading to Aggresome Formation;</b> <u>Yan Wang</u> ; Anatoli B. Meriin; Michael Y. Sherman; Catherine E. Costello; <i>Boston University School of Medicine, Boston, MA</i>
TP 483	<b>Monitoring Procaspase-3 Activation in the Presence of PAC-1 by LC-MS;</b> <u>Stone D.-H. Shi</u> ; Michael J. Greig; Jeff X. Zhu; Cathy D. Moore; Zhengwei Peng; Hieu T. Lam; Dawn M. Nowlin; <i>Pfizer, San Diego, CA</i>
TP 484	<b>Charge State Dependent Fragmentation of Gaseous Alpha-Synuclein Ions via Ion Trap CID, Beam-Type CID, and ETD;</b> <u>Chamnongsak Chanthamongrui</u> ; Jian Liu; Scott A. McLuckey; <i>Purdue University, West Lafayette, IN</i>
TP 485	<b>Identification of Binding Partners of hDSS1 using MALDI and LC-ESI Based Mass Spectrometry;</b> Sung-Jen Wei <sup>1</sup> ; <u>Katina Johnson</u> <sup>1</sup> ; Hong Dang <sup>2</sup> ; Thomas Darden <sup>1</sup> ; Bryan Betz <sup>1</sup> ; Margaret Humble <sup>1</sup> ; Carol Trempus <sup>1</sup> ; Jason Williams <sup>1</sup> ; Ronald Cannon <sup>1</sup> ; Raymond Tennant <sup>1</sup> ; <sup>1</sup> NIEHS/NIH/DHHS, Research Triangle Park, NC; <sup>2</sup> Alpha-Gamma Technologies Inc., Raleigh, NC
TP 486	<b>Peptide Products of Vsc1 and hSMR3A as Markers for Erectile Dysfunction (ED) in Diabetic and Non-Diabetic Etiologies;</b> <u>Giridharan Gokulrangan</u> <sup>1</sup> ; Jinsook Chang <sup>1</sup> ; Janna Kiselar <sup>1</sup> ; Kelvin Davies <sup>2</sup> ; Mark Chance <sup>1</sup> ; <sup>1</sup> Case Proteomics Center, Cleveland, OH; <sup>2</sup> Albert Einstein College of Medicine, Cleveland, OH
TP 487	<b>Protein Microheterogeneity and the Need for Population Proteomics for Protein Characterization: Case Study of Vitamin D Binding Protein;</b> <u>Chad R. Borges</u> ; Jason W. Jarvis; Paul E. Oran; Stephen P. Rogers; Randall Nelson; <i>Arizona State University, Tempe, AZ</i>
TP 488	<b>Total de novo Sequencing of Myelin P2 and Identification of its Lipid Ligand;</b> <u>Gianluca Maddalo</u> <sup>1</sup> ; Mohammadreza Shariatgorji <sup>1</sup> ; Chris Adams <sup>2</sup> ; Eva Fung <sup>2</sup> ; Jan Sedzik <sup>3</sup> ; Ulrika Nilsson <sup>1</sup> ; Roman Zubarev <sup>2</sup> ; Leopold L. Ilag <sup>1</sup> ; <sup>1</sup> Stockholm University, Stockholm, Sweden; <sup>2</sup> Uppsala University, Uppsala, Sweden; <sup>3</sup> Karolinska Institute, Stockholm, Sweden
TP 489	<b>Characterization of the Der4 Multiprotein Complex for the Elucidation of its Role in Acute Lymphoblastic Leukemia (ALL);</b> <u>Sabrina Baltruschat</u> ; Anne Benedikt; Adelheid Bursen; Tabiwang Arrey; Björn Meyer; Rolf Marschalek; Michael Karas; <i>Johann Wolfgang Goethe-University, Frankfurt, Germany</i>
TP 490	<b>Identification and Characterization of Structural Proteins in the Complex Phage 201phi2-1 by Mass Spectrometry;</b> <u>Susan T. Weintraub</u> ; Julie A. Thomas; Mandy Rolando; Stephen C. Hardies; Philip Serwer; <i>University of Texas HSC, San Antonio, TX</i>
TP 491	<b>Characterization of Intact Complexes of Anticancer Drugs and Serum Proteins, Enzymes and Antibodies using Electrospray Mass Spectrometry;</b> <u>Sool Yeon Cho</u> ; James F. Holland; John Roboz; <i>Mount Sinai School of Medicine, New York, NY</i>
TP 492	<b>Exploring the Functional Roles of BAG2 in Senescence with Identification of its Interaction Complexes;</b> <u>Ju Zhang</u> <sup>1</sup> ; Xiaomin Lou <sup>1</sup> ; Shangbin Yang <sup>2</sup> ; Siqi Liu <sup>1</sup> ; Ningzhi Xu <sup>1</sup> ; <sup>1</sup> Beijing Genomics Institute, CAS, Beijing, China; <sup>2</sup> Cancer Institute, CAMS, Beijing, China
TP 493	<b>A Detailed Characterisation of the Interaction between the PEBP/RKIP Protein and Locostatin, a Potential Antimetastatic Lead;</b> <u>Guillaume Gabant</u> <sup>1</sup> ; Martine Beaufour <sup>1</sup> ; Françoise Schoentgen <sup>2</sup> ; Martine Cadene <sup>1</sup> ; <sup>1</sup> CBM CNRS, Orleans, FRANCE; <sup>2</sup> IMPMC CNRS, Paris, France
TP 494	<b>Characterization of a Novel Subunit of the Drosophila Melanogaster Chromatin Remodeling Complex PBAP;</b> Gillian E Chalkley <sup>1</sup> ; Yuri M Moshkin <sup>1</sup> ; Karin Langenberg <sup>1</sup> ; Karel Bezstarosti <sup>1</sup> ; Andras Blastyak <sup>2</sup> ; Henrik Gyurkovics <sup>2</sup> ; <u>Jeroen AA Demmers</u> <sup>1</sup> ; C. Peter Verrijzer <sup>1</sup> ; <sup>1</sup> Erasmus Medical Center, Rotterdam, Netherlands; <sup>2</sup> Hungarian Academy of Sciences, Szeged, Hungary
PROTEIN CONFORMATION – OXIDATIVE AND COVALENT LABELING, 495 - 515	
TP 495	<b>Limited Proteolysis and Oxidative Surface Mapping for Characterization of the DNA-Binding Domain of Mismatch Repair Protein Pms1 by Mass Spectrometry;</b> <u>Allison N Schorzman</u> <sup>1</sup> ; Jenny M Cutalo <sup>2</sup> ; Lars C Pedersen <sup>1</sup> ; Thomas A Kunkel <sup>1</sup> ; Kenneth B. Tomer <sup>1</sup> ; <sup>1</sup> NIEHS, Research Triangle Park, NC; <sup>2</sup> Federal Bureau of Investigation, Quantico, VA
TP 496	<b>Conformational Studies of a Monoclonal Antibody, IgG1, by Chemical Oxidation: Structural Analysis by Ultra Performance LC-ESI-ToFMS and Multivariate Data Analysis;</b> <u>Leila Zamani</u> <sup>1</sup> ; Fredrik O. Andersson <sup>2</sup> ; Yang Yang <sup>2</sup> ; Per Edebrink <sup>2</sup> ; Sven P. Jacobsson <sup>2</sup> ; <sup>1</sup> Stockholm University, Stockholm, Sweden; <sup>2</sup> AstraZeneca, Södertälje, Sweden
TP 497	<b>Experimental and Informatic Aspects of Electrochemical Oxidation as a Surface Mapping Probe for Higher Order Protein Structure;</b> <u>Carlee McClintock</u> ; Vilmos Kertesz; Susie Dai; Robert Hettich; <i>Oak Ridge National Laboratory, Oak Ridge, TN</i>
TP 498	<b>FPK Labels Proteins Faster than they Unfold;</b> <u>Brian C. Gau</u> <sup>1</sup> ; Joshua S. Sharp <sup>2</sup> ; Don L. Rempel <sup>1</sup> ; Michael L. Gross <sup>1</sup> ; <sup>1</sup> Washington University, St. Louis, MO; <sup>2</sup> University of Georgia, Athens, GA
TP 499	<b>Monitoring Conformational Changes of the Bacillus anthracis Protective Antigen with Differential Oxidative Surface Mapping;</b> <u>James G. Smedley, III</u> <sup>1</sup> ; Joshua S. Sharp <sup>2</sup> ; Jeffrey F. Kuhn <sup>3</sup> ; Kenneth B. Tomer <sup>1</sup> ; <sup>1</sup> NIEHS, Durham, NC; <sup>2</sup> University of Georgia, Athens, GA; <sup>3</sup> Varian Analytical Instrum, Cary, NC
TP 500	<b>Use of Oxidation and Mass Spectrometry to Elucidate the Function Mechanism of a DNA-Architecture Protein;</b> Françoise Culard; Corinne Bure; Melanie Spothem; <u>Martine Cadene</u> ; <i>CBM du CNRS, Orleans, FRANCE</i>
TP 501	<b>Probing the Structure of Short-Lived Protein Folding Intermediates by Hydroxyl-Radical-Mediated Oxidative Labeling and ESI-MS;</b> <u>Bradley B. Stocks</u> ; Lars Konermann; <i>Univ. of Western Ontario, London, ON</i>
TP 502	<b>Substrate Binding Inhibits Chemical Modification of Human Bile Acid CoA:Amino Acid N-acyltransferase</b>

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- TP 503 **Structural Characterization of the Calcium Binding Protein Calbindin-D28k**; Carey A. Hobbs<sup>1</sup>; Leesa J. Deterding<sup>2</sup>; Richele J. Thompson<sup>1</sup>; Benjamin G. Bobay<sup>1</sup>; Kenneth Tomer<sup>2</sup>; John Cavanagh<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>NIEHS, Research Triangle Park, NC
- TP 504 **Protein Surface Mapping by Employing Hydroxyl Radicals, Mass Spectrometry and Molecular Dynamics Simulations**; Olga Charvatova<sup>1</sup>; B. Lachele Foley<sup>1</sup>; Marshall W. Bern<sup>2</sup>; Joshua S. Sharp<sup>1</sup>; Ron Orlando<sup>1</sup>; Robert J. Woods<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Palo Alto Research Center, Palo Alto, CA
- TP 505 **Surface Mapping of  $\beta$ -2-Microglobulin Oligomers using Covalent Labeling and Top-down Sequencing**; Mark Olbris; Vanessa Leah Mendoza; Richard Vachet; *University of Massachusetts, Amherst, MA*
- TP 506 **Probing the Structure of Serpin/Protease Complexes by Structural Mass Spectrometry Method**; Xiaojing Zheng; Patrick Wintrod; Mark Chance; *Case Western Reserve Univ, Cleveland, OH*
- TP 507 **Combining Structural Mass Spectrometry and Rosetta: Experimental Data Constrained de novo Structure Inference**; Keiji Takamoto<sup>1</sup>; Xiaojing Zheng<sup>1</sup>; Janna Kiselar<sup>1</sup>; Rhiju Das<sup>2</sup>; Robert Vernon<sup>2</sup>; David Baker<sup>2</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>University of Washington, Seattle, WA
- TP 508 **Pulsed Electron Beam Water Radiolysis: A Novel Method for Sub-Microsecond Hydroxyl Radical Protein Footprinting**; Caroline Watson<sup>1</sup>; Deanna O'Donnell<sup>2</sup>; Ireneusz Janik<sup>2</sup>; Tiandi Zhuang<sup>1</sup>; James H. Prestegard<sup>1</sup>; Joshua S. Sharp<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>University of Notre Dame, Notre Dame, IN
- TP 509 **Structural Probing of Snap-Frozen Proteins by X-ray radiolysis and Mass Spectrometry: Radiation Damage at Work**; Sayan Gupta; Rhijuta D'Mello; Mark R. Chance; *CWRU-Center for Proteomics, Upton, NY*
- TP 510 **Probing Native Structures of Homologous Large Proteins with Differential Covalent Labeling and Mass Spectrometry Characterization**; Susie Dai; Carlee McClintock; Robert Hettich; *Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 511 **A Novel Approach to Characterizing Prion Protein Structures using Chemical Labelling, Microwave-Assisted Acid Hydrolysis and MALDI-MS**; Josephine S.W. Tsang; Adina Bujold; David Wishart; Liang Li; *University of Alberta, Edmonton, Canada*
- TP 512 **Extension of Fast Photochemical Oxidation of Proteins (FPOP) to Mapping Calmodulin and Calmodulin-Peptide Complexes**; Hao Zhang; Michael L. Gross; *Washington University, Saint Louis, MO*
- TP 513 **Synthesis and Structural Characterization of Polyubiquitin Conjugates using High Resolution Mass Spectrometry**; Jieun Jung<sup>1</sup>; Marilena Manea<sup>1</sup>; Hans-Peter Wollscheid<sup>2</sup>; Martin Scheffner<sup>2</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>Laboratory of Analytical Chemistry, Konstanz, Germany; <sup>2</sup>Laboratory of Cellular Biochemistry, Konstanz, Germany
- TP 514 **Surface Mapping of rmetG-CSF to Determine Oligomerization Induced Difference in Surface Solvent Exposure at Neutral pH and 37 C**; Shabnam Farahmand; David M. Hambly; Himanshu S. Gadgil; Gerd R. Kleemann; Michael J. Treuheit; *Amgen, Inc., Seattle, WA*
- TP 515 **Ubiquitin Conformation and Dynamics Revealed using Selective Noncovalent Adduct Protein Probing MS and Site-Directed Mutagenesis**; Zhenjiu Liu; Shijun Cheng; Daniel Gallie; Ryan R. Julian; *University of California Riverside, Riverside, CA*
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- TP 549 **Differential Proteomic Analysis of C. Metalidurans Cultured under Simulated Microgravity: Application and Comparison of Three Isotope Coded Protein Labelling Strategies**; Baptiste Leroy<sup>1</sup>; Natalie Leys<sup>2</sup>; Caroline Rosier<sup>1</sup>; Max Mergeay<sup>2</sup>; Ruddy Wattiez<sup>1</sup>; <sup>1</sup>University of Mons-Hainaut, Mons, Belgium; <sup>2</sup>Belgian Nuclear Research Center, Mol, Belgium
- TP 550 **Simultaneous Measurement of Protein Half-life and Precursor Pool Enrichment in C. elegans**; Gennifer Merrihew; Michael Hoopmann; Michael J. Maccoss; *University of Washington, Seattle, WA*
- TP 551 **Probing for Huntingtin Interacting Proteins using iTRAQ Technology**; Marjan Gucek; Tamara Ratovitski; Christopher A. Ross; Robert N. Cole; *Johns Hopkins School of Medicine, Baltimore, MD*
- TP 552 **Effect of Hexa-carboxy Fullerenes on Differentiated Macrophages: Analysis by iTRAQ**; Timothy Sanchez<sup>1</sup>; Rashi Iyer<sup>1</sup>; Gao Jun<sup>1</sup>; Srinivas Iyer<sup>1</sup>; Sanjeev Bhardwaj<sup>2</sup>; James E. Carlson<sup>3</sup>; Shixin Sun<sup>3</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Merck & Co., Inc., West Point, PA; <sup>3</sup>Applied Biosystems, Framingham, MA
- TP 553 **Measurement of in vivo Protein Turnover from Tracheal Aspirates using Targeted Proteomics**; Daniela Tomazela<sup>1</sup>; Michael J. Maccoss<sup>1</sup>; Kimberly Spencer<sup>2</sup>; Cole F. Sessions<sup>2</sup>; Elizabeth Reed<sup>2</sup>; Bruce Patterson<sup>2</sup>; Aaron Hamvas<sup>2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Washington University, St Louis, MO
- TP 554 **Expression Analysis of the Subsarcolemal Mitochondrial Proteome**; Jing Wang; Claudia Maier; *Oregon State University, Corvallis, OR*
- TP 555 **Survey of Estrogen-Induced Differential Protein Expression in Zebrafish Embryos using 2D-LC-MS-MS and Label-Free Relative Quantitation**; Tatjana Talamantes; Stanley M. Stevens, Jr.; Navin Rauniyar; Laszlo Prokai; *University of North Texas Health Science Center, Fort Worth, TX*
- TP 556 **Quantification of Synaptosomes during Postnatal Development using 15N Labeled Rat Brain**; Daniel B. McClatchy; Lujian Liao; John R. Yates III; *The Scripps Research Institute, La Jolla, CA*
- TP 557 **Spatial Mapping of the Neurite and Soma Proteomes Reveals a Functional Cdc42/Rac Regulatory Network**; Feng Yang<sup>1</sup>; Olivier C. Pertz<sup>2</sup>; yingchun wang<sup>2</sup>; Marina A. Gristenko<sup>1</sup>; Tao Liu<sup>1</sup>; David G. Camp II<sup>1</sup>; Richard L. Klemke<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of California, San Diego, CA
- TP 558 **Considerations in Designing Experiments for the Absolute Quantification of Proteins**; Angela K. Walker; John R. Strahler; Michael Imperiale; Philip C. Andrews; *University of Michigan, Ann Arbor, MI*
- TP 559 **SILIP: A Novel Method for Stable Isotope Labeling of Proteins in planta for Quantitative Proteomic Analysis**; Flaubert Mbeunkui; Jennifer E. Schaff; Kevin Blackburn; David McK. Bird; Michael B. Goshe; *NC State University, Raleigh, NC*
- TP 560 **Characterization and Quantification of Surfactant Proteins and Lipids in INFASURF® by Fourier Transform Ion Cyclotron Resonance Mass**



## TUESDAY POSTERS

- Spectrometry (FTICR); Kevin D. Quinn;** Troy Wood; *University at Buffalo, Buffalo, NY*
- TP 561 **Relative Quantification of Acrolein-Modified Cys-Containing Mitochondrial Peptides using MRM;** Jianyong Wu; Claudia Maier; *Oregon State University, Corvallis, OR*
- TP 562 **Robust and Absolute Quantitation of PSA in Clinical Human Sera using Protein Reaction Monitoring (PRM);** Tanguy Fortin<sup>1</sup>; Arnaud Salvador<sup>2</sup>; Jean-Philippe Charrier<sup>1</sup>; Christof E. Lenz<sup>3</sup>; Genevieve Choquet-Kastylevsky<sup>1</sup>; Xavier Lacoux<sup>1</sup>; Jerome Lemoine<sup>2</sup>; <sup>1</sup>*Biomerieux, Marcy L'etoile, France*; <sup>2</sup>*UMR 5180 Sciences Analytiques, Université Claude B, Villeurbanne, France*; <sup>3</sup>*Applied Biosystems Germany, Darmstadt, Germany*
- TP 563 **Ultra Sensitive and Exact Quantification of Complex Protein Mixtures using MeCAT – Metal Coded Tagging;** Robert Ahrends<sup>2</sup>; Stefan Pieper<sup>2</sup>; Christian Scheler<sup>1</sup>; Michael W. Linscheid<sup>2</sup>; <sup>1</sup>*Proteome Factory AG, Berlin, Germany*; <sup>2</sup>*Humboldt-Universitaet Zu Ber, Berlin, Germany*
- TP 564 **Establishing a Targeted Label-Free Protein Quantification Workflow Based on an Integrated Mass Spectrometry and Bioinformatics Platform;** Wolfgang Jabs<sup>1</sup>; Markus Lubeck<sup>1</sup>; Marina Behrens<sup>1</sup>; Daniel C. Chamrad<sup>2</sup>; Klaus Marquart<sup>2</sup>; Martin Blueggel<sup>2</sup>; Barbara Sitek<sup>3</sup>; Birgit Korte<sup>3</sup>; Sebastian Link<sup>3</sup>; Christian Stephan<sup>3</sup>; Kai Stühler<sup>3</sup>; Helmut E. Meyer<sup>3</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*Protagen AG, Dortmund, Germany*; <sup>3</sup>*Ruhr-University Bochum, Bochum, Germany*
- TP 565 **Quantitation of Protein Phosphorylation using Multiple Reaction Monitoring;** Ning Tang; Christine Miller; Keith Waddell; *Agilent Technologies, Santa Clara, CA*
- TP 566 **Proteomic Analysis of the Anterior Pituitary from Long-Lived Snell Dwarf and Wild Type Mice by Q-ToF and Orbitrap FT-MS;** Jenny M. Alderman<sup>1</sup>; Linhong Jing<sup>1</sup>; Carol E. Parker<sup>1</sup>; Sneha Naik<sup>1</sup>; Natasha L. Brooks<sup>1</sup>; Urmila Srinivas<sup>1</sup>; David E. Harrison<sup>2</sup>; Kevin Flurkey<sup>2</sup>; Gunnar Boysen<sup>1</sup>; James A. Swenberg<sup>1</sup>; Xian Chen<sup>1</sup>; Terry P. Combs<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*Jackson Laboratories, Bar Harbor, ME*
- TP 567 **A Novel Strategy for Biomarker Discovery: ICPLQuant - A New Software Suite for Isotope-Labeling Based Proteomics;** Achim Brunner<sup>1</sup>; Eva-Maria Keidel<sup>1</sup>; Silke Martin<sup>3</sup>; Michael Kersten<sup>2</sup>; Josef Kellermann<sup>1</sup>; Friedrich Lottspeich<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Biochemistry, Martinsried, Germany*; <sup>2</sup>*Toplab GmbH, Martinsried, Germany*; <sup>3</sup>*Blutspendedienst des BRK, Munich, Germany*
- TP 568 **An iTRAQ-RPLC-MS-MS Approach for Protein Differential Expression Profiling of MCF7 Breast Cancer Cells: Towards Biomarker Discovery;** Jenny M. Armenta; Maria Iuliana Lazar; *Virginia Bioinformatics, Blacksburg, VA*
- TP 569 **Identification and Comparative Quantitation of Protein Variants in the Ethanol-Dosed Rat Liver Mitochondrial Proteome;** Peggi M Angel<sup>1</sup>; Punit Shah<sup>1</sup>; Marshall W. Bern<sup>3</sup>; Marie E. Csete<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*Emory University School of Medicine, Atlanta, GA*; <sup>3</sup>*Palo Alto Research Center, Palo Alto, CA*
- TP 570 **SILAC and iTRAQ Quantitation on an Orbitrap using Protein Prospector;** Peter R Baker<sup>2</sup>; Xiaorong Wang<sup>1</sup>; Nelson Jen<sup>1</sup>; Lan Huang<sup>3</sup>; <sup>1</sup>*University of California, Irvine, CA*; <sup>2</sup>*UCSF, San Francisco, CA*; <sup>3</sup>*University of California, Irvine, CA*
- TP 571 **Quantitative Proteome Changes during Differentiation of Murine Erythroleukemia (MEL) Cells Assessed by SILAC Labeling and nanoLC-MS;** Gerhard Mittler; Ravi Krovvidi; *Max Planck Institute of Immunobiology, Proteomics, Freiburg, Germany*
- TP 572 **Quantitative Proteomic Characterization of Colorectal and Intestinal Tumors from the *Apc*<sup>Min</sup> Mouse via Metabolic Labeling;** Edward L. Huttlin<sup>1</sup>; Xiaodi Chen<sup>1</sup>; Gregory Barrett-wilt<sup>1</sup>; Adrian D. Hegeman<sup>2</sup>; Amy C. Harms<sup>1</sup>; William F. Dove<sup>1</sup>; Michael R. Sussman<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*University of Minnesota, Saint Paul, MN*
- TP 573 **SILAC Reveals Heterogeneous Nuclear Ribonucleoprotein U as a Caspase Substrate in Human Colorectal Carcinoma Cells;** Fanyu Meng; Maarten Hoek; Meizhen Wu; Katie Southwick; Nathan Yates; Huseyin Mehmet; Ronald Hendrickson; *Merck & Co., Inc, Rahway, NJ*
- TP 574 **Mass Spectrometry-Based Protein Localization Study to Identify New Constituents of Human Liver Peroxisomes;** Sebastian Wiese<sup>1</sup>; Thomas Gronemeyer<sup>1</sup>; Rob Ofman<sup>2</sup>; Martin Eisenacher<sup>1</sup>; Christian Stephan<sup>1</sup>; Heiko Hayen<sup>3</sup>; Ronald JA Wanders<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Bettina Warscheid<sup>1</sup>; <sup>1</sup>*Medizinisches Proteom-Center, Bochum, Germany*; <sup>2</sup>*Amsterdam Medical Center, Amsterdam, Netherlands*; <sup>3</sup>*ISAS - Institute For Analytical Sciences, Dortmund, Germany*
- TP 575 **Quantitating Changes in Protein Carbonylation in Aging Rat Skeletal Muscle;** Juan Feng<sup>1</sup>; Hongwei Xie<sup>2</sup>; LaDora V Thompson<sup>1</sup>; Tim Griffin<sup>1</sup>; Edgar A. Arriaga<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*Waters Corporation, Milford, MA*
- TP 576 **Intelligent Use of Retention Time for Higher Order Multiple Reaction Monitoring Multiplexing – Scheduled MRM;** Jose Meza; Christie L Hunter; *Applied Biosystems, Foster City*
- TP 577 **Conquering the Challenges of iTRAQ-based Relative and Absolute Quantitation of Protein Biomarkers Indicative of Dehalorespiration;** Jeffrey J Werner; Celeste Ptak; Ruth E Richardson; Sheng Zhang; *Cornell University, Ithaca, NY*
- TP 578 **Comparison of Mass Spectrometry Methods for Relative Quantitative Analysis in Protein Mixtures;** John E Klimek<sup>1</sup>; Christine Henderson<sup>1</sup>; Lucinda Robertson<sup>1</sup>; Leif Rustvold<sup>1</sup>; Kerry Maddox<sup>2</sup>; Phillip Wilmarth<sup>1</sup>; Debra Mcmillen<sup>1</sup>; Ashok Reddy<sup>3</sup>; Klaus Frueh<sup>1</sup>; Larry David<sup>1</sup>; <sup>1</sup>*Oregon Health & Science University, Portland, OR*; <sup>2</sup>*Shriners Hospital, Portland, OR*; <sup>3</sup>*Proteogenix, Inc., Tigard, OR*
- TP 579 **Development of an MRM-based Label-free Quantitative Analysis for SDS-PAGE Separated Protein Complex Samples;** Sabine Baumgart; Celeste Ptak; Amber Krauchunas; Mariana Wolfner; Sheng Zhang; *Cornell University, Ithaca, NY*
- TP 580 **Stable Isotope Labeling Tandem MS (SILT) using MS2 Significantly Improves Quantitative Proteomics over Methods that Rely on Quantitation using MS1;** Kwasi G. Mawuenyega; Donald L. Elbert; Kristin R. Wildsmith; Karen R. Browning; Randall J. Bateman; *Washington University, Saint Louis, MO*
- TP 581 **Relative Quantification on a Subset of the Murine Hepatic Proteome using ESI QTOF and MALDI TOF/TOF;** Richard C. Scheri; Junga Lee; Douglas F.



## TUESDAY POSTERS

- Barofsky; Larry R. Curtis; *Oregon State University, Corvallis, OR*
- TP 582 **A Method for Rapid Differential Protein Expression Profiling from Tissue using 'Shotgun-based' LC-MS-MS and Spectral Counting;** Stanley M. Stevens, JR.; Navin Rauniyar; Vien Nguyen; Laszlo Prokai; *University of North Texas Health Science Center, Fort Worth, TX*
- TP 583 **Effect of False Positive Rate and Replication Number on Identification of Proteins by UPLC-MSE;** Chongfeng Xu<sup>1</sup>; Thomas Neubert<sup>2</sup>; <sup>1</sup>*NYU Medical Center, New York, NY*; <sup>2</sup>*Skirball Institute, Nyumc, New York, NY*
- TP 584 **Identification and Label-Free Relative Quantification of Acetylation, and Other Post-Translational Modifications using Multiple Reaction Monitoring;** Richard D Unwin; John R Griffiths; Anthony D Whetton; *University of Manchester, UK, Manchester, UK*
- TP 585 **Comparison of TA-CID, HASTE CID and IRMPD for Analysis of ITRAQ & Trade; Peptides in a Quadrupole Ion Trap Mass Spectrometer;** Atim Enyenihi<sup>1</sup>; John R Griffiths<sup>2</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*Manchester University, Withington, UK*
- TP 586 **Quantitative Analysis of Receptor Tyrosine Signaling in Stimulated Human Mammary Epithelial Cells;** Tyler H Heibeck<sup>1</sup>; Shi-jian Ding<sup>2</sup>; Lee Opresko<sup>1</sup>; Rui Zhao<sup>1</sup>; Athena Schepmoes<sup>1</sup>; David G Camp<sup>1</sup>; Richard D. Smith<sup>1</sup>; Steven Wiley<sup>1</sup>; Weijun Qian<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*University of Nebraska Medical Center, Omaha, NE*
- TP 587 **Label Free Relative Quantification of Map Kinase Phosphorylation Degree by UPLC-MS;** Dominic Winter; Marcel Schilling; Ursula Klingmueller; Wolf Dieter Lehmann; *German Cancer Research Center, Heidelberg, Germany*
- TP 588 **High Resolution Mass Spectrometry Proteomics Profiling of the Platelet Sheddome;** Colin G. Barry<sup>1</sup>; Karen P. Fong<sup>2</sup>; Lawrence F. Brass<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Div of Hematology Oncology Univ of Penn, Philadelphia, PA*
- TP 589 **A High Sensitivity Analytical Platform for Targeted Quantitative Proteomics using Multiple Reaction Monitoring;** Tao Liu; David T. Kaleta; Errol W. Robinson; Wei-Jun Qian; Ryan T. Kelly; Jason S. Page; Keqi Tang; Heather M. Mottaz; David G. Camp II; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 590 **Label-Free Relative Quantification using MS-MS TIC Compared to SILAC and Spectral Counting;** John M Asara<sup>1</sup>; Heather Christofk<sup>2</sup>; Jeffrey Engelman<sup>3</sup>; Bin Zheng<sup>1</sup>; Lisa Freimark<sup>1</sup>; Lewis Cantley<sup>2</sup>; <sup>1</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*Massachusetts General Hospital, Boston, MA*
- TP 591 **The Effect of Dynamic Exclusion on Label-Free Protein Quantification using MudPIT;** Ying Zhang; Zhihui Wen; Laurence Florens; Michael Washburn; *Stowers Institute For Medical Research, Kansas City, MO*
- TP 592 **Refinements to Proteome Quantitation Based on Spectral Counting: How to Deal with Peptides Shared by Multiple Proteins;** Zhihui Wen; Ying Zhang; Michael Washburn; Laurence Florens; *Stowers Institute for Medical Research, Kansas City, MO*
- TP 593 **Quantification of Protein Expression at CEM Cells during Anti-Cancer Therapy;** Petr Pompach<sup>1</sup>; Petr Novak<sup>1</sup>; Petr Man<sup>1</sup>; Jan Nedved<sup>1</sup>; Vladimír Havlicek<sup>1</sup>; Petr Dzubak<sup>2</sup>; Marian Hajduch<sup>2</sup>; <sup>1</sup>*Institute of Microbiology, Prague 4, Czech Republic*; <sup>2</sup>*Faculty of Medicine, Palacky University, Olomouc, Czech Republic*
- TP 594 **Effects of Trypsin on Spiked Isotope-labeled Tryptic Peptide Standards Used in Quantitative Proteomic Analysis;** Thomas A. Shaler<sup>1</sup>; Steve E. Kaiser<sup>2</sup>; Shanhua Lin<sup>1</sup>; Christopher Becker<sup>1</sup>; <sup>1</sup>*PPD Biomarker Discovery Sciences, Menlo Park, CA*; <sup>2</sup>*Stanford University, Stanford, CA*
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- PROTEINS: MODIFIED, METHODOLOGY AND IN VITRO MODIFICATIONS, 595 - 604**
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- TP 595 **Study of DNA-Protein Cross-Links Formation between Lysozyme and Oxanine by Mass Spectrometry;** Wen-Pong Lin; Wei-Loong Chiu; Hauh-Jyun Candy Chen; *National Chung Cheng Univers, Chia-Yi, Taiwan*
- TP 596 **The Cisplatin-Cytochrome C Interaction Studied by Electrospray Mass Spectrometry and MSn Analysis;** Ting Zhao; Fred King; *West Virginia University, Morgantown, WV*
- TP 597 **Assessing the Quality and Precision of Therapeutic Antibody LC-MS Data Acquired and Processed using Automated Workflows;** Scott Berger; Asish Chakraborty; *Waters Corporation, Milford, MA*
- TP 598 **Towards More Quantitative Evaluation of PEGylated Therapeutics and Protein Aggregates by MALDI TOF MS;** Ryan Wenzel; Benoit Plet; Alexis Nazabal; *CovalX AG, Zürich, Switzerland*
- TP 599 **Determining Peptide Susceptibilities to Deamidation by FTICR-MS;** Li Zhou<sup>1</sup>; Terry J. Amiss<sup>2</sup>; Carol E. Parker<sup>1</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>*University of North Carolina - Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*BD Technologies, Research Triangle Park, NC*
- TP 600 **Studies Towards the Development of Milliseconds Timescale Kinetics Chips for Quantitative Monitoring of Enzyme Catalysis by MS;** Allen W. Tsang<sup>1</sup>; Kevin Killeen<sup>2</sup>; William T. Lowther<sup>1</sup>; Thomas J. Jönsson<sup>1</sup>; Cristina M. Furdui<sup>1</sup>; <sup>1</sup>*Wake Forest University School of Medicine, Winston Salem, NC*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- TP 601 **In-gel Chemical Labeling: A Strategy for Characterization of the N-terminus and Phosphorylation Sites of Gel-Separated Proteins;** Joseph P Fernandez; Allison Russo; Abey Tharian; Haiteng Deng; *Proteomics Resource Center, Rockefeller University, New York, NY*
- TP 602 **Beta-Elimination of Disulfide Bridges: A Common Sample Preparation Induced Protein Modification;** Tomas Rejtar; Christian Baumgartner; Majlinda Kullolli; Barry L. Karger; *Northeastern University, Boston, MA*
- TP 603 **LC-MS and LC-MS-MS Characterization of CMC-544: A CD22-Targeted Immunoconjugate of Calicheamicin;** Jason X. Tang; Eugene Vidunas; Fang (anna) Wang; Justin Moran; *Wyeth Research, Pearl River, NY*
- TP 604 **Gas-Phase Ion/Ion Chemistry and Mass Spectrometry for the Determination of Alpha-1-Anti Trypsin Inhibitor Oxidation Sites;** Harsha P. Gunawardena; *Talecris Biotherapeutics, Research Triangle Park, NC*

## TUESDAY POSTERS

**PROTEOMICS: NEW APPROACHES TO DATA ANALYSIS,  
605 - 621**

- TP 605 **An Alternative Peptide Precursor Ion Selection Strategy for Protein Identification by Mass Spectrometry;** David A. Barnett; Rodney J. Ouellette; *Atlantic Cancer Research Institute, Moncton, Canada*
- TP 606 **A New Approach to Achieving a Fast, In-depth Biological Overview of MS-Based Proteomics Data;** Christian Ravnsborg Ingrell; Martin Damsbo; Peter Venø; Morten Bern; *Proxeon A/S, Odense, Denmark*
- TP 607 **Complementary Mass Spectrometry or Just Questionable Identifications?;** Scott Geromanos; *Waters Corporation, Milford, MA*
- TP 608 **High Resolution Analysis of the Human Proteome by Middle down Mass Spectrometry: A LC-FT-ICR-MS-MS Platform Bringing Sanity to Proteomics;** Michael T. Boyne II; Mingxi Li; Cong Wu; Leonid Zamdborg; Shannee Babai; Neil L. Kelleher; *University of Illinois, Urbana-Champaign, IL*
- TP 609 **The PeptideAtlas as a Tool for Targeted Proteomics;** David S Campbell<sup>1</sup>; Eric Deutsch<sup>2</sup>; Vinzenz Lange<sup>3</sup>; Paola Picotti<sup>4</sup>; Nichole King<sup>2</sup>; Simon Letarte<sup>2</sup>; Henry Lam<sup>2</sup>; Ning Zhang<sup>2</sup>; Ruedi Aebersold<sup>5</sup>; <sup>1</sup>ISB, *Seattle, WA*; <sup>2</sup>Institute For Systems Biology, *Seattle, WA*; <sup>3</sup>3M, *Ham Lake, MN*; <sup>4</sup>Institute For Molecular Systems Biology, *Zuerich, Switzerland*; <sup>5</sup>Swiss Federal Institute of Technology, *Zurich, Switzerland*
- TP 610 **Single-Hit and Biochemical Pathway Directed Proteomic Profiling;** Brook L. Nunn<sup>1</sup>; Shawna Hengel<sup>1</sup>; Theodore Larson Freeman<sup>1</sup>; Soyoung Ryu<sup>1</sup>; Eric J. Foss<sup>2</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, *Seattle, WA*; <sup>2</sup>University of Washington and Fred Hutchinson Cancer Center, *Seattle, WA*
- TP 611 **Intelligent Data Annotation Workflows Applied to the Characterization of Human Cerebrospinal Fluid;** Roger G. Biringer<sup>1</sup>; Zhiqi Hao<sup>1</sup>; Helen Tran<sup>1</sup>; Michael G. Harrington<sup>2</sup>; Andreas F. R. Hühmer<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, *San Jose, CA*; <sup>2</sup>Huntington Medical Research Institutes, *Pasadena, CA*
- TP 612 **Cross-Sample and Cross-Platform Training of Peptide Detectability;** Randy J. Arnold; Yong F. Li; Predrag Radivojac; Haixu Tang; *Indiana University, Bloomington, IN*
- TP 613 **SMART-Directed LC-MALDI Protein Identification using a MALDI-Ion Trap-TOF Mass Spectrometer;** Matthew E. Openshaw<sup>1</sup>; Rachel L. Martin<sup>1</sup>; John M. Allison<sup>2</sup>; Victor Spicer<sup>3</sup>; Werner Ens<sup>3</sup>; Oleg V. Krokhin<sup>3</sup>; <sup>1</sup>Shimadzu Biotech, *Manchester, UK*; <sup>2</sup>Kratos Analytical Ltd., *Manchester, UK*; <sup>3</sup>University of Manitoba, *Winnipeg, Canada*
- TP 614 **Mining in a MudPIT: Digging Deeper with PLGEM;** S Swanson; N Pavelka; L Florens; M Washburn; *Stowers Institute For Medical Research, Kansas City, MO*
- TP 615 **Targeted Peptide Identification Based on Selected Reaction Monitoring;** Bruno Domon; Paola Picotti; Nathalie Selevsek; Ruedi Aebersold; *IMSB - ETH Zurich, Zurich, Switzerland*
- TP 616 **Efficient Mining by Optimizing Acquisition Time and Sample Consumption: MALDI-TOF MS-MS Analysis of Low and High Complexity Protein Digests;** Patrick Pribil; Aaron Booy; Suzanne Ackloo; Gordana Ivosev; Min J. Yang; *MDS Sciex, Concord, ON*
- TP 617 **Determining Unassignable Peptides in Accurate Mass Measurement Shotgun Proteomics;** Chunyan Li;

Melissa Warren; William B. Whitman; Jon Amster; Yuchen liu; *University of Georgia, Athens, GA*

- TP 618 **A Bayesian Approach for Addressing the Protein Inference Problem in Shotgun Proteomics;** Yong F. Li; Randy J. Arnold; Predrag Radivojac; Haixu Tang; *Indiana University, Bloomington, IN*
- TP 619 **Iterative MS-MS Sampling of Proteomics Mixtures: Software and Methodology to Maximize Sampling of Detectable Components in Mixture;** Michael R. Hoopmann; Daniela Tomazela; Michael J. Maccoss; *University of Washington, Seattle, WA*
- TP 620 **Posterior Peptide Identification for Proteomics Data Analysis;** Haixu Tang; Yong F. Li; Randy J. Arnold; Predrag Radivojac; *Indiana University, Bloomington, IN*
- TP 621 **Duty Cycle and MRM Prediction Improvements for Protein ID Validation using the MIDAS Workflow on a QqLIT Mass Spectrometer;** Christof E. Lenz<sup>1</sup>; Henning Urlaub<sup>2</sup>; Matthias Glueckmann<sup>1</sup>; <sup>1</sup>Applied Biosystems, *Darmstadt, Germany*; <sup>2</sup>Max Planck Institute, *Goettingen, Germany*

**PROTEOMICS: BIOMARKER DISCOVERY 2, 622 - 646**

- TP 622 **Discovery of Wound Healing Markers: MALDI-MS Methodology for Wound Fluid Analysis and In Situ Imaging of Formalin-Fixed Paraffin Embedded Tissues;** Katri Huikko; Stephanie F Bernatchez; Patrick J Parks; Bathsheba Chong Conklin; *3M, St Paul, MN*
- TP 623 **The Application of MALDI-TOF MS Plasma Protein Profiling for Discrimination of Patients with Squamous Cell Carcinomas from Healthy Controls;** Valeriy E. Shevchenko; Natalia E. Arnotskaya; Sergei S. Aushkap; Valentina A. Yurchenko; David G. Zaridze; *N. N. Blokhin Russian Cancer Research Center, Moscow, Russia*
- TP 624 **Biomarker Discovery Of Amniotic Fluid From Patients with Posterior Urethral Valve Syndrome using Proteomics Strategies;** Jenny Albanese<sup>3</sup>; Olga Miroshnychenko<sup>2</sup>; H. Eva Witkowska<sup>2</sup>; Haichuan Liu<sup>2</sup>; Hanmin Lee<sup>1</sup>; Marjorie Minkoff<sup>3</sup>; Susan Fisher<sup>2</sup>; Raul Cortes<sup>1</sup>; <sup>1</sup>UC San Francisco Fetal Treatment Center, *San Francisco, CA*; <sup>2</sup>Department of Cell and Tissue Biology, *San Francisco, CA*; <sup>3</sup>Applied Biosystems in Foster City, *San Francisco, CA*
- TP 625 **A Non-Parametric Statistical Method to Assess Humoral Response in Pancreatic Cancer;** Tasneem H. Patwa; Huy Vuong; Laila Poisson; Debashis Ghosh; David E. Misek; Diane M. Simeone; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- TP 626 **Detection of Tumor-Derived Peptides in Pancreas Cancer Patient Plasma;** Kwasi Antwi; *The Biodesign Institute, Arizona State University, Tempe, AZ*
- TP 627 **LC-MS(E) Analysis of Human Urine Proteome;** Martin Gilar; Petra Olivova; Scott Geromanos; John Gebler; *Waters Corporation, Milford, MA*
- TP 628 **Proteomic Analysis of Membrane Glycoproteins using a Lectin Affinity Approach;** Yanfei Wang; Huy Vuong; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- TP 629 **Proteomic Markers in Prostate Tissue by Histology Directed Profiling Mass Spectrometry and LC-MS(MS)<sup>2</sup>, Malignant Vs. Adjacent Benign Tissue Sections;** Sean Clark; Jared Cox; Donald Shipman; Colleen Martin; Greg Bowersock; Christopher Amling; James Mobley; *University of Alabama at Birmingham, Birmingham, AL*
- TP 630 **Enhanced Biomarker Discovery using Pathway Markers, Density Based Fractionation and MALDI-**

## TUESDAY POSTERS

- MS-MS; WenKui Lan;** Marc Horn; *Prospect Biosystems, LLC, Newark, NJ*
- TP 631 **Programmable Proteomics for High Throughput Validation of Salivary Oral Cancer Protein Biomarkers;** Ebbing de Jong<sup>1</sup>; Hongwei Xie<sup>2</sup>; Getiria Onsongo<sup>1</sup>; John V Carlis<sup>1</sup>; Nelson L Rhodus<sup>1</sup>; Frank G Ondrey<sup>1</sup>; Tim Griffin<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN;* <sup>2</sup>*Waters Corporation, Milford, MA*
- TP 632 **Comparison Proteome Analysis of Two Closely-Related Ovarian Endometrioid Adnocarcinoma(OEA)-Derived Cell Lines;** Lan Dai; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- TP 633 **Discovery of O-linked Glycoprotein Cancer Biomarkers in Human Sera by Multi-Lectin Enrichment and Lectin Microarray Binding Patterns with MALDI QIT;** Chen Li<sup>1</sup>; David M Lubman<sup>1</sup>; Fan Xiang<sup>2</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI;* <sup>2</sup>*Shimadzu, Pleasanton, CA*
- TP 634 **Identification of 4-Hydroxynonenol Targets in Plasma Proteins using Click Chemistry;** Hye-Young H. Kim; Simona G. Codreanu; Keri A. Tallman; Ned A. Porter; Daniel C. Liebler; *Vanderbilt University, Nashville, TN*
- TP 635 **Identifying Candidate Protein Markers for Colorectal Cancer from Human Stool;** Patrick S. Quint; Douglas W. Mahoney; Ann L. Oberg; Garth D. Nelson; Jonathan J. Harrington; David A. Ahlquist; H. Robert Bergen, III; *Mayo Clinic College of Medicine, Rochester, MN*
- TP 636 **Pancreatic Cancer Biomarkers: Post-Translational State of Nuclear and Cytosolic High Mobility Group Box Protein-1 [HMGB1] as Determined by MALDI-TOF MS;** L.J. Sparvero<sup>1</sup>; Shelly A. Kucherer<sup>2</sup>; Herbert J. Zeh<sup>1</sup>; Michael T. Lotze<sup>1</sup>; Andrew A. Amoscato<sup>1</sup>; <sup>1</sup>*University of Pittsburgh, Pittsburgh, PA;* <sup>2</sup>*Carnegie Mellon University, Pittsburgh, PA*
- TP 637 **Proteomic Approaches for Detection of Metabolic Syndrome in Obese Adults;** Jacob A. Galan; Corrie Whisner; Stacy L. Mobely; W. Andy Tao; *Purdue University, West Lafayette, IN*
- TP 638 **Discovery of Pancreatic Cancer Biomarker for Early Detection: Proteomic Analysis of Human Pancreatic Duct Fluid (Juice);** Vadiraja B. Bhat; Lei Shi; Christopher Thompson; Rebecca Wiatrek; Mohsen Shabahang; Arundhati Rao; Alexzander A. Asea; *Scott & White Memorial Hospital, Temple, TX*
- TP 639 **Discovery of Schizophrenia Biomarker Proteins in Eccrine Sweat;** Mark M. Ross<sup>1</sup>; Michelle Raiszadeh<sup>1</sup>; Weidong Zhou<sup>1</sup>; Emanuel Petricoin<sup>1</sup>; Lance Liotta<sup>1</sup>; April Dickson<sup>2</sup>; Cindy Dickson<sup>2</sup>; Adam Freeberg<sup>2</sup>; Mary Ann Schaepper<sup>2</sup>; Wolff Kirsch<sup>2</sup>; <sup>1</sup>*George Mason University, Manassas, VA;* <sup>2</sup>*Loma Linda University, Loma Linda, CA*
- TP 640 **Comparative Proteomics of Human Intraductal Carcinoma and Matched Normal Breast Tissues: Biomarkers and Insights into Molecular Basis of DCIS Development;** Lambert C. Ngoka; *Virginia Commonwealth Univ., Richmond, VA*
- TP 641 **Nonporous Silica Reverse-Phase High-Performance Liquid Chromatography -Electrospray Tandem Mass Spectrometry (NPS-HPLC-ESI-MS-MS) with ExacTag Labeling for Lung Cancer Plasma Protein Characterization;** Karan Bedi<sup>3</sup>; Xiaoping Ao<sup>2</sup>; Fengming Kong<sup>2</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI;* <sup>2</sup>*University of Michigan, Medical Center, Ann Arbor, MI;* <sup>3</sup>*School of Public Health, University of Michigan, Ann Arbor, MI*
- TP 642 **Quantitative Analysis of the Malignant Glioma Secretome;** Catherine Formolo; Tobey J MacDonald; Yatrib Hathout; *Children's National Medical Center, Washington, DC*
- TP 643 **Differential Proteomics of Secreted Proteins for Melanoma Biomarker Discovery;** Mathur Rajesh; Lalita A. Shevde; Rajeev S. Samant; Adam I. Riker; Lewis K. Pannell; *Mitchell Cancer Institute, Mobile, AL*
- TP 644 **Site-Specific Identification of Protein Markers of Organophosphorus Compounds Exposure using Monomeric Avidin Purification;** Shi-Jian Ding<sup>1</sup>; Bin Li<sup>1</sup>; John Carr<sup>2</sup>; Larry Schopfer<sup>1</sup>; Steven Hinrichs<sup>1</sup>; Oksana Lockridge<sup>1</sup>; <sup>1</sup>*University of Nebraska Medical Center, Omaha, NE;* <sup>2</sup>*Missouri Southern State University, Joplin, MO*
- TP 645 **Biomarker Discovery using Low Enrichment Stable Isotope Labeling of Amino Acids in Cells;** Jing Xiao<sup>1</sup>; Wai-Nang Paul Lee<sup>2</sup>; Shu Lim<sup>2</sup>; Yingchun Zhao<sup>1</sup>; Robert Recker<sup>1</sup>; Gary Guishan XIAO<sup>1</sup>; <sup>1</sup>*Creighton University Medical Center, Omaha, NE;* <sup>2</sup>*Mass Spectrometry Core Facility, Pediatrics, Los Angeles, California*
- TP 646 **Biomarker Discovery by Stable Isotope Labeling and Quantitative Mass Spectrometry in a Trait Anxiety Mouse Model;** Christoph W. Turck; Katrin Haegler; Elisabeth Frank; Melanie Kessler; Boris Hamsch; Yuji Odagaki; Birgit Bisle; Rainer Landgraf; Christian Webhofer; *Max Planck Institute of Psychiatry, Munich, Germany*
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- BIOINFORMATICS 2, 647 - 671**
- TP 647 **A Program to Statistically Evaluate Mass Spectra for Identification of Differentiating Features and Biomarker Discovery;** Sean Beecroft<sup>1</sup>; Scott Kronewitter<sup>1</sup>; Maria Lorna A de Leoz<sup>1</sup>; Nannan Tao<sup>1</sup>; Suzanne Miyamoto<sup>2</sup>; Ruth Vinall<sup>2</sup>; Ralph deVere White<sup>2</sup>; Kit Lam<sup>2</sup>; Hyun Joo An<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, CA;* <sup>2</sup>*UC Davis Cancer Center, Sacramento, CA*
- TP 648 **Multi-Spectra Peptide Sequencing and its Applications to Multistage Mass Spectrometry;** Nuno Bandeira<sup>1</sup>; Jesper V Olsen<sup>2</sup>; Matthias Mann<sup>2</sup>; Pavel Pevzner<sup>1</sup>; <sup>1</sup>*University of California, San Diego (UCSD), La Jolla, CA;* <sup>2</sup>*Max Planck Institute For Biochemistry, D Martinsried, Germany*
- TP 649 **The MCW Automated Proteomics Workflow (MAPW);** Brian D. Halligan; Andrew Vallejos; Simon Twigger; Andrew Greene; *Medical College Of Wisconsin, Milwaukee, WI*
- TP 650 **Absolute Protein Quantification Estimated by Spectral Counting using Large Datasets in PeptideAtlas;** Ning Zhang<sup>1</sup>; Eric Deutsch<sup>1</sup>; Henry Lam<sup>1</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>*Institute for Systems Biology, Seattle, WA;* <sup>2</sup>*Swiss Federal Institute of Technology, Zurich, Switzerland*
- TP 651 **Spectral Clustering of MS-MS Data to Identify Unknown Peptide Modifications and Estimate Identifiable Spectra;** Jayson A Falkner; Anastasia K Yocum; Pratik D Jagtap; Philip C Andrews; *University of Michigan, Ann Arbor, MI*
- TP 652 **Chemical Contaminants in Proteomics LC-MS Data;** Xinjian Yan; Stephen Stein; *NIST, Gaithersburg, MD*
- TP 653 **Better Protein Quantification by Combining Peptide Identification Confidence and Retention-Time Prediction;** Lei Xin<sup>1</sup>; Weiwu Chen<sup>2</sup>; Weijie Yang<sup>2</sup>; Sean

## TUESDAY POSTERS

- Bendall<sup>1</sup>; BIN MA<sup>1</sup>; Gilles Lajoie<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, ON, Canada; <sup>2</sup>Bioinformatics Solutions Inc., Waterloo, ON, Canada
- TP 654 **Planets, Proteins, and Portability: A Common API and Desktop Environment for Proteomics Data Analysis;** Manor Askenazi<sup>1</sup>; Jignesh Parikh<sup>2</sup>; Tanya Cashorali<sup>3</sup>; Yi Zhang<sup>2</sup>; Scott Ficarro<sup>2</sup>; Nathaniel C. Blank<sup>4</sup>; Jarrod Marto<sup>2</sup>; <sup>1</sup>Dana-Farber Cancer Institute and Hebrew University, Boston, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA; <sup>3</sup>Northeastern University, Boston, MA; <sup>4</sup>Centre College, Danville, KY
- TP 655 **A Public Network for Publishing Proteomics Data and Tools;** Philip C Andrews; Bryan E Smith; James A Hill; Mark A Gjukić; Jayson A Falkner; *University of Michigan, Ann Arbor, MI*
- TP 656 **Two-phase Filtering Strategy for Identification of Peptide with Post-Translational Modifications;** Kang Ning<sup>1</sup>; Xia Cao<sup>1</sup>; Hoong Kee Ng<sup>2</sup>; Hon Wai Leong<sup>2</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>National University of Singapore
- TP 657 **Molecular Fragmentation Query Language for Shotgun Lipidomics;** Ronny Herzog; Dominik Schwudke; Andrej Shevchenko; *Max Planck Institute CBG, Dresden, Germany*
- TP 658 **Automated Evaluation of Peptide Identifications from Shotgun Proteomics Data by Use of Peptide Hydrophobicity and Reversed-Phase LC Retention Time;** Hua Xu; Lanhao Yang; Michael A. Freitas; *Ohio State University, Columbus, OH*
- TP 659 **AB3D: A Suite of Algorithms for Biomarker Discovery in Diagnostics and Drug Development using LC-MS;** Ken Aoshima<sup>1</sup>; Satoshi Tanaka<sup>2</sup>; Yuji Miura<sup>1</sup>; Yoshiya Oda<sup>1</sup>; Tatsuji Nakamura<sup>1</sup>; Hiromi Ohashi<sup>1</sup>; Masataka Ueda<sup>1</sup>; Akiyoshi Suganuma<sup>1</sup>; Junro Kuromitsu<sup>1</sup>; <sup>1</sup>Eisai Co., Ltd, Tsukuba, Japan; <sup>2</sup>CREST, Japan Science and Technology, Saitama, Japan
- TP 660 **Evaluating Efficiency of Cross-Species Comparisons;** A. Podtelejnikov; D. Potter; C. R. Ingrell; S. Larsen; *Proxeon A/S, Odense, Denmark*
- TP 661 **Mascot Percolator: Improved Peptide and Protein Identification;** Markus Brosch; Tim Hubbard; Jyoti Choudhary; *Wellcome Trust Sanger Institute, Cambridge, UK*
- TP 662 **How Stable are Peptide Identifications with Regards to Variations in MS-MS Spectra?;** Pierre-Alain Binz<sup>1,2</sup>; Markus Müller<sup>2</sup>; Frederique Lisacek<sup>2</sup>; David Bouyssié<sup>3</sup>; <sup>1</sup>Genebio, Geneva, Switzerland; <sup>2</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland; <sup>3</sup>IPBS, Toulouse, France
- TP 663 **Methods to Estimate the Precision of False Positive Rate Measured by Decoy Protein Database Searching;** Roger Moore; Mary K. Young; Terry Lee; *City of Hope, Duarte, CA*
- TP 664 **Alternative Splicing Database for Bottom-up and Top-down Protein Identification;** Kung-Yen Chang; D. Ryan Georgianna; Steffen Heber; Gary A. Payne; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- TP 665 **ABRF iPRG 2008 Study: Characterization of Protein Inference Reporting from Proteomics Studies;** Brian C. Searle<sup>1</sup>; David L. Tabb<sup>2</sup>; Alexey I. Nesvizhskii<sup>3</sup>; William S. Lane<sup>4</sup>; Jeffery A. Kowalak<sup>5</sup>; Jayson A. Falkner<sup>3</sup>; Sean L. Seymour<sup>6</sup>; <sup>1</sup>Proteome Software, Portland, OR; <sup>2</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>3</sup>University of Michigan, Ann Arbor, MI; <sup>4</sup>Harvard University, Cambridge, MA; <sup>5</sup>National Institute of Mental Health, Bethesda, MD; <sup>6</sup>Applied Biosystems, Foster City, CA
- TP 666 **Monte Carlo Simulation Based Algorithms for Scoring Ion Abundance and Peptide Sequence Tags in Database Searches of Shotgun-Proteomic Data;** Michael A. Freitas; Hua Xu; *Ohio State University, Columbus, OH*
- TP 667 **Identification of Peptides from Data-Independent Tandem MS;** Marshall W. Bern<sup>1</sup>; Gregory Finney<sup>2</sup>; Michael J. Maccoss<sup>3</sup>; Michael Hoopmann<sup>3</sup>; <sup>1</sup>Palo Alto Research Center, Palo Alto, CA; <sup>2</sup>Univ of Washington, Genome S, Seattle, WA; <sup>3</sup>University of Washington, Seattle, WA
- TP 668 **iProphet: A New Tool for Combining PeptideProphet Results from Multiple Search Engines Improves Spectrum Validation;** David Shteynberg<sup>1</sup>; Alexey Nesvizhskii<sup>2</sup>; Eric Deutsch<sup>1</sup>; Henry Lam<sup>1</sup>; Ruedi Aebersold<sup>3</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>University of Michigan, Ann Arbor, MI; <sup>3</sup>Swiss Federal Institute of Technology, Zurich, Switzerland
- TP 669 **New Developments for Open-Source Shotgun Proteomics Analysis with the Trans-Proteomic Pipeline;** Joshua Tasman<sup>1</sup>; Luis Mendoza<sup>1</sup>; David Shteynberg<sup>1</sup>; James Eddes<sup>1</sup>; Ning Zhang<sup>1</sup>; Chee-Hong Wong<sup>3</sup>; Brian S Pratt<sup>2</sup>; Henry Lam<sup>1</sup>; Jimmy Eng<sup>4</sup>; Eric Deutsch<sup>1</sup>; Ruedi Aebersold<sup>5</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Insilicos Llc, Seattle, WA; <sup>3</sup>Bioinformatics Institute, Singapore, Singapore; <sup>4</sup>University of Washington, Seattle, WA; <sup>5</sup>Swiss Federal Institute of Technology, Zurich, Switzerland
- TP 670 **Rapid Cyberinfrastructure Evolution for Proteomics Research;** Claudiu Farcas; To-ju Huang; Sam Payne; Nuno Bandeira; Ari Frank; Nitin Gupta; Pavel Pevzner; Ingolf Krueger; Vineet Bafna; *UCSD, La Jolla, CA*
- TP 671 **Empirical Evaluation of Algorithm Consensus Methods to Peptide Identification;** Tamanna Sultana; Rick Jordan; James Lyons-Weiler; *University of Pittsburgh, Pittsburgh, PA*
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- SYSTEMS BIOLOGY: DISCOVERY, 672 - 683**
- TP 672 **Interpretation of Proteomic 2D Electrophoresis and MALDI TOF/TOF Data using Pathway Analysis Tools to Understand Muscle Development;** Matthew Mcdonagh; Matthew Knight; *Biosciences Research Division, DPI Victoria, Melbourne, Australia*
- TP 673 **Comprehensive Analysis of Murine Adipose Tissue by Detergent-Free Pressure Cycling Protein Extraction and High Resolution Tandem Mass Spectrometry;** Emily Freeman<sup>1</sup>; Vera Gross<sup>2</sup>; Gary Smejkal<sup>2</sup>; Alexander Lazarev<sup>2</sup>; Haiming Cao<sup>1</sup>; Gokhan S. Hotamisligil<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Harvard University, Boston, MA; <sup>2</sup>Pressure Biosciences, Inc, Woburn, MA
- TP 674 **Mapping the Entamoeba Histolytica Proteome using Subcellular Fractionation, One-Dimensional Polyacrylamide Gel Electrophoresis and Liquid Chromatography-Tandem Mass Spectrometry;** Barbora Maralikova; Jorge Tovar; *Royal Holloway University of London, Egham, Surrey*
- TP 675 **Novel Insights into Platelet Biochemical Processes by a Combination of Unbiased, Comprehensive Proteomic Analysis by Mass Spectrometry and Pathway Analysis;** Geraldine M Walsh; Michael D Hoffman; Dana V Devine; Ronald C. Beavis; Juergen Kast; *University of British Columbia, Vancouver, Canada*

## TUESDAY POSTERS

- TP 676 **The Study of *Botrytis cinerea* Interaction with Tomatoes;** Punit Shah<sup>1</sup>; Gerardo Gutierrez-sanchez<sup>2</sup>; James A Atwood Iii<sup>2</sup>; Ann Powell<sup>3</sup>; Ron Orlando<sup>2</sup>; Carl Bergmann<sup>1</sup>; <sup>1</sup>*Complex Carbohydrate Research Center, Athens, GA*; <sup>2</sup>*University of Georgia, Athens, GA*; <sup>3</sup>*University of California, Davis, California*
- TP 677 **Proteogenome Profiling of *Acholeplasma Laidlawii*;** Vadim Govorun; *Institute of Physico-Chemical Medicine, Moscow, Russian Federation*
- TP 678 **The Human Saliva Proteome: Collection, Stability, and Analysis;** Timothy Britt Langston; Rebecca R. Secrist; Gaurav S.J.B. Rana; Michael J. Oldham; Jason W. Flora; *Philip Morris USA, Richmond, VA*
- TP 679 **The Secretomes on the Interface of *Magnaporthe grisea*-Rice Leaf Interaction;** Gerardo Gutierrez-Sanchez; Punit Shah; James A Atwood III; Denise Lennon; Peter Albersheim; Alan Darvill; Ron Orlando; Sheng-Cheng Wu; *Complex Carbohydrate Research Center, Athens, GA*
- TP 680 **Gauging Complementary Proteomics Discovery of *Nostoc punctiforme* PCC 73102 using a Combination of FFE, SCX, Ion-Trap and QTOF-MS;** Saw Yen Ow<sup>1</sup>; Nishikant Wase<sup>1</sup>; Mikkel Nissum<sup>2</sup>; Phillip C Wright<sup>1</sup>; <sup>1</sup>*University of Sheffield, Sheffield, UK*; <sup>2</sup>*BD Diagnostics, Martinsried, Germany*
- TP 681 **Processing of High Mass Accuracy MS-Data from Large-Scale Proteomics Experiments and Construction of Proteotypic Library for the *Arabidopsis Thaliana* Proteome;** Boris Zybailov; Giulia Friso; Paul Dominic B. Olinares; Heidi Rutschow; Klaas van Wijk; Qi Sun; *Cornell University, Ithaca, NY*
- TP 682 **Identification of Cancer Specific Protein Classes using Non-Tagged Proteomics Combined with Systems Biology Applied to Murine Models of Breast Cancer;** Anton Poliakov; Yuelong Liu; Gregory Bowersock; Huang-Ge Zhang; James Mobley; *University of Alabama at Birmingham, Birmingham, AL*
- TP 683 **Deciphering Pluripotency of Embryonic Stem Cells through Transcriptome, Proteome and Modificome;** Rong Zeng; Qing-Run Li; Jiu-Hong Kang; Jie Dai; Xiao-Bin Xing; Yi-Xue Li; *Shanghai Institutes for Biological Sciences, Shanghai, China*

## WEDNESDAY POSTERS

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- INSTRUMENTATION: TOF, 004 - 021**
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- WP 004 **Surface Probing Mass Spectrometry as a Differential Biomarker Monitoring Method;** Mariam S ElNaggar; Richard A Mathies; Evan R. Williams; *University of California, Berkeley, CA*
- WP 005 **Method to Improve the Dynamic Range Characteristics of Microchannel Plate-Based Ion Detectors, and Its Effect on Performance of TOF-MS;** Masahiro Hayashi<sup>1</sup>; Hisanao Hazama<sup>2</sup>; Yasuhide Naito<sup>3</sup>; Masahiko Iguchi<sup>4</sup>; Akio Suzuki<sup>1</sup>; Toshiyuki Uchiyama<sup>1</sup>; Katsutoshi Nonaka<sup>1</sup>; Kunio Awazu<sup>2</sup>; <sup>1</sup>*Hamamatsu Photonics K.K., Iwata, Shizuoka, JAPAN*; <sup>2</sup>*Graduate School of Engineering, Osaka University, Suita, Osaka, Japan*; <sup>3</sup>*GPI, Hamamatsu, Shizuoka, Japan*; <sup>4</sup>*Hamamatsu Corporation, Bridgewater, NJ*
- WP 006 **The Impact of Resolution on Accurate Mass Measurements of Complex Samples;** Doug McIntyre; Patrick D. Perkins; Edgar Naegel; *Agilent Technologies, Santa Clara, CA*
- WP 007 **A continuous Beam, Time of Flight Mass Spectrometer for Secondary Ion Mass Spectrometry;** Stephen P. Thompson; *SAI Ltd., Manchester, UK*
- WP 008 **A High Dynamic Range Ion Detector with Bipolar Post-Acceleration and Sub-Nanosecond Pulse Widths;** Stephen Ritzau<sup>1</sup>; Bruce Laprade<sup>1</sup>; Paul Mitchell<sup>2</sup>; <sup>1</sup>*Photonis USA, Inc., Sturbridge, MA*; <sup>2</sup>*Burle Industries, Lancaster, PA*
- WP 009 **Introducing a New High Sensitivity Benchtop Reflectron Time of flight Mass Spectrometer (BenchTOF-dx), Incorporating On-Line Spectral Dynamic Background Compensation (DBC);** Gerhard Horner<sup>1</sup>; Gareth Roberts<sup>2</sup>; <sup>1</sup>*ALMSCO Ltd, Munich, Germany*; <sup>2</sup>*Markes International Ltd, Cardiff, UK*
- WP 010 **Imaging Time-of-Flight Mass Spectrometry and Pattern Analysis for Characterizing Transient Gaseous Phenomena on the Moon;** Daniel E Austin; *Brigham Young University, Provo, UT*
- WP 011 **Evaluation of IR Multi Photon Dissociation as a Method for High Mass Protein Clean Up;** Ayman El-Faramawy<sup>1</sup>; Yuzhu Guo<sup>2</sup>; Udo H. Verkerk<sup>2</sup>; Bruce Thomson<sup>3</sup>; K W Michael Siu<sup>4</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>*Crms, York University, Toronto, ON*; <sup>3</sup>*Mds Sciex, Concord, ON*; <sup>4</sup>*York University, Toronto, ON*
- WP 012 **Design of a New Multi-Turn Ion Optical System for High-Performance Time-of-Flight Mass Spectrometers;** Masaru Nishiguchi<sup>1</sup>; Yoshihiro Ueno<sup>1</sup>; Osamu Furuhashi<sup>1</sup>; Michisato Toyoda<sup>2</sup>; Mitsutoshi Setou<sup>3</sup>; <sup>1</sup>*Shimadzu corporation, Kyoto, JAPAN*; <sup>2</sup>*Osaka University, Toyonaka, Osaka, Japan*; <sup>3</sup>*Hamamatsu Medical School, Hamamatsu, Shizuoka, Japan*
- WP 013 **Increased Throughput and Reduced Carry-Over of Mass Spectrometry Based Proteomics using High Efficiency Non-Split Nano-Flow Parallel Dual-Column Capillary HPLC System;** Hong Wang; Sam Hanash; *PHS, Fred Hutchinson Cancer Research Center, Seattle, WA*
- WP 014 **Development of a Stigmatic Mass Microscope using a Multi-Turn Time-of-Flight Mass Spectrometer, MULTUM-IMG;** Hisanao Hazama<sup>1</sup>; Jun Aoki<sup>2</sup>; Hirofumi Nagao<sup>1</sup>; Ren Suzuki<sup>1</sup>; Yasuhide Naito<sup>3</sup>; Michisato Toyoda<sup>2</sup>; Katsuyoshi Masuda<sup>4</sup>; Kenichi Fujii<sup>5</sup>; Toshio Tashima<sup>6</sup>; Kunio Awazu<sup>1</sup>; <sup>1</sup>*Graduate School of Engineering, Osaka University, Suita, Osaka, Japan*; <sup>2</sup>*Graduate School of Science, Osaka University, Toyonaka, Osaka, Japan*; <sup>3</sup>*GPI, Hamamatsu, Shizuoka, Japan*; <sup>4</sup>*Suntory Institute for Bioorganic Research, Mishima-gun, Osaka, Japan*; <sup>5</sup>*Osaka Institute of Technology, Hirakata, Osaka, Japan*; <sup>6</sup>*Japan Tobacco Inc., Takatsuki, Osaka, Japan*
- WP 015 **Ion Trajectory Simulation of Multi-Turn TOF using Surface Charge Method Accelerated by a Special Purpose Computer;** Jun Aoki<sup>1</sup>; Michisato Toyoda<sup>1</sup>; Ayumi Kubo<sup>1</sup>; Hisanao Hazama<sup>1</sup>; Kunio Awazu<sup>1</sup>; Yasuhide Naito<sup>2</sup>; <sup>1</sup>*Osaka University, Osaka, Japan*; <sup>2</sup>*GPI, Hamamatsu, Japan*
- WP 016 **A High Performance, Folded Geometry oa-ToF Mass Analyser Combining Single Stage and Dual Stage Reflectrons;** Jason L Wildgoose; *Waters Corporation, Manchester, UK*
- WP 017 **Performance of an ESI Linear Ion Trap/Orthogonal TOF Mass Spectrometer for UV Photodissociation of Biomolecules;** Tae-Young Kim; James P. Reilly; *Indiana University, Bloomington, IN*
- WP 018 **A Prototype High-Performance Axial-Time-of-Flight Mass Spectrometer for Electrospray Mass Spectrometry;** Robert Jackson; Bronson Crothers; Zhongyu Yang; Stephen Lammert; *Stillwater Scientific Instruments, Inc., Orono, ME*
- WP 019 **Miniature Laser Ablation Time-of-Flight Mass Spectrometry with Reversible Polarity Capability for Analysis of Planetary Samples;** Timothy J. Cornish<sup>1</sup>; Catherine M. Corrigan<sup>1</sup>; Scott A. Ecelberger<sup>1</sup>; William B. Brinckerhoff<sup>2</sup>; <sup>1</sup>*Jhu/apl, Laurel, MD*; <sup>2</sup>*NASA/Goddard Space Flight Center, Greenbelt, MD*
- WP 020 **The Effect of Ion Mobility Processes on the Mass Calibration of Analytes in MALDI TOFMS;** Renata Szyszka<sup>1</sup>; William J. Erb<sup>2</sup>; Kevin G. Owens<sup>1</sup>; <sup>1</sup>*Drexel University, Springfield, PA*; <sup>2</sup>*Ethicon, Somerville, Nj, NJ*
- WP 021 **Electron Transfer Dissociation within a RF Travelling Wave Ion Guide Collision Cell of a QTOF;** Jeff Brown; Iain Campuzano; Steven Pringle; Richard Chapman; *Waters Micromass MS Technologies, Manchester, UK*
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- INSTRUMENTATION: QUADRUPOLES AND TRAPS 1, 022 - 039**
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- WP 022 **Advanced Modeling of a QMS to Include Ion Source and Mass Filter;** Boris Brkic; Neil France; Thomas J. Hogan; Stephen Taylor; *University of Liverpool, Liverpool, UK*
- WP 023 **Comparison of a Ring Ion Guide and a Quadrupole Collision Cell for Threshold Collision-Induced Dissociation Ag+(N-(methyl)N acetamide)(solvent) Bond-Energy Determinations;** Vladimir Romanov; Udo H. Verkerk; Alan C. Hopkinson; K.W. Michael Siu; *York University/ Chemistry Department, Toronto, Canada*
- WP 024 **New Approaches to Supercomputer Modeling of Fields and Ion Cloud Dynamics with Total Account for Ion-Ion and image Charge Interactions;** Eugene Nikolaev<sup>1</sup>; Ivan Boldin<sup>2</sup>; Pavel Ryumin<sup>1</sup>; Gleb Vladimirov<sup>2</sup>; Ron M.a. Heeren<sup>4</sup>; Alexander Pozdnev<sup>3</sup>; Dmitriy Avtonomov<sup>1</sup>; <sup>1</sup>*The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation*; <sup>2</sup>*The Institute of Biochem. Phys. Russian Acad.Sc., Moscow, Russia*; <sup>3</sup>*Moscow State University, Dptm. of comp. math., Moscow, Russia*; <sup>4</sup>*Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands*

## WEDNESDAY POSTERS

- WP 025 **Reduction of Nonlinear Resonance Effects in the 3D quadrupole Ion Trap with Microscreened Endcap Holes and Optimized Endcap-to-Endcap Spacing;** Dodge L. Baluya; Richard A. Yost; *University of Florida, Gainesville, FL*
- WP 026 **Off-Resonance Excitation for Ejection or Fragmentation in a Linear Ion Trap Mass Spectrometer;** James Hager; *MDS Sciex, Concord, Canada*
- WP 027 **Geometrical Effect on the Performance of Ion Trap Array(ITA);** Xiao-Xu Li<sup>1</sup>; Gong-yu Jiang<sup>1</sup>; Chan Luo<sup>1</sup>; Fuxin Xu<sup>1</sup>; Peng Yang<sup>1</sup>; An Hu<sup>1</sup>; Yuan-yuan Wang<sup>1</sup>; Chuan-fan Ding<sup>1</sup>; Li Ding<sup>2</sup>; <sup>1</sup>*Fudan University, Shanghai, China*; <sup>2</sup>*Shimadzu Research Lab (shanghai), Shanghai, China*
- WP 028 **Linear Quadrupole Ion Trap for Fourier-Transform Mass Spectrometry;** Albrecht Glasmachers; Alexander Laue; *Universität Wuppertal, Wuppertal, Germany*
- WP 029 **Improving the Analytical Performance of the ESI Mass Spectrometer by Coupling 2D and 3D Digital Ion Traps;** Li Ding<sup>1</sup>; Xiaohui Yang<sup>1</sup>; Jiangong Zhu<sup>1</sup>; Andrew Entwistle<sup>2</sup>; Ikuo Konishi<sup>2</sup>; <sup>1</sup>*Shimadzu Research Lab (Shanghai) Ltd., Shanghai, China*; <sup>2</sup>*Shimadzu Research Laboratory (Europe) Ltd., Manchester, UK*
- WP 030 **Adaptation of a Triple-Quadrupole Mass Spectrometer for Threshold Collision-Induced Dissociation (TCID) Measurements using a Ring Ion Guide;** Vladimir Romanov; Udo H. Verkerk; Alan C. Hopkinson; K W Michael Siu; *CRMS, Chemistry, York University, Toronto, Canada*
- WP 031 **High Throughput Mass-Selective Soft Landing with Rectilinear Ion Trap in RF/DC isolation Mode;** Zongxiu Nie; Mike Goodwin; Wen-ping Peng; Michael Volny; Zheng Ouyang; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- WP 032 **Studies of Space Charge Effects in the Orbitrap Mass Analyzer;** Richard Perry<sup>1</sup>; Gary Abdiel Salazar<sup>1</sup>; Robert J. Noll<sup>1</sup>; Wolfgang Plass<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Justus-liebig-universitaet Giessen, Giessen, Germany*
- WP 033 **Transmission Mode Ion/Ion Reactions in the Q0 Cell of a Hybrid Triple Quadrupole/Linear Ion Trap Instrument;** Joshua Emory; Scott A. Mcluckey; *Purdue University, West Lafayette, IN*
- WP 034 **Design and Performance of a Halo Ion Trap Mass Analyzer;** Miao Wang<sup>1</sup>; Daniel E Austin<sup>1</sup>; Samuel Tolley<sup>2</sup>; Aaron Hawkins<sup>1</sup>; Edgar Lee<sup>2</sup>; Milton Lee<sup>1</sup>; <sup>1</sup>*Brigham Young University, Provo, UT*; <sup>2</sup>*Torion Technologies, Inc, Pleasant Grove, UT*
- WP 035 **Mass Selective Axial Ion Ejection from a Linear Quadrupole with an 8% Added Hexapole Field;** Zilan Xiao; Donald J. Douglas; *University of British Columbia, Vancouver, BC*
- WP 036 **High Pressure and Fabrication Imperfection Effects on Performance of Miniature Ion Trap and Ion Trap Array;** Wei Xu; Qingyu Song; Jeffrey Maas; Miriam Fico; Liang Gao; William Chappell; Graham Cooks; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- WP 037 **Metrological Characterization of the Fourier-Transform Ion Trap Mass Spectrometer;** Alexander Laue; Albrecht Glasmachers; Klaus Brockmann; *Universität Wuppertal, Wuppertal, Germany*
- WP 038 **A dynamic Pressure MALDI Source Interfaced to a 3D digital Ion Trap using a Linear Ion Trap;** Andrew Entwistle<sup>1</sup>; Ikuo Konishi<sup>2</sup>; Li Ding<sup>3</sup>; Shinichi Iwamoto<sup>4</sup>; Koichi Tanaka<sup>4</sup>; <sup>1</sup>*Shimadzu Research Lab, Manchester, UK*; <sup>2</sup>*Shimadzu Research Laboratory Ltd, Manchester, UK*; <sup>3</sup>*Shimadzu Research Lab (shanghai), Shanghai, China*; <sup>4</sup>*Shimadzu Corporation, Kyoto, Japan*
- WP 039 **A New Dual Cell Linear Ion Trap Configuration for Improved Quadrupole Ion Trap Performance;** Jae C. Schwartz; John E. P. Syka; Scott Quarmby; *Thermo Fisher Scientific, San Jose, CA*
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- ION MOBILITY, 040 - 064**
- WP 040 **Mass Accuracy and Dynamic Range in Ion Mobility-Mass Spectrometry Measurements: ADC vs. TDC;** Brian H. Clowers; Mikhail Belov; David Prior; William F. Danielson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 041 **Ion Mobility Orthogonal Time-of-Flight Mass Spectrometry (IMS- $\alpha$ TOF-MS) for the Analysis of Small Molecules using an Atmospheric Solids Analysis Probe;** Martin Green; Steven D Pringle; Kevin Giles; Hilary Major; *Waters Corporation, Manchester, UK*
- WP 042 **A High Flow Rate DMA with High Transmission and Resolution Designed for New API Instruments;** Juan Rus<sup>1</sup>; David Moro<sup>1</sup>; Juan A. Sillero<sup>1</sup>; Jordi Freixa<sup>1</sup>; Juan Fernandez De La Mora<sup>2</sup>; <sup>1</sup>*SEADM, Boecillo, SPAIN*; <sup>2</sup>*Yale University - Mechanical Engineering Departmen, New Haven, CT*
- WP 043 **Determining Ion Mobility Values using a Travelling Wave Separator;** Kevin Giles; Jason L Wildgoose; David Langridge; *Waters Corporation, Manchester, UK*
- WP 044 **A Next Generation MALDI-Ion Mobility-Surface-induced Dissociation-Time-of-Flight Mass Spectrometer with Novel Collision Source Configurations;** Wenjian Sun<sup>1</sup>; Kent Gillig<sup>2</sup>; Liuxi Chen<sup>2</sup>; David H. Russell<sup>2</sup>; <sup>1</sup>*Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China*; <sup>2</sup>*Texas A&M University, College Station, TX*
- WP 045 **Protein and Protein Complex Conformation Studies by Ion/Ion Reaction Coupled with Ion Mobility MS;** Qin Zhao<sup>1</sup>; Matthew Soyk<sup>1</sup>; Gregg Schieffer<sup>1</sup>; Ethan R. Badman<sup>2</sup>; R. S. Houk<sup>1</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Hoffmann-la Roche Inc., Nutley, NJ*
- WP 046 **Separation Factors for Rapid Gas Phase Chiral Separation;** Christopher Hilton<sup>1</sup>; Alison E. Holliday<sup>2</sup>; Clinton Krueger<sup>1</sup>; Herbert H Hill<sup>3</sup>; Ching Wu<sup>1</sup>; Mark Osgood<sup>1</sup>; <sup>1</sup>*Excellims Corporation, Maynard, MA*; <sup>2</sup>*Swarthmore College, Swarthmore, PA*; <sup>3</sup>*Washington State University, Pullman, WA*
- WP 047 **Comparative Study of Positive/Negative Ion Gas-Phase Conformations by MALDI-IM-TOFMS;** Liuxi Chen; Kent Gillig; David H. Russell; *Texas A&M University, College Station, TX*
- WP 048 **Ion Mobility Spectrometry at Pressures above Atmospheric;** Eric J. Davis; Maggie Tam; Prabha Dwivedi; Bill Siems; Herbert H Hill; *Washington State University, Pullman, WA*
- WP 049 **Evaluation of Nanoelectrospray – Ion Mobility Spectrometry – Condensation Particle Counting for Determining the Size and Molecular Mass of Biomolecules;** Efthymios Kapellios; Chiara Carazzone; Spiros Pergantis; *University of Crete, Heraklion, Greece*
- WP 050 **Clustering Analysis of IM-MS Data;** Lei Tao<sup>1</sup>; David B. Dahl<sup>2</sup>; Lisa M. Pérez<sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>*Texas A&M University, Department of Chemistry, College Station, Tx*; <sup>2</sup>*Texas A&M University, Department of Statistics, College Station, TX*
- WP 051 **Overtone Mobility Spectrometry and Its Utility for Biomolecule Analysis;** Ruwan T. Kurulugama; Fabiane

## WEDNESDAY POSTERS

- M. Nachtigall; David E. Clemmer; *Indiana University, Bloomington, IN*
- WP 052 **Evaluation of Linear Injection and Orthogonal Injection into Planar FAIMS-MS;** Leonard Rorrer; Marilyn Prieto; Richard A. Yost; *University of Florida, Gainesville, FL*
- WP 053 **Effect of FAIMS Electrode Shape on Transmission Efficiency;** Michael Belford; Jean-jacques Dunyach; Mark Hardman; *Thermo Fisher Scientific, San Jose, CA*
- WP 054 **A Dual-Source Electrospray/MALDI Ion Mobility-Mass Spectrometer for Biomolecular Structural Characterization;** Sevugarajan Sundarapandian; Michal Kilman; John A. Mclean; *Vanderbilt University, Nashville, TN*
- WP 055 **Using LC-IMS-MS to Increase High-Throughput Peptide Identifications;** Eric A. Livesay<sup>1</sup>; Erin S. Baker<sup>1</sup>; Daniel J. Orton<sup>1</sup>; Ronald J. Moore<sup>1</sup>; William F. Danielson<sup>1</sup>; Brian L. LaMarche<sup>2</sup>; Athena A. Schepmoes<sup>1</sup>; Derek F. Hopkins<sup>2</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Environmental Molecular Sciences Laboratory, Richland, WA*
- WP 056 **Gas-Phase Structure Dependence on the Ion Temperature in IMS. Experimental and Theoretical Results;** Francisco Alberto Fernandez Lima; Christopher Becker; Lisa M. Perez; Kent Gillig; Shane Tichy; William K. Russell; David H. Russell; *Texas A&M University, College Station, TX*
- WP 057 **Determining the Structures of Macromolecular Assemblies using Restraints from Gas-Phase Measurements;** Brandon T. Ruotolo<sup>1</sup>; Ah Young Park<sup>1</sup>; Daniel Hirschberg<sup>1</sup>; Daniel Barsky<sup>2</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>*Cambridge University, Cambridge, UK*; <sup>2</sup>*Lawrence Livermore National Laboratory, Livermore, CA*
- WP 058 **NanoES Charge Reduction Ion Mobility and Parallel Ion Mobility Spectrometry: New Tools for Analytical and Preparative Applications of Nano(Bio)Objects;** Christian Laschober<sup>1</sup>; Anne Maisser<sup>2</sup>; Dieter Blaas<sup>3</sup>; Wladyslaw Szymanski<sup>2</sup>; Guenter Allmaier<sup>1</sup>; <sup>1</sup>*Vienna University of Technology, Vienna, Austria*; <sup>2</sup>*University of Vienna, Vienna, Austria*; <sup>3</sup>*Medical University of Vienna, Vienna, Austria*
- WP 059 **Design of a Hemispherical FAIMS Cell;** Marilyn Prieto; Jennifer Bryant; Todd Prox; Richard A. Yost; *University of Florida, Gainesville, FL*
- WP 060 **Optimization of Parameters for Protein and Peptide Analysis using High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS);** Jonathan C. McNally<sup>2</sup>; Sucharita Dutta<sup>1</sup>; Julie Horner<sup>3</sup>; <sup>1</sup>*Thermo Fisher, San Jose, CA*; <sup>2</sup>*ThermoFisher Scientific, San Francisco, CA*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- WP 061 **Evaluation of the Analytical Characteristic of a Differential Mobility Analysis Coupled to a Triple Quadrupole System (DMA-MSMS);** Hassan Javaheri<sup>1</sup>; Yves Le Blanc<sup>1</sup>; Bruce A. Thomson<sup>1</sup>; Juan Fernandez de la Mora<sup>2</sup>; Juan Rus<sup>3</sup>; Juan Antonio Sillero Sepúlveda<sup>3</sup>; <sup>1</sup>*Mds Sciex, Concord, ON*; <sup>2</sup>*Yale University, New Haven, CT*; <sup>3</sup>*SEADM, Valladolid, Spain*
- WP 062 **Characterization and Use of Drift Times from Features in LC-IMS-MS Experiments;** Erin Baker; Anoop M. Mayampurath; Navdeep Jaitly; Brian H. Clowers; Rui Zhao; Keqi Tang; Eric A. Livesay; Daniel J. Orton; William F. Danielson III; Mikhail Below; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 063 **Increased Performance in Dual-Gate Ion Mobility Spectrometry Through the Use of a Novel Gate Pulse Sequence;** Brian Webb; Nathan Kaiser; James E. Bruce; *Washington State University, Pullman, WA*
- WP 064 **Simulation of Ion Motion in a Travelling Wave Mobility Separator using a Hard-Sphere Collision Model;** David Langridge; Kevin Giles; John B Hoyes; *Waters Corporation, Manchester, UK*
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- ELEMENTAL ANALYSIS AND SPECIATION, 065 - 071**
- WP 065 **Lanthanide and Actinide Nitrate Behavior in Water/Alcohol Media Studied by ESI-MS and ESI-MSn;** Jean Jacques Gaumet<sup>1</sup>; Anita K. Gianotto<sup>2</sup>; Gary Groenewold<sup>2</sup>; Christopher M Leavitt<sup>3</sup>; Michael J. Van Stipdonk<sup>3</sup>; Frédéric Aubriet<sup>1</sup>; <sup>1</sup>*Lsmcl, Metz University, Metz, France*; <sup>2</sup>*Ineel, Idaho Falls, ID*; <sup>3</sup>*Wichita State University, Wichita, KS*
- WP 066 **TOF SIMS Analysis of Zirconium Metals;** Handong Liang; Wenpan Li; Dongxu Sun; *China University of Mining and Technology, Beijing, CHINA*
- WP 067 **Pulsed Glow Discharge Mass Spectrometry: An Ionization Source for Aerosol Analysis;** Farzad Fani-Pakdel; Benjamin W. Smith; James D. Winefordner; Nicolò Omenetto; *University of Florida, Gainesville, FL*
- WP 068 **Speciation of Divalent and Trivalent Metals by ESI-MS: Comparison of Some Characteristics Among Hydrolyzed Metal Species;** Tatsuya Urabe<sup>1</sup>; Takahisa Tsugoshi<sup>2</sup>; Michihiro Aimoto<sup>3</sup>; Miho Tanaka<sup>1</sup>; <sup>1</sup>*Tokyo University of Marine Science and Technology, Tokyo, Japan*; <sup>2</sup>*AIST, Ibaraki, Japan*; <sup>3</sup>*Nippon Steel Corp., Chiba, Japan*
- WP 069 **Determination of Toxic Heavy Metals in Feminine Hygiene Products;** Jeoung Hwa Shin<sup>1</sup>; Kyu Keon Lee<sup>2</sup>; Yun Gyong Ahn<sup>1</sup>; <sup>1</sup>*korea Basic Science Institute, Seoul, South Korea*; <sup>2</sup>*Seojeong College, Yang-Ju, South Korea*
- WP 070 **Qualitative and Quantitative Analysis of Antisense Oligonucleotides by Oxygen Reaction in an Octopole Collision Cell via ICPMS;** Kirk Lokits; Patrick A. Limbach; Joseph A. Caruso; *University of Cincinnati, Cincinnati, OH*
- WP 071 **Analysis of Arsenic Compounds in Fish by CE/ESI-ToF-MS and CE/ICP-MS;** Björn Meermann; Marc Bartel; Andy Scheffer; Martin Vogel; Uwe Karst; *University of Münster, Münster, Germany*
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- AGRICULTURE, 072 - 084**
- WP 072 **Analysis of Aminoglycoside Residues in Milk by Electrospray LC-MSn after Derivatization with Phenyl Isocyanate;** Sheri B. Turnipseed<sup>1</sup>; Susan B. Clark<sup>1</sup>; Christine M. Karbiwnyk<sup>1</sup>; Wendy C. Andersen<sup>1</sup>; Keith E. Miller<sup>2</sup>; Mark R. Madson<sup>1</sup>; <sup>1</sup>*FDA, Denver Federal Center, Denver, CO*; <sup>2</sup>*University of Denver, Denver, CO*
- WP 073 **Quantitative Assay of Dimethoate in Foods by Liquid Chromatography Tandem Mass Spectrometry and Isotope Dilution;** Leonardo Di Donna<sup>1</sup>; Barbara Macchione<sup>1</sup>; Fabio Mazzotti<sup>1</sup>; Enzo Perri<sup>2</sup>; Giovanni Sindona<sup>1</sup>; <sup>1</sup>*Università della Calabria Dipartimento di Chimica, Arcavacata di Rende, ITALY*; <sup>2</sup>*Istituto Sperimentale per l'Olivicoltura, Arcavacata di Rende, Italy*
- WP 074 **DESI-MS Analysis of Mycotoxins from Grain Matrices;** Mark Busman; *USDA-ARS, Peoria, IL*



## WEDNESDAY POSTERS

- WP 075 **Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry of Citric Fruit Juices and Peel Oils: Characterization and Comparison;** Alan G. Marshall<sup>1</sup>; Mark R Crosswhite<sup>2</sup>; <sup>1</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL;* <sup>2</sup>*Florida State University, Tallahassee, FL*
- WP 076 **Proteome Evaluation of Medicago Truncatula Cell Cultures using Monolithic Capillary 2D-LC-MS-MS;** Mohamed Bedair<sup>1</sup>; Zhentian Lei<sup>1</sup>; Bonnie S. Watson<sup>1</sup>; Lloyd W. Sumner<sup>2</sup>; <sup>1</sup>*Samuel Roberts Noble Foundation, Ardmore, OK;* <sup>2</sup>*The Noble Foundation, Ardmore, OK*
- WP 077 **Detection and Validation of a Retrotransposon-Like Protein, PEG11, Over-Expressed in Callipyge Sheep Skeletal Muscle;** Michelle Colgrave<sup>1</sup>; Keren Byrne<sup>1</sup>; Tony Vuocolo<sup>1</sup>; Roger Pearson<sup>1</sup>; Noelle Cockett<sup>2</sup>; Chris Bidwell<sup>3</sup>; Ross Tellam<sup>1</sup>; <sup>1</sup>*CSIRO, St Lucia, Australia;* <sup>2</sup>*Utah State University, Logan, UT;* <sup>3</sup>*Purdue University, West Lafayette, IN*
- WP 078 **Identification and Label-Free Quantification of Medicago truncatula Vacuolar Membrane Proteins using 2D LC-MS-MS;** Zhentian Lei<sup>1</sup>; Narumon Sawasdipuksa<sup>2</sup>; Polkit Sangvanich<sup>2</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>*The Samuel Roberts Noble Foundation, Ardmore, OK;* <sup>2</sup>*Chulalongkorn University, Bangkok, Thailand*
- WP 079 **Monitoring the Degradation of the Insecticides Thiamethoxam and Imidacloprid by Zero-Valent Metals in Water by Electrospray Ionization Mass Spectrometry;** Rodinei Augusti; Renata Pereira Lopes; Ana Paula Fonseca Maia de Urzedo; Clésia Cristina Nascentes; *Federal University of Minas Gerais, Belo Horizonte/ MG, Brazil*
- WP 080 **Proteomic Analysis of Pithecellobium dulce (Manila Tamarind) Seeds using Two-Dimensional Gel Electrophoresis and Tandem Mass Spectrometry;** Narumon Sawasdipuksa<sup>1</sup>; Zhentian Lei<sup>2</sup>; Lloyd W. Sumner<sup>2</sup>; Polkit Sangvanich<sup>1</sup>; <sup>1</sup>*Chulalongkorn University, Bangkok, Thailand;* <sup>2</sup>*The Samuel Roberts Noble Foundation, Ardmore, OK*
- WP 081 **Ultra Fast Quantifications of Sulfamerazine, Sulfamethoxazole, Sulfadimethoxine and Sulfamethazine Residues in Milk using LDTD-APCI-MS-MS;** Sébastien Sauv  <sup>1</sup>; Patrice Tremblay<sup>2</sup>; Pedro A. Segura<sup>1</sup>; Pierre Picard<sup>2</sup>; Serge Fortier<sup>3</sup>; Luc Gagnon<sup>3</sup>; <sup>1</sup>*Universit   de Montr  al, Montreal, QC, Canada;* <sup>2</sup>*Phytonix Technologies, Quebec, QC, Canada;* <sup>3</sup>*MAPAQ, Sainte-Foy, QC, Canada*
- WP 082 **Chemical Analysis and Identification of Compounds Present in Stable Fly (Stomoxys calcitrans L.) Feces;** Brian P. Quinn; Ulrich R. Bernier; Jerome A. Hogsette; *USDA-ARS-CMAVE, Gainesville, FL*
- WP 083 **Developing a Method for Rapid Detection of Wheat Insects using MALDI QqTOF Mass Spectrometry with HPLC;** Yuwei Qian<sup>1</sup>; Ke Sun<sup>2</sup>; Victor Spicer<sup>1</sup>; Werner Ens<sup>1</sup>; Digvir Jayas<sup>2</sup>; Noel White<sup>3</sup>; Oleg Krokhin<sup>1</sup>; <sup>1</sup>*Physics and Astronomy, University of Manitoba, Winnipeg, Manitoba, Canada;* <sup>2</sup>*Biosystems Engineering, University of Manitoba, Winnipeg, Manitoba, Canada;* <sup>3</sup>*Agriculture and Agri-Food Canada, Winnipeg, Manitoba, Canada*
- WP 084 **Analysis of Clenbuterol in Meat and Feedstuff by LC-MS-MS;** N.T. Thu Thuy<sup>1</sup>; L.V. Xu<sup>1</sup>; P. T. Anh<sup>1</sup>; T. K. Tinh<sup>1</sup>; C.P. Ngoc Son<sup>1</sup>; Kefei Wang<sup>2</sup>; <sup>1</sup>*Center for Education and Development in Chromatogr, Ho Chi Minh City, Vietnam;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
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- ION ACTIVATION, 085 - 101**
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- WP 085 **CID Fragmentation Rearrangement of Buspirone Confirmed by LTQ-Orbitrap FT Mass Spectrometer;** Austin Li<sup>1</sup>; Xiang-yu Jiang<sup>2</sup>; <sup>1</sup>*Covance Laboratory, Inc., Sun Prairie, WI;* <sup>2</sup>*Covance - 08, Waunakee, WI*
- WP 086 **Ultraviolet Photodissociation of Fluorescently-Labeled Oligosaccharides in a Quadrupole Ion Trap Mass Spectrometer;** Jeff Wilson; Jennifer Brodbelt; *University of Texas at Austin, Austin, TX*
- WP 087 **Experimental Strategies for Determining Inner Shell Hydration Energies of Alkaline Earth Metal Dications;** Damon R Carl<sup>1</sup>; Robert M. Moision<sup>2</sup>; Peter B. Armentrout<sup>1</sup>; <sup>1</sup>*University of Utah, Salt Lake City, UT;* <sup>2</sup>*University of California San Diego, La Jolla, CA*
- WP 088 **Identification of Bis-aryl Hydrazone Crosslinked Peptides by Ultraviolet Photodissociation Mass Spectrometry;** Myles Gardner; Jennifer Brodbelt; *University of Texas - Austin, Austin, TX*
- WP 089 **Ultraviolet (355 nm) Photodissociation of Small Chromophore-Containing Molecules on a Hybrid QqTOF Mass Spectrometer;** Changtong Hao<sup>1</sup>; Yves Le blanc<sup>2</sup>; Udo Verkerk<sup>1</sup>; Alexandre Loboda<sup>2</sup>; Bruce Thomson<sup>2</sup>; K W Michael Siu<sup>1</sup>; <sup>1</sup>*CRMS, York University, Toronto, ON, Canada;* <sup>2</sup>*MDS Analytical Technologies, Concord, ON, Canada*
- WP 090 **Measuring the Effective Temperature of Vibrationally Excited Ions;** Alessandra L. Ferzoco; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- WP 091 **Fragmentation Mechanistic Study of TRA Analogs using High Resolution High Mass Accuracy Multistage Orbitrap Mass Spectrometer;** Wendy Zhong; *Schering-Plough, Summit, NJ*
- WP 092 **Coupling of an FT-ICR Mass Spectrometer with a VUV Beamline;** Roland Thissen<sup>1</sup>; Jean-Marc Bizau<sup>6</sup>; Joel Lemaire<sup>2</sup>; Christophe Blancard<sup>3</sup>; Marcello Coreno<sup>4</sup>; Christophe Dehon<sup>2</sup>; Christophe Nicolas<sup>1</sup>; Pietro Franceschi<sup>5</sup>; Alexandre J. Giuliani<sup>1</sup>; <sup>1</sup>*Synchrotron Soleil, Gif-sur-Yvette, France;* <sup>2</sup>*Laboratoire De Chimie Physique, Orsay, France;* <sup>3</sup>*CEA-DAM, Bruy  res-le-Ch  tel, France;* <sup>4</sup>*CNR-Lab. Naz. TAS-INFN, Basovizza, ITALY;* <sup>5</sup>*Sincrotrone Trieste, Basovizza, Italy;* <sup>6</sup>*LIXAM-CNRS, Orsay, France;* <sup>7</sup>*Lab. Plan  tologie, Grenoble, France*
- WP 093 **Laser-Induced Dissociation of Peptide Ions using Shaped Femtosecond Laser Pulses;** Christine L. Kalcic; Tissa C. Gunaratne; Nelson Winkler; Gavin E. Reid; A. Daniel Jones; Marcos Dantus; *Michigan State University, East Lansing, MI*
- WP 094 **ESI Tandem Mass Spectrometry Investigation of Gas-Phase Phosphoric Acid Clusters;** Ryan Dain; Vy Pham; Michael J. Van Stipdonk; *Wichita State University, Wichita, KS*
- WP 095 **A Study on Oxygenated Uranium and Cerium Clusters and Their Reactivity in the Gas Phase Followed by FTICRMS;** Fr  d  ric Aubriet<sup>1</sup>; Anita K. Gianotto<sup>2</sup>; Gary Groenewold<sup>2</sup>; Jean Jacques Gaumet<sup>1</sup>; <sup>1</sup>*LSMCL, Metz University, Metz, FRANCE;* <sup>2</sup>*INEEL, Idaho Falls, ID*
- WP 096 **Radical Directed Dissociation: A New Paradigm in Protein Identification;** Ryan R. Julian; Tony Ly; *University of California, Riverside, Riverside, CA*

## WEDNESDAY POSTERS

- WP 097 **Unimolecular Decay of Negatively Charged, Deoxynucleosides and Nucleosides in the Gas Phase Studied by Matrix Assisted Laser Desorption/Ionization;** Helga Dögg Flosadóttir; Benedikt Ómarsson; Oddur Ingólfsson; *University of Iceland, Reykjavik, Iceland*
- WP 098 **Revealing the Mechanism Behind Selective Dissociation at Tyrosine Residues Following Photodissociative Generation of Peptide Radical Cations;** Tony Ly; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- WP 099 **Protonated Carbamic Acid in the Gas Phase. The Aminodihydroxyethyl Radical Studied by Neutralization-Reionization Mass Spectrometry and ab initio/RRKM Calculations;** Joshua A Gregersen<sup>1</sup>; Changtong Hao<sup>2</sup>; Frantisek Turecek<sup>1</sup>; *<sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>York University, Toronto, ON*
- WP 100 **Microsolvation of Co<sup>2+</sup> by acetonitrile and water: Photodissociation dynamics of Co<sup>2+</sup>(CH<sub>3</sub>CN)<sub>n</sub>(H<sub>2</sub>O)<sub>m</sub>;** Manori Gunawardhana; *University of Massachusetts Amherst, Amherst, MA*
- WP 101 **Isomeric Distinction Based on Regiospecific Collision-Induced Dissociations in Tandem Mass Spectrometry;** Aura Tintaru<sup>1</sup>; Yohann Benchabane<sup>2</sup>; Gérard Boyer<sup>2</sup>; Stéphane Humbel<sup>2</sup>; Laurence Charles<sup>1</sup>; *<sup>1</sup>Université de Provence, Marseille, France; <sup>2</sup>Université Paul Cézanne, Marseille, France*
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- ION MOLECULE REACTIONS 1, 102 - 117**
- WP 102 **Big Time Scale Ion-Molecule Reactions Investigation in Segmented Gas-Filled RFQ Interfaced to O-TOF MS;** Ilya V. Soulimentkov; Alexey V. Chudinov; Alexander R. Pikhtev; Ella V. Chardakova; Viacheslav I. Kozlovskiy; *Institute for Energy Problems of Chemical Physics, Chernogolovka, Russian Federation*
- WP 103 **General Recognition of Isomeric  $\alpha$ ,  $\beta$  or  $\gamma$ -mono-Substituted Pyridines by Mass Spectrometry;** Yuri E Corilo<sup>1</sup>; Marcos N Eberlin<sup>2</sup>; *<sup>1</sup>State University of Campinas, Campinas, Brazil; <sup>2</sup>Thomson Lab Unicamp, Campinas, Sp, Brazil*
- WP 104 **Intermolecular Hydrogen Bonding in Noncovalent Complexes of Cavitands Studied by Gas-Phase Ion-Molecule Reactions and Theoretical Calculations;** Elina Kalenius<sup>1</sup>; Raisa Neitola<sup>1</sup>; Enrico Dalcanale<sup>2</sup>; Pirjo Vainiotalo<sup>1</sup>; *<sup>1</sup>University of Joensuu, Joensuu, Finland; <sup>2</sup>University of Parma, Parma, Italy*
- WP 105 **Evidence for the Existence of an  $\alpha$ -Effect in the Gas Phase Reactions of the Hydroperoxide Anion with Dimethyl Methylphosphonate;** Andrew M. McAnoy<sup>1</sup>; Martin R.L. Paine<sup>2</sup>; Stephen J Blanksby<sup>2</sup>; *<sup>1</sup>Defence Science and Technology Organisation, Melbourne, Australia; <sup>2</sup>University of Wollongong, Wollongong, Nsw, Australia*
- WP 106 **Elimination Reactions of Microsolvated Fluoride: A Comprehensive Study of Different Solvents;** Nicole Eyt; Stephanie M. Villano; Veronica M. Bierbaum; *University of Colorado, Boulder, CO*
- WP 107 **Reactivity and Thermochemistry of a Series of  $\alpha$ ,n-Dehydropicolines and Picoline N-Oxides;** Paul G. Wenthold; Bonnie Schafman-Janowiak; *Purdue University, West Lafayette, IN*
- WP 108 **Modeling Oxidative Damage of Peptides in the Gas Phase;** Christopher K Barlow<sup>1</sup>; Satish Chand<sup>2</sup>; Christopher J. Easton<sup>2</sup>; Richard A. J. O'Hair<sup>1</sup>; *<sup>1</sup>University of Melbourne, Melbourne, Australia; <sup>2</sup>Australian National University, Canberra, ACT, Australia*
- WP 109 **Directly Observing the Gas Phase Reactions of Carbon-Centred Radicals using Distonic Anions;** Benjamin B Kirk; David G Harman; Stephen J Blanksby; *University of Wollongong, Wollongong, Australia*
- WP 110 **A Novel  $\sigma, \sigma, \sigma$ -Triradical Cation: The 3,4,5-Tridehydropyridinium Ion;** Bartłomiej J. Jankiewicz; Jennifer N. Reece; Nelson R. Vinuesa; John J. Nash; Hilikka I. Kenttämä; *Purdue University, West Lafayette, IN*
- WP 111 **Gas-Phase Charge Inversion of Drug and Drug Metabolites Ions via Ion/Ion Reactions;** Kerry M. Hassell<sup>1</sup>; Yves LeBlanc<sup>2</sup>; Scott A. McLuckey<sup>1</sup>; *<sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>MDS Sciex, Concord, Canada*
- WP 112 **Gas Phase Hydrogen/Deuterium Exchange of Peptides: Effect of Intramolecular Interactions;** Young Lee; Laura Simpson; Elaine M. Marzluff; *Grinnell College, Grinnell, IA*
- WP 113 **Fragmentation of Nanoparticles under keV Cluster Bombardment;** Sidhartharaja Rajagopalachary; Stanislav Verkhotoirov; Emile A. Schweikert; *Texas A&M University, College Station, TX*
- WP 114 **Spatial Distribution and Identification of Terminal Negative Ions in Inhomogeneous Electric Field Established by Corona Needle;** Kanako Sekimoto; Mitsuo Takayama; *Yokohama City University, Yokohama, Japan*
- WP 115 **Gas Phase Hydrogen/Deuterium Exchange of Peptides Containing Acidic Sidechains;** Elaine M. Marzluff; Ning-Shiuan Lee; Spring Knapp; *Grinnell College, Grinnell, IA*
- WP 116 **Gas-Phase H/D Exchange of Lysine-Containing Peptides: Impact of Conformational Changes and Intramolecular Interactions;** Byoung Joon Ko<sup>1</sup>; Jennifer Brodbelt<sup>2</sup>; *<sup>1</sup>UT-Austin, Austin, TX; <sup>2</sup>The University of Texas, Austin, TX*
- WP 117 **Investigation of Deprotonation Reactions on Peptides, Proteins and DNA at Atmospheric Pressure by ESSI-MS;** David Touboul; Matthias Conradin Jecklin; Renato Zenobi; *ETH Zurich, Zurich, Switzerland*
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- EMERGING CONTAMINANTS 2, 118 - 138**
- WP 118 **Parabens and Sunscreens in the Environment: Determination by HPLC-ESI-MS-MS and GC-MS and Calculation of Phototoxicity;** Charlita Rosal; Leon D. Betowski; *US EPA, Las Vegas, NV*
- WP 119 **Analysis of Polybrominated Diphenyl Ethers (PBDEs) in GC Triple Linear Quadrupole Mass Spectrometer;** Byungchul (BC) Cha; Nigel Gore; Dipankar Ghosh; *Thermo Fisher Scientific, San Jose, CA*
- WP 120 **Occurrence of Pharmaceuticals and Personal Care Products (PPCPs) from Environmental Aqueous Samples by LC/ESI-MS-MS;** Seung-Woon Myung; *Kyonggi University, Suwon-Si, South Korea*
- WP 121 **Profiling Analysis of the Degradation Products of Alkylphenol Polyethoxylates by LC-MS using an Acclaim Surfactant Column with Mass Spectrometric Detection;** Jinyuan Wang; Stacy Henday; Xiaodong Liu; William C. Schnute; *Dionex Corporation, Sunnyvale, CA*
- WP 122 **Analysis of Melamine and Related Compounds using MALDI/TOF;** James A. Campbell; Catherine E Petersen; David Wunschel; *Pacific Northwest National Laboratory, Richland, WA*

## WEDNESDAY POSTERS

- WP 123 **Investigation of LC-MS-MS for Analysis of Current-Use Flame Retardants;** Gordia MacInnis<sup>1</sup>; Gregg Tomy<sup>2</sup>; Gilles Arsenault<sup>3</sup>; Eric Reiner<sup>4</sup>; Frank Dorman<sup>5</sup>; Chris Marvin<sup>1</sup>; <sup>1</sup>*Environment Canada, Burlington ON, Canada*; <sup>2</sup>*Department of Fisheries & Oceans, Winnipeg MB, Canada*; <sup>3</sup>*Wellington Laboratories Inc., Guelph ON, Canada*; <sup>4</sup>*Ontario Ministry of the Environment, Toronto ON, Canada*; <sup>5</sup>*Restek Corporation, Bellefonte PA, USA*
- WP 124 **Comparison of Turbulent-Flow Chromatography and Conventional Reversed-Phase Liquid Chromatography for the On-Line Preconcentration of Anti-Infectives in Wastewaters;** Pedro A. Segura<sup>1</sup>; Christian Gagnon<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montréal, QC*; <sup>2</sup>*Environnement Canada, Montréal, QC*
- WP 125 **Determination of Pharmaceuticals and Personal-Care Products using Polar Organic Chemical Integrative Samplers and Liquid Chromatography Tandem Mass Spectrometry;** Stephen L. Werner<sup>1</sup>; Edward T. Furlong<sup>2</sup>; David A. Alvarez<sup>2</sup>; <sup>1</sup>*US Geological Survey, National Water Quality Labo, Lakewood, CO*; <sup>2</sup>*U.S. Geological Survey, Denver, CO*
- WP 126 **Endocrine Disruptors Adsorbed on Macro and Micro Plastic Debris in the Ocean;** Lorena M. Rios<sup>1</sup>; Patrick R. Jones<sup>1</sup>; O. David Sparkman<sup>1</sup>; Charles Moore<sup>2</sup>; <sup>1</sup>*University of the Pacific, Stockton, CA*; <sup>2</sup>*Algalita Marine Research Foundation, Long Beach, CA*
- WP 127 **Characterization of EE2 Metabolite in Bioreactors with Pure Cultures of *Nitrosomonas europaea* and in Activated Sludge using LC/ITMS;** Jolanta Skotnicka-Pitak<sup>1</sup>; Jolanta Skotnicka-Pitak<sup>5</sup>; Diana S. Aga<sup>1</sup>; Wendell O. Khunjar<sup>2</sup>; Nancy G. Love<sup>3</sup>; Taewoo Yi<sup>4</sup>; Willie F. Harper Jr.<sup>4</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*Virginia Tech, Blacksburg, VA*; <sup>3</sup>*University of Michigan, Ann Arbor, MI*; <sup>4</sup>*University of Pittsburgh, Pittsburgh, PA*; <sup>5</sup>*Cracow University of Technology, Krakow, Poland*
- WP 128 **Automated Online SPE-LC-MS-MS Analysis of Pharmaceuticals with Variable Hydrophobicities in Municipal Wastewaters;** Araceli Garcia Ac<sup>1</sup>; Sebastien Sauve<sup>1</sup>; Christian Gagnon<sup>2</sup>; <sup>1</sup>*Université de Montréal, Montreal, Canada*; <sup>2</sup>*Ecosystem Research Division, Environment Canada, Montreal, Quebec, Canada*
- WP 129 **Simultaneous Determination of Pharmaceuticals in Water by Liquid Chromatography Tandem Mass Spectrometry;** Hye-seoung Shin<sup>1</sup>; Ji Hye Gil<sup>1</sup>; Su-won Lee<sup>2</sup>; <sup>1</sup>*Hankyong National University, Ansung, South Korea*; <sup>2</sup>*The Office of Waterworks, Seoul, South Korea*
- WP 130 **LC-MS Characterization of Golden Alga (*Prymnesin parvum*) Toxin in Natural Waters;** Pamela Hamlett; *TX Parks & Wildlife Dept., San Marcos, TX*
- WP 131 **Activity-directed Analytical Tools Based on Hormone Receptor-Affinity Extraction for Isolating EDCs from complex Mixtures Prior to Detection by LC-MS-MS;** Lauren Shaw; Patrick Lee Ferguson; *University of South Carolina, Columbia, SC*
- WP 132 **Combination of NanoESI-QqTOF-MS-MS and LC-MS-MS for Identification of Photolytic Degradation Products of Antibiotic Sulfamethoxazole in Aqueous Solutions;** Despina Tsipi<sup>1</sup>; Panagiota Mpourou<sup>1</sup>; Spiros Antoniou<sup>1</sup>; Eleni Botitsi<sup>1</sup>; Spiros D. Garbis<sup>2</sup>; Silvia Lacorte<sup>3</sup>; <sup>1</sup>*General Chemical State Laboratory, Athens, Greece*; <sup>2</sup>*Academy of Athens - Biomedical Foundation, Athens, Greece*; <sup>3</sup>*CID-CSIC, Barcelona, Spain*
- WP 133 **Online SPE-LC-APPI-MS-MS for the Quantification of Estrogenic Endocrine Disruptors in Water;** Liza Viglino<sup>1</sup>; Khadija Aboufadi<sup>1</sup>; Michèle Prévost<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>*Université de Montreal, Montreal, CANADA*; <sup>2</sup>*École Polytechnique de Montréal, Montréal, Canada*
- WP 134 **Novel Determination Method of Anti-Infectives and Estrogenic Endocrine Disruptors in Wastewater and Drinking Water using LDTD-APCI-MS-MS;** Paul Favad<sup>1</sup>; Pedro A. Segura<sup>1</sup>; Pierre Picard<sup>2</sup>; Michèle Prévost<sup>3</sup>; Christian Gagnon<sup>4</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montréal, QC*; <sup>2</sup>*Phytonix Technologies, Inc., Quebec, QC*; <sup>3</sup>*École Polytechnique de Montréal, Montréal, QC*; <sup>4</sup>*Environnement Canada, Montréal, QC*
- WP 135 **Mass Spectrometric Analysis of Human Urine for 22 Phthalate Metabolites by using a Novel Reversed HPLC Gradient;** Manori J Silva; Ella Samandar; John Reidy; James Preau; Needham Larry; Antonia Calafat; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 136 **Trace Analysis of Polar Pharmaceuticals in Wastewater after Treatment with Membrane Bioreactor by LC-MS;** Mary Dawn Celiz<sup>1</sup>; Sandra Perez<sup>2</sup>; Damia Barcelo<sup>2</sup>; Diana Aga<sup>1</sup>; <sup>1</sup>*The State University of New York at Buffalo, Buffalo, NY*; <sup>2</sup>*Department of Environmental Chemistry, IIQAB-CSIC, Barcelona, Spain*
- WP 137 **Determination of Bisphenol A, Selected Alkylphenols and Related Ethoxylates in Water Samples using Solid Phase Extraction and GC-EI-MSMS;** Ivana Kosarac; Brian Stewart; Cariton Kubwabo; *Health Canada, Ottawa, ON, Canada*
- WP 138 **Comparison of ESI,APPI,APCI and APCI/APPI for Determining Estrogenic Chemicals in Water by UPLC-MS-MS with Chemical Derivatizations;** Guang-Wen Lien; Chia-Yang Chen; *National Taiwan University, Taipei, TAIWAN*
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- HYDROCARBON & PETROCHEMICAL, 139 - 160**
- WP 139 **Elestrospray Ionization Mass Spectrometry Characterization of Sorption of Oilsands Naphthenic Acids to Engineered Polymers;** John Headley; Kerry M. Peru<sup>2</sup>; Mohamed Mohamed<sup>3</sup>; Lee Wilson<sup>3</sup>; <sup>1</sup>*Environment Canada, WSTD, Saskatoon, CANADA*; <sup>2</sup>*Environment Canada, Saskatoon, SK*; <sup>3</sup>*Department of Chemistry, 110 Science Place, Saskatoon, Sk, Canada*
- WP 140 **Can Naphthenic Acids Be used as Molecular Monitors of Crude Oil Biodegradation in the Environment? A Field Investigation;** Christine A. Hughey<sup>1</sup>; Carina S. Minardi<sup>1</sup>; Mmilili M. Mapolelo<sup>2</sup>; Ryan P. Rodgers<sup>3</sup>; Alan G. Marshall<sup>3</sup>; Dan Ruderman<sup>4</sup>; <sup>1</sup>*Chapman University, Orange, CA*; <sup>2</sup>*Florida State Univ, Dept of Chemistry, Tallahassee, FL*; <sup>3</sup>*Ion Cyclotron Resonance Prog, Tallahassee, FL*; <sup>4</sup>*Applied Proteomics, Inc., Glendale, CA*
- WP 141 **Analyses of Kamchatka Crude Oil by FTICR Mass Spectrometry;** Alexey Kononikhin<sup>1</sup>; Gleb Vladimirov<sup>2</sup>; Erast Kunenkov<sup>2</sup>; Igor Popov<sup>1</sup>; Irina Perminova<sup>2</sup>; Andrey Garmash<sup>2</sup>; Gennadij Karpov<sup>3</sup>; Sergey Varfolomeev<sup>1</sup>; Eugene Nikolaev<sup>4</sup>; <sup>1</sup>*Institute for Biochemical Physics RAS, Moscow, Russia*; <sup>2</sup>*Lomonosov Moscow State University, Moscow, Russia*; <sup>3</sup>*Institute of Volcanology and Seismology RAS, Petropavlovsk-Kamchatsky, Russia*; <sup>4</sup>*The Institute For Energy Problems of Chemical Phys, Moscow, Russian Federation*

## WEDNESDAY POSTERS

- WP 142 **Classification and Differentiation of Crude oil by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry using Electrospray Ionization;** Matthias Witt<sup>1</sup>; Jens Fuchser<sup>1</sup>; Victor Fursey<sup>2</sup>; <sup>1</sup>Brüker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Brüker Daltonics, Billerica, MA
- WP 143 **Evolved Gas Analysis in Thermogravimetry by a Novel Photo-Ionisation Mass Spectrometer: Organic Signatures of Polymer Pyrolysis and Crude Oil Distillation;** Ralf Zimmermann<sup>1</sup>; Mohammed Saraji-Bozorgzad<sup>2</sup>; Thorsten Streibel<sup>2</sup>; Martin Sklorz<sup>2</sup>; Robert Geißler<sup>2</sup>; <sup>1</sup>University of Augsburg, Augsburg, Germany; <sup>2</sup>Helmholtz Zentrum München, Oberschleissheim, Germany
- WP 144 **Characterization of B100 Biodiesel and Biodiesel Precipitants by GCMS and LC-MS;** Ryan C Shea<sup>1</sup>; Rick E Pauls<sup>1</sup>; Phyllis S Munowitz<sup>1</sup>; Michael Foster<sup>2</sup>; <sup>1</sup>BP Global Aromatics Technology, Naperville, IL; <sup>2</sup>BP Global Fuels Technology, Naperville, IL
- WP 145 **Petroleum Molecular Speciation Comparisons by ASAP, APPI, and APCI Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Jeremiah M. Purcell<sup>1</sup>; Ryan P. Rodgers<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>; Charles N. McEwen<sup>2</sup>; Barbara S. Larsen<sup>2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL 32310; <sup>2</sup>DuPont Corporate Center for Analytical Sciences, Wilmington, DE 19880
- WP 146 **Electrospray Ionization FT-ICR Mass Spectrometry of "ARN" Naphthenic acids in Crude Oil: Extraction and Quantification;** Mmili Myles Mapolelo<sup>1</sup>; Ryan P. Rodgers<sup>2</sup>; Andrew T Yen<sup>3</sup>; Sam Asomaning<sup>3</sup>; Justin Debord<sup>3</sup>; Alan G. Marshall<sup>4</sup>; <sup>1</sup>Florida State Univ, Dept of Chemistry, Tallahassee, FL; <sup>2</sup>Natl High Magnetic Field Lab, Tallahassee, FL; <sup>3</sup>BakerPetrolite, Sugarland, TX; <sup>4</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL
- WP 147 **Biodiesel and Diesel Fuel Analysis with the Supersonic GC-MS;** Aviv Amiray; Marina Poliak; Alexander Gordin; Alexander B. Fialkov; *Tel-Aviv University, Tel-Aviv, Israel*
- WP 148 **Effect of Source Rock Type and Maturity on Polar Chemical Composition Derived from FT-ICR Mass Spectrometry;** G. Eric Michael<sup>2</sup>; Ryan P. Rodgers<sup>3</sup>; Alan G. Marshall<sup>3</sup>; Donald F. Smith<sup>1</sup>; <sup>1</sup>Fom Inst. Atomic/Molecular Physics, Amsterdam, The Netherlands; <sup>2</sup>ConocoPhillips, Houston, TX; <sup>3</sup>National High Magnetic Field Laboratory/FSU, Tallahassee, FL
- WP 149 **Hydrocarbon Type Analysis of Individual Fractions Depending on the Boiling Range of Lube Oil by GC-MSD;** Myoung-Han No; Eunkyoun Kim; *Skenergy Institute Of Technology, Daejeon, South Korea*
- WP 150 **Characterization of Asphaltene Emulsion Interfacial Material by Ultrahigh Resolution FT-ICR Mass Spectrometry;** Brandie M. Ehrmann<sup>1</sup>; Priyanka Juyal<sup>2</sup>; Ryan P. Rodgers<sup>2</sup>; Alan G. Marshall<sup>3</sup>; <sup>1</sup>National High Magnetic Field Laboratory/FSU, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL
- WP 151 **Biodiesel Typification and Quality Control by Direct Infusion Electrospray Ionization Mass Spectrometry Fingerprinting;** Sérgio Adriano Saraiva; Marcos N Eberlin; Rodrigo R. Catharino; Humberto M. Milagre; *ThoMSon Lab Unicamp, Campinas, SP, Brazil*
- WP 152 **Analysis of Petrochemicals in Seafood after Oil Spills using Electronic Nose and High-Speed Gas Chromatography-Mass Spectrometry;** F. Aladar Bencsath<sup>1</sup>; Paul P. Eilers<sup>2</sup>; <sup>1</sup>FDA, Gulf Coast Seafood Lab, Dauphin Island, AL; <sup>2</sup>Prairie Dog Pals, Albuquerque, New Mexico
- WP 153 **ESI FT-ICR MS in the Speciation of Recalcitrant Sulfur Aromatic Compounds in Desulfurized Vacuum Gas Oils;** Saroj Panda<sup>1</sup>; Jan T. Andersson<sup>2</sup>; Wolfgang Schrader<sup>1</sup>; <sup>1</sup>Max-Planck Inst Coal Res., Mülheim / Ruhr, Germany; <sup>2</sup>Westfälische Wilhelms-Universität Münster, Münster, Germany
- WP 154 **Characterization of an Oily Mixture of Reactive Cyclo-[Mo(CO)<sub>4</sub>(Sb<sub>4</sub>EtnPr(6-n))] Complexes by LIFDI-MS;** H Bernhard Linden; *Linden CMS, Leeste, Germany*
- WP 155 **Rapid Hydrocarbon Analysis using a Miniature Rectilinear Ion Trap Mass Spectrometer;** Ewa Sokol; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- WP 156 **Characterization of Naphthenic Acids from Athabasca Oil Sands for Environmental Analysis using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Mark P. Barrow<sup>1</sup>; Kerry M. Peru<sup>2</sup>; John V. Headley<sup>2</sup>; Peter J. Derrick<sup>3</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Environment Canada, Saskatoon, Canada; <sup>3</sup>Inst of Fundamental Sciences, Palmerston North, New Zealand
- WP 157 **First Generation Biofuels: Simple Mixtures - Complex Analytics;** G. John Langley<sup>1</sup>; Julie Herniman<sup>1</sup>; Martin Gower<sup>1</sup>; Steven Lamond<sup>1</sup>; Pearl McMahon<sup>1</sup>; Tom Lynch<sup>2</sup>; Hugh Preston<sup>2</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>BP Castrol Global Lubricants Technology, Pangbourne, UK
- WP 158 **Multidimensional On-Line HPLC<sub>x</sub>GC for Characterization of Hydrocarbon Fractions in Petrochemical Samples;** Nieves Sarrion<sup>1</sup>; Joseph Gibert<sup>2</sup>; J. Antonio Muñoz<sup>1</sup>; Ariadna Galve<sup>3</sup>; <sup>1</sup>Konik-Tech, S.A., Sant Cugat del Vallés, SPAIN; <sup>2</sup>Konik Instruments, Inc., Miami, FL; <sup>3</sup>IKAI, Sant Cugat Del Vallès, Spain
- WP 159 **Applications of Atmospheric Pressure Photoionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Analysis of Asphaltenes and Heavy Crude Oil;** Amy Mckenna; Jeremiah M. Purcell; Tanner M. Schaub; Ryan P. Rodgers; Alan G. Marshall; *National High Magnetic Field Laboratory, Tallahassee, FL*
- WP 160 **Electrospray Ionization FT-ICR Mass Spectrometric Mapping of Petroleum Compound Classes by Simple Silver Adduction;** Priyanka Juyal; Ryan P. Rodgers; Alan G Marshall; *National High Magnetic Field Laboratory/FSU, Tallahassee, FL*
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- IMAGING MS PROTEINS & PEPTIDES, 161 - 175**
- WP 161 **Monitoring Tumor Progression in a Mouse Model of Malignant Pleural Effusion by MALDI IMS;** Joey C. Latham; Pierre Chaurand; Kirk B. Lane; Taylor Sherrill; Richard M. Caprioli; *Vanderbilt Univ Sch of Med, Nashville, TN*
- WP 162 **Protein Markers of Survival in Metastatic Melanoma by Histology Directed MALDI MS;** William Hardesty<sup>1</sup>; Mark C. Kelley<sup>1</sup>; Deming Mi<sup>1</sup>; Robert L. Low<sup>2</sup>; Richard M. Caprioli<sup>3</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>UCDHSC, Aurora, CO; <sup>3</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- WP 163 **Efficient Strategies for Identification of Proteins in MALDI Tissue Images;** Barbara Leinweber<sup>1</sup>; George Tsaprailis<sup>1</sup>; Linda A. Breck<sup>2</sup>; Cynthia L. David<sup>1</sup>; Yelena Feinstein<sup>1</sup>; Serrine S. Lau<sup>1</sup>; <sup>1</sup>College of Pharmacy, University of Arizona, Tucson, AZ; <sup>2</sup>College of Science, University of Arizona, Tucson, AZ

## WEDNESDAY POSTERS

- WP 164 **Exploring the Assembly of an Organism using MALDI Imaging: A Systems Approach to Understanding Embryonic Development;** Maxence Wisztorski<sup>1</sup>; Jocelyne Bruand<sup>2</sup>; Julien Franck<sup>1</sup>; David Bonnel<sup>1</sup>; Vineet Bafna<sup>2</sup>; Eduardo Macagno<sup>2</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>MALDI Imaging Team, University of Lille, Villeneuve d'Ascq, FRANCE; <sup>2</sup>University of California, La Jolla, San Diego, CA
- WP 165 **Imaging Mass Spectrometry Clocking in with Proteomics: On-Tissue MS-MS for Proteins Identification;** Luke MacAleese; Erika R. Amstalden Van Hove; Jonathan Stauber; Ron M.A. Heeren; *FOM Inst. Atomic/Molecular Physics, Amsterdam, NETHERLANDS*
- WP 166 **Measuring HIV Protease Inhibitors in Cytocentrifuged Leukocyte Sub-Types using Mass Spectrometry Imaging Techniques;** Lennard Dekker; Jeroen van Kampen; Peter Burgers; Marleen Reedijk; Rob Gruters; Ab Osterhaus; Theo Luider; *Erasmus Medical Center, Rotterdam, Netherlands*
- WP 167 **MALDI-MSI of Prostate Tissues for Detection of Cancer and Micrometastatic Disease;** Lisa H. Cazares; Raymond S. Lance; Savvas E. Mendrinou; Michael B. Williams; MaryAnn Clements; Richard R. Drake; O. John Semmes; *EVMS Norfolk, VA, Norfolk, VA*
- WP 168 **MALDI MSI Analysis of Rat Hearts from Animals Treated with Isoprenaline;** Alan Barnes<sup>1</sup>; Jatin Burniston<sup>2</sup>; <sup>1</sup>Shimadzu Biotech, Manchester, UK; <sup>2</sup>Liverpool John Moore's University, Liverpool, UK
- WP 169 **Visualisation and in situ Characterisation of Proteins in Adenocarcinoma tissue sections by Direct MALDI-Mass Spectrometry Imaging;** Marie-Claude Djidja<sup>1</sup>; Chris W. Sutton<sup>2</sup>; Paul M. Loadman<sup>2</sup>; Peter Scriven<sup>3</sup>; Marten F. Snel<sup>4</sup>; Emmanuelle Claude<sup>4</sup>; Malcolm R. Clench<sup>1</sup>; <sup>1</sup>Sheffield Hallam Uni, UK, Sheffield, UK; <sup>2</sup>Institute of Cancer Therapeutics, Bradford, UK; <sup>3</sup>University of Sheffield, Sheffield, UK; <sup>4</sup>Waters Corporation, Manchester, UK
- WP 170 **Brain MS Imaging after Ischemic Stroke in Mice – Insight for Brain Injury by Abnormal Proteolysis;** ZeZong Gu<sup>1</sup>; Fanjun Meng<sup>1</sup>; Wei Wu<sup>2</sup>; Joseph P. Fox<sup>3</sup>; Jiankun Cui<sup>2</sup>; Gongyi Shi<sup>3</sup>; <sup>1</sup>Univ. Missouri-Columbia School of Medicine, Columbia, MO; <sup>2</sup>Burnham Institute for Medical Research, La Jolla, CA; <sup>3</sup>Bruker Daltonics Inc., Fremont, CA
- WP 171 **From Lipids to Proteins in one Single Tissue;** Erika R. Amstalden Van Hove<sup>1</sup>; Ivo Klinkert<sup>1</sup>; Tiffany Greenwood<sup>2</sup>; Kristine Glunde<sup>2</sup>; Ron M.a. Heeren<sup>1</sup>; <sup>1</sup>FOM Inst. Atomic/molecular Physics, Amsterdam, Netherlands; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- WP 172 **What Lies Beneath: In Situ Assessment of Endogenous Enzyme Activity using Imaging Mass Spectrometry;** Kristen Herring<sup>1</sup>; Kristin E. Burnum<sup>1</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- WP 173 **MALDI Tissue Imaging of the Chick Heart;** Angus C. GreY; Jarren Section; Ricardo A. Moreno-Rodriguez; Edward L. Krug; Kevin L. Schey; *Medical University of SC, Charleston, SC*
- WP 174 **Mining Tissue Microarrays of Disease: Detection of Molecular Features using MALDI Imaging Mass Spectrometry;** Reid Groseclose<sup>2</sup>; Pierre P. Massion<sup>1</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>2</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- WP 175 **Correlation of a Tyrosine Kinase Inhibitor Distribution with Proteome Response in a Glioma Mouse Model by MALDI Imaging Mass Spectrometry;** Sara L. Frappier<sup>1</sup>; Michael L. Edgeworth<sup>1</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt Univ Sch of Med, Nashville, TN
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- COMPUTER APPLICATIONS: PROTEOMICS, 176 - 188**
- WP 176 **Enhanced Identification of Biotin-Derivatized Peptides;** Peter G. Slade<sup>1</sup>; Erin S. D. Bolstad<sup>2</sup>; Michelle Williams<sup>1</sup>; Ioannis Papayannopoulos<sup>1</sup>; John S. Wishnok<sup>1</sup>; Steven R. Tannenbaum<sup>1</sup>; <sup>1</sup>MIT, Cambridge, MA; <sup>2</sup>University of Connecticut, Storrs
- WP 177 **IPEP: A Computational Tool for Designing Proteomics Experiments around PTM Motifs;** Victoria Izumi<sup>1</sup>; Dihui Lu<sup>2</sup>; Eric Haura<sup>2</sup>; David Fenstermacher<sup>2</sup>; Steven Eschrich<sup>2</sup>; John Koomen<sup>2</sup>; <sup>1</sup>Moffitt Cancer Center & Research Institute, Tampa, FL; <sup>2</sup>H. Lee Moffitt Cancer Center, Tampa, FL
- WP 178 **Accurate Extraction of MS-MS Scans – Database Search Enhancement;** Ilan Vidavsky; Michael L. Gross; *Washington University, St Louis, MO*
- WP 179 **Swift: Automated Submission to Five MS-MS Search Engines with Unified Parameters;** Christopher Mason; Roman Ženka; Eric Winter; David Lentz; H. Robert Bergen III; *Mayo Proteomics Research Center, Rochester, MN*
- WP 180 **PRIME: Proteome Research Information Management Environment For High-Throughput Proteomics Laboratories;** Panagiotis G Papoulias<sup>1</sup>; David Lentz<sup>2</sup>; Philip Andrews<sup>3</sup>; <sup>1</sup>National Resource For Proteomics And Pathways, Ann Arbor, MI; <sup>2</sup>Mayo Clinic, Rochester, MN; <sup>3</sup>University of Michigan, Ann Arbor, MI
- WP 181 **Adaptable Enterprise Pipeline for the Computational Proteomics Analysis System (CPAS);** Brendan Maclean<sup>1</sup>; Parag Mallick<sup>2</sup>; <sup>1</sup>LabKey.com, Seattle, WA; <sup>2</sup>Cedars-Sinai, Los Angeles, CA
- WP 182 **New Methods in Peptide de novo Sequencing Software with Manual Intervention Feature for Tandem Mass Spectral Data;** Jingwen Yao<sup>1</sup>; Matthew J. Kelly<sup>1</sup>; Kiriko Kamiya<sup>1</sup>; Jennifer Broughton<sup>1</sup>; Shigeki Kajihara<sup>2</sup>; <sup>1</sup>Shimadzu Research Lab. (Europe) Ltd., Manchester, UK; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- WP 183 **Enhancing and Automating the Maximum Entropy Deconvolution of Protein Spectra Acquired on High-Resolution TOF Mass Spectrometers;** Keith Richardson<sup>1</sup>; John Skilling<sup>2</sup>; Jason Wildgoose<sup>1</sup>; Iain Campuzano<sup>1</sup>; Scott Berger<sup>3</sup>; Robert Bateman<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Maximum Entropy Data Consultants Ltd, Kenmare, Ireland; <sup>3</sup>Waters Corporation, Milford, MA
- WP 184 **Software for the Automated Processing of Data from <sup>15</sup>N-Metabolic Labeling Proteomics and Accurate Mass Peptide Identification;** Li Jing; Jon Amster; *University of Georgia, Athens, GA*
- WP 185 **HERMES Novel Aspect: Platform Independent Open Source Project for submitting Data Files to MASCOT;** John Philip<sup>1</sup>; Panagiotis G Papoulias<sup>2</sup>; Paul Tempst<sup>1</sup>; Philip Andrews<sup>3</sup>; <sup>1</sup>Memorial Sloan-Kettering Cancer Center, New York, NY; <sup>2</sup>National Resource For Proteo, Ann Arbor, MI; <sup>3</sup>University of Michigan, Ann Arbor, MI

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- WP 186 **Exploring Benefits of High Mass Accuracy Tandem Spectra in Proteomics**; Tom Patterson<sup>1</sup>; Alexander R. Ivanov<sup>2</sup>; <sup>1</sup>*nScan, Medford, MA*; <sup>2</sup>*Harvard School of Public Health, Boston, MA*
- WP 187 **MS-Scout: a Tool for Assessing Proteomic Data Quality in LC-MS and LC-FAIMS-MS Experiments**; Jesse Canterbury; Michael Hoopmann; Michael J. Maccoss; *University of Washington, Seattle, WA*
- WP 188 **B-Fabric - An Infrastructure for Integrated Management and Analysis of Proteomic and Transcriptomic Derived Data**; Bertran Gerrits; Christian panse; Can Tuerker; Dieter Joho; Simon Barkow; Ralph Schlapbach; *ETH / UZH Zurich, Zurich, Switzerland*
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- MATERIALS AND POLYMERS, 189 - 219**
- WP 189 **LC-MS<sup>n</sup> Determination of Non-Ionic Surfactants, Structure Analysis of Poly(Oxyethylene-Co-Oxypropylene) Fatty Ethers and Poly(Oxyethylene) Fatty Esters**; Andreas Nasioudis<sup>1</sup>; Jan W. van Velde<sup>1</sup>; Ron M.a. Heeren<sup>2</sup>; Oscar F. Van Den Brink<sup>1</sup>; <sup>1</sup>*Akzo Nobel Chemicals, Arnhem, Netherlands*; <sup>2</sup>*Fom Inst. Atomic/molecular Physics, Amsterdam, Netherlands*
- WP 190 **Structural Analysis of PEG by ESI-QIT and MALDI-QToF**; Nilufer Solak; Chrys Wesdemiotis; *University of Akron, Akron, OH*
- WP 191 **Gold Nanoparticle Surface-Assisted Laser Desorption/Ionization (SALDI) Time-of-Flight MS of Low Molecular Weight Polymers**; Justin Engle; S. Kim R. Williams; *Colorado School of Mines, Golden, CO*
- WP 192 **Characterization of Linear and Branched Polyacrylates by Tandem Mass Spectrometry**; Kittisak Chaicharoen<sup>1</sup>; Michael J. Polce<sup>2</sup>; Anirudha Singh<sup>1</sup>; Coleen Pugh<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*University of Akron, Akron, OH*; <sup>2</sup>*Lubrizol Advanced Materials, Brecksville, OH*
- WP 193 **Study of Cycling and Ring-Forming Reactions of Multiple Functional Chemicals During the APCI Ionization to Synthesize Novel Large Crown Chemicals**; Wenjie Cao; *CRYOVAC, Sealed Air Corp., Duncan, SC*
- WP 194 **Characterization of Fatty Alcohol Ethoxylate n(2-23) EO by ESI-MS and APCI-MS**; Monica Cecilia Vargas Mamani<sup>1</sup>; Sergio Adriano Saraiva<sup>1</sup>; Heliara Nascimento<sup>1</sup>; Gilberto Silva<sup>2</sup>; Marcos N Eberlin<sup>1</sup>; <sup>1</sup>*Thomson Laboratory Mass Spectrometry, Campinas, Brazil*; <sup>2</sup>*Oxiteno Industria Comercio SA, Maua-SP, Brazil*
- WP 195 **An Absolute Molecular Mass Distribution Standard: SRM 2881**; Charles M. Guttman; Kathleen M. Flynn; Anthony J. Kearsley; William E. Wallace; *National Institute of Standards & Technology, Gaithersburg, MD*
- WP 196 **UPLC/ESI-TOF Mass Spectrometry for a Fast Determination of "Critical Conditions" of Adsorption of Copolymers**; Jana Falkenhagen; Andreas Thuenemann; Steffen M. Weidner; *Fed.Inst.Mat.Research, Berlin, Germany*
- WP 197 **LDI-FTMS Analysis of Thin Films Deposited on Silicon by Plasma Polymerization of Acetylene**; Sasa Miladinovic<sup>1</sup>; Valerie De Vriendt<sup>2</sup>; Stephane Lucas<sup>2</sup>; Charles L. Wilkins<sup>1</sup>; <sup>1</sup>*University of Arkansas, Fayetteville, AR*; <sup>2</sup>*University of Namur-FUNDP, Namur, Belgium*
- WP 198 **Analysis of Poly(styrene-co-allyl alcohol) using MS and MS-MS Methods**; Bethany Subel; Chrys Wesdemiotis; *University of Akron, Akron, OH*
- WP 199 **Molecular Identification of Nitro-Tyrosine Modification in Human Eosinophil Proteins by Proteolytic Affinity Extraction- Mass Spectrometry (PROFINEX)**; Petre AlinA<sup>1</sup>; Martina Ulrich<sup>2</sup>; Gerd Doering<sup>2</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*University of Konstanz, Konstanz, Germany*; <sup>2</sup>*Institut für Allgemeine Hygiene, Tuebingen, Germany*
- WP 200 **MALDI Mass Spectrometry as a Novel Tool for Molecular Weight and Polydispersity Analysis on Low Molecular Weight Polyamino Acids**; Ettigounder Ponnusamy; Justin Wildsmith; *Sigma-Aldrich, St. Louis, MO*
- WP 201 **Cryodetection of Nanoparticles in the MegaDalton Range using MALDI-TOF Mass Spectrometry**; David M. Sipe; Alexander A. Aksenov; Mark E. Bier; *Carnegie Mellon University, Pittsburgh, PA*
- WP 202 **Matrix-Assisted Laser Desorption/Ionization Tandem Mass Spectra of Synthetic Polymers using the Low and the High-Energy Fragmentation**; Hiroki Nakajima<sup>1</sup>; Martin Resch<sup>2</sup>; Leren Wan<sup>3</sup>; Fan Xiang<sup>4</sup>; <sup>1</sup>*Shimadzu Corporation, Life Science Laboratory, Kyoto, JAPAN*; <sup>2</sup>*Shimadzu Europa GmbH, Duisburg, Germany*; <sup>3</sup>*Shimadzu Beijing Office, Beijing, CHINA*; <sup>4</sup>*Shimadzu Biotech, Pleasanton, CA*
- WP 203 **Ionizing Polymers with Protonated Amino Acids: New Fragmentation Pathways and Thermochemistry**; Abdulrahman Alhazmi; Paul Michael Mayer; *University of Ottawa, Ottawa, Canada*
- WP 204 **Characterization of Polymers by MALDI TOF Mass Spectrometry for REACH Compliance. Does Different Matrix Have Any Influence on Mass Accuracy?**; Heliara Nascimento<sup>1</sup>; Sergio Saraiva<sup>2</sup>; Jerusa Simone Garcia<sup>2</sup>; Monica Vargas<sup>2</sup>; Marcos N Eberlin<sup>2</sup>; <sup>1</sup>*Thomson Mass Spectrometry Laboratory, Campinas, Brazil*; <sup>2</sup>*Thomson Lab Unicamp, Campinas, Sp, Brazil*
- WP 205 **Derivatization of Silsesquioxanes for Structure Elucidation by MALDI-TOF Mass Spectrometry**; Roman Borisov<sup>1</sup>; Nikolai Yu. Polovkov<sup>1</sup>; Vjacheslav V. Kireev<sup>2</sup>; Vladimir Zaikin<sup>1</sup>; <sup>1</sup>*Topchiev Institute of Petrochemical Synthesis, Moscow, Russian Federation*; <sup>2</sup>*D.Mendeleev University of Chemical Technology, Moscow, Russia*
- WP 206 **Comprehensive Two-Dimensional Gas Chromatography/High-Resolution Time-of-flight Mass Spectrometry for Polymer Analysis Coupled with Pyrolyzer**; Junichi Osuga<sup>1</sup>; Masaaki Ubukata<sup>1</sup>; Kazutetsu Nojima<sup>1</sup>; Takatoshi Noguchi<sup>2</sup>; Hisae Miyamoto<sup>2</sup>; Kristie Hoyt<sup>3</sup>; Yasuyuki Shibata<sup>4</sup>; Yoshikatsu Takazawa<sup>4</sup>; <sup>1</sup>*JEOL Ltd., Akishima, JAPAN*; <sup>2</sup>*Nissan Chemical Industries, LTD., Funabashi, JAPAN*; <sup>3</sup>*JEOL USA, Inc., Boston, MA*; <sup>4</sup>*National Institute for Environmental Studies, Tsukuba, Japan*
- WP 207 **Effect of the Cation Used in Electrospray Ionization of Living Polymers on the Release of End-Groups during Collision-Induced Dissociations**; Michaël Mazarin<sup>1</sup>; Marion Girod<sup>1</sup>; Trang Phan<sup>1</sup>; Stéphane Humbel<sup>2</sup>; Laurence Charles<sup>1</sup>; <sup>1</sup>*Universités Aix-Marseille, Marseille, France*; <sup>2</sup>*Université Paul Cézanne, Marseille, France*
- WP 208 **MALDI-TOF MS of N-Substituted Fulleropyrrolidines**; Eun Su Park; Kathleen M. Flynn; Mickey C. Richardson; Gale A. Holmes; Charles M. Guttman; William E. Wallace; *National Institute of Standards & Technology, Gaithersburg, MD*

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- WP 209 **Mass Spectral Characterization of a Sorbitan Oleate Ethoxylate Surfactant**; Michael J. Polce<sup>1</sup>; Mark Szewc<sup>2</sup>; Giovanni A. Pallante<sup>2</sup>; Robert P. Lattimer<sup>1</sup>; <sup>1</sup>Lubrizol Advanced Materials, Brecksville, OH; <sup>2</sup>Thermo Scientific, Brunswick, OH
- WP 210 **Electrospray Ionization-Mass Spectrometry in the Analysis of a Wide Range of Polymer Additives**; Rob Burkhalter; Liepin Huang; *Corning, Inc., Corning, NY*
- WP 211 **Tandem Mass Spectrometry of Poly(Methacrylic Acid) Anions and Cations Produced by Electrospray Ionization**; Rémi Giordanengo<sup>1</sup>; Beatrice Allard-Breton<sup>2</sup>; Laurence Charles<sup>1</sup>; <sup>1</sup>Universités Aix-Marseille, Marseille, France; <sup>2</sup>ARKEMA, Centre de Recherche Rhône Alpes, Pierre-Bénite, France
- WP 212 **Direct Probe - Atmospheric Pressure Chemical Ionization (DP-APCI) of Amphiphilic Conetworks**; Chrys Wesdemiotis<sup>1</sup>; Sara Whitson<sup>1</sup>; Gabor Erdodi<sup>1</sup>; Joseph Kennedy<sup>1</sup>; Robert P. Lattimer<sup>2</sup>; <sup>1</sup>The University of Akron, Akron, OH; <sup>2</sup>Lubrizol Advanced Materials, Cleveland, OH
- WP 213 **High and Low Energy Fragmentation of Polymers in MALDI TOF/TOF and ESI FT-ICR Instruments**; Arpad Somogyi; Todd Mize; Peng Shu; Robert Bates; Henry Hall, Jr.; *University of Arizona, Tucson, AZ*
- WP 214 **Fourier Transform Analysis of Unresolved Electrospray Mass Spectra of Poly(ethylene glycol): Evidence of Polymer Blending**; Huifang Yao; Kelsey D. Cook; *University of Tennessee, Knoxville, TN*
- WP 215 **Time-of-Flight Secondary Ion Mass Spectrometric Analysis for Tertiary Structure of Poly(methylphenylsiloxane) in Monolayer Film**; Hye Kyoung Moon; Joseph A. Gardella, Jr.; *State University of New York at Buffalo, Buffalo, NY*
- WP 216 **Investigation of Oxidative Degradation Products from Aged Nylon**; Steven M. Thornberg; Michael I. White; Donald R. Bradely; Robert Bernstein; James M. Hochrein; *Sandia National Laboratories, Albuquerque, NM*
- WP 217 **Characterization of Poly(dichlorophosphazene)s and Their Reactions to Poly(organophosphazene)s**; Alyson Leigh; Sujeewani Ekanayake; Supat Moolsin; Matthew Panzer; Wiley Youngs; Claire Tessier; Chrys Wesdemiotis; *The University of Akron, Akron, OH*
- WP 218 **Optimization of MALDI-TOF-MS Sample Preparation for Synthetic Polymers via Nanoliter Deposition and Novel Matrix Formulations**; Julie Harmon<sup>1</sup>; Charles M. Guttman<sup>2</sup>; Drew Sauter<sup>3</sup>; Brent Hilker<sup>1</sup>; Kevin Clifford<sup>1</sup>; Andrew D. Sauter III<sup>3</sup>; Kathleen Flynn<sup>2</sup>; <sup>1</sup>University of South Florida, Tampa, FL; <sup>2</sup>NIST, Polymers Division, Gaithersburg, MD; <sup>3</sup>Nanoliter, Llc, Henderson, NV
- WP 219 **Sequencing of a Living Poly(Ethylene Oxide)/Polystyrene Block Copolymer by Tandem Mass Spectrometry**; Marion Girod; Trang N. T. Phan; Laurence Charles; *Universités Aix-Marseille, Marseille, France*
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- CARBOHYDRATES/OLIGOSACCHARIDES – STRUCTURAL CHARACTERIZATION, 220 -233**
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- WP 220 **Methodology and Characterization of Non-Covalent Protein Bound Heparin Oligosaccharides by Mass Spectrometry**; Hicham Naimy; Nancy Leymarie; Joseph Zaia; *Boston University, Boston, MA*
- WP 221 **Heparin-Like Glycosaminoglycan Peptide Non Covalent Complexes Studies using ECD: A New Potential Tool for HLGAGs Structure Elucidation**; Coraline Desbans<sup>1</sup>; Patrick Soubayrol<sup>2</sup>; Jean-claude Tabet<sup>3</sup>; <sup>1</sup>Université Paris VI (UPMC), Paris, France; <sup>2</sup>Sanofi-aventis, Chilly-mazarin, France; <sup>3</sup>University Paris Vi (upmc), Paris Cedex 05, France
- WP 222 **Influence of Charge State and Sodium Cationization on EDD and IRMPD of Glycosaminoglycan Oligosaccharides**; Jeremy Wolff<sup>1</sup>; Tatiana Laremore<sup>2</sup>; Robert J. Linhardt<sup>2</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Rensselaer Polytechnic Institute, Guilderland, NY
- WP 223 **Fully Automated Chip-Based Electrospray Ionization Multistage Mass Spectrometry of Long Chain Polysaccharides Functionalized with Aromatic Amines**; Valentina L. Udrescu<sup>1</sup>; Eugen N. Sisu<sup>2</sup>; Ioana Sisu<sup>2</sup>; Lucian Rusnac<sup>3</sup>; Mark Allen<sup>4</sup>; Reinaldo Almeida<sup>4</sup>; Alina D. Zamfir<sup>1</sup>; <sup>1</sup>National Institute for R&D in Electrochemistry, Timisoara, Romania; <sup>2</sup>Institute of Chemistry, Romanian Academy, Timisoara, Romania; <sup>3</sup>University "Politehnica", Timisoara, Romania; <sup>4</sup>Advion BioSciences, Norfolk, UK
- WP 224 **Wavelength-Resolved Fragmentation of Methyl-Glucopyranoside Anomers by Infrared Multiple-Photon Dissociation with a CO<sub>2</sub> Laser and Fourier Transform Ion Cyclotron Mass Spectrometry**; Sarah Stefan; John R. Eyler; *University of Florida, Gainesville, FL*
- WP 225 **Structure Characterization of Carbohydrates by Electrospray Mass Spectrometry**; Yufang Zheng; Mark A Wingerd; Kirill V Tret'yakov; Quan-long Pu; Stephen E. Stein; *NIST, Gaithersburg, MD*
- WP 226 **Electron Capture Dissociation of Metal-Adducted N-Linked Oligosaccharides Released from Bovine Thyroid Stimulating Hormone**; Wen Zhou; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WP 227 **Energy Dependence for Fragmentations of Sodium Ion Adducts of Sialyllactose Isomers, N-Neuraminic Acid and Lactose**; Takae Takeuchi<sup>1</sup>; Junko Fujita<sup>1</sup>; Michiko Tajiri<sup>2</sup>; Yoshinao Wada<sup>3</sup>; <sup>1</sup>Nara Women's University, Nara, JAPAN; <sup>2</sup>Crest, Jst, Izumi, Osaka, JAPAN; <sup>3</sup>Osaka MCHRI, Izumi, Japan
- WP 228 **Fragmentation Mechanism of Negatively-Charged Lewis-Type Trisaccharides in the Gas Phase: Experimental and Theoretical Studies**; Hiroaki Suzuki<sup>1</sup>; Tohru Yamagaki<sup>1</sup>; Kazuo Tachibana<sup>1</sup>; Kazuhiko Fukui<sup>2</sup>; <sup>1</sup>University of Tokyo, School of science, Tokyo, JAPAN; <sup>2</sup>CBRC, AIST, Tokyo, Japan
- WP 229 **Determination of Sialic Acid Linkage by Sequential Mass Spectrometry**; David Ashline; Vernon N. Reinhold; *University of New Hampshire, Lee, NH*
- WP 230 **Analysis of Carbohydrate Fragment Ion Spectra by MALDI TOF/TOF Mass Spectrometry and MS-MS Database Searching**; Matthias Glueckmann<sup>1</sup>; Christof Lenz<sup>1</sup>; Lydia Nuwaysir<sup>2</sup>; Ningombam Sanjib Meitei<sup>3</sup>; Radha Nigam<sup>3</sup>; Kamal Kishore<sup>3</sup>; <sup>1</sup>Applied Biosystems, Germany, Darmstadt, Germany; <sup>2</sup>Applied Biosystems, U.S.A., Foster City, CA; <sup>3</sup>PREMIER Biosoft International, Palo Alto, CA
- WP 231 **Structural Characterization of Pyridylaminated Oligosaccharides by High-Sensitive Capillary Electrophoresis-ESI-QIT-TOF Mass Spectrometry**; Emi Ito<sup>1</sup>; Kazuki Nakajima<sup>1</sup>; Akio Tominaga<sup>2</sup>; Hiroaki Waki<sup>2</sup>; Hiroto Itoi<sup>2</sup>; Kazuaki Kakehi<sup>3</sup>; Kozo Miseki<sup>2</sup>; Minoru Suzuki<sup>1</sup>; <sup>1</sup>The Institute of Physical and Chemical Research, Saitama, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Kinki University, Osaka, Japan



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- WP 232 **Structural Characterization of Sulfated Glycans from High Molecular Weight Salivary Mucins using Rapid, Robust Methods of Sample Preparation and Analysis;** Sarah Robinson<sup>1</sup>; Akraporn Prakobphol<sup>1</sup>; Simon Allen<sup>1</sup>; Nancy J. Phillips<sup>2</sup>; Birgit Schilling<sup>3</sup>; Bradford W. Gibson<sup>3</sup>; Susan J. Fisher<sup>1</sup>; Penelope M. Drake<sup>1</sup>; <sup>1</sup>Department of Cell and Tissue Biology, UCSF, San Francisco, CA; <sup>2</sup>Department of Pharmaceutical Chemistry, UCSF, San Francisco, CA; <sup>3</sup>Buck Institute For Age Research, Novato, CA
- WP 233 **Structural Characterization of Carboxymethylcellulose by Gas Chromatography-Mass Spectrometry;** Huiming Wang; Darryl H. Samuels; Tuyen T. Nguyen; Patrick J. Cowan; *Hercules Incorporated, Wilmington, DE*
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- NON-COVALENT INTERACTIONS 2, 234 - 250**
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- WP 234 **Gas-Phase Foot-Printing of Nucleic Acids and Protein-Nucleic Acids by EDD;** Joshua Wilhide; Kevin B. Turner; Daniele Fabris; *University of Maryland Baltimore County, Baltimore, MD*
- WP 235 **Mass Spectrometry Reveals the Non-Covalent Interaction Network in Yeast Translation Initiation Factors;** Alan M. Sandercock; Dijana Matak-Vinkovic; Alex J. Painter; Carol V. Robinson; *University of Cambridge, Cambridge, UK*
- WP 236 **Structure and Stability of Micelles in the Gas Phase;** Jacquelyn R Jhingree; John S Klassen; *University of Alberta, Edmonton, Canada*
- WP 237 **Analysis of an Intact Dissimilatory Sulfite Reductase Protein Complex from *Desulfovibrio vulgaris* using an Ion Mobility QTOF Analyzer;** Ming Dong<sup>1</sup>; Michael Daly<sup>2</sup>; Haichuan Liu<sup>3</sup>; Simon Allen<sup>3</sup>; Evelin Szakal<sup>3</sup>; Steven C. Hall<sup>3</sup>; Susan J. Fisher<sup>3</sup>; Lee L. Yang<sup>1</sup>; Julie Dearnley<sup>2</sup>; Terry C. Hazen<sup>1</sup>; Jil T. Geller<sup>1</sup>; Mary E. Singer<sup>1</sup>; Jian Jin<sup>1</sup>; Mark D. Biggin<sup>1</sup>; H. Ewa Witkowska<sup>3</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>Waters Corporation, Dublin, CA; <sup>3</sup>UCSF Core Mass Spectrometry Facility, San Francisco, CA
- WP 238 **Chemokine-Glycosaminoglycan Interactions: Composition, Orientation, and Specificity Studied by Mass Spectrometry;** Matthew Schenauer; Matthew D. Sweeney; Julie A. Leary; *UC Davis, Davis, CA*
- WP 239 **Comparison of CID, ECD, and ETD in the Dissociation of Noncovalent Complexes;** Sucharita Dutta<sup>1</sup>; Shelley N Jackson<sup>2</sup>; Amina S. Woods<sup>3</sup>; <sup>1</sup>Thermo Fisher, San Jose, CA; <sup>2</sup>Nida-irp, Nih, Baltimore, MD; <sup>3</sup>Nida Irp, Nih, Baltimore, MD
- WP 240 **Epitope Mapping for Carbohydrate-Protein Interaction by Nanoprobe-Based Affinity Mass Spectrometry;** Han-Tsung Huang<sup>1</sup>; Shu-Hua Chen<sup>1</sup>; Mei-Chun Tseng<sup>1</sup>; Po-Chiao Lin<sup>2</sup>; Ching-Wen Ho<sup>1</sup>; Der-Lii Tzou<sup>1</sup>; Chun-Cheng Lin<sup>2</sup>; Chun-Hung Lin<sup>1</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Chemistry, Tsing Hua University, Hsinchu, Taiwan
- WP 241 **Investigating Conformational Changes of Protein-Nucleic Acid and Protein-Ligand-Nucleic Acid Complexes by Tandem Mass Spectrometry;** Kevin B. Turner; Daniele Fabris; *University of Maryland Baltimore County, Baltimore, MD*
- WP 242 **The Binding Interface of LexA/RecA Investigated by Solution Phase H/D Exchange, Cross-linking and Mass Spectrometry;** Brittany R. Perkins; Guilong Cheng; Kim Giese; Vicki H. Wysocki; John W. Little; *University of Arizona, Tucson, AZ*
- WP 243 **Insight into the Subunit Interactions of 20S Proteasome using Chemical Cross-Linking and MALDI Tandem Mass Spectrometry;** Guoqiang Chen; ZHILI LI; *Chinese Academy of Medical Sciences, Beijing, CHINA*
- WP 244 **Genome Inspired G-quadruplex DNA Binding Ligands for Affinity MALDI-TOF Mass Spectrometry;** Junfeng Xiao; Linda McGown; *Rensselaer Polytechnic Institute, Troy, NY*
- WP 245 **Probing Allosteric Regulation of the 20S Proteasome with Mass Spectroscopy;** Monika Tokmina-Lukaszewska; Lydia S. Endel; Srividya Madabhushi; Maria E. Gaczynska; Pawel A. Osmulski; *University of Texas HSC, San Antonio, TX*
- WP 246 **Investigating Non-covalent Interactions using Isoelectric Trapping and Mass Spectrometry;** Stephanie Cologna; Peniel Lim; William K. Russell; Gyula Vigh; David H. Russell; *Texas A&M University, College Station, TX*
- WP 247 **High-Mass MALDI ToF Mass Spectrometry and Chemical Cross-linking for the study of Intact Protein Complexes;** Alexis Nazabal; Benoit Plet; Ryan Wenzel; *CovalX, Zürich, Switzerland*
- WP 248 **Analysis of Major Protein Complexes of Erythrocytes Directly from Cell Lysate Utilizing Capillary Electrophoresis Mass Spectrometry;** Mehdi Moini; An Nguyen; *University of Texas at Austin, Austin, TX*
- WP 249 **Electron Transfer Dissociation of Protein-Protein Complexes in a Quadrupole Ion Trap Mass Spectrometer;** Srikanth Rapole<sup>1,3,4</sup>; Jonathan Wilson<sup>2</sup>; Mark Olbris<sup>1,3,4</sup>; Richard Vachet<sup>1,3,4</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA; <sup>3</sup>University of Massachusetts, Amherst, MA; <sup>4</sup>University of Massachusetts, Amherst, MA
- WP 250 **Deconvoluting Heterogenous Macromolecular Assemblies;** Justin LP Benesch<sup>1</sup>; J Andrew Aquilina<sup>2</sup>; Carol V Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, UK; <sup>2</sup>University of Wollongong, Wollongong, Australia
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- NUCLEIC ACIDS, 251 - 272**
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- WP 251 **Characterization of Platinum-Based Quadruplex Intercalating Ligands Studied by ESI-MS;** Sarah Pierce<sup>1</sup>; Roxanne Kieltyka<sup>2</sup>; Hanadi Sleiman<sup>2</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>The University of Texas, Austin, TX; <sup>2</sup>McGill University, Montreal, Canada
- WP 252 **Determination of Ligand-Induced Changes in DNA Conformations by Chemical Probes and Tandem Mass Spectrometry;** Carol E. Parr; Jennifer Brodbelt; *The University of Texas, Austin, TX*
- WP 253 **Analysis of post-Transcriptionally Modified RNA in Heat Shocked Bacteria using LC-MS;** Susan Russell; Patrick A. Limbach; *University of Cincinnati, Cincinnati, OH*
- WP 254 **Using <sup>13</sup>C-Enriched dGTP for Unambiguous Base Composition Determination from Accurate and Precise Mass Measurement with an ESI-TOF Mass Spectrometer;** Kristin A. Sannes-Lowery; Amy Schink; Thomas A. Hall; Yun Jiang; Steven A. Hofstadler; *Ibis Biosciences, Inc., Carlsbad, CA*
- WP 255 **Towards a Mass Spectrometry Based Platform for Screening Mutations of the Fragile X Gene;** Eric D. Dodds; Flora Tassone; Paul J. Hagerman; Carlito B. Lebrilla; *University of California, Davis, CA*
- WP 256 **UPLC-MS Analysis of RNAi Oligonucleotides;** Vera Ivleva; Ying-qing Yu; Martin Gilar; John Gebler; *Waters Corporation, Milford, MA*



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- WP 257 **The Optimal Properties of Cross-Linked RNA:Protein for Electron Capture Dissociation;** Kady Krivos; Larry Sallans; Patrick A. Limbach; *University of Cincinnati, Cincinnati, OH*
- WP 258 **Green Tea Catechins Bound to DNA and RNA Observed by using Cold Spray Ionization Mass Spectrometry;** Kentaro Yamaguchi<sup>1</sup>; Takashi Kuzuhara<sup>1</sup>; Yoshihisa Sei<sup>2</sup>; Hirota Fujiki<sup>1</sup>; Mayumi Shibuta<sup>1</sup>; Masasmi Suganuma<sup>3</sup>; Natsuko Yamashita<sup>1</sup>; <sup>1</sup>*Tokushima Bunri University, Sanuki-city, Kagawa, Japan*; <sup>2</sup>*Tokushima Bunri University, Sanuki-city, Japan*; <sup>3</sup>*Saitama Cancer Center, Kitaadachi-gun, Saitama, Japan*
- WP 259 **Fragmentation Pathways of PNAs and Chemically Modified RNAs in Gas-Phase Ion-Electron Reactions and Vibrational Activation;** Hangtian Song; Jiong Yang; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WP 260 **Characterization of Degradation Pathways of Modified Therapeutic Oligonucleotides using Mass Sequencing via UPLC-MS;** Anthony Leone; Peter Yehl; Ann O'Brien; *Merck Co Inc, West Point, PA*
- WP 261 **Identification of Possible rRNA Modifications Resulting in Antibiotic Resistance;** Rebecca Rohlfs; Patrick A. Limbach; *University of Cincinnati, Cincinnati, OH*
- WP 262 **Novel G-Quadruplex Higher Order Assemblies Revealed by Electro Spray Ionization Mass Spectrometry;** Nicolas Smargiasso<sup>1</sup>; Frederic Rosu<sup>1</sup>; Erin Baker<sup>2</sup>; Michael T. Bowers<sup>3</sup>; Pierre Colson<sup>1</sup>; Edwin De Pauw<sup>1</sup>; Valerie Gabelica<sup>1</sup>; <sup>1</sup>*University of Liege, Liege, Belgium*; <sup>2</sup>*Pnnl, Richland, WA*; <sup>3</sup>*University of California, Santa Barbara, CA*
- WP 263 **High Throughput Purification and Analysis of PCR-Generated Oligonucleotides on a Fully Automated ESI-TOF-Based Platform;** Jared Drader; Jose Gutierrez; Thomas A. Hall; Kristin A. Sannes-lowery; Jose Alcala; James C. Hannis; Amy Schink; Maria Tobar-Mosquera; Sheri Manalili; Lendall C. Cummins; David Moore; Ranga Sampath; Lawrence Blyn; David J. Ecker; Steven A. Hofstadler; *Ibis Biosciences, Inc., Carlsbad, CA*
- WP 264 **Exploring the Formation Pathways of DNA G-Quadruplex Architectures;** Frederic Rosu<sup>1</sup>; Harmonie Poncelet<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Pierre Colson<sup>1</sup>; Edwin De Pauw<sup>2</sup>; Valerie Gabelica<sup>1</sup>; <sup>1</sup>*University of Liege, Liege, BELGIUM*; <sup>2</sup>*Liege University, Liege, Belgium*
- WP 265 **Discovery of A New Type of DNA Photoproduct Containing a mC⇌A Dimer;** Dian Su; John-Stephen Taylor; Michael L. Gross; *Washington University, St Louis, MO*
- WP 266 **RNA Mass Spectrometry: a Platform Technology for Non-Coding RNA Research;** Yuriko Sakaguchi; Hiroki Ueda; Takeo Suzuki; Takayuki Katoh; Takeshi Seguchi; Kenjyo Miyauchi; Tsutomu Suzuki; *The University of Tokyo, Tokyo, Japan*
- WP 267 **Quantitative Analysis of DNA Interstrand Cross-Links and Mono-Adducts Formed in Human Cells Induced by Psoralens and UVA Irradiation;** Congfang Lai<sup>1</sup>; Huachuan Cao<sup>3</sup>; Hai Luo<sup>2</sup>; Yinsheng Wang<sup>2</sup>; <sup>1</sup>*Riverside, CA*; <sup>2</sup>*University of California, Riverside, CA*; <sup>3</sup>*University of California, Riverside, Riverside, CA*
- WP 268 **LC-MS-MS for the Quantification of Cytosine Methylation in DNA;** Hongxia Wang; Yinsheng Wang; *Department of Chemistry, UC Riverside, Riverside, CA*
- WP 269 **Top-Down Analysis of siRNA via Ion Trap Collision-Induced Dissociation;** Teng-Yi Huang; Jian Liu; Xiaorong Liang; Brittany Hodges; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- WP 270 **LC-MS-MS Quantification and in-vitro Replication Studies of Thymidine Glycol/8-Oxo-2'-Deoxyguanosine Tandem Lesions;** Yong Jiang; Yinsheng Wang; *University of California, Riverside, Riverside, CA*
- WP 271 **Reactivity of Nitrogen Mustards towards Guanines Adjacent to Methylated Cytosines in Oligonucleotides;** Suncerae Smith; Jennifer Brodbelt; *The University of Texas, Austin, TX*
- WP 272 **Decoy Oligonucleotides: Analysis and Use in Head and Neck Carcinogenesis;** Rita Casadonte<sup>1</sup>; Lisa Manier<sup>1</sup>; David Carbone<sup>1</sup>; Jennifer Grandis<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*University of Pittsburgh School of Medicine, Pittsburgh, PA*
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- WP 273 **A Novel Approach for Electron Ionization LC-MS with Supersonic Molecular Beams;** Tal Alon; Kfir Gil; Alexander B. Fialkov; Aviv Amirav; *Tel-Aviv University, Tel-Aviv, Israel*
- WP 274 **Direct Analysis of Aqueous Samples Containing Explosives at Picogram Level by LC-MS;** Olivier Vigneau; Xavier Machuron-Mandard; *CEA, Arpajon Cedex, France*
- WP 275 **Sensitive LC-MS-MS Method for the Determination of Diclofenac in Human EDTA Plasma;** Aimin Tan; Jun Li; Harshvardhan Patel; Jacky Lee; Saleh Hussain; François Vallée; *Anapharm Inc., Richmond Hill, Canada*
- WP 276 **Simultaneous Evaluation by Mass Spectroscopy of Multiple Formulation Ingredients in Dissolution Studies;** Audrey Tournant; Louis-Philippe Labranche; Daniel Abran; Alain Carrier; *Sandoz Canada Inc., Boucherville, Canada*
- WP 277 **Simulation of Phase I and II Metabolism of Toremfene using On-Line Electrochemistry/Immobilized Enzymes/Liquid Chromatography/Mass Spectrometry;** Wiebke Lohmann; Uwe Karst; *University of Münster, Münster, Germany*
- WP 278 **Determination of Vincristine and Vinblastine in C. Roseus Leaves by Liquid Chromatography Mass Spectrometry;** Qishan Lin; Jinghua Zhu; *University at Albany, Rensselaer, NY*
- WP 279 **Cob(D)alamin as an Analytical Tool for identifying Sucralose by using LC-MS-MS;** Hitesh V Motwani<sup>1</sup>; Henrik Kylin<sup>2</sup>; Bernard Golding<sup>3</sup>; Margareta Törnqvist<sup>1</sup>; <sup>1</sup>*Stockholm University, Stockholm, Sweden*; <sup>2</sup>*Norwegian Institute for Air Research, Tromsø, Norway*; <sup>3</sup>*Newcastle University, Newcastle upon Tyne, UK*
- WP 280 **A LC-MS-MS Method for Quantitative Determination of Topotecan [(S)-9-di-methylaminomethyl-10-hydroxy-camptothecin] in Human Plasma;** Claudia Meek<sup>1</sup>; Daniel Bowers<sup>2</sup>; Richard Leff<sup>1</sup>; <sup>1</sup>*Texas Tech University, Dallas, TX*; <sup>2</sup>*UT Southwestern Medical Center, Dallas, TX*
- WP 281 **Fast Identification of Anthocyanins in Blueberries Comparing Reverse Phase and HILIC High Performance Liquid Chromatography Coupled with ESI-IT-TOF-MS Detection;** Jeremy S Barnes; Hien Nguyen; Kevin Schug; *University of Texas At Arlington, Arlington, TX*

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- WP 282 **A Faster and More Environmentally Friendly Approach to Quantitating Amotosalen HCl in Human Plasma;** Kelly Balla<sup>1</sup>; Roy Bogseth<sup>2</sup>; Todd Wielgos<sup>2</sup>; <sup>1</sup>*Baxter Healthcare Corp., Round Lake, IL*; <sup>2</sup>*Baxter Healthcare, Round Lake, IL*
- WP 283 **Utilizing the Electrospray Membrane Probe to Map Electrospray Signal Response in Gradient LC/ES/MS;** Thomas P. White; Craig M. Whitehouse; *Analytica of Branford, Inc., Branford, CT*
- WP 284 **Establishing Regression Model of Calibration Curve in a LC-MS-MS Method;** Rong Yi; Dunmin Mao; *Can Test Ltd., Burnaby, Canada*
- WP 285 **Comparison of Different Ionization Techniques (ESI, DART, APGD) for Coupling of Mass Spectrometry with Planar Chromatography (HPTLC-MS);** Gertrud E. Morlock; *University of Hohenheim, Stuttgart, Germany*
- WP 286 **Simultaneous Determination of Rosuvastatin and N-Desmethylrosuvastatin in Human Plasma using Negative Ion ESI-LC-MS-MS;** Linge Li; William R. Mylott; Bruce J. Hidy; Rand G. Jenkins; *PPD, Richmond, VA*
- WP 287 **Role of LC Mobile Phase Additives in Mass Spectrometry Signal Responses in Pesticide Analysis;** yaorong qian; *US EPA, Ft. Meade, MD*
- WP 288 **Polymer-Coated C18 Stationary Phase Designed for High-Sensitivity and High-Throughput Analyses in LC-MS;** Osamu Shirota; Hiroko Arai; Miho Ebata; *Shiseido, Yokohama, Japan*
- WP 289 **Phosphorylated Compounds and Electrospray : an unmatched Couple?;** Filip Lemiere<sup>1</sup>; Thomas De Vijlder<sup>2</sup>; Jasper Boschmans<sup>1</sup>; Erwin Witters<sup>1</sup>; <sup>1</sup>*University of Antwerp, Antwerp, Belgium*; <sup>2</sup>*University of Antwerp; Dept. Biology, Antwerp, Belgium*
- WP 290 **Enhanced Sensitivity and Selectivity in LC-MS-MS Bioanalysis of Basic Analytes using High pH Mobile Phases with 'Wrong-Way-Round' Positive-Ion ESI;** Laura Nakovich; Linge Li; Moucun Yuan; James Creegan; William R. Mylott; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- WP 291 **Trace Pd Analysis in Drug Substance with LC-MS;** Min Yang; Patrick Drumm; Donald Drinkwater; *Novartis Pharmaceuticals, East Hanover, NJ*
- WP 292 **Detection of Potential Ion Suppression in Quantitative LC-MS Analysis;** Atsumu Hirabayashi<sup>1</sup>; Masako Ishimaru<sup>1</sup>; Naomi Manri<sup>1</sup>; Toshiyuki Yokosuka<sup>2</sup>; Hiroko Hanzawa<sup>1</sup>; <sup>1</sup>*Hitachi, Ltd., Central Research Laboratory, Tokyo, Japan*; <sup>2</sup>*Hitachi, Ltd., Hitachi Research Laboratory, Hitachi, Japan*
- WP 293 **Qualitative Analysis of Tea by Ion Chromatography-Time-of-Flight Mass Spectrometry with High Sensitivity and Resolution;** Kazuko Tanaka<sup>1</sup>; Kazutetsu Nojima<sup>1</sup>; Toshinobu Honda<sup>2</sup>; <sup>1</sup>*JEOL Ltd., Akishima, Tokyo, Japan*; <sup>2</sup>*JEOL USA Inc., Modesto, CA*
- WP 294 **Advantages and Drawbacks of Silver Coordination Ion-Spray Ionisation of Vitamin D3 and Metabolites;** Evgueni Fedorov; Michel Coutu; John Chapdelaine; Jean-François Larocque; Laurentiu Ciochina; Michael Mancini; *Warnex Bioanalytical Services, Laval, QC*
- WP 295 **Evaluation of Column Retentivity with Large Injection Volume for High Sensitive and High-Throughput LC-MS-MS Quantitative Analysis;** Jun Watanabe<sup>1</sup>; Hiroshi Hike<sup>2</sup>; Masazumi Yasumoto<sup>1</sup>; Seiji Horie<sup>1</sup>; Yasuhiko Bando<sup>2</sup>; <sup>1</sup>*Takara Bio Inc., Kusatsu, Japan*; <sup>2</sup>*AMR, Inc., Tokyo, Japan*
- WP 296 **Determination of Stavudine in Rat Plasma, Amniotic Fluid, Fetal and Placental Tissues using LC-MS-MS;** Meng Xu; Catherine A. White; Michael G. Bartlett; *University of Georgia, Athens, GA*
- WP 297 **Evaluation of uHPLC Column Efficiency (N) vs Flow Rate: Implications of the Unexpected van Deemter Plot Obtained;** Yuan-Qing Xia<sup>1</sup>; Mohammed Jemal<sup>2</sup>; <sup>1</sup>*Bristol-Myers Squibb Company, Princeton, NJ*; <sup>2</sup>*Bristol-Myers Squibb, Princeton, NJ*
- WP 298 **Identification of Darbepoetin Alfa in Human Plasma by LC-MS-MS for Doping Control;** Fuyu Guan<sup>1</sup>; Cornelius E. Uboh<sup>2</sup>; Lawrence R. Soma<sup>1</sup>; Eric K. Birks<sup>1</sup>; Jinwen Chen<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Kennett Square, PA*; <sup>2</sup>*PA Equine Toxicology and Research Center, West Chester, PA*
- WP 299 **Application of On-Line Column Switching to Eliminate Phospholipids and Other Matrix Interferences in UPLC-MS-MS Bioanalysis;** Moucun Yuan<sup>1</sup>; James Waltrip<sup>1</sup>; William R. Mylott<sup>1</sup>; Bruce Hidy<sup>1</sup>; Rand Jenkins<sup>1</sup>; Grace O'Maille<sup>2</sup>; Sudhakar M. Pai<sup>2</sup>; <sup>1</sup>*PPD, Richmond, VA*; <sup>2</sup>*Akros Pharma Inc., Princeton, NJ*
- WP 300 **Identification of Four Unknown Peaks in the Forced Degradation Study of Betamethasone Sodium Phosphate by LC-MSn and NMR;** Xin Wang; Bin Chen; Min Li; Rustum Abu; *Schering Plough, Union, NJ*
- WP 301 **Simultaneous Determination of 17a-Hydroxyprogesterone Caporate (17-OHPC), Hydroxyprogesterone (17-OHP) and Progesterone (P) in Human Plasma using LC-MS-MS;** Shimin Zhang<sup>3</sup>; Sripal Reddy Mada; Marilynn Torch; Don Mattison<sup>1</sup>; Steve Caritis<sup>2</sup>; Raman Venkataramanan; OPRU Network<sup>1</sup>; <sup>1</sup>*Center for Research for Mothers and Children, Bethesda, MD*; <sup>2</sup>*Magee Womens Hospital, Pittsburgh, PA*; <sup>3</sup>*University of Pittsburgh, Pittsburgh, PA*
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- CLINICAL CHEMISTRY – SMALL MOLECULE, 302 - 322**
- WP 302 **Quantitation of Glutathione by Liquid Chromatography/Positive Electrospray Tandem Mass Spectrometry;** Fagen Zhang; Michael J. Bartels; David R. Geter; Yo-Chan Jeong; Melissa R. Schisler; Amanda J. Wood; B. Bhaskar Gollapudi; *The Dow Chemical Company, Midland, MI*
- WP 303 **Biomonitoring of Caffeine Exposure and Enzyme Activity Phenotyping by LC-MS-MS;** Michael e. Rybak; Ching-I Pao; Christine M. Pfeiffer; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 304 **Quantification of Free and Bound N-Acetylneuraminic Acids in Blood Serum of Disease-Free and Breast Cancer Patients;** Guangxiang Wu; Loubna Hammad; Milos V. Novotny; Yehia Mechref; *Indiana University, Bloomington, IN*
- WP 305 **Amino Acid Quantitation in Plasma, Urine and CSF by iTRAQ™ Reagent Amino Acid Analysis Kit and MS-MS;** Jean Lacey<sup>1</sup>; Bruno Casetta<sup>2</sup>; Scott B. Daniels<sup>3</sup>; Subodh Nimkar<sup>4</sup>; Mark J. Magera<sup>1</sup>; Dietrich Matern<sup>1</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*; <sup>2</sup>*Applied Biosystems, Monza, ITALY*; <sup>3</sup>*Applied Biosystems, Framingham, MA*; <sup>4</sup>*Applied Biosystems, Foster City, CA*
- WP 306 **Commutability of NIST SRM 1955 Homocysteine and Folate in Frozen Human Serum with Selected Total Homocysteine Immunometric or Enzymatic Assays;** Bryant C. Nelson<sup>1</sup>; Christine M. Pfeiffer<sup>2</sup>; Mindy Zhang<sup>2</sup>; David L. Duewer<sup>1</sup>; Katherine E. Sharpless<sup>1</sup>; Katrice A. Lippa<sup>1</sup>; <sup>1</sup>*National Institute of*

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- Standards and Technology, Gaithersburg, MD; <sup>2</sup>Centers for Disease Control and Prevention, Atlanta, Georgia*
- WP 307 **Quantitation of Steroid Hormones in Tissue Sections;** Xia Xu<sup>1</sup>; Josip Blonder<sup>1</sup>; Donald J. Johann<sup>2</sup>; Larry K. Keefer<sup>2</sup>; Regina G. Ziegler<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>National Cancer Institute, Bethesda, MD
- WP 308 **Simultaneous Quantitation of Testosterone and Androstenedione in Serum by Online Extraction and LC-MS-MS;** Valdemir Melechco Carvalho; Odete H. Nakamura; Jose G. H. Vieira; *Fleury Institute, São Paulo, Brazil*
- WP 309 **Simultaneous Analysis of Newer Antiepileptic Drugs by Rapid Resolution LC/ Triple Quadrupole Mass Spectrometry;** Uta Juerges<sup>1</sup>; Bernhard J. Steinhoff<sup>1</sup>; Juergen Wendt<sup>2</sup>; <sup>1</sup>Epilepsiezentrum Kork, Kehl, Germany; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- WP 310 **SACI and Ion Exchange Chromatography: a New Way for Biomarker Discovery;** Simone Cristoni<sup>1</sup>; Luigi Rossi Bernardi<sup>2</sup>; <sup>1</sup>ISB, Milan, ITALY; <sup>2</sup>Multimedica Laboratories, Milan, Italy
- WP 311 **Determination of Isoprenoid Biosynthesis Intermediates using HPLC- and UPLC-MS-MS;** Willem Kulik<sup>1</sup>; Linda Henneman<sup>1</sup>; Arno G. van Cruichten<sup>1</sup>; Simone W. Denis<sup>1</sup>; Richard A. Gibbs<sup>2</sup>; Hans R. Waterham<sup>1</sup>; <sup>1</sup>AMC, Amsterdam University, Amsterdam, netherlands; <sup>2</sup>School of Pharmacy and Pharmaceutical Sciences, West Lafayette, IN
- WP 312 **Determination of Total Homocysteine, Methylmalonic Acid, and 2-Methylcitric Acid in Dried Blood Spots by Tandem Mass Spectrometry;** Coleman T Turgeon<sup>1</sup>; Mark J. Magera<sup>1</sup>; Carla D. Cuthbert<sup>2</sup>; Perry R Loken<sup>1</sup>; Dimitar Gavrilov<sup>1</sup>; Devin Oglesbee<sup>1</sup>; Kimiyo Raymond<sup>1</sup>; Silvia Tortorelli<sup>1</sup>; Piero Rinaldo<sup>1</sup>; Dietrich Matern<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>University of Miami, Miami, FL
- WP 313 **Determination of Homovanillic Acid and 5-Hydroxyindoleacetic Acid in Human Cerebrospinal Fluid using Solid Phase Extraction and LC-MS-MS;** Rene Gagnon<sup>1</sup>; Bernard Échenne<sup>2</sup>; Régén Drouin<sup>1</sup>; <sup>1</sup>CHUS-Service de Génétique, Sherbrooke, Canada; <sup>2</sup>CHUS-Service de Neuropédiatrie, Sherbrooke, Canada
- WP 314 **Rapid Analysis of Bile Acids in Serum by LC-MS-MS;** Bingfang Yue<sup>1</sup>; William L. Roberts<sup>2</sup>; Alan L. Rockwood<sup>2</sup>; <sup>1</sup>ARUP Laboratories, Salt Lake City, UT; <sup>2</sup>Department of Pathology, University of Utah, Salt Lake City, UT
- WP 315 **Analysis of Gadolinium-based MRI Contrasting Agents by CE/ESI-ToF-MS and HILIC/ESI-MS;** Jens Künnemeyer; Lydia Terborg; Uwe Karst; *University of Münster, Münster, Germany*
- WP 316 **Multicenter Validation of the MassTrak<sup>®</sup> Reagent Kit for the Quantification of Tacrolimus in Whole Blood using LC-MS-MS;** Donald P Cooper<sup>1</sup>; Kimberly L Napoli<sup>2</sup>; Paul J Taylor<sup>3</sup>; Catherine Hammett-Stabler<sup>4</sup>; Quynhmai Nguyen<sup>2</sup>; Webb S Lowe<sup>4</sup>; Mike E Franklin<sup>3</sup>; Kendon S Graham<sup>1</sup>; Gareth W Hammond<sup>1</sup>; Michael R Morris<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>University of Texas Medical School at Houston, Houston, TX; <sup>3</sup>Princess Alexandra Hospital, Brisbane, Australia; <sup>4</sup>University of North Carolina Hospitals, Chapel Hill, NC
- WP 317 **Detection of Volatile Metabolites of High Molecular Weight in Urine by Atmospheric Pressure Ionization-Mass Spectrometry;** Pablo Martinez-Lozano Sinues<sup>2</sup>; Juan Fernandez de la Mora<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>SEADM, Valladolid, Spain
- WP 318 **Estrone Sulfate and Estradiol Sulfate: a New Highly Sensitive LC-MS-MS Assay;** Brian C. Netzel; Ravinder J. Singh; *Mayo Clinic, Rochester, MN*
- WP 319 **Detection of Amphetamines in urine Samples via Direct Infusion Electrospray Ionization Mass Spectrometry: a Fast Screening Method for Doping Control;** Patricia Bergo<sup>1</sup>; Joane M Correa<sup>4</sup>; Tanus J Nagem<sup>3</sup>; Mario C Guerreiro<sup>2</sup>; Luiz C A Oliveira<sup>2</sup>; Rodinei Augusti<sup>4</sup>; Clesia C Nascentes<sup>4</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>Federal University of Lavras, Lavras/MG, Brazil; <sup>3</sup>Federal University of Ouro Preto, Ouro Preto/MG, Brazil; <sup>4</sup>Federal University of Minas Gerais, Belo Horizonte/MG, Brazil
- WP 320 **Reducing Analytical Time for Urine Organic Acid Profiling using GC-MSD and Deconvolution Reporting Software (DRS);** Jie Chen<sup>1</sup>; Chin-Kai Meng<sup>2</sup>; Srinivas Narayan<sup>1</sup>; Michael Bennett<sup>1</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA; <sup>2</sup>Agilent Technologies, Wilmington, DE
- WP 321 **Mass Spectrometric Characterization of New Drugs and Designer Analogs in Sports Drug Testing;** Mario Thevis<sup>1</sup>; Maxie Kohler<sup>1</sup>; Nils Schlörer<sup>2</sup>; Wilhelm Schänzer<sup>1</sup>; <sup>1</sup>German Sport University, Cologne, Germany; <sup>2</sup>University of Cologne, Cologne, Germany
- WP 322 **Extractive Electrospray Ionization Mass Spectrometry of Breath for Monitoring Intake of Pharmaceuticals in Real-Time: Valproic Acid;** Gerardo Gamez<sup>1</sup>; Liang Zhu<sup>1</sup>; Konstantin Chingina<sup>1</sup>; Huanwen Chen<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>College of Chemistry, Jilin University, Changchun, China
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- SMALL MOLECULE ANALYSIS – DATA PROCESSING/INSTRUMENTATION, 323 - 340**
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- WP 323 **Approaching Universal Detection: High Throughput Drug Discovery Analysis using LC-MS Multimode Source/ELSD/CLND;** Wayne Duncan<sup>1</sup>; Ken Lewis<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Opans, Llc, Durham, NC
- WP 324 **Use of Deconvolution Reporting Software for the Analysis of Pesticide Residues in High Fat Content Foodstuffs;** Petra Kopecka<sup>1</sup>; Jas Oliver-Kang<sup>2</sup>; Matthew J. Almond<sup>1</sup>; <sup>1</sup>The University of Reading, Reading, UK; <sup>2</sup>CEMAS, North Ascot, UK
- WP 325 **Probing the Effects of Popular Substrates on Laser Desorption of Ions and Neutrals;** Irene L. Anestis-Richard; Yanfeng Chen; Christopher D. Lane; Thomas M. Orlando; *Georgia Institute of Technology, Atlanta, GA*
- WP 326 **Critical Experimental Parameters for Preparing a High-Sensitivity Nanostructure-Initiator Mass Spectrometry (NIMS) Surface;** Hin-Koon Woo<sup>1</sup>; Trent Northen<sup>2</sup>; Oscar Yanes<sup>3</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>The Scripps Research Inst., La Jolla, CA; <sup>3</sup>Thescrippsresearchinstitute, La Jolla, CA
- WP 327 **Determination of Proton Affinities of trans-2-Aminocyclohexanol and Its Related Compounds;** Sumit Mukherjee; Eric Wang; Jianhua Ren; Vyacheslav V. Samoshin; *University of The Pacific, Stockton, CA*
- WP 328 **Investigations of the Use of Carbon-Based Materials as Matrixes for LDI-MS Profiling and Imaging of Small Molecule;** Aoshuang Xu; Sangwon Cha; Hui Zhang; Edward S Yeung; *Iowa State University, Ames, IA*

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- WP 329 **SALDI-Screening of Samples Prior to LC-MS Analysis;** Nahid Amini; Mohammadreza Shariatgorji; Gunnar Thorsen; Carlo Crescenzi; Leopold L. Ilag; *Stockholm University, Stockholm, Sweden*
- WP 330 **Determination of the Ion Structures of Isomers using Precursor Ion Fingerprinting;** Michelle Sheldon<sup>3</sup>; Robert Mistrik<sup>2</sup>; Timothy R. Croley<sup>1</sup>; <sup>1</sup>*Commonwealth of Virginia, Richmond, VA*; <sup>2</sup>*Highchem, Ltd., Bratislava, SLOVAKIA*; <sup>3</sup>*Div of Consolidated Lab, Richmond, VA*
- WP 331 **Laser Desorption of Organic Molecules in Different Irradiation Arrangement;** Alexander Zinovev; Igor Veryovkin; Michael Pellin; *ANL, Argonne, IL*
- WP 332 **The Rapid Identification of the Impurities of Simvastatin using UPLC<sup>TM</sup>-Q-ToF<sup>TM</sup> Technology and an Intelligent Data Mining Approach;** Warren Potts Iii<sup>1</sup>; Rob Plumb<sup>2</sup>; Michael D Jones<sup>2</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters, Milford, MA*
- WP 333 **Complete Characterization of Isobaric Impurities by Chromatographic Data Dependent Scan with Simultaneous Two Collision Induced Dissociation Methods on LTQ Orbitrap;** Shigeru Sakamoto; Mihoko Yamaguchi; *Thermo Fisher Scientific, Yokohama, Japan*
- WP 334 **Gas Phase Hydrogen Deuterium Exchange of Compounds Introduced by HPLC to a Commercial Mass Spectrometer at mL/min Flow Rates;** David Black; David J. Burinsky; *Glaxosmithkline, Rtp, NC*
- WP 335 **On-Line Concentration of Small Molecules by Microfluidic Electrocapture for ESI-MS Analysis;** Juan Astorga-Wells<sup>1</sup>; Tomas Bergman<sup>1</sup>; Peter Michelsen<sup>2</sup>; Hans Jörnvall<sup>1</sup>; <sup>1</sup>*Karolinska Institutet, Stockholm, Sweden*; <sup>2</sup>*Stockholm University, Hässleholm, Sweden*
- WP 336 **Advantages of a High-Resolution Multi-Reflecting Time-of-Flight Mass Spectrometer for the Analysis of Small Molecules;** Matthew Giardina; Viatcheslav Artaev; *LECO Corporation, St. Joseph, MI*
- WP 337 **Selecting the Right HPLC for a Mass Spectrometer using the Linear Compensatory Model as an Evaluation Technique;** Catherine Fontaine; Simon Robert; Valérie Vincent; Milton Furtado; Troy Bradley; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, CANADA*
- WP 338 **Statistical Evaluation of the Benefit of combined Use of Accurate Mass and Isotopic Pattern;** Marcus Macht<sup>1</sup>; Petra Decker<sup>1</sup>; Aiko Barsch<sup>1</sup>; Ilmari Krebs<sup>1</sup>; Catherine Stacey<sup>2</sup>; <sup>1</sup>*Bruker Daltonik, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*
- WP 339 **Applying Isotopic Profile Analysis to Metabolite Detection and Identification using High Mass Accuracy MSn Analysis;** Neil J Loftus<sup>1</sup>; Simon Ashton<sup>1</sup>; John Warrander<sup>1</sup>; Gerard Hopfgartner<sup>2</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*University of Geneva, Geneva, Switzerland*
- WP 340 **Development of a Molecular Formula Machine;** Richard Joyce; Donald S Richards; *Pfizer Ltd, Sandwich, UK*
- WP 343 **Automated Screening System for Solvent and Column Selections to Minimize Sample Carryover during LC-MS-MS Method Development;** Joseph Whitson<sup>1</sup>; Dale F. Schoener<sup>1</sup>; Patrick Lin<sup>2</sup>; <sup>1</sup>*Alta Analytical Laboratory, El Dorado Hills, CA*; <sup>2</sup>*Intertek-alta Analytical, El Dorado Hills, CA*
- WP 344 **LC-MS-MS Analysis of 8-Isoprostane-PGF2a as a Measure of the Antioxidant Activity of Lycopene *in vivo*;** Jeff Dahl; Richard B. Van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- WP 345 **Methods for Quantitative Measurements using a Helium Metastable-Beam Open-Air-Ion-Source Mass Spectrometer;** O. David Sparkman; Patrick R. Jones; Matthew Curtis; Teresa Vail; *University of the Pacific, Stockton, CA*
- WP 346 **Quantitative Analysis of Perfluorooctanoic Acid by LC-MS-MS;** Yanan Yang<sup>1</sup>; Naoto Shimizu<sup>2</sup>; Doug Mcintyre<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc, Santa Clara, CA*; <sup>2</sup>*Agilent Technologies, Hachioji-shi, Tokyo, Japan*
- WP 347 **Employing Higher Resolution to Obtain Better Selectivity for Quantitation Experiments on a Triple-Quadrupole Instrument Platform (API 5000<sup>TM</sup> LC-MS System);** Anthony Romanelli; Jefferey Miller; Xavier Misonne; *Applied Biosystems, Framingham, MA*
- WP 348 **IS Response Variations in Incurred Sample Analysis by LC-MS-MS: Case by Case Trouble-Shooting;** Aimin Tan; Saleh Hussain; François Vallée; *Anapharm Inc., Richmond Hill, Canada*
- WP 349 **The Development of Quantitative Real-Time Detection of Flavors During Fermentation by Fused-Droplet Electrospray Ionization (FD-ESI) Mass Spectrometry;** Chang-nan Chen<sup>1</sup>; Jentaie Shiea<sup>2</sup>; Yi-Feng Lin<sup>1</sup>; Patrick R. Jones<sup>3</sup>; <sup>1</sup>*Chaoyang University of Technology, Taichung, Taiwan*; <sup>2</sup>*National Sun Yat-sen Univ., Kaohsiung, Taiwan*; <sup>3</sup>*University of The Pacific, Stockton, CA*
- WP 350 **Increasing Specificity in MALDI Quantitative Analysis by using MS<sup>3</sup> on a Hybrid Quadrupole-Linear Ion Trap;** Bruce Collings<sup>1</sup>; Pauline J. Vollmerhaus<sup>2</sup>; Yves G. Leblanc<sup>3</sup>; <sup>1</sup>*Mds Sciex, Concord, ON*; <sup>2</sup>*Applied Biosystems/mds Sciex, Concord, ON*; <sup>3</sup>*Mds Analytical Technologies, Concord, ON*
- WP 351 **Benefits of a Scheduled Multiple Reaction Monitoring Experiment for Pesticide Screening in Food using LC-MS-MS;** Loïc Beyet<sup>1</sup>; Michel Cam<sup>2</sup>; Nadine Lamour<sup>2</sup>; Nadia Pace<sup>3</sup>; <sup>1</sup>*Applied Biosystems, Courtaboeuf Cedex, FRANCE*; <sup>2</sup>*Capinov, Landernau, France*; <sup>3</sup>*Applied Biosystems/MDS Sciex, Toronto, Canada*
- WP 352 **Importance of Co-eluting Analyte and Internal Standard in Quantitative LC-ESI-MS;** Martin Ahnoff; Ia Hultman; Mathias Liljebblad; *AstraZeneca R&D, Molndal, SWEDEN*
- WP 353 **Measurement of Vitamin D in Infant Formula by Liquid Chromatography Tandem Mass Spectrometry (LC-MS-MS);** Min Huang; Paul Laluzerne; Doug Winters; *Covance, Food and Drug Analysis, Madison, WI*
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- QUANTITATION OF SMALL MOLECULES,341 - 353**
- WP 341 **Performance Comparison of Standard Electrospray Versus Nanospray for the Quantification of Nucleotides and Their Phosphorolated Metabolites;** John D. Lennon<sup>1</sup>; Ken Lewis<sup>1</sup>; Gary Valaskovic<sup>2</sup>; <sup>1</sup>*OpAns, LLC, Durham, NC*; <sup>2</sup>*New Objective, Inc., Woburn, MA*
- WP 342 **Optimized Conditions for the Simultaneous Determination of Vitamins D<sub>3</sub> and D<sub>2</sub> by UPLC-MS-**

## WEDNESDAY POSTERS

## IMMUNOLOGY, 354 - 374

- WP 354 **Mass Spectrometric Characterization of Apheresis Samples from Rheumatoid Arthritis Patients - Approaching the Principles of Function of Immunomodulation Therapy;** Mike Kienbaum<sup>1</sup>; Cornelia Koy<sup>1</sup>; Helen Montgomery<sup>3</sup>; Susanne Drynda<sup>2</sup>; Koichi Tanaka<sup>4</sup>; Joern Kekow<sup>2</sup>; Reinhard Guthke<sup>5</sup>; Hans-Juergen Thiesen<sup>6</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, Rostock, GERMANY*; <sup>2</sup>*Otto von Guericke University, Magdeburg, Germany*; <sup>3</sup>*Shimadzu, Koichi Tanaka Ms Research Laboratory, Manchester, UK*; <sup>4</sup>*Shimadzu Corporation, Kyoto, JAPAN*; <sup>5</sup>*Hans Knoell Institute, Jena, Germany*; <sup>6</sup>*University of Rostock, Rostock, Germany*
- WP 355 **Activation State of Primary Human B Cells Measured by Quantitation of Phosphorylation on Syk Kinase Linker Region Tyrosines;** Anita Izrael-Tomasevic; Andrew C. Vendel; Jill Calamine-Fenaux; Dan L. Eaton; David P. Arnott; *Protein Chemistry Department, Genentech, Inc., South San Francisco, CA*
- WP 356 **Analysis of Naturally Processed Splenic and Thymic Peptides from the NOD Mouse;** Henry W. Rohrs<sup>1</sup>; Anish Suri<sup>2</sup>; Emil Unanue<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>*Washington University, St Louis, MO*; <sup>2</sup>*Bristol-Myers Squibb, Princeton, NJ*
- WP 357 **Comparison of Mass Spectrometry and Hemagglutinin Inhibition Assays to Assess the Antigenicity of the Influenza Virus;** Alexander Schwahn; Bethny Morrissey; Kevin Downard; *University of Sydney, Sydney, Australia*
- WP 358 **Fast de novo Sequencing of a Monoclonal Antibody via Shotgun Protein Sequencing;** Jennie Lill<sup>1</sup>; Nuno Bandeira<sup>2</sup>; Victoria Pham<sup>1</sup>; David Arnott<sup>1</sup>; Pavel Pevzner<sup>2</sup>; <sup>1</sup>*Genentech Inc, South San Francisco, CA*; <sup>2</sup>*University of California, San Diego, La Jolla, CA*
- WP 359 **Characterization of Plasma Derived and Recombinant Immunoglobulins G by MALDI Mass Spectrometry;** Omar Belgacem<sup>1</sup>; Emmanuel Raptakis<sup>1</sup>; Andrea Buchacher<sup>2</sup>; Katharina Pock<sup>2</sup>; <sup>1</sup>*Shimadzu Biotech, Manchester, UK*; <sup>2</sup>*Octapharma Pharmazeutika, Vienna, Austria*
- WP 360 **Proteomic Strategies for the Identification of potential Drug Targets within the T Cell mTOR-Raptor Mediated Signal Transduction Pathway;** Christine A. Jelinek<sup>1</sup>; Greg M. Delgoffe<sup>1</sup>; Thomas P. Kole<sup>1</sup>; Dawn Chen<sup>1</sup>; Robert O'meally<sup>3</sup>; Jonathan Powell<sup>1</sup>; Robert J. Cotter<sup>2</sup>; <sup>1</sup>*Johns Hopkins School of Medicine, Baltimore, MD*; <sup>2</sup>*Middle Atlantic Ms Laboratory, Baltimore, MD*; <sup>3</sup>*Johns Hopkins School of Medi, Baltimore, MD*
- WP 361 **De novo Determination of Primary Structure, Sequence Microheterogeneities and N-Linked Glycosylation of an Epitope Specific Anti-Beta-Amyloid Monoclonal Antibody;** Irina Perdivara<sup>1</sup>; Leesa Deterding<sup>1</sup>; Adrian Moise<sup>2</sup>; Kenneth B. Tomer<sup>1</sup>; Michael Przybylski<sup>2</sup>; <sup>1</sup>*Niehs, Rtp, NC*; <sup>2</sup>*University of Konstanz, Konstanz, Germany*
- WP 362 **Identification of HLA Class I-Presented Peptides from Vaccinia Virus By Multi-Dimensional Liquid Chromatography and Tandem Mass Spectrometry;** Kenneth L. Johnson; Inna G. Ovsyannikova; Christopher J. Mason; H. Robert Bergen, III; Gregory A. Poland; *Mayo Clinic, Rochester, MN*
- WP 363 **Characterization of the Epitope Between IL-13 and 13C5 using Surface Plasmon Resonance, Covalent Labeling and Epitope Excision Mass Spectrometry;** Shaun McLoughlin; Yan Chen; Enrico DiGiammarino; Eric Hebert; Suzanne Scesney; Denise Karaoglu-Hanzatian; Laura Miesbauer; Tanveer Ahmed; Robert Johnson; John Harlan; Chengbin Wu; *Abbott Laboratories, Abbott Park, IL*
- WP 364 **Proteomic Characterization of Natural Killer Cell Surface Proteins in the Avian Immune System;** Georgios S. Katselis<sup>1</sup>; Lei Zhang<sup>2</sup>; Ronald M. Goto<sup>2</sup>; Roger E. Moore<sup>1</sup>; Helen Ge<sup>1</sup>; Marcia M. Miller<sup>2</sup>; Terry D. Lee<sup>1</sup>; <sup>1</sup>*Immunology, City of Hope, Duarte, CA*; <sup>2</sup>*Molecular Biology, City of Hope, Duarte, CA*
- WP 365 **Monitoring Chemical Modification of an Antibody using Different LC-MS Approaches;** Eef Dirksen<sup>1</sup>; Arjan Mank<sup>1</sup>; Roland Vulders<sup>2</sup>; Marc Robillard<sup>2</sup>; <sup>1</sup>*Philips Research, MiPlaza, Eindhoven, Netherlands*; <sup>2</sup>*Philips Research, Biomolecular Engineering, Eindhoven, Netherlands*
- WP 366 **Epitope Identification of a Monoclonal Antibody to the H1-Carbohydrate Recognition Domain of the Asialoglycoprotein Receptor;** Raluca Stefanescu<sup>1</sup>; Rita Born<sup>2</sup>; Beat Ernst<sup>2</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*University of Konstanz, Konstanz, Germany*; <sup>2</sup>*Institute of Molecular Pharmacy, Basel, Switzerland*
- WP 367 **MALDI TOF-MS Analysis of High-Mass Impurities in Immunoglobulin G Solution using Kinetic Energy Discrimination with Superconducting Detectors;** Kaori Chiba-Kamoshida; Masahiro Ukibe; Shigetomo Shiki; Yiner Chen; Masataka Ohkubo; *National Institute of Advanced Industrial Science, Tsukuba, JAPAN*
- WP 368 **Mass Spectrometry-Based Characterization of the Role between an ICPF-Related Angiogenic Peptidic Complex and Chronic Wound Healing;** Bart H.J van den Berg<sup>1</sup>; Charles J Matyi<sup>2</sup>; Ashli E Brown<sup>2</sup>; William E. Holmes<sup>3</sup>; Kenneth O Willeford<sup>2</sup>; <sup>1</sup>*College of Veterinary Medicine, Mississippi State, MS*; <sup>2</sup>*Biochemistry and Molecular Biology, Mississippi State, MS*; <sup>3</sup>*Mississippi State Chemical Laboratory, Mississippi State, MS*
- WP 369 **Immuno-Affinity Based Detection of Small GTPases by MALDI TOF MS using Glyco-Affi MALDI Plate;** Rituparna Ghosh<sup>1</sup>; Shambhunath Bose<sup>1</sup>; Mi Kyung Son<sup>2</sup>; Jeong won Seo<sup>2</sup>; Yangsun Kim<sup>1</sup>; Jihee Chang<sup>3</sup>; Heung Bin Lim<sup>3</sup>; <sup>1</sup>*Hudson Surface Technology, Newark, NJ*; <sup>2</sup>*Applied Surface Technology Asia Inc., Suwon, South Korea*; <sup>3</sup>*Dankook University, Yong-in, South Korea*
- WP 370 **Identification of Proteins Present in Circulating Immune Complexes in Patients with Autoimmune Disease;** Leticia Cano<sup>1</sup>; Howard Jaffe<sup>2</sup>; Anil K. Chauhan<sup>3</sup>; Henry M. Fales<sup>1</sup>; <sup>1</sup>*NHLBI, NIH, Bethesda, MD*; <sup>2</sup>*NINDS, NIH, Bethesda, MD*; <sup>3</sup>*ProGen Biologics LLC, Ballwin, MO*
- WP 371 **The Cross-Presented HLA-Peptidome;** Michal Bassani-Sternberg; Arie Admon; *Technion - Israel Institute of Tech, Haifa, Israel*
- WP 372 **The mTOR Signaling Pathway and Its Influence on the MHC Class I Peptide Repertoire;** Marie-Helene Fortier; Etienne Caron; Mathieu Courcelles; Claude Perreault; Pierre Thibault; *IRIC, Universite de Montreal, Montreal, Canada*
- WP 373 **Monoclonal Antibody Degradation: Formation of a Thioether Cross-Link Between Heavy and Light Chains is pH Dependent;** Maggie Huang; Mingfang Hong; Michael Lewis; Michael Bond; Qing Mike Tang; *Centocor - Johnson & Johnson, Radnor, PA*

## WEDNESDAY POSTERS

- WP 374 **The Identification of MHC Class II Peptides Expressed *in vivo* by B-cell Leukemias and Lymphomas**; Andrew Norris<sup>1</sup>; Mark Cobbold<sup>2</sup>; Dina Bai<sup>1</sup>; Michael E. Williams<sup>1</sup>; Victor H. Engelhard<sup>1</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>University of Birmingham, Birmingham, UK
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- DRUG METABOLISM QUANTITATION 2, 375 - 387**
- WP 375 **Stabilization of Troglitazone Extracts with Ascorbic Acid for the LC-MS-MS Analysis of Blood and Plasma Samples**; Bahau Habulihaz; Lawrence Colwell; *Merck Research Laboratories, Rahway, NJ*
- WP 376 ***In vitro* Identification and Quantification of 6 Novel Phase I / Phase II Metabolites of Galangin using Human Liver S9**; Sheng Liu; Susan Dearborn; Sarah Mitchell; Patty Walton; Adrian Sheldon; *Charles River Laboratories Preclinical Services, Shrewsbury, MA*
- WP 377 **Is Standard-Free Quantitation of Metabolites Possible?**; Asoka Ranasinghe; Bogdan Slecza; Jian Wang; Celia Darienzo; Timothy Olah; *Bristol-Myers Squibb Company, Princeton, NJ*
- WP 378 **HPLC-MSMS Assay for Aprepitant: A Case Study Utilizing Mobile Phase Containing Ethylenediaminetetraacetic Acid to Solve Non-Linearity of Calibration Curves**; Cynthia M. Chavez-Eng; Ryan W. Lutz; Marvin L. Constanzer; Eric J. Woolf; *Merck & Co., West Point, PA*
- WP 379 **Studies on the Degradation and Stabilization of 17-Valerate Betamethasone in Rat Serum**; Jie Zhang; Shimin Wei; Weiyi Zheng; Wenkui Li; Tom Smith; Francis Tse; *Novartis Pharmaceuticals Corp, East Hanover, NJ*
- WP 380 **Automated Liquid-Liquid Extraction Method for High-Throughput Analysis of Tolterodine and 5-Hydroxymethyl Tolterodine in Human EDTA Plasma by LC-MS-MS**; Samuel Gu; Nuno Santos; Saleh Hussain; François Vallée; *Anapharm, Richmond Hill, Canada*
- WP 381 **High Throughput Strategies for Metabolite Identification in Drug Discovery Pharmacokinetic Studies**; Yung-Hsiang Chen; Melis Arslan Coraggio; Qin Yue; Patrick J. Rudewicz; *Genentech, Inc., South San Francisco, CA*
- WP 382 **Investigation of Adenosine and Its Precursors and Metabolites in Perfused Mouse Kidneys using LC-SRM**; Jin Ren; Zaichuan Mi; Ek Jackson; *University of Pittsburgh, Pittsburgh, PA*
- WP 383 **Simultaneous Determination of Creatinine, Uric Acid and Its Metabolites in Urine, Plasma and Cell Lysates using Liquid Chromatography-Mass Spectrometry**; Kyung Mee Kim; Xiaosen Ouyang; Reginald F. Frye; Cheryl D. Galloway; Richard J. Johnson; George N. Henderson; *University of Florida, Gainesville, FL*
- WP 384 **UPLC-MS-MS Determination of Cortisol and 6 $\beta$ -Hydroxycortisol in Human Urine – Comparison with HPLC-MS-MS Method**; Yuwen Zhao<sup>1</sup>; Lina Tang<sup>1</sup>; Jamie Zhao<sup>1</sup>; Yuan-Shek Chen<sup>1</sup>; Benjamin Chien<sup>1</sup>; Ken Blakeslee<sup>2</sup>; <sup>1</sup>Quest Pharmaceutical Services, Newark, DE; <sup>2</sup>Waters Corporation, Milford, MA
- WP 385 **Trouble-Shooting Non-specific Binding (NSB) of Analyte in a Quantitative LC-MS-MS Urine Assay**; Wenkui Li; Suyi Luo; Harold T Smith; Francis LS Tse; *Novartis Pharmaceuticals, East Hanover, NJ*
- WP 386 **Selective Removal of Phospholipids from Plasma in LC-MS-Based Quantitative Bioanalysis**; Steven T. Wu<sup>1</sup>; Dale F. Schoener<sup>2</sup>; Mohammed Jemal<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Alta Analytical Laboratory, El Dorado Hills, CA
- WP 387 **Simultaneous Quantitative and Qualitative Measurements of *in vitro* Microsomal Metabolism Assays by Orbitrap LC-MS Methods**; Mustafa Varoglu; Xiaowei He; Scott Coleman; Min Chu; *Cubist Pharmaceuticals, Lexington, MA*
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- DRUG METABOLISM: REACTIVE METABOLITES, 388 - 402**
- WP 388 ***In vitro* Evidence for Formation of Reactive Intermediates of Resveratrol in Human Liver Microsomes**; Rick Steenwyk; Beijing Tan; *Pfizer, Groton, CT*
- WP 389 **Evaluation of Neutral Loss, Precursor Ion Scan and Exact Mass Measurement for Identification and Characterization of GSH-Trapped Reactive Metabolites**; Xavier Czeszak<sup>1</sup>; Valerie Mancel<sup>2</sup>; Alvaro Jesus Cardenas Armesto<sup>1</sup>; Jean-Marie Nicolas<sup>2</sup>; Steven Smith<sup>2</sup>; Claude Delatour<sup>2</sup>; <sup>1</sup>UCB Pharma SA - Research DMPK, Braine l'Alleud, Belgium; <sup>2</sup>UCB Pharma SA - Non-Clinical Development DMPK, Braine l'Alleud, Belgium
- WP 390 **Detection and Characterization of Reactive Metabolites using Ultra-Performance Liquid Chromatography and High Resolution Mass Spectrometry**; Hung-Ysiang Chen; Teresa Dong; Qin Yue; Patrick J. Rudewicz; *Genentech, Inc., South San Francisco, CA*
- WP 391 **Enhanced Duty Cycle on a Hybrid Quadrupole oa-TOF Instrument to Improve the Limit of Detection for Reactive Metabolite Screening**; Jose Castro-Perez<sup>1</sup>; John Shockcor<sup>1</sup>; Kate Yu<sup>1</sup>; Henry Shion<sup>1</sup>; Jeff Goshawk<sup>3</sup>; Kevin Bateman<sup>2</sup>; <sup>1</sup>Waters Corp., Milford, MA; <sup>2</sup>Merck Frosst, Kirkland, Canada; <sup>3</sup>Waters MS Technology Center, Manchester, UK
- WP 392 **Determination of the Hemoglobin Adduct 2-Hydroxyethylvaline by HPLC with Electrospray Ionization and High Resolution Time-of-Flight Mass Spectrometry Quantitation**; Kathy A. Brzak; Fagen Zhang; *The Dow Chemical Company, Midland, MI*
- WP 393 **A High-Throughput Screening of Glutathione Conjugates using Stable-Isotope Labeling and Liquid Chromatography / Negative ESI Precursor Ion Tandem Mass Spectrometry**; Shengkai Liao; Nigel P. Ewing; Brian Boucher; Hong Gao; Olivier Materne; Nagendra Chemuturi; Christopher L Brummel; *Vertex Pharmaceuticals, Inc., Cambridge, MA*
- WP 394 **P450 Bioactivation of Analogs of Fluoro-Iodoaniline Assessed by GSH Trapping Studies: Insight into Mechanism of P450 Oxidation**; Chenghong Zhang; Cornelis Hop; Cyrus Khojasteh; *Genentech, South San Francisco, CA*
- WP 395 **Identification and Characterization of a New Metabolite of Amodiaquine by Electrochemistry On-Line with ESI/MS**; Tove Johansson<sup>1</sup>; Ulrik Jurva<sup>3</sup>; Collen Masimirembwa<sup>2</sup>; <sup>1</sup>Department of Chemistry, Gothenburg, Sweden; <sup>2</sup>African Institute of Biomedical Science & Technolo, Harare, Zimbabwe; <sup>3</sup>Astrazeneca R&d Mölndal, Mölndal, Sweden
- WP 396 **MALDI TOF/TOF Identification of Alkylation Sites in Recombinant Carbonyl Reductase Inactivated by Electrophilic Metabolites of a Lung Tumor Promoter**; Kristofer Fritz; Colin Shearn; Jose Gomez; John A. Thompson; *University of Colorado Health Sciences Center, Denver, CO*

## WEDNESDAY POSTERS

- WP 397 **The Detection and Identification of Unforeseeable Reactive Metabolites: A Strategy to Avoid Missing Metabolites or Their Degradants;** Don Laudicina; *Neurocrine Biosciences, San Diego, CA*
- WP 398 **Mapping of Covalently Modified Peptides by Reactive Metabolites from Liver Microsomal Proteins;** Manuel Tzourros; Axel Paehler; F. Hoffmann-La Roche, Ltd., Basel, Switzerland
- WP 399 **Combining NanoESI LC-MS with Fraction Collection and MS<sup>n</sup> Experiments to Assess Bioactivated Electrophiles by Glutathione Trapping;** Geoffrey S. Rule<sup>1</sup>; Laurance Lee<sup>2</sup>; Yan Chen<sup>2</sup>; Chenghong Zhang<sup>3</sup>; Cyrus Khojasteh<sup>3</sup>; <sup>1</sup>Advion BioSystems, Ithaca, NY; <sup>2</sup>Thermo Fisher Scientific, Inc., San Jose, CA; <sup>3</sup>Genentech, Inc., South San Francisco, CA
- WP 400 **An Algorithm for Thorough Background Subtraction from High Resolution LC-MS Data: Application to Unbiased Detection of Glutathione-Trapped Reactive Metabolites;** Haiying Zhang<sup>4</sup>; Yanou Yang<sup>2</sup>; Li Ma<sup>3</sup>; Kan He<sup>3</sup>; Mingshe Zhu<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol Myers Squibb, Pennington, NJ; <sup>3</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>4</sup>Bristol-Myers Squibb R&d, Pennington, NJ
- WP 401 **Comparative Analysis of QQQ/LIT Scan Modes for *in vitro* GSH Assessment and Screening for Reactive Metabolites;** Claire Bramwell-German<sup>1</sup>; Hua-Fen Liu<sup>1</sup>; Jennie Lill<sup>2</sup>; Elliott Jones<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Genentech Inc, South San Francisco, CA
- WP 402 **Identification of Stable Oxidative Metabolites and Iminium Ion Reactive Intermediates using High Mass Accuracy MS<sup>n</sup> Analysis;** Masatoshi Takahashi<sup>1</sup>; Ichiro Hirano<sup>2</sup>; Simon Ashton<sup>3</sup>; John Warrander<sup>3</sup>; Neil Loftus<sup>3</sup>; <sup>1</sup>Shimadzu Scientific, Columbia, MA; <sup>2</sup>Shimadzu Corporation, Tokyo, JAPAN; <sup>3</sup>Shimadzu, Manchester, UK
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- PTMs – SULFATION, NTRATION AND STRATEGIES, 403 - 418**
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- WP 403 **Characterization of Tyrosine Sulfation for Chemokine Receptor Peptides;** Connie Jen; Julie A. Leary; *UC Davis, Davis, CA*
- WP 404 **Proteome Profiling using an Integrated Top-Down and Bottom-Up Strategy;** Si Wu<sup>1</sup>; Natacha M. Lourette<sup>1</sup>; Rui Zhao<sup>1</sup>; Nikola Tolic<sup>1</sup>; Nathan P. Manes<sup>1</sup>; Ryan D. Estep<sup>2</sup>; Scott W. Wang<sup>2</sup>; Joshua N. Adkins<sup>1</sup>; Richard D. Smith<sup>1</sup>; Ljiljana Pasa-Tolic<sup>1</sup>; <sup>1</sup>PNNL, Richland, WA; <sup>2</sup>OHSU, Portland, OR
- WP 405 **Metal Oxide-Based Enrichment of Sulfated Peptides and Sulfated Oligosaccharides;** Yibing Kong; Wen Zhou; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WP 406 **NitroDIGE: A New Method to Investigate the Subproteome of the S-Nitrosylated Proteins in Neurological Diseases;** Fanjun Meng; Zezong Gu; *Univ. Missouri-Columbia School of Medicine, Columbia, MO*
- WP 407 **Structural Characterization of Intact Proteins by Complementary LC-MS Linear Ion Trap Mass Spectrometry;** Kiyonaga Fujii<sup>1</sup>; Shingo Nakamura<sup>1</sup>; Kazuya Honbou<sup>1</sup>; Kiyohiro Takahashi<sup>1</sup>; Toshihide Nishimura<sup>2</sup>; Fuyuhiko Inagaki<sup>1</sup>; <sup>1</sup>Hokkaido University, Sapporo, JAPAN; <sup>2</sup>Tokyo Medical University, Tokyo, JAPAN
- WP 408 **Top Down Proteomic Study of Human Salivary Proteins using LTQ-Orbitrap;** Xuemei Han<sup>1</sup>; Tao Xu<sup>1</sup>; Aaron Aslanian<sup>2</sup>; Fred K. Hagen<sup>3</sup>; John Yates<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Salk Institute, La Jolla, CA; <sup>3</sup>University of Rochester Medical Center, Rochester, NY
- WP 409 **Automated 1D to 6D Multi-Dimensional LC Separation of Proteins and Peptides Prior to Analysis by Mass Spectrometry For Functional Proteomics;** Peter Kent<sup>1</sup>; Kerry Nugent<sup>2</sup>; Laurence M. Brill<sup>3</sup>; <sup>1</sup>Michrom Bioresources, Auburn, CA; <sup>2</sup>Michrom Bioresources, Inc., Auburn, CA; <sup>3</sup>Burnham Inst For Med Res, La Jolla, CA
- WP 410 **Use of a Data-Independent Acquisition Strategy with Dual Stages of Fragmentation for PTM Characterization;** Craig Dorschel<sup>1,3</sup>; Kevin Blackburn<sup>2</sup>; Scott Geromanos<sup>13</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>North Carolina State University, Raleigh, NC; <sup>3</sup>Waters Corporation, Milford, MA
- WP 411 **An integrated Computational and Experimental Approach to Characterize the extracellular Proteome from a natural Extremophilic Microbial Community;** Brian Erickson<sup>1</sup>; Nathan C. Verberkmoes<sup>2</sup>; Manesh Shah<sup>2</sup>; Steven Singer<sup>3</sup>; Michael Thelen<sup>3</sup>; Jill Banfield<sup>4</sup>; Robert Hettich<sup>2</sup>; <sup>1</sup>University of Tennessee - Oak Ridge National Lab, Knoxville, TN; <sup>2</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>3</sup>Lawrence Livermore National Laboratory, Livermore, CA; <sup>4</sup>University of California, Berkeley, CA
- WP 412 **Identification and Characterization of 3-Nitrotyrosine Modified Proteins in Cerebrospinal Fluid;** Ashley Beasley; Avindra Nath; Robert J. Cotter; *Johns Hopkins University School of Medicine, Baltimore, MD*
- WP 413 **Development of a Mass Spectrometric Method for the Identification and Characterization of HNO-induced Cysteine Nitroxilation on Platelet Proteins;** Michael D. Hoffman; Geraldine M. Walsh; Dana V. Devine; **Juergen KasT**; *University of British Columb, Vancouver, Canada*
- WP 414 **Assessing Dynamic Change of Protein S-Nitrosylation by Label-Free Quantitative Proteomics;** Yi-Ju Chen; Hsiao-Chiao Chou; Wei-Chi Ku; Yu-Ju Chen; *Institute of Chemistry, Academia Sinica, Taipei, Taiwan*
- WP 415 **Identification of Oxidative Stress Induced Post-Translational Modifications via an Intact Protein Separation Space;** Mark E. Mccomb; David H. Perlman; Wantao Ying; Claire Dauly; Giuseppe Infusini; Weiwei Tong; James West; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- WP 416 **First Round and Second Round Search Engines for Analyzing Post-Translational Modifications Such as Phosphorylation;** Martin Blueggel<sup>1</sup>; L M Freimark<sup>3</sup>; R J Shaw<sup>2</sup>; D Chamrad<sup>1</sup>; R Garretson<sup>4</sup>; J M Asara<sup>3</sup>; <sup>1</sup>Protagen AG, Dortmund, GERMANY; <sup>2</sup>The Salk Institute for Biological Studies, San Diego, CA; <sup>3</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>4</sup>Protagen Inc., Chester, NJ
- WP 417 **The Development and Evaluation of Protein Standards for the Analysis of Tyrosine Nitration and 4-Hydroxynonenal Modifications in Human Plasma;** Bensheng Li; Birgit Schilling; Jason Held; Emily A. Gaman; Bradford W. Gibson; *Buck Institute For Age Research, Novato, CA*
- WP 418 **Improved Validation Protocol for Identification of Peptide Modifications using MS-MS Spectra Based on Detailed Investigation of *in vivo* Tyrosine Nitration;** Stanley M. Stevens, Jr.; Katalin Prokai-Tatrai; **Laszlo Prokai**; *University of North Texas Health Science Center, Fort Worth, TX*



## WEDNESDAY POSTERS

- PHOSPHO-PROTEOMICS, 419 - 452**
- WP 419 **An Integrated Workflow for Identification and Quantitation of Intact Phosphoproteins;** Ljiljana Pasa-Tolic<sup>1</sup>; Si Wu<sup>1</sup>; Feng Yang<sup>1</sup>; Rui Zhao<sup>1</sup>; Natacha M. Lourette<sup>1</sup>; Nikola Tolic<sup>1</sup>; Kim K. Hixson<sup>1</sup>; Stephen J. Callister<sup>1</sup>; Samuel Kaplan<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific NW Nat'l Lab, Richland, WA*; <sup>2</sup>*UT-Houston Medical School, Houston, Texas*
- WP 420 **Protein Phosphorylation Changes in Human Microvascular Endothelial Cells Induced by cigarette Smoke Exposure;** Jason W. Flora; Jeffery S. Edmiston; Timothy Britt Langston; Gaurav S.J.B. Rana; Rebecca R. Secrist; Willie J. McKinney; *Philip Morris USA, Richmond, VA*
- WP 421 **Differential Phosphotyrosine-dependent Signaling by Neurotrophins Analyzed via Primary Neuronal SILAC;** Daniel S. Spellman<sup>1</sup>; Catia C. Proenca<sup>2</sup>; Katrin Deinhardt<sup>1</sup>; Francis S. Lee<sup>2</sup>; Moses V. Chao<sup>1</sup>; Thomas A. Neubert<sup>1</sup>; <sup>1</sup>*Skirball Institute, NYU School of Medicine, New York, NY*; <sup>2</sup>*Weill Medical College of Cornell University, New York, NY*
- WP 422 **Mitochondrial Phosphoproteome;** Angel Aponte<sup>1</sup>; Darci Phillips<sup>2</sup>; Ksenia Blinova<sup>2</sup>; Stephanie French<sup>2</sup>; Robert S. Balaban<sup>2</sup>; <sup>1</sup>*NHLBI, Proteomics Core Facility, NIH, Bethesda, MD*; <sup>2</sup>*NHLBI, Laboratory of Cardiac Energetics, NIH, Bethesda, MD*
- WP 423 **Quantitative Phosphoproteome Analysis Applied to the Human Neural Stem Cell;** Kun Cho<sup>1</sup>; Eunmin Kim<sup>1</sup>; Gun Wook Park<sup>1</sup>; Jeong Hwa Lee<sup>1</sup>; Yeong Hee Ahn<sup>1</sup>; Kyung-Hoon Kwon<sup>1</sup>; Jin Young Kim<sup>1</sup>; Kyung Hee Byun<sup>2</sup>; Bong Hee Lee<sup>2</sup>; Jong Shin Yoo<sup>1</sup>; <sup>1</sup>*Korea Basic Science Institute, Daejeon, South Korea*; <sup>2</sup>*Gachon University Medical Center, Incheon, South Korea*
- WP 424 **Analysis by Blue Native PAGE and Mass Spectrometry of Protein-Protein Interactions within EphB2-NG108 Cells in Response to EphrinB1-Fc Stimulation;** Costel Darie<sup>1</sup>; Daniel Spellman<sup>2</sup>; Guoan Zhang<sup>3</sup>; Vivekananda Shetty<sup>3</sup>; Thomas Neubert<sup>4</sup>; <sup>1</sup>*Skirball Institute/New York University, New York, NY*; <sup>2</sup>*New York University School, New York, NY*; <sup>3</sup>*New York University, New York, NY*; <sup>4</sup>*Skirball Institute, Nymc, New York, NY*; <sup>5</sup>*Immunotope, Inc., Doylestown, PA*
- WP 425 **Hydroxy Acid-Modified Metal Oxide Chromatography (HAMMOC) for Plant Phosphoproteomics;** Naoyuki Sugiyama; Sumiko Ohnuma; Yutaka Kyono; Masaru Tomita; Yasushi Ishihama; *Keio University, Tsuruoka, Japan*
- WP 426 **Development of a Phosphoproteomics Approach to Study GPCR-Mediated Signaling Events in a Human Prostate Carcinoma Cell Line;** Heike Piechura<sup>1</sup>; Sebastian Wiese<sup>2</sup>; Eva M. Neuhaus<sup>2</sup>; Hanns H. Hatt<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Bettina Warscheid<sup>1</sup>; <sup>1</sup>*Medizinisches Proteom-Center, Ruhr-Universität, Bochum, Germany*; <sup>2</sup>*Department of Cell Physiology, Ruhr-Universität, Bochum, Germany*
- WP 427 **SEMI-Quantitation Strategy for Label-Free Quantitative Profiling of Phosphoproteome in Lung Cancer of Different Invasive Potential;** Yi Ting Wang<sup>1</sup>; Chia-feng Tsai<sup>1</sup>; Pei-Yi Lin<sup>1</sup>; Tzu-Chan Hong<sup>4</sup>; Chih-Chiang Tsou<sup>2</sup>; Wen-Lian Hsu<sup>2</sup>; Ting-Yi Sung<sup>2</sup>; Tse-Ming Hong<sup>3</sup>; Pan-Chyr Yang<sup>4</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Institute of information, science, Academia Sinica, Taipei, Taiwan*; <sup>3</sup>*Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan*; <sup>4</sup>*Department of Internal Medicine, NTU, Taipei, Taiwan*
- WP 428 **Phosphoproteome Analysis of Trastuzumab (Herceptin) Resistant Breast Cancer Cells by Electron Transfer Dissociation Mass Spectrometry;** Li-Rong Yu<sup>1</sup>; Zhongyu Zhu<sup>2</sup>; Ricky D. Holland<sup>1</sup>; Dimiter S. Dimitrov<sup>2</sup>; <sup>1</sup>*National Center for Toxicological Research, FDA, Jefferson, AR*; <sup>2</sup>*Nanobiology Program, NCI-Frederick, Frederick, MD*
- WP 429 **Phosphorylation of Transmembrane Proteins in Plants in Response to Two Different Nitrogen Stimuli;** Wolfgang Engelsberger; Waltraud Schulze; *Mpi F. Molecular Plantphysio, Potsdam, Germany*
- WP 430 **Phosphoproteomic Analysis of Human Glioma Cells using Titanium Dioxide Enrichment and Mass Spectrometry;** Li-Rong Yu<sup>1</sup>; Luke H. Stockwin<sup>2</sup>; Dianne L. Newton<sup>2</sup>; Timothy D. Veenstra<sup>2</sup>; <sup>1</sup>*National Center for Toxicological Research, FDA, Jefferson, AR*; <sup>2</sup>*SAIC-Frederick, Inc., NCI-Frederick, Frederick, MD*
- WP 431 **Tenderness of Fresh Lamb Correlates with Phosphorylation of Key Structural Proteins in the Sarcomere;** Christopher J. Buck; Angus Tester; Matthew McDonagh; *Biosciences Research Division, DPI Victoria, Melbourne, Australia*
- WP 432 **Changes in Arabidopsis Phosphorylation during Drought Response: Quantitative Phosphoproteomics via Metabolic Labeling;** Gregory A. Barrett-Wilt<sup>1</sup>; Edward L. Huttlin<sup>1</sup>; Amy C. Harms<sup>2</sup>; Michael R. Sussman<sup>1</sup>; <sup>1</sup>*University of Wisconsin Department of Biochemistry, Madison, WI*; <sup>2</sup>*University of Wisconsin Biotechnology Center, Madison, WI*
- WP 433 **Enrichment of Phosphopeptides at Low pH using Phos SpinTrap Fe;** Ann-Marie Nissfolk; Johan Ohman; Gabriella Risberg; Marianne Albenius; Marika Sjobahl; *GE Healthcare Bio-Sciences AB, Uppsala, Sweden*
- WP 434 **A Tandem Phosphoprotein / Phosphopeptide Enrichment Strategy for the Characterization of Signaling Proteins in Chronic Lymphocytic Leukemia;** Liwen Wang; Raj Muthusamy; Michael A. Freitas; John C. Byrd; *Ohio State University, Columbus, OH*
- WP 435 **Phosphoproteomic Approaches to Profiling of T-lymphocytes Activated via beta-2 integrins;** Erol E. Gulcicek; Christopher M. Colangelo; Kathryn L. Stone; Kenneth R. Williams; Jeffrey R. Bender; Mark Collinge; *Yale University, New Haven, CT*
- WP 436 **Analyzing Phosphorylation Patterns in Human Platelets;** René P. Zahedi<sup>1</sup>; Urs Lewandrowski<sup>1</sup>; Julia Wiesner<sup>1</sup>; Stepan Gambaryan<sup>2</sup>; Albert Sickmann<sup>1</sup>; <sup>1</sup>*Rudolf Virchow Center for Experimental Biomedicine, Wuerzburg, Germany*; <sup>2</sup>*University of Wuerzburg, Wuerzburg, Germany*
- WP 437 **Quantitative Proteomics Reveals Stoichiometric Changes in Phosphorylation in the mTOR Pathway Following Mitogenic Stimulation;** Audrey Carriere; Carnello Marie; Louis-Andre Julien; Huanhuan Gao; Eric Bonneil; Pierre Thibault; Philippe Roux; *IRIC-Universite de Montreal, Montreal, QC, Canada*
- WP 438 **A Quantitative Approach towards the Phosphoproteome of Osmotically Challenged Yeast Cells;** Ilse Dohnal<sup>1</sup>; Dorothea Anrather<sup>2</sup>; Jiri Veis<sup>2</sup>; Christoph Stingl<sup>3</sup>; Karin Grosstessner-Hain<sup>3</sup>; Karl Mechtler<sup>3</sup>; Gustav Ammerer<sup>1</sup>; <sup>1</sup>*Christian Doppler Laboratory for Proteome Analysis, Vienna, Austria*; <sup>2</sup>*University of Vienna, Vienna, Austria*; <sup>3</sup>*Research Institute for Molecular Pathology, Vienna, Austria*
- WP 439 **Phosphotyrosine Profiling in Lung Cancer Cell Lines;** Bin Fang<sup>1</sup>; Jiannong Li<sup>1</sup>; Jingchun Gao<sup>1</sup>; Guolin



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- Zhang<sup>1</sup>; Arthur Edwards<sup>1</sup>; John Koomen<sup>2</sup>; Eric Haura<sup>1</sup>; <sup>1</sup>*H. Lee Moffitt Cancer Center, Tampa, FL*; <sup>2</sup>*H. Lee Moffitt Cancer Center, Tampa, FL*
- WP 440 **Screening for EphB signaling Effectors using SILAC and a Hybrid Linear Ion Trap-Orbitrap Mass Spectrometer**; Guoan Zhang<sup>1</sup>; David Fenyo<sup>2</sup>; Thomas A. Neubert<sup>1</sup>; <sup>1</sup>*New York University, New York, NY*; <sup>2</sup>*The Rockefeller University, New York, NY*
- WP 441 **A See-and-Catch Strategy for Studying Dynamics of Molecular Assemblies in Cells with Fluorescence Microscopy and Mass Spectrometry**; Changhui Deng; Andrew Krutchinsky; *UCSF, San Francisco, CA*
- WP 442 **Changes in the PTM Profile of the MRN Complex in Response to DNA Double Strand Breaks**; Andrea M De Santis<sup>1</sup>; Karen M. Cersaletti<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; Patrick Concannon<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, VA*; <sup>2</sup>*Benaroya Research Institute, Seattle, WA*
- WP 443 **Quantitative Phosphoproteomics for Identification of Factors Controlling Osteoblast Differentiation of Human Mesenchymal Stem Cells**; Kristoffer T. G. Rigbolt; Blagoy Blagoev; *University of Southern Denmark, Odense, Denmark*
- WP 444 **Defining the Dynamic Phosphoproteome during *Xenopus Laevis* Development by electron Transfer Dissociation (ETD) Mass Spectrometry**; Jered V. Mcgivern; Michael D. Sheets; *UW-Madison BMC, Madison, WI*
- WP 445 **Phosphoproteomics Analysis of Cellular Proteins in Response to *Helicobacter Pylori***; Chih-Jie Chang<sup>1</sup>; Li-Chia Yang<sup>1</sup>; Sung-Fang Chen<sup>2</sup>; Lu-Ping Chow<sup>1</sup>; <sup>1</sup>*Institute of Biochemistry, Taipei, Taiwan*; <sup>2</sup>*Biomedical engineering center, Hsinchu, Taiwan*
- WP 446 **Phosphoproteome Analysis of *Drosophila melanogaster* Embryos**; Bo Zhai; Judit Villen; Sean Beausoleil; Julian Mintseris; Steven Gygi; *Department of Cell Biology, Harvard Medical School, Boston, MA*
- WP 447 **Proteomics Analysis of Early Signaling Events in Response to Ordered Tyrosine Phosphorylation in PDGFR**; Allen W. Tsang; Revati Wani; Cristina M. Furdulj; *Wake Forest University School of Medicine, Winston Salem, NC*
- WP 448 **Quantitative Phosphoproteomics of Depolarization-Dependent Protein Phosphorylation in Nerve Terminals**; Martin R. Larsen<sup>1</sup>; Mark Graham<sup>2</sup>; Phillip J. Robinson<sup>2</sup>; <sup>1</sup>*Univ. Southern Denmark, Odense, DENMARK*; <sup>2</sup>*Childrens Medical Research Institute (CMRI), westmade, Sydney, Australia*
- WP 449 **Monitoring Phosphorylation Sites using LC/MRM/MS-MS: Trials and Tribulations of Targeting Biologically Important but Poorly Ionized Phosphopeptides**; Lorne E. B. Taylor<sup>1</sup>; Andreas Traweger<sup>1</sup>; Brett Larsen<sup>1</sup>; David Cox<sup>2</sup>; Stephen A Tate<sup>2</sup>; Tony Pawson<sup>1</sup>; <sup>1</sup>*Samuel Lunenfeld Research Institute, Toronto, Canada*; <sup>2</sup>*MDS Sciex, Concord, ON*
- WP 450 **The Phosphoproteome of Human Primary T-Lymphocytes: A Database Creation**; Montserrat Carrascal; Vanessa Casas; David Ovelheiro; Marina Gay; Joaquín Abian; *IIBB-CSIC, Barcelona, SPAIN*
- WP 451 **Investigation of Phosphoproteome of Human Skeletal Muscle by Global and Targeted HPLC-ESI-MS-MS**; Zhengping Yi<sup>1</sup>; Benjamin Bowen<sup>1</sup>; Hyonson Hwang<sup>1</sup>; Natalie Lefort<sup>1</sup>; Kurt Højlund<sup>2</sup>; Charles R. Flynn<sup>1</sup>; Elena De Filippis<sup>1</sup>; Christian Meyer<sup>1</sup>; Lawrence J. Mandarino<sup>1</sup>; <sup>1</sup>*Arizona state university, Tempe, AZ*; <sup>2</sup>*Odense University Hospital, Odense, Denmark*
- WP 452 **Profiling of mTOR Phosphorylation Pathway in Rat Liver using Mass Spectrometry**; Gokhan Demirkan; Arthur Salomon; Philip Gruppuso; *Brown University, Providence, RI*
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- PROTEINS: GLYCOPROTEINS, 453 - 479**
- WP 453 **The Comparative Profiling of Glycosylation in a mouse Model of Human Ovarian Endometrioid Adenocarcinoma Based on Genetic Defects using MALDI-QIT-TOF-MS**; Hyeveung Kim<sup>1</sup>; Fan Xiang<sup>2</sup>; Kathleen R. Cho<sup>3</sup>; Rong Wu<sup>3</sup>; David M. Lubman<sup>4</sup>; <sup>1</sup>*Department of Chemistry, University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Shimadzu Biotech, Pleasanton, CA*; <sup>3</sup>*Department of Pathology, University of Michigan, Ann Arbor, MI*; <sup>4</sup>*Department of Surgery, University of Michigan, Ann Arbor, MI*
- WP 454 **Purification and Characterization of a Therapeutic Monoclonal Antibody from Patient Serum Samples**; Camille Strachan; Mike Bond; Mike Lewis; Qing Tang; *Centocor R&D, Radnor, PA*
- WP 455 **Extension of Microwave-Accelerated Residue-Specific Acid Cleavage to Glycoproteins**; Jinxi Li<sup>1</sup>; Kevin J. Shefcheck<sup>2</sup>; John H. Callahan<sup>2</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>*University of Maryland, College Park, MD*; <sup>2</sup>*FDA/CFSAN, College Park, MD*
- WP 456 **Characterization of Isolated Glycans via MALDI Mass Spectrometry using the New Matrix 1,5-DAN**; Susanne Mette; Stephanie Felske-Mueller; Nicola Klare; Andreas Wattenberg; *Protagen AG, Dortmund, Germany*
- WP 457 **Glycoproteomics of the Protozoan *Toxoplasma Gondii* using Serial Lectin Affinity Chromatography and Tandem Mass Spectrometry**; Qilie Luo; Sam H Zhang; Edward Nieves; Louis Weiss; Ruth H Angeletti; *Albert Einstein College of Medicine, Bronx, NY*
- WP 458 **Effect of Metal Cations on Non-Enzymatic Glycation in Human Serum Albumin**; Zheling Zhang; David H. Powell; Nicolas Polfer; *University of Florida, Gainesville, FL*
- WP 459 **The Nature of Glycosylation in the Yeast *Kluyveromyces lactis***; Catherine L. Swaim; Michelle L. Cushing; Lauren Fields; Julie Canovas; Christopher H. Taron; Jack S. Benner; *New England BioLabs, Ipswich, MA*
- WP 460 **Analysis of IgA1 N-glycans towards Understanding Their Role in Binding Fc receptor FcαRI**; Stephanie B. Wall<sup>1</sup>; Michelle M. Gomes<sup>2</sup>; Jan Novak<sup>1</sup>; Andrew B. Herr<sup>2</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*University of Cincinnati College of Medicine, Cincinnati, OH*
- WP 461 **Probing the Effect of Glycosylation on IgG Conformation using controlled Proteolysis and LC-MS Analysis**; Himanshu Gadgil; Kimberly Westland; Gary Pipes; Michale Treuheit; Bruce Kerwin; *Amgen, Thousand Oaks, WA*
- WP 462 **Effectiveness of Glycoprotein Enrichment by Lectin Affinity Chromatography**; Milan Madera<sup>2</sup>; Benjamin Mann<sup>1</sup>; Yehia Mechref<sup>2</sup>; Milos Novotny<sup>2</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*National Center for Glycomics and Glycoproteomics, Bloomington, IN*
- WP 463 **Mass Spectrometry-Based Analysis of HIV-1 Envelope Protein Glycosylation Profiles and its Correlation with Envelope Immunogenicity**; Eden P. Go<sup>1</sup>; Janet Irungu<sup>1</sup>; Ying Zhang<sup>1</sup>; Dilusha S. Dalpathado<sup>1</sup>; Qing Chang<sup>1</sup>; Hua-Xin Liao<sup>2</sup>; Laura L. Sutherland<sup>2</sup>; S. Munir Alam<sup>2</sup>; Barton F. Haynes<sup>2</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>*Chemistry Department of University*

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- of Kansas, Lawrence, KS; <sup>2</sup>Duke University Medical Center, Durham, NC
- WP 464 **Comparative Studies of Protein Glycosylation using Isotope Labeling and Electrospray Linear Ion Trap Mass Spectrometry;** Zhi-Yu Lin; Guor-Rong Her; National Taiwan University, Taipei, TAIWAN
- WP 465 **Characterization of the Glycosylation Pattern of Therapeutic Antibodies using a Centrifugal Microfluidic Platform in Combination with MALDI-MS Detection;** Thuy T Tran; Gunnar E Thorsén; Department of Analytical Chemistry, Stockholm, Sweden
- WP 466 **Analysis of E-Cadherin Mediated Cell-Cell Adhesion;** Krystyn Blackmon-Ross<sup>1</sup>; Mihai Nita-Lazar<sup>2</sup>; Maria A. Kukuruzinska<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>BU School of Medicine, Boston, MA; <sup>2</sup>BU Goldman School of Dental Medicine, Boston, MA
- WP 467 **Characterization of Recombinant Bovine Trypsin Derived from Transgenic Maize and Elucidation of Its Oligosaccharide Composition;** Pegah Jalili; Gordon Nicol; Janet Irungu; Kevin Ray; Sigma-Aldrich, St. Louis, MO
- WP 468 **Effort of Glycosylation on Ca<sup>2+</sup>-dependent Human Serum Amyloid P using Mass Spectrometry;** Jiaxi Wang; Kirk Green; Brian McCarry; MRCMS, McMaster University, Hamilton, Canada
- WP 469 **Profiling Protein Specific-Changes in Glycosylation in Human Milk by MALDI-FTICR Mass Spectrometry;** Mariana Barboza; John Froehlich; Carlito Lebrilla; University of California, Davis, CA
- WP 470 **A Methodology for the Analysis of Temporal Changes in the Composition of N-Linked Glycans in Human Milk using HPLC-Chip/TOF MS;** Larry Lerno<sup>1</sup>; Richard Seipert<sup>1</sup>; Rudolf Grimm<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 471 **Differences in N-Linked Carbohydrates of the Simian Immunodeficiency Virus Envelope Protein (gp120) are Associated with Progression to Neurological Disease;** David R Graham; Johns Hopkins University, Baltimore, MD
- WP 472 **Process Optimization for Magnetic Beads Purification of Glycoproteins;** Ulrike Schweiger-Hufnagel<sup>1</sup>; Arndt Asperger<sup>1</sup>; Stefan Weise<sup>3</sup>; Katrin Sparbier<sup>1</sup>; Irina Kessler<sup>1</sup>; Markus Kostrzewa<sup>1</sup>; Jonathan Wilson<sup>2</sup>; Carsten Baessmann<sup>1</sup>; Peter Hufnagel<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Protagen AG, Dortmund, Germany
- WP 473 **Structural Characterization of a Renal Biomarker NGAL;** Cheng Zhao; Carol Ramsay; Panfilo Ozaeta; Jeffrey Fishpaugh; Kevin Rupprecht; Abbott Laboratories, Abbott Park, IL
- WP 474 **Dynamic Glycosylation of Human Milk Proteins;** John Froehlich; Eric D. Dodds; Richard Seipert; Mariana Barboza; Carlito Lebrilla; University of California, Davis, California
- WP 475 **A Comprehensive Strategy to Characterize N-, O-Glycans and Glycoproteins;** HUI ZHOU<sup>1</sup>; Yunping Huang<sup>2</sup>; Mei Lin<sup>2</sup>; Michael Grace<sup>2</sup>; David Ashline<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>University of New Hampshire, Durham, NH; <sup>2</sup>Bristol-myers Squibb Company, Pennington, NJ
- WP 476 **The Ion Trap; Critical Component for a Comprehensive Evaluation of Metastatic Glycan Biomarkers;** Vernon N. Reinhold; Justin M Prien; David Ashline; Anthony Lapadula; University of New Hampshire, Durham, NH
- WP 477 **Glycoprotein Discovery in a Gram-Negative Pathogenic Bacterium *Francisella tularensis* through Two-Dimensional Electrophoresis, Lectin Affinity, and Mass Spectrometry Approaches;** Lucie Balonova<sup>1</sup>; Lenka Hernychova<sup>1</sup>; Jiri Stulik<sup>1</sup>; Zuzana Bilkova<sup>2</sup>; William R. Alley<sup>3</sup>; Milos V. Novotny<sup>3</sup>; <sup>1</sup>University of Defence, Hradec Kralove, Czech Republic; <sup>2</sup>University of Pardubice, Pardubice, Czech Republic; <sup>3</sup>Indiana University, Bloomington, IN
- WP 478 **Structural Analysis of the Outer-Core of *Yersinia enterocolitica* O:9 Lipopolysaccharide using Glycoengineering and Mass Spectrometry;** Messele A. Fentabil; Jeremmy Iwashkiw; Amirreza Faridmoayer; Mario F. Feldman; John S. Klassen; University of Alberta, Edmonton, Canada
- WP 479 **Quantitation of the cardiac Glycoproteome using iTRAQ;** Jennifer E. Grant<sup>1</sup>; Amy D. Bradshaw<sup>2</sup>; John H. Schwacke<sup>3</sup>; Catalin F. Baicu<sup>2</sup>; Michael R. Zile<sup>2</sup>; Kevin L. Schey<sup>1</sup>; <sup>1</sup>Dept. of Cell and Mol. Pharmacology, MUSC, Charleston, SC; <sup>2</sup>Cardiology Division, Dept. of Medicine, MUSC, Charleston, SC; <sup>3</sup>Dept. of Biostatistics and Bioinformatics, MUSC, Charleston, SC
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- PROTEIN CONFORMATION HD EXCHANGE 1, 480 - 498**
- WP 480 **Hydrogen exchange Shows That Phosphorylation of c-Abl Tyr 89 Disrupts Downregulatory Intramolecular Interactions;** Shugui Chen<sup>1</sup>; Thomas E Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA
- WP 481 **Mg<sup>2+</sup> Concentration-Dependence of 70S Ribosomal-Protein Dynamics Revealed by H/D Exchange and Mass Spectrometry;** Tatsuya Yamamoto; Yoshitsugu Shiro; RIKEN, Sayo-gun, Japan
- WP 482 **Development of a Structure Based Assay for Characterization of Synthetic Rexinoids by Use of Hydrogen Deuterium Exchange Mass Spectrometry;** LeeAnn J. Boerma; Gang Xia; Sebyung Kang; Donald Muccio; Matthew B. Renfrow; UAB at Birmingham, Birmingham, AL
- WP 483 **Probing Conformational Dynamics of PEGylated Proteins with Hydrogen/Deuterium Exchange and Mass Spectrometry;** Rinat R. Abzalimov; Igor A. Kaltashov; University of Massachusetts, Amherst, MA
- WP 484 **Identification of the Oligomerization Surface of the gp3 Subunit of the Bacteriophage P22 using Hydrogen Exchange;** Lisa M. Jones<sup>1</sup>; Daniel Nemecek<sup>2</sup>; Matthew B. Renfrow<sup>1</sup>; George J. Thomas, Jr.<sup>2</sup>; Peter E. Prevelige, Jr.<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Missouri-Kansas City, Kansas City, Missouri
- WP 485 **Conformational Changes in HIV Nef upon Myristoylation as Determined by Hydrogen Exchange Mass Spectrometry;** Chris R. Morgan<sup>1</sup>; Purushottam Narute<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA
- WP 486 **The Effects of Mutation and Inhibitor Binding on Abl kinase Conformation by Hydrogen Deuterium Exchange Mass Spectrometry;** Roxana E. Iacob<sup>1</sup>; Teodora Pene-Dumitrescu<sup>2</sup>; Nathanael S. Gray<sup>3</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>4</sup>; <sup>1</sup>Barnett Institute, NEU, Boston, MA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA; <sup>3</sup>Dana-Farber Cancer Institute, Harvard Medical, Boston, MA; <sup>4</sup>Northeastern University, Boston, MA

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- WP 487 **Characterization of the Modular Organization of p47phox by Hydrogen/Deuterium Exchange;** Julien Marcoux<sup>1</sup>; Petr Man<sup>1</sup>; Corinne Vives<sup>2</sup>; Franck Fieschi<sup>2</sup>; Eric Forest<sup>1</sup>; <sup>1</sup>LSMP - Institut de Biologie Structurale, Grenoble, France; <sup>2</sup>LPM - Institut de Biologie Structurale, Grenoble, France
- WP 488 **Conformational Analysis of the HIV-1 Viral Infectivity Factor (Vif) Protein using Hydrogen Exchange Mass Spectrometry;** Sean R. Marcisin<sup>1</sup>; Dana Gabuzda<sup>2</sup>; K.S. Rajendran<sup>2</sup>; Andrew J. Brazier<sup>2</sup>; John Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA
- WP 489 **Local Unfolding of hWT and Three ALS-mutant SOD1 Apoproteins at Physiological Temperatures Monitored by Hydrogen/Deuterium Exchange Mass Spectrometry;** Armando Durazo<sup>1</sup>; Bryan F. Shaw<sup>4</sup>; Madhuri Chattopadhyay<sup>1</sup>; Julian Whitelegge<sup>2</sup>; Kym Faull<sup>3</sup>; Joan S. Valentine<sup>1</sup>; <sup>1</sup>UCLA Chemistry, Los Angeles, CA; <sup>2</sup>University of California La, Los Angeles, CA; <sup>3</sup>Ucla, Los Angeles, CA; <sup>4</sup>Harvard University, Cambridge, MA
- WP 490 **Structural Investigation of C-Kit Tyrosine Kinase by Hydrogen/Deuterium Exchange Coupled with FT-ICR Mass Spectrometry;** Huimin Zhang<sup>1</sup>; Xiu Yu<sup>2</sup>; Michael Greig<sup>2</sup>; Wade Diehl<sup>2</sup>; Ketan Gajiwala<sup>2</sup>; You-Ai He<sup>2</sup>; Elizabeth Lunney<sup>2</sup>; Alan G. Marshall<sup>1</sup>; Mark R. Emmett<sup>1</sup>; <sup>1</sup>Nat'l High Magnetic Field Lab, Florida State Univ., Tallahassee, FL; <sup>2</sup>Pfizer Global, R&D- La Jolla, San Diego, CA
- WP 491 **Probing an Integrin I Domain Structure with Enhanced H/D Exchange Mass Spectrometry (DXMS) and Differential Scanning Calorimetry (DSC);** Sheng Li<sup>2</sup>; Tong Liu<sup>2</sup>; Paul H. Weinreb<sup>1</sup>; Samantha Phan<sup>1</sup>; Stephen Demarest<sup>1</sup>; Alexander Buko<sup>1</sup>; R. Blake Pepinsky<sup>1</sup>; Virgil Woods, Jr.<sup>2</sup>; Sharon Gao<sup>1</sup>; <sup>1</sup>Biogenidec, Inc., San Diego, CA 92121; <sup>2</sup>University of California, La Jolla, CA 92093
- WP 492 **Semi-Automated Hydrogen Deuterium Exchange (HDX) for the Analysis of Dynamics and Structure of Viral Poly(A) Polymerase;** Marek Daniel Kotler; Paul David Gershon; *University of California, Irvine, CA*
- WP 493 **Assembly of Matrix Protein VP40 of Ebola Virus by Hydrogen-Deuterium Exchange Mass Spectrometry;** Leslie Silva<sup>1</sup>; M. Javad Aman<sup>2</sup>; David Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, Canada; <sup>2</sup>U.S. Medical Research Inst. of Infectious Disease, Fredrick, MD
- WP 494 **Towards the Identification of the CRABP II and RAR Regions Involved in RA Transfer using HDX and Chemical Crosslinking;** Virginie Sjoelund; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- WP 495 **How Do Infectious Bacteria Protect Themselves? H/D Exchange Mass Spectrometry Probes the Answer;** Justin B. Sperry; Craig L. Smith; Michael G. Caparon; Scott J. Hultgren; Thomas E. Ellenberger; Michael L. Gross; *Washington University in St. Louis, St. Louis, MO*
- WP 496 **The Iron Binding Mechanism of Human Transferrin Examined by Hydrogen Deuterium Exchange Mass Spectrometry;** Cedric Bobst<sup>1</sup>; Igor A. Kaltashov<sup>2</sup>; <sup>1</sup>University of Massachusetts, Amherst, Amherst, MA; <sup>2</sup>University of Massachuset, Amherst, MA
- WP 497 **Factors Affecting Hydrogen-Deuterium Exchange at the MHC-Peptide Binding Interface;** Sachin Patil; Hermann von Grafenstein; *University of Toledo, Toledo, OH*
- WP 498 **Using HX-ESI-MS to Investigate the Amyloidogenic Protein Beta-2-Microglobulin in Its Monomeric State and When Bound Within the Major Histocompatibility Complex;** John P. Hodkinson<sup>1</sup>; Thomas R. Jahn<sup>2</sup>; Sheena E. Radford<sup>1</sup>; Alison E. Ashcroft<sup>1</sup>; <sup>1</sup>University of Leeds, Leeds, UK; <sup>2</sup>University of Cambridge, Cambridge, UK
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- PROTEIN QUANTITATION 3, 499 - 538**
- WP 499 **An Attempt to Quantitative Analysis for Clinical Proteomics by Two-Dimensional Electrophoresis and MALDI-TOF-MS using Stable Isotope-Labeled Small Organic Molecules;** Sadamu Kurono<sup>1</sup>; Takeshi Ueda<sup>2</sup>; Masayuki Maruoka<sup>2</sup>; Hanjoung Cho<sup>3</sup>; Satomi Niwayama<sup>3</sup>; <sup>1</sup>Iberica Holdings Co., Ltd., Kurume-shi, Fukuoka, Japan; <sup>2</sup>Chiba Cancer Center, Chuo-ku, Chiba, Japan; <sup>3</sup>Texas Tech University, Lubbock, TX
- WP 500 **Combining Isotope Coded Protein Labelling (ICPL) and TiO<sub>2</sub> Phosphopeptide Enrichment: a Novel Strategy for Quantitative Phosphoproteomics;** Nicolien FA Nagtzaam<sup>1</sup>; Martijn W. H. Pinkse<sup>3</sup>; Michael Kersten<sup>1</sup>; Christian Recktenwald<sup>2</sup>; Barbara Seliger<sup>2</sup>; Thomas M. Halder<sup>1</sup>; Peter D.E.M. Verhaert<sup>3</sup>; <sup>1</sup>Toplab GmbH, Martinsried, Germany; <sup>2</sup>University of Halle, Halle, Germany; <sup>3</sup>Delft University of Technology, Delft, The Netherlands
- WP 501 **Yeast Heat-Shock Response Studied by Label-Free Quantitative Proteomics;** Hannah Scott<sup>1</sup>; Hans C. Dalebout<sup>2</sup>; Davinia J. Mills<sup>1</sup>; Magnus Palmblad<sup>2</sup>; <sup>1</sup>The University of Reading, Reading, UK; <sup>2</sup>Leiden University Medical Center, Leiden, The Netherlands
- WP 502 **Utilization of SILAC Labeling for Comparative Analyses of Protein Expression in Planktonic Versus Biofilm-Grown Bacteria;** Nancy J. Phillips<sup>1</sup>; Deborah M. B. Post<sup>2</sup>; Birgit Schilling<sup>2</sup>; Christopher T. Steichen<sup>3</sup>; Margaret R. Ketterer<sup>3</sup>; Jason W. Johnston<sup>3</sup>; Megan L. Falsetta<sup>3</sup>; Michael A. Apicella<sup>3</sup>; Bradford W. Gibson<sup>2</sup>; <sup>1</sup>The University of California San Francisco, San Francisco, CA; <sup>2</sup>The Buck Institute For Age Research, Novato, CA; <sup>3</sup>The University of Iowa, Iowa City, IA
- WP 503 **Quantitative Proteomic Analysis of TLR Agonist-Mediated Synergy and Tolerance;** Ying Du; Yanbao Yu; Carol E. Parker; Xian Chen; *University of North Carolina, Chapel Hill, NC*
- WP 504 **Quantitation of Native Catalytically Active Spliceosomal B- and C-Complexes by Chemical (iTRAQ) and Metabolic (SILAC) Labeling;** Carla Schmidt; Mads Gronborg; Jochen Deckert; Sergey Bessonov; Ira Lemm; Reinhard Lührmann; Henning Urlaub; *MPI for Biophysical Chemistry, Göttingen, Germany*
- WP 505 **Absolute Quantification for Clinical-Resistant BCR-ABL Mutants from CML;** Jung Ok Park<sup>1</sup>; Gum Young Kang<sup>1</sup>; Sun Kyu Choi<sup>3</sup>; Dong Wook Kim<sup>2</sup>; Young Hwan Kim<sup>3</sup>; Kwang Pyo Kim<sup>1</sup>; <sup>1</sup>Konkuk University, Seoul, South Korea; <sup>2</sup>The Catholic University, Seoul, South Korea; <sup>3</sup>Korea Basic Science Institute, Daejeon, South Korea
- WP 506 **Characterization of Membrane-Bound Protein Complexes in Yeast using SILAC and Quantitative MS;** Silke Oeljeklaus; Benedikt Reintartz; Michael Kohl; Christian Stephan; Ralf Erdmann; Helmut E. Meyer; Bettina Warscheid; *Ruhr-University Bochum, Bochum, Germany*

## WEDNESDAY POSTERS

- WP 507 **Label-Free Comparative Proteomics of Arabidopsis Clp Protease Mutants and Absolute Quantification of Subunit Composition of the Clp Core Complex;** Paul Dominic B. Olinares<sup>1</sup>; Giulia Friso<sup>1</sup>; Boris Zybailov<sup>1</sup>; Andrea Rudella<sup>2</sup>; Verence Ramirez-Rodriguez<sup>1</sup>; Qi Sun<sup>3</sup>; Klaas J. Van Wijk<sup>1</sup>; <sup>1</sup>Plant Biology, Cornell University, Ithaca, NY; <sup>2</sup>Waters, Barcelona, SPAIN; <sup>3</sup>Computational Biology Unit, Cornell University, Ithaca, NY
- WP 508 **Validating and Quantifying Effects of siRNA Based RNA Interference on GAPDH at the Protein Level using Targeted Mass Spectrometry;** Sahana Mollah; Katherine Williams; Laura Chapman; Richard Fekete; Joseph Krebs; Christie L Hunter; *Applied Biosystems, Foster City, CA*
- WP 509 **Importance of Transmission Window Selection in Quadrupole-Based Mass Spectrometers to Increase Signal Intensities in iTRAQ-Based Quantitation;** Jesse B. Hines<sup>1</sup>; Maria E. Warren<sup>2</sup>; Carol E. Parker<sup>2</sup>; Xian Chen<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Durham, NC; <sup>2</sup>University of North Carolina - Chapel Hill, Chapel Hill, NC
- WP 510 **Profiling Real-Time MyD88 Interactions in a TLR-agonist-Specific pathway by using iTRAQ and SILAC;** Sun Yong Jeong; Yanbao Yu; Linhong Jing; Nedyalka Dicheva; Carol E. Parker; Xian Chen; *University of North Carolina, Chapel Hill, NC*
- WP 511 **Identification of Drosophila Melanogaster Low Abundance Membrane Glycoproteins using Off-Line Multidimensional Chromatography-Mass Spectrometry;** Jong Hee Song<sup>1</sup>; David E. Clemmer<sup>2</sup>; <sup>1</sup>SKenergy R&D Center, Daejeon, South Korea; <sup>2</sup>Indiana University, Bloomington, IN
- WP 512 **Comparative Quantitative Analysis of Mouse Adipose Tissue using LC-MALDI TOF/TOF and LTQ Orbitrap XL;** Dorothea Rutishauser<sup>1</sup>; Bernd Roschitzki<sup>2</sup>; Albert Johan Gerrits<sup>3</sup>; Peter M. Gehrig<sup>4</sup>; Hadi Al Hasani<sup>5</sup>; Ralph Schlapbach<sup>6</sup>; <sup>1</sup>Functional Genomic Center Zurich, Zurich, Switzerland; <sup>2</sup>University of Zurich, Zurich, Switzerland; <sup>3</sup>University Zurich / Eth Z, Zurich, Switzerland; <sup>4</sup>Functional Genomics Center, Zurich, Switzerland; <sup>5</sup>German Institute for Human Nutrition, Nuthetal, Germany; <sup>6</sup>Eth Zurich Fgcz, Zurich, Switzerland
- WP 513 **Direct Multiplexed Peptide Immunoaffinity-Based Quantification of Biomarkers using SISCAPA;** Eric Kuhn; Hasmik Keshishian; Veronica Saenz-vash; Michael Burgess; Terri Addona; Steven A. Carr; *Broad Institute of MIT and Harvard, Cambridge, MA*
- WP 514 **Quantitative Mass Spectrometry of the Astrocyte Secretome by SILAC;** Todd M. Greco; Adrian Mak; Lynn Spruce; Steven H. Seeholzer; Harry Ischiropoulos; *Children's Hospital of Phila, Philadelphia, PA*
- WP 515 **Global Quantitative Proteomic Analyses of Nostoc Punctiforme PCC 73102 under Diazotrophic Conditions using iTRAQ and Label-Free Techniques;** Saw Yen Ow<sup>1</sup>; Wolfgang Jabs<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Karin Stensjo<sup>3</sup>; Phillip C Wright<sup>1</sup>; <sup>1</sup>University of Sheffield, Sheffield, UK; <sup>2</sup>Bruker Daltonik, Bremen, Germany; <sup>3</sup>Uppsala University, Uppsala, Sweden
- WP 516 **Quantification of Proteome Changes in L6 cells Containing Giant Mitochondria;** Rongxiao Sa; Marian Navratil; Edgar A. Arriaga; *University of Minnesota, Minneapolis, MN*
- WP 517 **Identification and Absolute Quantification of Proteins in Retina Synaptic Ribbon Preparations by UPLC and MS<sup>E</sup> Approaches;** Karin Green<sup>1</sup>; William F. Sewell<sup>3</sup>; Craig Dorschel<sup>2</sup>; James E. Evans<sup>1</sup>; <sup>1</sup>Univ. of Mass Med. Sch., Worcester, MA; <sup>2</sup>Waters Corporation, Ms Ct, Milford, MA; <sup>3</sup>Massachusetts Eye and Ear, Boston, MA
- WP 518 **High-Throughput Mass Spectrometric Quantification of Glycolytic Proteins in the Yeast Proteome;** Ronald Aardema; Henk L. Dekker; Jaap Willem Back; Leo J. de Koning; Chris G. de Koster; *University of Amsterdam, Amsterdam, The Netherlands*
- WP 519 **Pioneering Off-Gel Methodology for Protein Quantification using a Dual Channel (Cy3, Cy5) Laser Induced Fluorescence Detector and NanoESI-Qq-FT-ICR ECD-MS-MS;** Caroline Tokarski<sup>1</sup>; Claude Netter<sup>2</sup>; Jocelyne Tahar<sup>3</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Univ. des Science/Tech de Lille, Villeneuve d'Ascq, FRANCE; <sup>2</sup>Dionex, Voisin-le-Bretonneux, France; <sup>3</sup>Picometrics, Toulouse, France
- WP 520 **A Facile New Protocol for Multiplexed Quantitation of Membrane Proteomes;** Andrew J Thompson; Ritchie Williamson; Emma L Schofield; John Stephenson; Diane P Hanger; Brian H Anderton; *MRC Centre For Neurodegeneration Research, London, UK*
- WP 521 **Multiplexed Quantitative Proteomics Assessment of Radiation-Induced Lung Damage using ExacTag Labeling;** Xiaoping Ao<sup>1</sup>; Li Wang<sup>1</sup>; Ming Zhang<sup>1</sup>; Theodore S. Lawrence<sup>1</sup>; David M. Lubman<sup>2</sup>; <sup>1</sup>University of Michigan Medical Center, Ann Arbor, MI; <sup>2</sup>University of Michigan, Ann Arbor, MI
- WP 522 **Micropreparative Liquid Chromatographic Fractionation and Differential Expression Analysis of Protein Extracts from Endothelial Cells Treated with Vascular Endothelial Growth Factors;** John Flensburg<sup>1</sup>; Fuad Bahram<sup>2</sup>; Lena Claesson-Welsh<sup>2</sup>; <sup>1</sup>GE Healthcare Bio-Sciences AB, Uppsala, Sweden; <sup>2</sup>Uppsala University, Rudbeck Laboratory, Uppsala, Sweden
- WP 523 **Label Incorporation Kinetics in SILAC Cultured Rat Cortical Primary Neuron Proteins, and its Application to Amyloid-beta Toxicity Study;** Stefano Gotta; Gianluca Sardone; Davide Franceschini; Claus Andersen; Roberto Raggiaschi; *Siena Biotech SpA, Siena, Italy*
- WP 524 **FLEXIQuant – a Full-Length Stable Isotope-Labeled Quantitation Method;** Sasha A. Singh<sup>1</sup>; Michael Springer<sup>2</sup>; Marc W. Kirschner<sup>2</sup>; Judith Jejanathirajah<sup>1</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Harvard Medical School/Children's Hospital Boston, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- WP 525 **Analysis of Proteins in Native Cerebrospinal Fluid by Multiple Reaction Monitoring;** Yong Seok Choi; Kelvin H. Lee; *University of Delaware, Newark, DE*
- WP 526 **The Development of a Targeted MRM Assay for Quantitation of Low Abundance Cytochrome P450 Proteins;** Amy Bartlett<sup>1</sup>; Therese Mckenna<sup>1</sup>; Christopher Hughes<sup>1</sup>; Johannes P. C. Vissers<sup>1</sup>; Scott Geromanos<sup>2</sup>; Catalin Donneanu<sup>2</sup>; James Langridge<sup>1</sup>; <sup>1</sup>Waters Corporation MS Technologies Centre, Manchester, UK; <sup>2</sup>Waters Corporation, Milford, MA
- WP 527 **Quantitation of Protein Expression in Human IPS Cells using iTRAQ, ETD, and Beam-Type CAD on an Orbitrap Mass Spectrometer;** Doug Phanstiel; Justin Brumbaugh; James A Thomson; Joshua J. Coon; *University of Wisconsin, Madison, WI*

## WEDNESDAY POSTERS

- WP 528 **Comparison of Non-labeling Quantitative Proteomics Techniques using Ion Trap and QTOF Mass Spectrometers;** Roger Powell; Nichole Reisdorph; Rick Reisdorph; *National Jewish Medical Res, Denver, CO*
- WP 529 **Quantitative MudPIT Analysis of the Eukaryotic RNA Polymerases;** Amber L Mosley; Samantha G Pattenden; Mihaela E Sardi; Laurence Florens; Jerry L Workman; Michael P Washburn; *Stowers Institute, Kansas City, MO*
- WP 530 **Identifying and Quantifying Novel Biochemical Pathways in Newly Discovered Prokaryotes;** Vibhuti Patel<sup>1</sup>; Andrew Crombie<sup>1</sup>; Konstantinos Thalassinos<sup>1</sup>; Joanne B. Connolly<sup>2</sup>; J. Colin Murrell<sup>1</sup>; Susan E. Slade<sup>1</sup>; James Scrivens<sup>3</sup>; <sup>1</sup>*University of Warwick, Coventry, UK;* <sup>2</sup>*Waters, Manchester, UK;* <sup>3</sup>*Univ of Warwick, Coventry, UK*
- WP 531 **Quantitation of Tandem MS Ion Data for Hypothesis Driven Structural MS in Protein Footprinting Experiments;** Janna Kiselar<sup>1</sup>; Sayan Gupta<sup>2</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>*Case Western reserve University, Cleveland, OH;* <sup>2</sup>*Cwru-center For Proteomics, Upton, NY*
- WP 532 **A Two-Stage Design for Rapid and Reliable Quantitation Applied to Knock-Out Mice: Combining Shotgun and Targeted iTRAQ Measurements;** Peter Pichler<sup>1</sup>; Peter Hasselblatt<sup>2</sup>; Erwin Wagner<sup>2</sup>; Goran Mitulovic<sup>3</sup>; Gustav Ammerer<sup>1</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>*Christian Doppler Laboratory for Proteome Analysis, Vienna, Austria;* <sup>2</sup>*Research Institute of Molecular Pathology (IMP), Vienna, Austria;* <sup>3</sup>*Inst. of Mol. Biotech. (IMBA), Vienna, Austria*
- WP 533 **Quantitative Proteome Analysis of Lung Carcinoma Cells Performed by Label-Free and DIGE Techniques;** Barbara Sitek<sup>1</sup>; Gereon Poschmann<sup>1</sup>; Birgit Korte<sup>1</sup>; Sebastian Link<sup>1</sup>; Christian Stephan<sup>1</sup>; Wolfgang Jabs<sup>3</sup>; Daniel C. Chamrad<sup>2</sup>; Klaus Marquardt<sup>2</sup>; Marina Behrens<sup>3</sup>; Kathy Pfeiffer<sup>1</sup>; Martin Blueggel<sup>2</sup>; Carsten Baessmann<sup>3</sup>; Helmut E. Meyer<sup>1</sup>; Kai Stuehler<sup>1</sup>; <sup>1</sup>*Ruhr Universitaet Bochum, Bochum, GERMANY;* <sup>2</sup>*Protagen Ag, Dortmund, GERMANY;* <sup>3</sup>*Bruker Daltonik GmbH, Bremen, Germany*
- WP 534 **Label-Independent Quantitative Analysis of Rat Mitochondrial Proteomes using Quadrupole Time-of-Flight Mass Spectrometry;** Rick Reisdorph<sup>1</sup>; Roger Powell<sup>1</sup>; Matthew Jackman<sup>2</sup>; Michael Armstrong<sup>1</sup>; Nichole Reisdorph<sup>1</sup>; <sup>1</sup>*National Jewish Medical and Research Center, Denver, CO;* <sup>2</sup>*UCHSC, Denver, CO*
- WP 535 **Tracking the Modifications of  $\beta$ -cells Proteome and Transcriptome Induced by Glucotoxicity;** Yohann Couté<sup>1</sup>; Yannick Brunner<sup>1</sup>; Domitille Schvartz<sup>1</sup>; Feliciano Priego-Capote<sup>1</sup>; Céline Hernandez<sup>2</sup>; Ron D. Appel<sup>2</sup>; Jean-Charles Sanchez<sup>1</sup>; <sup>1</sup>*Biomedical Proteomics Group, Geneva, Switzerland;* <sup>2</sup>*Proteome Informatics Group, SIB, Geneva, Switzerland*
- WP 536 **Quantifying Histone Variants and Modifications for Senescence by Label-Free LC-MS;** Hye R Jung<sup>1</sup>; Johannes P.C. Vissers<sup>2</sup>; Jim Langridge<sup>2</sup>; Lise C Rudkjaer<sup>3</sup>; Kristian Helin<sup>3</sup>; Ole N. Jensen<sup>1</sup>; <sup>1</sup>*University of Southern Denmark, odense, Denmark;* <sup>2</sup>*Waters Corporation, Manchester, UK;* <sup>3</sup>*Biotech Research and Innovation Centre, Copenhagen, Denmark*
- WP 537 **Profiling of Proliferating and Differentiated Mes-c-myc A1 Cell Line from Mouse Embryonic Mesencephalon by 2D LC-MS-MS and Alternate Scanning LC-MS;** Angela Chambery<sup>2</sup>; Johannes P.C. Vissers<sup>1</sup>; Jim I. Langridge<sup>1</sup>; Luca Colucci-D'Amato<sup>2</sup>; Simona Scarpella<sup>1</sup>; Augusto Parente<sup>2</sup>; <sup>1</sup>*Waters Corporation, Manchester, UK;* <sup>2</sup>*Dipartimento di Scienze della Vita, Caserta, Italy*
- WP 538 **MudPIT as a Tool for the Separation and Quantification of Proteins for GM Crop Safety Assessments;** Kaisa M. Koistinen<sup>1</sup>; Paul D. Fraser<sup>1</sup>; John M. Halket<sup>2</sup>; Raj K. P. Patel<sup>1</sup>; Peter M. Bramley<sup>1</sup>; <sup>1</sup>*Royal Holloway, University of London, Egham, UK;* <sup>2</sup>*King's College London, London, UK*
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- PROTEINS: MODIFIED, BIOLOGICAL APPLICATIONS, 549 - 566**
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- WP 549 **Characterization of Tyrosine Nitration in Mouse 3-Oxoacid CoA-Transferase;** Yuan Wang; Liang Shi; Fuli Peng; Jianmin Shao; Ningzhi Xu; Siqi Liu; *Beijing Genomics Institute, CAS, Beijing, China*
- WP 550 **Mass Spectrometric and Biophysical Investigation of a Conformational Disease “Antithrombin III Aalborg”;** Allan Stensballe<sup>1</sup>; Marie Thomsen<sup>2</sup>; Shona Pedersen<sup>2</sup>; Soren Risom Kristensen<sup>2</sup>; Daniel Otzen<sup>1</sup>; <sup>1</sup>*Aalborg University, Aalborg, Denmark;* <sup>2</sup>*Aalborg University Hospital, Aalborg, Denmark*
- WP 551 **Modification of Carbonic Anhydrase II with Acetaldehyde - The First Metabolite of Ethanol;** Janne Janis<sup>1</sup>; Fatemeh Ahmad<sup>5</sup>; Jarkko Valjakka<sup>5</sup>; Abdul Waheed<sup>3</sup>; William Sly<sup>3</sup>; Claudiu Supuran<sup>2</sup>; Onni Niemelä<sup>4</sup>; Daniela Vuollo<sup>2</sup>; Seppo Parkkila<sup>5</sup>; Pirjo Vainiotalo<sup>1</sup>; <sup>1</sup>*University of Joensuu, Joensuu, Finland;* <sup>2</sup>*Università degli studi di Firenze, Firenze, Italy;* <sup>3</sup>*Saint Louis University School of Medicine, St Louis, MO;* <sup>4</sup>*Seinäjoki Central Hospital, Seinäjoki, Finland;* <sup>5</sup>*University of Tampere, Tampere, Finland*
- WP 552 **Application of FT-MS to Elucidate Degradation Pathways of Therapeutic Proteins;** Anne Zeck; Joerg Thomas Regula; *Roche Diagnostics GmbH, Penzberg, Germany*
- WP 553 **Using Isotopic Labelling to Investigate Serum Albumin Modifications;** Klaus C Rumpel; Mireia Fernandez-Ocana; Hendrik Neubert; *Pfizer Global Research And Development, Sandwich, Kent, UK*
- WP 554 **Analysis of Post Translational Modifications of the Scaffolding Protein Homer in 6 Brain Regions;** Wallace Helton<sup>1</sup>; Karen K. Szumlinski<sup>2</sup>; Christine Wu<sup>1</sup>; <sup>1</sup>*Univ. of Colorado Health, Aurora, CO;* <sup>2</sup>*Univ. California Santa Barbara, Santa Barbara, CA*
- WP 555 **Systematic Investigation of Carbonylation in Human Serum Albumin;** Diogo Oliveira-Silva; David Simpson; Zafer Ugur; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- WP 556 **Characterization of an N-linked Glycosylated Kappa Urinary Light Chain from a Patient with Primary Systemic Amyloidosis;** Yan Jiang; Roger Theberge; Amareth Lim; Tatiana Prokaeva; Lawreen H. Connors; Martha Skinner; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- WP 557 **Detection of Post Translational Modifications on Distinct Mediator Complexes;** Andrew Paoletti; Ronald Conaway; Joan Conaway; Laurence Florens; Michael Washburn; *Stowers Institute for Medical Research, Kansas City, MO*
- WP 558 **The Analysis of Post-Translational Modification of High Mobility Group Box (HMGB) Proteins in HL-60 Cells;** Lei Xiong<sup>1</sup>; Yinsheng Wang<sup>2</sup>; <sup>1</sup>*Department of Chemistry, UC-Riverside, Riverside, CA;* <sup>2</sup>*University of California, Riverside, CA*

## WEDNESDAY POSTERS

- WP 559 **Studying the Structure of the Escherichia Coli Ribosome by Mass Spectrometry**; Xiaohui Liu; James P. Reilly; *Indiana University, Bloomington, IN*
- WP 560 **Towards Comprehensive Sequence Mapping and Identification of novel Post-Translational Modifications in Human Estrogen Receptor by Tandem Mass Spectrometry**; Christian Atsriku; David Britton; Jason Held; Birgit Schilling; Crystal Berger; Gary Scott; Christopher Benz; Brad W. Gibson; Mike Baldwin; *Buck Institute for Age Research, Novato, CA*
- WP 561 **Site-Specific Identification of 3-Nitrotyrosine in Platelet Proteins**; Marissa Martinez; *University of Pennsylvania, Philadelphia, PA*
- WP 562 **Identification of Post-Translational Modifications of SOD-1 Purified from Control and sALS Patient Tissue**; Joshua L. Johnson<sup>1</sup>; Daryl A. Bosco<sup>2</sup>; Robert H. Brown Jr.<sup>2</sup>; Jeffrey N. Agar<sup>1</sup>; *Brandeis University, Waltham, MA*; <sup>2</sup>Mass. Gen. Hspitl. and Harvard Medical School, Boston, MA
- WP 563 **Posttranslational Modifications of Proteins Identified by LC-Mass Spectrometry**; Benlian Wang; Masaru Miyagi; Ram H. Nagaraj; krzysztof Palczewski; Mark Chance; *Case Western Reserve University, Cleveland, OH*
- WP 564 **Reactions of Biogenic VOCs with Peptides and Proteins**; Simin D. Maleknia; Mark A Adams; *The University of New South Wales, Sydney, Australia*
- WP 565 **Beta B2 Crystallin: Study of Glutamine and Glutamic Acid Conversion**; Xiaojuan Li; Jason J Cournoyer; Cheng Lin; Chunxiang Yao; Peter B. O'connor; *Boston University Medical School, Boston, MA*
- WP 566 **Investigating the Mechanism of Bacterioferritin Co-migratory Protein, a Cysteine Dependant Peroxidase, using High Resolution Mass Spectrometry**; David J Clarke; Alan R. Brown; John R. Govan; Dominic J. Campopiano; Pat R. R. Langridge-Smith; C. Logan Mackay; *University of Edinburgh, Edinburgh, UK*
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- PROTEOMICS: BIOMARKER ASSAYS 1, 567 - 583**
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- WP 567 **Improved MRM Assay Design using Previously Acquired MS-MS from Multiple Instruments**; David M Cox<sup>1</sup>; Anthony Hung<sup>2</sup>; Stephen A Tate<sup>1</sup>; Brigitte Simons<sup>1</sup>; Min Du<sup>2</sup>; John C McDermott<sup>2</sup>; *MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>York University, Department of Biology, Toronto, Canada
- WP 568 **Developing Reliable MRM Assay for Protein Quantification Based on Parallel Multiplexing LC-MS-MS Analysis**; Asish Chakraborty; Catalin Doneanu; Weibin Chen; Scott Geromanos; Gordon Fujimoto; John Gebler; *Waters Corporation, Milford, MA*
- WP 569 **Increasing the Range of Targeted SRM Transitions for Biomarker Quantitation: Combining SRM Building/Predicting with FAIMS Separation**; Josef Ruzicka<sup>1</sup>; Kevin J. Mchale<sup>1</sup>; Scott Peterman<sup>1</sup>; Amol Prakash<sup>2</sup>; *Thermo Fisher Scientific, Somerset, NJ*; <sup>2</sup>Thermo BRIMS, Cambridge, MA
- WP 570 **Proteomics and Novel Biomarkers in Bladder Carcinoma**; West Kassous; Jordan Steinberg; Lorne Budman; David Blank; Bernard F Gibbs; *McGill University, Montreal, Que Canada*
- WP 571 **The Roles of MALDI-TOF MS Quantification and Proteomics in the Study of Anthrax Toxemia**; Adrian R Woolfitt; Anne E Boyer; Maribel Gallegos; Maria I Solano; John R Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- WP 572 **A Computational Approach for the Differential Analysis of Proteomics Data Acquired by Selected Reaction Monitoring Mass Spectrometry**; Gregory Finney<sup>1</sup>; Kelli Kline<sup>3</sup>; Daniela Tomazela<sup>2</sup>; Christine Wu<sup>4</sup>; Michael J. Maccoss<sup>2</sup>; *<sup>1</sup>Univ of Washington, Genome Sciences, Seattle, WA*; *<sup>2</sup>University of Washington, Seattle, WA*; *<sup>3</sup>Univ. Colorado Hsc, Denver, CO*; *<sup>4</sup>University of Colorado, Aurora, CO*
- WP 573 **Quantification of Focal Adhesion Kinase Activation Loop Phosphorylation by LC-MS as a Biomarker for *in vivo* c-Src Activity**; Eugene F. Ciccamaro<sup>1</sup>; Ian A. Blair<sup>2</sup>; *<sup>1</sup>University of Pennsylvania, Philadelphia, PA*; *<sup>2</sup>Univ. of Penn/center For Cancer, Philadelphia, PA*
- WP 574 **Quantitative and Semi-Quantitative Analysis of Proteins from Controls' and Patients' Plasma for Biomarker Verification in Ovarian Cancer**; Umut Oguz; Yifan Huang; John Koomen; Rebecca Sutphen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- WP 575 **Multi-Site Phosphorylation Assays for Tau Protein and Their Relevance to Alzheimer's Disease and Other Neurological Disorders**; Malcolm Ward<sup>1</sup>; Mireia Fernandez-Ocana<sup>2</sup>; Richard Killick<sup>2</sup>; Diane Hanger<sup>2</sup>; Emma Schofield<sup>1</sup>; Helen Byers<sup>1</sup>; Simon Lovestone<sup>2</sup>; Brian Anderton<sup>2</sup>; *<sup>1</sup>Proteome Sciences PLC, London, UK*; *<sup>2</sup>MRC Centre for Neurodegeneration Research, London, UK*
- WP 576 **Verification of lung Cancer Protein Biomarker Candidates using a Label Free Quantification Mass Spectrometric Approach**; Qinfeng Liu; Takefumi Kikuchi; Jamsshedur Rahman; David Carbone; Pierre Massion; Daniel C. Liebler; *Vanderbilt University, Nashville, TN*
- WP 577 **Development of a MRM-Transition Workflow and Atlas for *S. Cerevisiae* and Other Model Organisms**; Ashley Eastham; Li Huang; Daniel Martin; *Institute for Systems Biolog, Seattle, WA*
- WP 578 **Highly Selective Enrichment of Fibrinopeptide A from Human Serum by Fe3O4@Al2O3 for MALDI MS Analysis**; Cheng-Tai Chen; Yu-Chie Chen; *National Chiao Tung Univ., Hsinchu, Taiwan*
- WP 579 **Biomarker Validation using *de novo* MRM Analysis – Something Borrowed and Something New**; Devanand M. Pinto; Susanne Penny; Kenneth Chisholm; Andrej Vasilj; *NRC, Halifax, Canada*
- WP 580 **Identification of Animal Furs and Feathers by MALDI-TOF Mass Spectrometry**; Thomas Ellsner<sup>1</sup>; Wolfgang Pusch<sup>1</sup>; Guido Mix<sup>1</sup>; Klaus Hollemeyer<sup>2</sup>; Wolfgang Altmeyer<sup>3</sup>; Elmar Heinzle<sup>2</sup>; Markus Kostrzewa<sup>1</sup>; *<sup>1</sup>Bruker Daltonics, Leipzig, Germany*; *<sup>2</sup>Biochemical Engineering, Saarbruecken, Germany*; *<sup>3</sup>Gene-Facts, Saarbruecken, Germany*
- WP 581 **Generation of Unique Protein Specific MRM Signatures; using Peptide Information from Alternate Scanning LC-MS Data to Drive MRM Development**; Therese Mckenna<sup>1</sup>; Amy Bartlett<sup>1</sup>; Christopher Hughes<sup>1</sup>; Kieran Neeson<sup>1</sup>; Johannes P.C. Vissers<sup>1</sup>; Scott Geromanos<sup>2</sup>; Catalin Doneanu<sup>2</sup>; James Langridge<sup>1</sup>; *<sup>1</sup>Waters, Manchester, UK*; *<sup>2</sup>Waters Corporation, Milford, MA*
- WP 582 **High-Resolution Biomarker Discovery: Targeted Tandem Mass Spectrometry Methods for Quantitative Validation of Transcription Factor Candidates**; Johannes Hewel; Charanjit Sandhu; Jian liu; Vincent Fong; Andrew Emili; *University of Toronto, Toronto, Canada*

## WEDNESDAY POSTERS

- WP 583 **Quantification of Protein Biomarkers of Preterm Birth by Stable Isotope Dilution LC-MS-MS Method;** Sumit Shah<sup>1</sup>; Eugene Ciccimaro<sup>1</sup>; Kenneth Yu<sup>1</sup>; Samuel I Parry<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>Univ of Penn/Center For Cancer Pharmacology, Philadelphia, PA; <sup>2</sup>Univ of Penn/Dept of OB-GYN, Philadelphia, PA
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- PROTEOMICS: NEW APPROACHES TO INSTRUMENTATION, 584 - 603**
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- WP 584 **Utilizing Experimentally -Generated Protein Ion Maps from Data-Independent LC-MS Acquisitions for Identifying Low Abundant Proteins in Complex Mixtures;** Roy Martin<sup>1</sup>; J. Will Thompson<sup>2</sup>; Arthur Moseley<sup>3</sup>; Scott Geromanos<sup>1</sup>; <sup>1</sup>Waters Corporation, Beverly, MA; <sup>2</sup>Duke University, Igsp, Morrisville, NC; <sup>3</sup>Duke University Medical Center, Raleigh, NC
- WP 585 **Combining CAF Labeling, Parallel MS-MS, and Sequence Tag Searching for High Throughput LC-MALDI Protein Identification;** Yong Chen; Ansgar Brock; *Novartis-GNF, San Diego, CA*
- WP 586 **Déjà vu LC-MS-MS: How to Replay an LC-MS-MS Chromatogram without Injecting the Sample Again!;** Daniel Eikel<sup>1</sup>; Simon J. Prosser<sup>1</sup>; Gary A. Schultz<sup>1</sup>; Reinaldo Almeida<sup>2</sup>; Mark Allen<sup>2</sup>; <sup>1</sup>Advion BioSystems, Ithaca, NY; <sup>2</sup>Advion BioSciences Ltd., Heathersett, UK
- WP 587 **Automated Integration of Multidimensional Protein Identification Technology (MudPit) with Accurate Mass and Time Tags (AMT) Proteomics;** Vilém Guryca; Sabine Brugière; Magalie Court; Christophe Bruley; Jérôme Garin; Christophe Masselon; *CEA Grenoble, IRTSV/EDyP, Grenoble, France*
- WP 588 **A Reproducible Method for Online RP/RP 2D Nanolc/MS for Analysis of Proteomic Samples;** James Murphy; Martha Stapels; Keith Fadgen; Scott Geromanos; *Waters Corporation, Milford, MA*
- WP 589 **Comparison of Protein Identifications from Complex Samples by Capillary and Nanoflow LC-MS;** Christine Miller; Ning Tang; *Agilent Technologies, Santa Clara, CA*
- WP 590 **A Novel Approach Enabling Dual MS-Analyses of a Single LC-Injection with Excellent Sensitivity;** Leonie F. Waanders<sup>1</sup>; Reinaldo Almeida<sup>3</sup>; Gary A. Schultz<sup>2</sup>; Peter Bandilla<sup>1</sup>; Mark Allen<sup>3</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>MPI for Biochemistry, Martinsried, GERMANY; <sup>2</sup>Advion Biosciences, Ithaca, USA; <sup>3</sup>Advion Biosciences Limited, Norfolk, UK
- WP 591 **Strong Cation Exchange LC Peptide Retention Time Prediction and Its Application in Proteomics;** Konstantinos Petritis; Lars J. Kangas; Navdeep Jaitly; Matthew Monroe; Daniel Lopez-Ferrer; Robert A. Maxwell; Anoop M. Mayampurath; Brianna O. Petritis; Heather M. mottaz; Mary S Lipton; David G. Camp; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 592 **Characterization of the Human COP9 Signalosome using a New Tandem Affinity Purification Strategy and Quantitative Mass Spectrometry;** Lei Fang; Xiaorong Wang; Phang-Lang Chen; Lan Huang; *University of California, Irvine, Irvine, CA*
- WP 593 **A Novel Configuration using Silica Monolithic Column Technology to Analyze Complex Protein Mixtures by LC-MS-MS;** Sandra Chu<sup>1</sup>; Almut Rapp<sup>2</sup>; Sven Andrecht<sup>2</sup>; Stephen A Tate<sup>1</sup>; David M Cox<sup>1</sup>; <sup>1</sup>MDS Analytical Technologies, Concord, CANADA; <sup>2</sup>Merck KGaA, Darmstadt, Germany
- WP 594 **Practical Applications of Top-Down Proteomics using a MALDI TOF-TOF Platform;** Kevin L. Schey; Susana Comte-Walters; Angus C. Grey; Ed Krug; John H. Schwacke; *Medical Univ of SC, Charleston, SC*
- WP 595 **Strategies for Obtaining Confident Identifications in High Coverage, High Throughput LC-MS Proteomics Measurements using Hybrid FT Instruments;** Aleksey V. Tolmachev; Matthew E. Monroe; Ronald J. Moore; Samuel O. Purvine; Joshua N. Adkins; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Lab, Richland, WA*
- WP 596 **Accessing Natural Product Biosynthesis through Selective Detection of a Distinctive Post-Translational Modification in Complex Proteomes;** Paul M. Thomas; Stefanie B. Bumpus; Bradley S. Evans; Neil L. Kelleher; *University of Illinois, Urbana-Champaign, Urbana, IL*
- WP 597 **Liquid Chromatography Coupled Electron Capture Dissociation in a Radio Frequency Linear Ion Trap for the Top-down Analysis of Protein Mixtures;** Takeshi Sakamoto; Naomi Manri; Hiroyuki Satake; Akihito Kaneko; Takashi Baba; *Central Research Laboratory, Hitachi, Ltd, Kokubunji, Japan*
- WP 598 **The Use of 25-50 cm Long Nano Columns in LC-MS-MS Proteomics Studies for Maximized Peak Capacity and Increased Protein Identification;** Goran Mitulovic<sup>1</sup>; Robert Van Ling<sup>2</sup>; Evert-Jan Sneekes<sup>2</sup>; Remco Swart<sup>2</sup>; Karl Mechtler<sup>3</sup>; <sup>1</sup>IMBA, Vienna, AUSTRIA; <sup>2</sup>Dionex Corp., Amsterdam, Netherlands; <sup>3</sup>Imp Research Institute of Mo, Vienna, Austria
- WP 599 **Application of Data-Independent Parallel Fragmentation for Label-Free Proteomic Analysis and Protein Characterization;** Kevin Blackburn; Michael B. Goshe; *NC State University, Raleigh, NC*
- WP 600 **Folding Inhibition by Electrospray Additives for Top-Down Mass Spectrometry of Larger Proteins;** Honghai Jiang<sup>1</sup>; Xianglei Kong<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Mahmud Hossain<sup>1</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, Austria
- WP 601 **Utilising Ion Mobility Spectrometry to Separate Precursors From Background Ions and Species with Different Charges in Automated Tandem MS Experiments;** Chris Hughes; Jim Langridge; Therese McKenna; Richard Tyldesley-Worster; *Waters MS Technologies Centre, Manchester, UK*
- WP 602 **High-Speed Proteomic Signature by Swift LC-MS-MS and Label-Free Quantitation;** Pei-Yi Lin<sup>1</sup>; Chia-Feng Tsai<sup>1</sup>; Chih-Chiag Tsou<sup>2</sup>; Chien-Peng Wu<sup>1</sup>; Yi-Ting Wang<sup>1</sup>; Ting-Yi Sung<sup>2</sup>; Wen-Lian Hsu<sup>2</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of information science, Academia Sinica, Taipei, Taiwan
- WP 603 **An Analytical Comparison of MS-MS Based Quantitation of stable Isotope Labeled Peptides on LC-ESI Qq-TOF and LC-MALDI TOF/TOF MS Platforms;** Leanne B Ohlund<sup>1</sup>; Michael A. Kuzyk<sup>1</sup>; Monica H. Elliot<sup>1</sup>; Derek Smith<sup>1</sup>; Hong Xian<sup>2</sup>; Allen Delaney<sup>2</sup>; Christie L. Hunter<sup>3</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of Victoria Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Michael Smith Genome Sciences Centre, Vancouver, Canada; <sup>3</sup>Applied Biosystems, Foster City, CA
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- PROTEOMICS: BIOMARKER DISCOVERY 3, 604 - 625**
- WP 604 **Maximizing the Feature Identities and Qualities Leads to Enhanced Quantitation in a Label-Free LC-MS Profiling Experiments;** Wen Yu; Leo E. Bonilla; Mike T. Davis; Alex Taylor; Chris B. Russell; Andy Welcher; Scott D. Patterson; *Amgen, Seattle, WA*



## WEDNESDAY POSTERS

- WP 605 **Multidimensional Separation and Stable Isotope Labeled Proteome for Identification of Serum Biomarkers of Pancreatic Cancer;** Kenneth Yu<sup>1</sup>; Colin G. Barry<sup>1</sup>; David Austin<sup>1</sup>; Anil K. Rustgi<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Univ. of Penn/center For Can, Philadelphia, PA
- WP 606 **Microcontact Printed Surfaces for Enrichment and Identification of Endogenous Cellular Adhesion Proteins;** Melanie Schroeder<sup>1</sup>; Richard A. Eigenheer<sup>2</sup>; Milan Mrksich<sup>1</sup>; <sup>1</sup>University of Chicago, Chicago, IL; <sup>2</sup>Uc Davis, Davis, CA
- WP 607 **Protein Biomarker Candidates for Coronary Artery Disease from a Mouse Model of Atherosclerosis using 2D-LC-MALDI and 2D-LC-ESI Based Quantitative Proteomics;** Linhong Jing<sup>1</sup>; David Seo<sup>2</sup>; Maria Warren<sup>1</sup>; Nedyalka Dicheva<sup>1</sup>; Yanbao Yu<sup>1</sup>; Carol Parker<sup>1</sup>; Debra Schwinn<sup>2</sup>; Geoffrey Ginsburg<sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Duke University, Durham, NC
- WP 608 **Normalization of Spectral Count Data using Zero-Inflated Poisson Regression;** Douglas W. Mahoney; Ann L. Oberg; Patrick S. Quint; Jonathan J. Harrington; Jeanette E. Eckel-Passow; Terry M. Therneau; David A. Ahlquist; H. Robert Bergen, Iii; Mayo Clinic College of Medicine, Rochester, MN
- WP 609 **Comparison of Tryptic Protein Digestion and Microwave-Accelerated Acetic Acid Protein Digestion for Identification of Markers for Egg in Adulterated Foods;** Kevin J. Shefcheck<sup>1</sup>; Jinxi Li<sup>2</sup>; Catherine Fenselau<sup>2</sup>; John H. Callahan<sup>1</sup>; Steve Musser<sup>1</sup>; <sup>1</sup>USFDA, College Park, MD; <sup>2</sup>University of Maryland, College Park, MD
- WP 610 **Population Based Proteomics Studies of Type 2 Diabetes;** Randall Nelson; Chad R. Borges; Paul Oran; Jason Jarvis; Arizona State University, Tempe, AZ
- WP 611 **Inter-/Intra-Person Urinary Protein Variations and the Impact of Bariatric Surgery on Kidney Function;** Yan Zhang; Todd Kellogg; Gary Nelsestuen; University of Minnesota, Minneapolis, MN
- WP 612 **Improving Resolution in Nanolc Separations for Proteomics and the Effect of Chromatographic Resolution on Peptide Identification;** Remco van Soest; David W. Neyer; Jia Eng Siow; Phillip H. Paul; Eksigent Technologies, Dublin, CA
- WP 613 **From Bench to Bedside: Mass Spectrometric Identification of an Alternatively Spliced Fibronectin Domain Strongly Expressed in Neovasculature of Liver Metastases;** Christoph Rösli<sup>1</sup>; Alessandra Villa<sup>2</sup>; Dario Neri<sup>1</sup>; <sup>1</sup>Institute of Pharmaceutical Sciences, ETH Zurich, Zurich, Switzerland; <sup>2</sup>Philochem AG, Zurich, Switzerland
- WP 614 **Xenobiotics Mediated Plasma Proteomics: Implications for Biomarker Discovery in Environmental Health;** Hongying Zhong; Central China Normal Univers, Wuhan, CHINA
- WP 615 **Applications of Proteomics to Evaluate Drug-Induced Liver Toxicity;** Charlotte Ip<sup>1</sup>; Josef S. Ozer<sup>1</sup>; Raymond J. Gonzalez<sup>1</sup>; Denny B. Christian<sup>1</sup>; Frank D. Sistare<sup>1</sup>; William H. Schaefer<sup>2</sup>; <sup>1</sup>Merck, West Point, PA; <sup>2</sup>Merck Research Labs, West Point, PA
- WP 616 **Profiling Low-Concentration Biomarkers of Human CNS Lymphoma in Cerebrospinal Fluid by Label-Free Quantitative Mass Spectrometry;** Sushmita Mimi Roy<sup>1</sup>; James Rubenstein<sup>2</sup>; Howard Schulman<sup>1</sup>; Christopher Becker<sup>1</sup>; <sup>1</sup>PPD Biomarker Discovery Sciences, LLC, Menlo Park, CA; <sup>2</sup>University of California San Francisco, San Francisco, CA
- WP 617 **: Hexapeptide Combinatorial Library for Reduction of Dynamic Range of Serum Prior to SELDI Analysis;** Steve Roth; Fiona Plows; Vanitha Thulasiraman; Mariana Rusa; Hongmin Zhang; Steven Gu; Bio-Rad Laboratories, Inc, Fremont, CA
- WP 618 **Discovery and Identification of Markers of Toxicity in a Multi-site, Multi-Compound Study: Selected Results from the EU PredTox Consortium;** Diane Mccarthy<sup>1</sup>; Ben Collins<sup>2</sup>; Alexandra Walijew<sup>3</sup>; Arnd Brandenburg<sup>4</sup>; Stephen Pennington<sup>2</sup>; Jean-Charles Gautier<sup>5</sup>; Philip Hewitt<sup>3</sup>; William Gallagher<sup>2</sup>; <sup>1</sup>Bio-Rad, Malvern, PA; <sup>2</sup>University College Dublin, Dublin, Ireland; <sup>3</sup>Merck KGaA, Darmstadt, Germany; <sup>4</sup>GeneData AG, Basel, Switzerland; <sup>5</sup>sanofi-aventis, Vitry sur Seine, France
- WP 619 **Proteome Analysis of Low Amount Clinical Samples Reveals Candidate Marker Proteins for Lung Squamous Cell Cancer;** Gereon Poschmann<sup>1</sup>; Anna Ulrich<sup>1</sup>; Barbara Sitek<sup>1</sup>; Bence Sipos<sup>3</sup>; Sebastian Wiese<sup>1</sup>; Christian Stephan<sup>1</sup>; Ann Vander Borgh<sup>2</sup>; Bettina Warscheid<sup>1</sup>; Frans Ramaekers<sup>2</sup>; Günther Klöppel<sup>3</sup>; Helmut E. Meyer<sup>1</sup>; Kai Stühler<sup>1</sup>; <sup>1</sup>Ruhr-Universitaet Bochum, Bochum, Germany; <sup>2</sup>University of Maastricht, Maastricht, The Netherlands; <sup>3</sup>Universitaet Kiel, Kiel, Germany
- WP 620 **N-Dimensional Grouping As a Tool for Mining Proteomic Expression Profiling Data;** Stephen A Tate<sup>1</sup>; Ron Bonner<sup>1</sup>; Devanand M. Pinto<sup>2</sup>; Gordana Ivosev<sup>1</sup>; Chris Lock<sup>1</sup>; Lyle Burton<sup>1</sup>; <sup>1</sup>MDS Sciex, Concord, CANADA; <sup>2</sup>Nrc, Halifax, NS
- WP 621 **Computational Reassembly of Fractionated Samples for Biomarker Discovery using Accurate Mass Pattern with Limited Identity;** D. R. Mani; Jacob Jaffe; Steven A. Carr; Broad Institute of MIT and Harvard, Cambridge, MA
- WP 622 **Development of a Fast and Simple One-Dimensional Separation Approach for the Detection of Low Abundance Plasma Proteins;** Michael Schirm; Dmitri Sitnikov; Enrique Escobar; Tam Lehuu; Chunyan Li; Joanna Hunter; Caprion Proteomics, Montreal, Canada
- WP 623 **Evaluation of Label-Free Proteome Profiling Method for the Analysis of Formalin Fixed Paraffin Embedded Tissues;** Javad Nazarian<sup>1</sup>; Brian D. Halligan<sup>2</sup>; Mariarita Santi<sup>1</sup>; Tobey MacDonald<sup>1</sup>; Yetrib Hathout<sup>1</sup>; <sup>1</sup>Children's Natl. Medical Center, Washington, DC; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI
- WP 624 **Proteomic Profiling of D-Serine-Induced Toxicity Biomarkers in Rat Urine;** Rhonda L. Pitsch<sup>1</sup>; Claude Grigsby<sup>2</sup>; Ronelito Perez<sup>3</sup>; Mitchell Meade<sup>2</sup>; Kari Greenchurch<sup>3</sup>; John J. Schlager<sup>2</sup>; Pavel Shiyonov<sup>2</sup>; <sup>1</sup>HJF, Wright-Patterson AFB, OH; <sup>2</sup>Afrl, Dayton, OH; <sup>3</sup>The Ohio State Universtiy, Columbus, OH
- WP 625 **Identification of Low Abundant Proteins in Human Plasma after HPLC and Electrophoretic Fractionation;** Xinli Yang; Brown University, Providence, RI
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- BIOINFORMATICS 3, 626 - 648**
- WP 626 **Large Scale Deamidation Quantification in Aged Lens Tissues;** Surendra Dasari<sup>1</sup>; Phillip A Wilmarth<sup>1</sup>; Ashok P. Reddy<sup>2</sup>; Lucinda J.G Robertson<sup>1</sup>; Srinivasa R. Nagalla<sup>2</sup>; Larry L. David<sup>1</sup>; <sup>1</sup>School of Medicine, Oregon Health and Science Univ, Portland, OR; <sup>2</sup>Proteogenix, Portland, OR



## WEDNESDAY POSTERS

- WP 627 **A Visual Programming Platform and Comprehensive Experimental Metadata Model for Diagnostic Workflows;** Maciek Sasinowski<sup>1</sup>; Krista Miller<sup>1</sup>; Jason Miller<sup>1</sup>; Heather Sasinowska<sup>1</sup>; Ryan Castillo<sup>1</sup>; David Coppit<sup>1</sup>; Dariya Malyarenko<sup>2</sup>; Haijien Chen<sup>2</sup>; Eugene R. Tracy<sup>2</sup>; William E. Cooke<sup>2</sup>; Dennis M. Manos<sup>2</sup>; Tina Bunai<sup>2</sup>; Oliver John Semmes<sup>3</sup>; Richard R. Drake<sup>4</sup>; <sup>1</sup>INCOGEN, Inc., Williamsburg, VA; <sup>2</sup>College of William and Mary, Williamsburg, VA; <sup>3</sup>Eastern Virginia Medical School, Norfolk, VA
- WP 628 **Data Processing Improvements in MS Peak Detection for Trace Quantitation from Accurate Mass LC-MS Peptide Maps;** Beth Gillece-Castro<sup>1</sup>; Marc V. Gorenstein<sup>1</sup>; Daniel Golick<sup>1</sup>; Keith Richardson<sup>2</sup>; Barry Dyson<sup>2</sup>; Scott Berger<sup>1</sup>; Jeff Mazzeo<sup>1</sup>; Thomas E. Wheat<sup>1</sup>; Diane Diehl<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters, Manchester, UK
- WP 629 **A Free MS-MS *de novo* Sequencing and Protein Identification Online Server;** Mingjie Xie<sup>1</sup>; Weiming Zhang<sup>1</sup>; Weijie Yang<sup>1</sup>; Weiwu Chen<sup>1</sup>; Gilles Lajoie<sup>2</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>Bioinformatics Solutions, Inc, Waterloo, CANADA; <sup>2</sup>University of Western Ontario, London, CANADA
- WP 630 **Computational Prediction of the Highest Responding Peptides Per Protein in Electrospray Mass Spectrometry;** Vincent A. Fusaro; D. R. Mani; Jacob D. Jaffe; Jill Mesirov; Steven A. Carr; *Broad Institute of MIT and Harvard, Cambridge, MA*
- WP 631 **Validating Database Search Results of ETD Spectra;** Rovshan Sadygov; Rovshan Sadygov; *Thermo Fisher Scientific, San Jose, CA*
- WP 632 **MS-Xelerator: Advanced Algorithms for LC-MS Data Processing Applied to Biomarker Discovery, Differential Analysis and Quantitative Proteomics;** Marco Ruijken; *MsMetrix, Maarssen, Netherlands*
- WP 633 **Discriminative Identification of Activation and IL-4 Stimulation Effects in the Microsomal Fraction of CD4+ Cells under Th2 Cell Promoting Conditions;** Robert Moulder<sup>1</sup>; Jan-Jonas Filén<sup>1</sup>; Petri Kouvonen<sup>2</sup>; Tuula Nyman<sup>3</sup>; Riitta Lahesmaa<sup>1</sup>; <sup>1</sup>Turku Centre For Biotechnology, Turku, Finland; <sup>2</sup>University of Turku / Centre For Biotechnology, Turku, Finland; <sup>3</sup>University of Helsinki, Helsinki, Finland
- WP 634 **IDEAL-Q: An automated Tool for High-Performance Label-Free Quantitative Analysis;** Chih-Chiang Tsou<sup>1</sup>; Chia-Feng Tsai<sup>2</sup>; Ethan Y. H. Tsui<sup>1</sup>; Paul C. Y. Yu<sup>1</sup>; Yi-Ting Wang<sup>2</sup>; Pei-Yi Lin<sup>2</sup>; Yu-Ju Chen<sup>2</sup>; Ting-Yi Sung<sup>1</sup>; Wen-Lian Hsu<sup>1</sup>; <sup>1</sup>Institute of Information Science, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- WP 635 **Simplified Extensive Peptide Identification using Sequence Temperature Values and Feature Probabilities;** Sean L. Seymour; Ignat Shilov; Alpesh Patel; Wilfred Tang; Alexander Loboda; Christie L Hunter; Lydia Nuwaysir; Dan Schaeffer; *Applied Biosystems|MDS Sciex, Foster City, CA*
- WP 636 **STRAP2: Reliable, Hierarchical Peak Identification for Multicomponent Mass Spectra;** Bernhard Y. Renard<sup>1</sup>; Marc Kirchner<sup>1</sup>; Ullrich Koethe<sup>1</sup>; Judith A. J. Steen<sup>2</sup>; Hanno Steen<sup>2</sup>; Fred A. Hamprecht<sup>1</sup>; <sup>1</sup>University of Heidelberg, Heidelberg, GERMANY; <sup>2</sup>Harvard Medical School/Children's Hospital Boston, Boston, MA
- WP 637 **Calibrating E-Values for MS-MS Database Search Methods;** Gelio Alves<sup>1</sup>; Aleksey Y Ogurtsov<sup>1</sup>; Wells Wu<sup>2</sup>; Guanghui Wang<sup>2</sup>; Rong-fong Shen<sup>2</sup>; Yi-Kuo Yu<sup>1</sup>; <sup>1</sup>National Center for Biotechnology Information, NLM, Bethesda, MD; <sup>2</sup>National Heart, Lung & Blood Institute, NIH, Bethesda, MD
- WP 638 **Automated Decoy Analysis in Proteomics Projects;** Peter Hufnagel<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Gerhard Koerting<sup>3</sup>; Ray Sanchez<sup>2</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Protagen AG, Dortmund, Germany
- WP 639 **NIST Reference Libraries of Peptide Fragmentation Spectra: 2008;** Paul Rudnick<sup>1</sup>; Niksa Blonder<sup>1</sup>; Yuri Mirokhin<sup>1</sup>; Lewis Geer<sup>2</sup>; Dmitrii Tchekhovskoi<sup>1</sup>; Jeri Roth<sup>1</sup>; Lisa E. Kilpatrick<sup>1</sup>; Qian Dong<sup>1</sup>; Stephen Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>Ncbi / Nlm / Nih, Bethesda, MD
- WP 640 **Boston University Protein Identifier (BUPID): Improved Probability-Based Protein Identification using Peptide Mass Fingerprint Data;** Weimei Tong; David H. Perlman; Catherine E. Costello; Mark E. McComb; *BU School of Medicine, Boston, MA*
- WP 641 **Concatenated or Separate? Using Sample Bias Validation to Decide between Competing Database Search Strategies and Meta-Engines;** John T. Prince; Edward M. Marcotte; *University of Texas at Austin, Austin, TX*
- WP 642 **Assessing Abundance Ratios in Large-Scale Proteomics Datasets: t-Tests, Q-Values, Variance Shrinkage and Missing Data;** Tiansong Wang<sup>1</sup>; Qiangwei Xia<sup>2</sup>; Fred Taub<sup>1</sup>; Gundula Bosch<sup>1</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Emory University, Atlanta, GA
- WP 643 **ProLuCID: Using Probability and Statistical Scores to Improve Sensitivity and Specificity of CID and ETD Database Search Results;** Tao Xu; John Venable; Sung Kyu Park; Daniel Cociorva; Bingwen Lu; Lujian Liao; Johannes Hewel; Catherine C L Wong; Xuemei Han; James Wohlschlegel; John Yates; *The Scripps Research Institute, La Jolla, CA*
- WP 644 **A Novel Feature Selection and Disease Classification Algorithm using Probabilistic Information of Peptide Peaks in MALDI proTOF Data;** Lin Zhang<sup>1</sup>; Jianqiu Zhang<sup>1</sup>; Yufei Huang<sup>1</sup>; Xiaobo Zhou<sup>2</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, TX; <sup>2</sup>The Methodist Hospital, Houston, TX
- WP 645 **New Method for the Validation of *de novo* Sequencing Results;** Lei Xin; Gilles Lajoie; Bin Ma; *University of Western Ontario, London, Canada*
- WP 646 **Controlling False Discovery Rates in Large-Scale Shotgun Proteomic Studies;** Phillip A. Wilmarth; Lucinda J.G. Robertson; Larry L. David; *Oregon Health & Sciences University, Portland, OR*
- WP 647 **C4-Based HPLC-MS-MS of Whole Proteins in an LTQ-Orbitrap;** Yihuan S. Tsai; Alexander Scherl; Scott A. Shaffer; David R. Goodlett; *University of Washington, Seattle, WA*
- WP 648 **DeepQuanTR: a Novel Software for the Targeted Identification of Quantitative Differences in Two-Dimensional Peptide Maps Created from Comparative LC-MALDI Experiments;** Tim Fugmann; Dario Neri; Christoph Rösli; *Institute of Pharmaceutical Sciences, ETH Zurich, Zurich, Switzerland*
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- SYSTEMS BIOLOGY: INTERACTIONS, 649 - 655**
- WP 649 **Systematic Investigation of Dose-Dependent Dynamics of a Histone H2AX-Associated Complex;** YuanYu Lee; Ling Xie; Yanbao Yu; Linhong Jing; Carol E. Parker; Xian Chen; *University of North Carolina, Chapel Hill, NC*

## WEDNESDAY POSTERS

- WP 650 **A Pipeline for Rapid Characterization of Human Protein Complexes Complementing esiRNA-Driven Screens;** Magno Junqueira<sup>1</sup>; Yusuke Toyoda<sup>1</sup>; Zoltan Maliga<sup>1</sup>; Mikolaj Slabicki<sup>1</sup>; Mirko Theis<sup>1</sup>; Frank Buchholz<sup>1</sup>; Antony Hyman<sup>1</sup>; Andrej Shevchenko<sup>2</sup>; <sup>1</sup>*Max Planck Institute, Dresden, Germany*; <sup>2</sup>*Mpi of Molecular Cell Biology And Genetics, Dresden, Germany*
- WP 651 **Local Structure of Protein Interaction Networks and Protein Complexes from Rhodopseudomonas Palustris Based on Global Analysis of Protein Affinity Isolations;** William Cannon<sup>1</sup>; Mudita Singhal<sup>1</sup>; Don S. Daly<sup>1</sup>; Kevin K. Anderson<sup>1</sup>; Lee Ann McCue<sup>1</sup>; Ronald Taylor<sup>1</sup>; Denise D. Schmoyer<sup>2</sup>; Manesh B. Shah<sup>2</sup>; Julia Sharp<sup>3</sup>; Greg Hurst<sup>2</sup>; Brian S. Hooker<sup>1</sup>; Dale A. Pelletier<sup>2</sup>; W. Hayes McDonald<sup>2</sup>; Michelle V. Buchanan<sup>2</sup>; H. Steven Wiley<sup>1</sup>; <sup>1</sup>*Pacific NW National Lab, Richland, WA*; <sup>2</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>3</sup>*Clemson University, Clemson, SC*
- WP 652 **Mapping *in vivo* Protein-Protein Interactions and Topology using Protein Interaction Reporter Technology;** Haizhen Zhang<sup>1</sup>; Xiaoting Tang<sup>1</sup>; Gerhard Munske<sup>1</sup>; Chunxiang Zheng<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Nikola Tolic<sup>2</sup>; Gordon A. Anderson<sup>2</sup>; James E. Bruce<sup>1</sup>; <sup>1</sup>*Washington State University, Pullman, WA*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*
- WP 653 **Developing Informatics Data Pipeline (IDP) Software to Decipher Transcriptional Coregulator Networks from Large-Scale Proteomic Profiling of Coregulator Complexes;** Anna Malovannaya; Rainer Lanz; Jun Qin; Bert W O'Malley; *Baylor College of Medicine, Houston, TX*
- WP 654 **Identification of Protein Complexes in Rhodopseudomonas palustris;** W. Hayes McDonald<sup>1</sup>; Dale A. Pelletier<sup>1</sup>; Michael S. Allen<sup>1</sup>; Trish K. Lankford<sup>1</sup>; Manesh B. Shah<sup>1</sup>; Denise D. Schmoyer<sup>1</sup>; Tse-Yuan S. Lu<sup>1</sup>; Linda J. Foote<sup>1</sup>; Catherine K. McKeown<sup>1</sup>; Elizabeth T. Owens<sup>1</sup>; Greg Hurst<sup>1</sup>; Keiji G. Asano<sup>1</sup>; Jenny L. Morrell-Falvey<sup>1</sup>; Mitchel J. Doktycz<sup>1</sup>; Brian S. Hooker<sup>2</sup>; William R. Cannon<sup>2</sup>; H. Steven Wiley<sup>2</sup>; Michelle V. Buchanan<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*
- WP 655 **A High Throughput Platform to Map the Cell Cycle Interactome: Its Pitfalls with Spectral Data, Protein Identification and Data Mining;** Erwin Witters<sup>1</sup>; Kris Laukens<sup>1</sup>; Kim Henderickx<sup>1</sup>; Filip Lemièrè<sup>1</sup>; Dominique Eeckhout<sup>2</sup>; Jelle Van Leene<sup>2</sup>; Geert De Jaeger<sup>2</sup>; <sup>1</sup>*University of Antwerp, Antwerp, Belgium*; <sup>2</sup>*Ghent University, Ghent, Belgium*

## THURSDAY POSTERS

INSTRUMENTATION – NEW CONCEPTS 2, 003 - 022	
ThP 003	<b>Detection and Analysis of Nitrogen-Containing Pesticide Residues in Food and the Environment by Surface-Ionization Methods;</b> <u>Usman Khasanov</u> <sup>1</sup> ; Dilshodbek Usmanov <sup>1</sup> ; Saida Iskhakova <sup>1</sup> ; Utkur Rasulev <sup>1</sup> ; Steven Lehotay <sup>2</sup> ; Aviv Amirav <sup>3</sup> ; <sup>1</sup> Arifov Institute of Electronics, Tashkent, Uzbekistan; <sup>2</sup> Eastern Regional Research Center, Wyndmoor, PA; <sup>3</sup> Tel Aviv University, Tel Aviv, Israel
ThP 004	<b>Optimization of a Penning Ionization Source on a FT-ICR Instrument for Identification of Chemical Warfare Agents;</b> <u>Clotilde Le Vot</u> <sup>1</sup> ; Carlos Afonso <sup>1</sup> ; Claude G. Beaugrand <sup>2</sup> ; Jean-Claude Tabet <sup>1</sup> ; <sup>1</sup> University Paris 6, Paris, France; <sup>2</sup> Abionix Sarl, Talence, France
ThP 005	<b>A New Liquid-Type Cluster-Ion-Beam Source for Secondary Ion Mass Spectrometry using an Electrospray Ionization Technique;</b> <u>Yukio Fujiwara</u> ; Kouji Watanabe; Hidehiko Nonaka; Naoaki Saito; Toshiyuki Fujimoto; Akira Kurokawa; Shingo Ichimura; National Institute of Advanced Industrial Science, Tsukuba, Japan
ThP 006	<b>Design of a Progressively Spaced Stacked Ring Ion Guide for Improved Ion Transmission at High Pressure;</b> <u>Eloy R. Wouters</u> ; Maurizio Splendore; Michael W. Senko; John E. P. Syka; Jean-Jacques Dunyach; Thermo Fisher Scientific, San Jose, CA
ThP 007	<b>High Throughput Preparative Mass Spectrometry with Continuous Mass Selective Waveform Isolation;</b> <u>Qingyu Song</u> ; Scott A. Smith; Michael Volny; Zheng Ouyang; R. Graham Cooks; Purdue University, West Lafayette, IN
ThP 008	<b>DRILL: Atmospheric Pressure Confining/Focusing Vortex Flow Structure and Method of Generating/Transmitting Dry Ions from Ion Source to Mass Analyzer;</b> <u>Andrei Fedorov</u> <sup>1</sup> ; Amod Jain <sup>2</sup> ; <sup>1</sup> Georgia Institute of Technology, Atlanta, GA; <sup>2</sup> Indian Institute of Technology, Kharagpur, India
ThP 009	<b>Development of Novel Mass Spectrometer Equipped with ECRIS;</b> Masanori Kidera <sup>1</sup> ; Masayoshi Toda <sup>2</sup> ; Shuichi Enomoto <sup>1</sup> ; <u>Kazuya Takahashi</u> <sup>1</sup> ; <sup>1</sup> RIKEN, Wako-shi, Japan; <sup>2</sup> Tokyo University of Marine Science and Technology, Tokyo, Japan
ThP 010	<b>Structural and Quantitative Determination of Soft/Reactively Landed Nucleobases and Nucleosides on Silver Surfaces using Surface-Enhanced Raman Scattering and Mass Spectrometry;</b> <u>Karl E. Jackson</u> <sup>1</sup> ; Michael Volny <sup>2</sup> ; Matthew Diener <sup>1</sup> ; Tim Elam <sup>1</sup> ; Frantisek Turecek <sup>1</sup> ; <sup>1</sup> University of Washington, Seattle, WA; <sup>2</sup> Purdue University, West Lafayette, Indiana
ThP 011	<b>Fabrication and Characterization of a Lateral, Microfabricated Carbon Nanotube Ionization Source for a Miniaturized Mass Spectrometer;</b> <u>Charles Parker</u> <sup>1</sup> ; Srividya Natarajan <sup>1</sup> ; Jeffrey Glass <sup>1</sup> ; Kristin Gilchrist <sup>2</sup> ; Jeffrey Piascik <sup>2</sup> ; Brian R. Stoner <sup>2</sup> ; <sup>1</sup> Duke University, Durham, NC; <sup>2</sup> Rti, International, Research Triangle Park, NC
ThP 012	<b>A Zero Dead Time Microfluidic System for Pre-Steady-State Kinetics by DIOS-TOF MS;</b> <u>Kevin P. Nichols</u> ; Han JGE Gardeniers; MESA+ Institute for Nanotechnology, Enschede, Netherlands
ThP 013	<b>From Atmosphere to Vacuum: New Approaches to Transporting Ions in Mass Spectrometry;</b> <u>Lisa Cousins</u> <sup>1</sup> ; Gholamreza Javahery <sup>1</sup> ; Heather Gamble <sup>1</sup> ; Serguei Savtchenko <sup>1</sup> ; Nasser Ashgriz <sup>2</sup> ; <sup>1</sup> Ionics Mass Spectrometry Group, Inc., Toronto, Canada; <sup>2</sup> University of Toronto, Toronto, Canada
ThP 014	<b>Preparation of Novel Catalysts using Soft Landing of Mass-Selected Ions on Surfaces;</b> <u>Julia Laskin</u> <sup>1</sup> ; Peng Wang <sup>1</sup> ; Zhibo Yang <sup>1</sup> ; Omar Hadjar <sup>2</sup> ; Wen-Ping Peng <sup>3</sup> ; R. Graham Cooks <sup>4</sup> ; <sup>1</sup> Pacific NW National Laboratory, Richland, WA; <sup>2</sup> O.i. Analytical, Pelham, AL; <sup>3</sup> National Dong Hwa University, Taiwan, China; <sup>4</sup> Purdue University, West Lafayette, IN
ThP 015	<b>Efficiently Transporting Ions from Viscous Flow to Ultra-High Vacuum with Minimal Loss;</b> <u>Patrick Roach</u> <sup>1</sup> ; Kevin Kuchta <sup>2</sup> ; William Woodward <sup>1</sup> ; A. Welford Castleman, Jr. <sup>1</sup> ; <sup>1</sup> Penn State, University Park, PA; <sup>2</sup> Extrel CMS, Pittsburgh, PA
ThP 016	<b>Milisecond Nanoliters, Moving Matter with Electric Fields for MALDI &amp; ESI using a New Integrated Device;</b> <u>Drew Sauter</u> <sup>1</sup> ; Andrew D. Sauter III <sup>1</sup> ; Julie Harmon <sup>2</sup> ; <sup>1</sup> Nanoliter, LLC, Henderson, NV; <sup>2</sup> University of South Florida, Tampa, FL
ThP 017	<b>Pulse Counting Detector with Near Simultaneous Detection of Negative and Positive Ions for Quadrupole Mass Spectrometry;</b> <u>Charles Jolliffe</u> <sup>1</sup> ; Lisa Cousins <sup>1</sup> ; Heather Gamble <sup>1</sup> ; Gholamreza Javahery <sup>1</sup> ; Kevin Hunter <sup>2</sup> ; Peter Raffin <sup>2</sup> ; Dick Stresau <sup>2</sup> ; <sup>1</sup> Ionics Mass Spectrometry Group Inc., Toronto, ON; <sup>2</sup> ETP Electron Multipliers, Division of SGE Analytic, Ermington, NSW, Australia
ThP 018	<b>Effects of Materials, Space-Charge, Surface-Charge, and Aberrations on Performance for Miniature Mass Spectrometry;</b> <u>Guido F. Verbeck</u> ; Richard C. Maxwell; David Birdwell; University of North Texas, Denton, TX
ThP 019	<b>Laser Desorption/Ionization Mass Spectrometry on Porous Silica and Alumina for Peptide Mass Fingerprinting;</b> <u>Christine Enjalbal</u> ; Jean Martinez; Nawar Shenar; University Montpellier 2, Montpellier, France
ThP 020	<b>Characterization of Soft-Landed (0.1 – 1.0 eV) Nanoclusters and Fullerenes on Au;</b> <u>Stephen Davila</u> ; David Birdwell; Guido F. Verbeck; University of North Texas, Denton, TX
ThP 021	<b>Reducing System Carry over with Novel Surface Coatings;</b> <u>Peter Kovarik</u> <sup>1</sup> ; Thomas Covey <sup>1</sup> ; Dan L. Bantz <sup>2</sup> ; <sup>1</sup> MDS Sciex, Concord, Canada; <sup>2</sup> Parker Life Sciences, Hollis, NH
INSTRUMENTATION: QUADRUPOLES AND TRAPS 2, 022 - 040	
ThP 022	<b>Fragmentation of Singly Charged Peptide Ions via Interaction with Metastable Helium Atoms;</b> Vadym Berkout; MassTech, Inc., Columbia, MD
ThP 023	<b>Simultaneous Detection of a Wide Mass Range of Product Ion Including Immonium Ions in MS-MS using MALDI-DIT MS;</b> <u>Sadanori Sekiya</u> <sup>1</sup> ; Shinichi Iwamoto <sup>1</sup> ; Li Ding <sup>2</sup> ; Ikuro Konishi <sup>3</sup> ; Koichi Tanaka <sup>1</sup> ; <sup>1</sup> Shimadzu Corporation, Kyoto, Japan; <sup>2</sup> Shimadzu Research Lab (Shanghai), Shanghai, China; <sup>3</sup> Shimadzu Research Laboratory Ltd, Manchester, UK
ThP 024	<b>Method for Improved Accuracy with Simion for Devices Having Curved Electrode Surfaces;</b> David G. Welkie; Analytica of Branford, Branford, CT
ThP 025	<b>Top-Down Protein Analysis with Ion-Ion Reactions on a Home-Built Linear Ion Trap Mass Spectrometer;</b> <u>Matthew Soyk</u> <sup>1</sup> ; Qin Zhao <sup>1</sup> ; Gregg Schieffer <sup>1</sup> ; R. Sam Houk <sup>1</sup> ; Ethan R. Badman <sup>2</sup> ; <sup>1</sup> Iowa State University, Ames, IA; <sup>2</sup> Hoffmann-La Roche Inc., Nutley, NJ
ThP 026	<b>Circular Array of Miniature Rectilinear Ion Traps;</b> <u>Scott A. Smith</u> ; Miriam Fico; Jeffrey D. Maas; William

## THURSDAY POSTERS

- J. Chappell; R. Graham Cooks; *Purdue University, West Lafayette*
- ThP 027 **Quantitative Analysis of Biomolecules in the Quadrupole Ion Trap via Pulsed Q DCID;** Unige Laskay; Shannon L. Cook; Glen P. Jackson; *Ohio University, Athens, OH*
- ThP 028 **A New Method for Digitally Producing Waveforms and its Use in Digital Ion Trap Mass Spectrometry;** Hideya Koizumi; Bruce Jatko; William H Andrews Jr; William B Whitten; Peter TA Reilly; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 029 **Pulsed Q DCID – A Faster, More Energetic Fragmentation Method for Analysis of Peptide Mixtures;** Shannon L. Cook; Unige Laskay; Glen P. Jackson; *Ohio University, Athens, OH*
- ThP 030 **Planar Electrode Array Ion Traps Including a Unique Coaxial Geometry;** Edgar D. Lee<sup>1</sup>; Samuel E. Tolley<sup>1</sup>; Aaron R. Hawkins<sup>2</sup>; Daniel E. Austin<sup>2</sup>; Brett J. Hansen<sup>2</sup>; Milton L. Lee<sup>2</sup>; Doug L. Later<sup>3</sup>; *Torion Technologies, American Fork, UT*; <sup>2</sup>*Brigham Young University, Provo, UT*; <sup>3</sup>*Torion Technologies Inc., American Fork, UT*
- ThP 031 **High Precursor Ion Isolation in a Pure Quadrupole Field;** Roger Giles; Kamlesh Jain; Ikuo Konishi; *SRL, Manchester, UK*
- ThP 032 **Ion Trap Triple Resonant Ejection: Relationships between Supplemental Waveform Phase / Amplitude and Effective Trap Capacity;** Ken Newton; August Specht; *Varian Inc., Walnut Creek, CA*
- ThP 033 **Novel Calibrant Injection Method with High-Vacuum MALDI Digital Ion Trap Mass Spectrometer;** Shinichi Iwamoto<sup>1</sup>; Hidenori Takahashi<sup>1</sup>; Kei Kodera<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Ikuo Konishi<sup>2</sup>; Li Ding<sup>3</sup>; Koichi Tanaka<sup>1</sup>; *<sup>1</sup>Shimadzu Corporation, Kyoto, Japan*; *<sup>2</sup>Shimadzu Research Laboratory Ltd, Manchester, UK*; *<sup>3</sup>Shimadzu Research Lab (Shanghai), Shanghai, China*
- ThP 034 **Fragmentation Efficiencies of Six Different Linear Quadrupole Ion Traps with Added Hexapole Fields;** Ori Granot; D. J. Douglas; *University of British Columbia, Vancouver, BC*
- ThP 035 **Ion Oscillation Frequency Shifts in Linear Radio Frequency Quadrupole Ion Traps with Added Hexapole Fields;** Xianzhen Zhao; D. J. Douglas; *Dept. of Chemistry, Univ. of British Columbia, Vancouver, Canada*
- ThP 036 **Development and Characterization of Laser Induced Fluorescence Spectroscopy Coupled with Ion Trap Mass Spectrometry;** Qunzhou Bian; Francis O. Talbot; Matthew Forbes; Rebecca Jockusch; *University of Toronto, Toronto, Canada*
- ThP 037 **An Ion Guide Study: Quadrupoles, Rectilinear Quadrupoles, Hexapoles, and Octopoles;** Christopher R. Taormina; Edward Nicolette; Ted Theodore Novak; Randall E. Pedder; *Ardara Technologies L.P., Ardara, PA*
- ThP 038 **Extending the Mass Range of Collision Activation Dissociation in a Low Pressure Linear Quadrupole Ion Trap;** Michael Guna<sup>1</sup>; Yves G. Leblanc<sup>2</sup>; *<sup>1</sup>Mds Sciex, Concord, ON*; *<sup>2</sup>Mds Analytical Technologies, Concord, ON, ON*
- ThP 039 **Curved Multipole Ion Guides, A Computational Study and Experimental Validation;** Felician Muntean<sup>1</sup>; Urs Steiner<sup>2</sup>; *<sup>1</sup>Varian Inc., Walnut Creek, CA*; *<sup>2</sup>Varian, Santa Clara, CA*
- ThP 040 **Development of a Low Power Ion Trap Mass Spectrometer for the Analysis of Organics on Mars;** Theresa Evans-Nguyen<sup>3</sup>; Robert J. Cotter<sup>3</sup>; Vladimir M. Doroshenko<sup>2</sup>; Becker Luann<sup>1</sup>; *<sup>1</sup>Johns Hopkins University, Baltimore, MD*; *<sup>2</sup>Masstech, Inc., Columbia, MD*; *<sup>3</sup>Middle Atlantic Ms Laboratory, Baltimore, MD*
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- ION MOBILITY APPLICATIONS, 041 - 068**
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- ThP 041 **Evaluation of an APCI-FAIMS-MS Method for the Detection of the Pyrethroids, Bifenthrin and Permethrin;** Erick Molina<sup>1</sup>; Ulrich R. Bernier<sup>2</sup>; Brian P. Quinn<sup>2</sup>; Richard A. Yost<sup>1</sup>; *<sup>1</sup>University of Florida, Gainesville, FL*; *<sup>2</sup>USDA-ARS-CMAVE, Gainesville, FL*
- ThP 042 **Ion Mobility of Serine Octamer Clusters using Tri-wave High-Definition Mass Spectrometry;** Gustavo Henrique M Ferreira Souza<sup>1</sup>; Diana Uria<sup>2</sup>; Marcos N. Eberlin<sup>3</sup>; *<sup>1</sup>ThoMSon MS Lab. UNICAMP / Waters Brazil, MS Lab., Campinas - Sao Paulo, Brazil*; *<sup>2</sup>Waters Corporation, Manchester, UK*; *<sup>3</sup>ThoMSon Mass Spectrometry Lab. - UNICAMP, Campinas, Brazil*
- ThP 043 **Comprehensive Profiling of N-Linked Serum Glycans by IMS-MS for Diagnosis of Disease States;** Dragan Isailovic<sup>1</sup>; Sarah T. Stokes<sup>1</sup>; Manolo D. Plasencia<sup>1</sup>; Ruwan Kurulugama<sup>1</sup>; Zuzana Kyselova<sup>2</sup>; Radoslav Goldman<sup>3</sup>; Yehia Mechref<sup>1</sup>; Milos Novotny<sup>1</sup>; David E. Clemmer<sup>1</sup>; *<sup>1</sup>Indiana University, Bloomington, IN*; *<sup>2</sup>IU Chemistry Dept, Bloomington, IN*; *<sup>3</sup>Georgetown University Medical Center, Washington, DC*
- ThP 044 **Distinguishing Isomers in N-Linked Glycan Profiles using Multidimensional Ion Mobility-Mass Spectrometry;** Manolo D. Plasencia; Dragan Isailovic; Sarah T. Stokes; David E. Clemmer; *Indiana University, Bloomington, IN*
- ThP 045 **Structure of Protein Aggregates in the Gas-Phase using MALDI-IM-MS;** Ryan Blase; Francisco Alberto Fernandez Lima; Christopher Becker; Lisa M. Perez; David H. Russell; *Texas A&M University, College Station, TX*
- ThP 046 **Interactions of Metals Species with Proteins and DNA: Investigated using nanoElectrospray Ion Mobility Spectrometry with Inductively Coupled Plasma Mass Spectrometry;** Chiara Carazzone; Efthymios Kapellios; Katerina Kanaki; SPIROS PERGANTIS; *University of Crete, Heraklion, Greece*
- ThP 047 **Coupling AFFF/MALS or SEC/MALS to Ion Mobility Spectrometry for Analysis of Antibodies, Fragments, Aggregates, Non-Covalent Complexes and Protein Conjugates;** Bruce A. Andrien; Christine A. Nowak; Adam W. Lucka; *Alexion Pharmaceuticals, Cheshire, CT*
- ThP 048 **Analysis of Lymph Metabolome from Dietary Stressed Rats by Electrospray Ionization-Ion Mobility/Mass Spectrometry;** Kimberly Kaplan<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Min Xu<sup>2</sup>; Sean Davidson<sup>2</sup>; Patrick Tso<sup>2</sup>; Bill Siems<sup>1</sup>; Herbert H Hill<sup>1</sup>; *<sup>1</sup>Washington State University, Pullman, WA*; *<sup>2</sup>University of Cincinnati, Cincinnati, OH*
- ThP 049 **Shape Selective Studies of Cationised Gas Phase Structures of Glucose Polymers using Travelling Wave-Based Ion Mobility Mass Spectrometry;** Richard Holland; Konstantinos Thalassinou; James Scrivens; *University of Warwick, Coventry, UK*
- ThP 050 **Evaluating Phosphopeptide Separation from a Tryptic Digest using High-Field Asymmetric-Waveform Ion Mobility Spectrometry (FAIMS);** Jennifer Bryant; Richard A. Yost; *University of Florida, Gainesville, FL*
- ThP 051 **Improved Characterisation of Phosphorylated Peptides utilising Travelling Wave-Based and Drift**

## THURSDAY POSTERS

- Cell Ion Mobility Mass Spectrometry with Molecular Modelling Studies;** Konstantinos Thalassinos<sup>1</sup>; Gillian R. Hilton<sup>1</sup>; Susan E. Slade<sup>1</sup>; Megan Grabenauer<sup>2</sup>; Michael T. Bowers<sup>2</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>UC Santa Barbara, Santa Barbara, CA
- ThP 052 **The Amazing Stability and Intensity of Noncovalent Complexes as Demonstrated by Ion Mobility Mass Spectrometry;** Amina S. Woods<sup>1</sup>; Shelley N Jackson<sup>2</sup>; J. Albert Schultz<sup>3</sup>; Thomas Egan<sup>4</sup>; <sup>1</sup>NIDA IRP, NIH, Baltimore, MD; <sup>2</sup>Nida-irp, Nih, Baltimore, MD; <sup>3</sup>Ionwerks, Inc., Houston, TX; <sup>4</sup>Ionwerks Inc, Houston, TX
- ThP 053 **Ion-Mobility to Measure the Length Distribution of Aerosol Nanowires: Experiment and Theory;** Soo Kim; George Mulholland; Michael R. Zachariah; Univ. of Maryland & NIST, College Park, MD
- ThP 054 **Ion Mobility Shift Reagents for Identification of Primary Amines;** Thomas J. Kerr; John A. Mclean; Vanderbilt University, Nashville, TN
- ThP 055 **Ion Mobility Shift Strategies for Structural Characterization of Carbohydrates;** Larissa S Fenn; John A. McLean; Vanderbilt University, Nashville, TN
- ThP 056 **Gas-Phase Conformation of Gramicidin A Ions: An Ion Mobility Mass Spectrometry/Gas-Phase H/D Isotope Exchange Study;** Kent J. Gillig; Chris Becker; Liuxi Chen; Lei Tao; Francisco Alberto Fernandez Lima; David H. Russell; Texas A&M University, College Station, TX
- ThP 057 **Structure and Energetics of Beta-Sheet Peptide Self-Assembly Studied by nano-Electrospray Ionisation Mass Spectrometry and Travelling-Wave Ion Mobility Spectrometry;** Tom W Knapman; Amalia Aggeli; Sarah A Harris; Alison E. Ashcroft; University of Leeds, Leeds, UK
- ThP 058 **Analysis of Proteins from Red Blood Cells by Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS);** Sunyoung Lee; Dragan Isailovic; David E. Clemmer; Indiana University, Bloomington, IN
- ThP 059 **Detection of Oligonucleotide Gas-Phase Conformers by Combined H/D Exchange and Ion Mobility;** Dorothee Balbeur<sup>1</sup>; Joëlle Widart<sup>1</sup>; Bernard Leyh<sup>2</sup>; Laetitia Cravello<sup>3</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>LSM at the ULg, Liège, Belgium; <sup>2</sup>Molecular Dynamics Laboratory, Liège, Belgium; <sup>3</sup>Waters Corporation, Manchester, UK
- ThP 060 **Effect of Site Specific Post-Translational Modification and Amino Acid Residue Position on the Ion Mobility of Peptides;** Prabha Dwivedi; Herbert H Hill; Washington State University, Pullman, WA
- ThP 061 **Characterization of Anhydrous Oligonucleotides by Ion Mobility Mass Spectrometry;** Ablatt Mahsut; Sophie Zhao; John A. Mclean; Vanderbilt University, Nashville, TN
- ThP 062 **Structural Characteristics of the Alzheimer's Disease Amyloid Beta Protein;** Megan M. Murray<sup>1</sup>; Summer L. Bernstein<sup>1</sup>; Mary Krone<sup>1</sup>; Margaret M. Condrón<sup>2</sup>; Thomas Wytenbach<sup>1</sup>; David B. Teplow<sup>2</sup>; Joan-Emma Shea<sup>1</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara, Santa Barbara, CA; <sup>2</sup>University of California, Los Angeles, Los Angeles, CA
- ThP 063 **Using Ion Mobility to Probe the Influence of Side-Chain Interactions on the Gas-Phase Structure of Peptides;** Zhaoxiang Wu; Lei Tao; David H. Russell; TAMU, College Station, TX
- ThP 064 **Native ESI Studies of Multimeric Metalloproteins using Ion Mobility Mass Spectrometry;** Peter A Faull<sup>1</sup>; Perdita E Barran<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Karoliina Korkeila<sup>1</sup>; Andrew Gray<sup>1</sup>; Bryan J McCullugh<sup>3</sup>; <sup>1</sup>The University of Edinburgh, Edinburgh, UK; <sup>2</sup>University of Innsbruck, Innsbruck, Austria; <sup>3</sup>University of Manchester, Manchester, UK
- ThP 065 **Ion Mobility Mass Spectrometry of the Products of Oligomerisation of Activated Nucleotides with Montmorillonite;** Michael F Aldersley<sup>1</sup>; James P Ferris<sup>1</sup>; Prakash C Joshi<sup>1</sup>; Michal Kliman<sup>2</sup>; John A. Mclean<sup>2</sup>; Sevugarajan Sundarapandian<sup>2</sup>; Dmitri Zagorevski<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute, Troy, NY; <sup>2</sup>Vanderbilt University, Nashville, TN
- ThP 066 **Traditional Chinese Medicine Analysis by UPLC/Ion Mobility Mass Spectrometry;** John P. Shockcor; Kate Yu; Jose Castro-perez; Henry Y. Shion; Waters Corporation, Milford, MA
- ThP 067 **The Use of Ion Mobility/Time-of-Flight Mass Spectrometry for the Study of Protein Conformations;** Frank Sobott<sup>1</sup>; Stephen J. Watt<sup>2</sup>; Iain Campuzano<sup>3</sup>; <sup>1</sup>Chemistry Department, Oxford, UK; <sup>2</sup>Waters Australia, Rydalmere, NSW; <sup>3</sup>Waters, Manchester, UK
- ThP 068 **Optimization of FAIMS Source Coupled to Nanoflow ESI for the Detection and Quantitation of a Leukemia Biomarker;** Susan E. Abbatiello<sup>1</sup>; Michael W. Belford<sup>2</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>University of Pittsburgh Cancer Institute, Pittsburgh, PA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
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- INSTRUMENTATION: ION SOURCES, GENERAL, 069 - 078**
- ThP 069 **New Atmospheric Pressure Desorption/Ionization Source for Mass Spectrometry;** Taeman Kim; Kevin Dixon; Desmond Kaplan; Catherine Stacey; Melvin Park; Bruker Daltonics Inc., Billerica, MA
- ThP 070 **In situ Mass Spectrometry of Levitated Droplets using Charge Assisted Laser Desorption Ionization;** Kaveh Jorabchi; Michael S. Westphall; Lloyd Smith; University of Wisconsin-Madison, Madison, WI
- ThP 071 **Selected Ion Monitoring (SIM) Mode Data Collection using the Laser Diode Thermal Desorption (LDTD) Source to Increase Sensitivity;** James M. Koers; JAMES KOERS; Thermo, Indianapolis, IN
- ThP 072 **Determination of Rapid H/D Exchange Number of Solid Peptides and Proteins by Electrospray-Assisted Laser Desorption Ionization (ELDI) Mass Spectrometry;** Li-Hua Lo<sup>1</sup>; Jingyueh Jeng<sup>2</sup>; Yi-Tzu Cho<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen Univ., Kaohsiung, TAIWAN; <sup>2</sup>Chia Nan University of Pharmacy & Science, Tainan, Taiwan
- ThP 073 **Studies of Ion Transmission From Atmospheric Pressure into Vacuum through Conductance Openings;** Ross C. Willoughby<sup>1</sup>; Edward Sheehan<sup>2</sup>; David Fries<sup>3</sup>; <sup>1</sup>Chem-Space Associates, Pittsburgh, PA; <sup>2</sup>Chem-Space Associates, Inc., Pittsburgh, PA; <sup>3</sup>U South Florida, St Petersburg, FL
- ThP 074 **Atmospheric Pressure Free Liquid Infrared MALDI Mass Spectrometry: Towards a Unified Liquid Chromatography ESI/MALDI MS Interface;** Erdmann Rapp<sup>1</sup>; Aleš Charvát<sup>2</sup>; Alexander Beinsen<sup>2</sup>; Henning Urlaub<sup>2</sup>; Bernd Abel<sup>3</sup>; <sup>1</sup>Max Planck Institute for Dyn. of Compl. Tech. Sys., Magdeburg, Germany; <sup>2</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>3</sup>IPC University of Goettingen, Goettingen, Germany
- ThP 075 **Laser Diode Thermal Desorption Ionization Source (LDTD): Fundamental Aspects;** Pierre Picard<sup>1</sup>; Patrice

## THURSDAY POSTERS

- Tremblay<sup>1</sup>; E. Real Paquin<sup>2</sup>; <sup>1</sup>Phytronix Technologies, Inc., Quebec, Canada; <sup>2</sup>Universite Laval, Quebec, QC
- ThP 076 **Investigating Gas Composition on Transport and Desolvation of High m/z Species in the First Vacuum Stages of a Mass Spectrometer;** Jain D G Campuzano<sup>1</sup>; Kevin Giles<sup>1</sup>; Manajit Hayer-Hart<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Max Plank Institute of Biochemistry, Martinsried, Germany
- ThP 077 **Development of New Microscope MALDI-Q-FTICR-MS;** Katsutoshi Takahashi; *Nat'l Institute Advan. Indus. Sci Tech, Tokyo, Japan*
- ThP 078 **Reactive Electrospray-Assisted Laser Desorption Ionization (ELDI) for Characterization of Peptides and Proteins;** Ivory Peng<sup>1</sup>; Rachel O. Loo<sup>1</sup>; Jentaie Shiea<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>National Sun Yat-sen Univ., Kaohsiung, Taiwan
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- IONIZATION MECHANISMS, 079 - 102**
- ThP 079 **Looking at a Supersonic Reactor: A Study of Reactions Occurring in the MALDI Plume;** William J. Erb<sup>1</sup>; Kevin G. Owens<sup>2</sup>; <sup>1</sup>Ethicon, Somerville, NJ; <sup>2</sup>Drexel University, Springfield, PA
- ThP 080 **Systematic Investigation of the Surface Morphology Influence on Ion Desorption/Ionization from Porous Silicon and its Implication in D/I Mechanism;** Yongsheng Xiao; Eric Tucker; Lin He; *North Carolina State University, Raleigh, NC*
- ThP 081 **A 'Hopping Proton' Model for Molecular Dynamics Simulations of Highly Charged Water Nanodroplets;** Elias Ahadi; Lars Konermann; *Univ. of Western Ontario, London, Canada*
- ThP 082 **Probing Ionization Behaviors for Isomers of Nitrophenol under APCI and ESI using LC-MS and Direction Infusion/ MS;** STEPHEN CHAN; *Roche Carolina, Inc., Florence, SC*
- ThP 083 **ESI Oxidation Artifacts Revisited: Solution Phase Electrochemistry or Gas Phase Radical Attack?;** Brian Boys<sup>1</sup>; Mark Kuprowski<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Canada
- ThP 084 **Behavior of Phosphorylated Peptide/Copper Complexes in the Gas Phase under CID and ECD Conditions;** Françoise Fournier<sup>1</sup>; Christiane Garbay<sup>2</sup>; Carlos Afonso<sup>1</sup>; Jean-claude Tabet<sup>1</sup>; <sup>1</sup>Université Paris 6, Paris, France; <sup>2</sup>Université Paris 5, Paris, France
- ThP 085 **Internal Energy Transfer in Carbon-Based Surface-Assisted Laser Desorption / Ionization: Graphite versus Diamond;** Ho-Wai Tang; Kwan-Ming Ng; Chi-Ming Che; *Dept of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong*
- ThP 086 **Atmospheric Pressure MALDI on a Compact FT-ICR Mass Spectrometer;** Vladimir M. Doroshenko; Andrey N. Vilkov; *MassTech Inc., Columbia, MD*
- ThP 087 **Assessment of the Limits to Sensitivity with ESI, APCI, and MALDI;** Bradley B. Schneider; Hassan Javaheri; Thomas R. Covey; *MDS Sciex, Concord, Canada*
- ThP 088 **Internal Energy of Preformed Ions and Peptides Produced by Laser Desorption/Ionization from Laser-Induced Silicon Microcolumn Arrays;** Jessica A. Stolee<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>The George Washington University, Washington, DC
- ThP 089 **Voltage-Flow Rate Tuning of Nanoelectrospray Mass-Spectrometry;** Willem Engel; *University Leiden, Leiden, The Netherlands*
- ThP 090 **4-Chloro- $\alpha$ -Cyanocinnamic Acid – Rational Selection of a Superior MALDI Matrix;** Thorsten Wolfgang Jaskolla; Michael Karas; *JW Goethe Univ. of Frankfurt, Frankfurt/Main, Germany*
- ThP 091 **The Effects of Water Content for Nanoparticulate Matrices on Ion Composition in LDI-TOFMS;** Katherine Stumpo; David H. Russell; *Texas A&M University, College Station, TX*
- ThP 092 **Redox-Free MALDI MS with a Laser using Tunable Mid-Infrared Generation;** Yoshinao Wada<sup>1</sup>; Michiko Tajiri<sup>2</sup>; Sachiko Suzuki<sup>3</sup>; <sup>1</sup>Osaka MCHRI & Osaka University, Izumi, Osaka, Japan; <sup>2</sup>JST-CREST & Osaka MCHRI, Izumi, Osaka, Japan; <sup>3</sup>Graduate School of Engineering, Osaka University, Suita, Osaka, Japan
- ThP 093 **Surface Effects and Electrochemical Cell Capacitance in Desorption Electrospray Ionization;** Michael Volny<sup>1</sup>; Andre Venter<sup>1</sup>; Scott A. Smith<sup>1</sup>; Marco Pazzi<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, Lafayette, IN; <sup>2</sup>Universita' Di Torino, Torino, Italy
- ThP 094 **Generation of Highly-Charged Peptide and Protein Ions by Atmospheric Pressure IR MALDI Ion Trap Mass Spectrometry;** Alexander Pirkel; Simone Koenig; Klaus Dreisewerd; *University of Muenster, Muenster, Germany*
- ThP 095 **Production of Multiply-Charged Aluminium Cluster Anions in a Penning Trap;** Lutz Schweikhard; Franklin Martinez; Gerrit Marx; Noelle Walsh; *University of Greifswald, Greifswald, Germany*
- ThP 096 **Study on the Influence of Laser Fluence and Spot Size on the Ion Desorption of MALDI;** Hui Qiao; Victor Spicer; Kenneth Standing; Werner Ens; *University of Manitoba, Winnipeg, Canada*
- ThP 097 **Field-Free Atmospheric Ionization: Electrospray and Atmospheric Pressure Chemical Ionization;** Edward Sheehan<sup>1</sup>; Ross C. Willoughby<sup>2</sup>; Robert Classon<sup>2</sup>; Daniel Dodgen<sup>2</sup>; <sup>1</sup>Chem-Space Associates, Inc., Pittsburgh, PA; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 098 **Protein Analysis from Polyacrylamide Gel using Mid-Infrared Nanosecond Pulsed Laser;** Sachiko Suzuki; Tamami Fujita; Kunio Awazu; *Osaka University, Osaka, Japan*
- ThP 099 **Resonance Electron Capture by Small Peptides;** Yury V Vasil'ev; Valery G Voinov; Douglas F. Barofsky; Max L. Deinzer; *Oregon State University, Corvallis, OR*
- ThP 100 **Computational Model of Droplet Ejection in Desorption Electrospray Ionization;** Anthony B. Costa; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- ThP 101 **SMALDI-MS: Characterization of Laser Optical Parameters;** Sabine Günther; Klaus-Peter Hinz; Martin Köstler; Oliver Schulz; Bernhard Spengler; *University of Giessen, Giessen, Germany*
- ThP 102 **Post-Ionization Characteristics by a Femto-Second Laser Combined with TOF-SIMS;** Ryo Mibuka<sup>1</sup>; Ryotaro Todokoro<sup>2</sup>; Safwat Hassaballa<sup>1</sup>; Kousuke Kumonai<sup>2</sup>; Morio Ishihara<sup>2</sup>; Hisayoshi Yurimoto<sup>3</sup>; Kiichiro Uchino<sup>1</sup>; <sup>1</sup>Kyushu Univ., Fukuoka, Japan; <sup>2</sup>Osaka Univ., Toyonaka, Japan; <sup>3</sup>Hokkaido Univ., Sapporo, Japan
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- ION STRUCTURES/ENERGETICS 2, 103 - 115**
- ThP 103 **Site-Specific Double-Hydrogen Transfer during CID Fragmentation of O-Alkyl Ethers of Ortho-Hydroxybenzoic Acids;** Athula B. Attygalle; Jason B. Bialecki; Upul Nishshanka; Carl S. Weisbecker; Josef Ruzicka; *Stevens Institute of Technology, Hoboken, NJ*
- ThP 104 **Gas Phase Chiral Recognition in Cucurbituril Cavities;** Nannan Fang; David V. Dearden; *Brigham Young University, Provo, UT*

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- ThP 105 **Strategies to Investigate Fuel Cell Catalysts and Labile Inorganic Complexes in the Gas Phase;** Bridgette J. Duncombe; Marianne Ogunoshun; Kathryn Wills; Jason B. Love; *University of Edinburgh, Edinburgh, UK*
- ThP 106 **Gas Phase Studies of Binding to Chiral Catalysts;** Guoping Wang; Kelly A. Hay; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- ThP 107 **Triuret (Carbonyldiurea) as a Potent Hypokalemic Agent: Structure Characterization of Triuret-Alkali Metal Adducts by Means of Mass Spectrometric Techniques;** Sergiu P. Paliu; Cesar S. Contreras; Nicolas C. Polfer; John R. Eyler; *University of Florida, Gainesville, FL*
- ThP 108 **Computational Modeling of the H/D Exchange Behavior of Asparagine and its O-Methyl Ester;** Brooklynd Saar<sup>1</sup>; Elise Dennis<sup>1</sup>; Brittany R. Perkins<sup>2</sup>; John Poutsma<sup>1</sup>; Vicki H. Wysocki<sup>2</sup>; <sup>1</sup>*College of William & Mary, Williamsburg, VA*; <sup>2</sup>*University of Arizona, Tucson, AZ*
- ThP 109 **Ruthenium and Enzyme Catalyzed Dynamic Kinetic Resolution of Secondary Alcohols. An ESI-MS-MS Mechanistic Study;** Humberto Márcio Santos Milagre; Boniek Gontijo Vaz; Marcos N Eberlin; *Thomson Lab Unicamp, Campinas, Sp, Brazil*
- ThP 110 **Selective Supramolecular Nanoboxes: Trapping of Small Molecules by Cucurbit[5]uril and Decamethylcucurbit[5]uril Characterized in the Gas Phase using FTICR/MS;** Jacob Voelkel; Jamie Olsen; McKay Allred; Chadin Dejsupa; David V. Dearden; *Brigham Young University, Provo, UT*
- ThP 111 **Comparison of the Proton Affinities of Peptides Containing Lysine and (L)-2,3-Diaminopropionic Acid;** Robert Harper; Jianhua Ren; *University of the Pacific, Stockton, CA*
- ThP 112 **Gas-Phase H/D Exchange of Deprotonated Glycine Oligomers (Gly)<sub>n</sub> (n=1-6);** Zhixin Tian; Steven R. Kass; *University of Minnesota, Minneapolis, MN*
- ThP 113 **Double Hydrogen Transfer on Unimolecular Dissociation for 1-Methyl-3-(*i*-phenylalkanoyl) Hydantoin Derivatives including Deuterium Labeled Ones using a Four Sector Tandem Mass Spectrometer;** Hiroshi Yamaoka<sup>1</sup>; Nahoko Hirakawa<sup>1</sup>; Kyoko Okada<sup>1</sup>; Kimio Isa<sup>2</sup>; Hiroki Kinoshita<sup>2</sup>; Tetsuya Maekawa<sup>2</sup>; Yoshio Takai<sup>3</sup>; Nico M.M. Nibbering<sup>4</sup>; <sup>1</sup>*Osaka Prefecture University, Sakai, Osaka, Japan*; <sup>2</sup>*University of Fukui, Fukui, Japan*; <sup>3</sup>*Osaka University, Osaka, Japan*; <sup>4</sup>*Vrije Universiteit, Amsterdam, The Netherlands*
- ThP 114 **Mass Spectrometric and Theoretical Study of Bonding in Iodine Fluorides IF<sub>n</sub><sup>-</sup> (n=2,4,6,8);** Lee Scott Sunderlin<sup>1</sup>; Calvin Gibson<sup>1</sup>; Thomas M. Gilbert<sup>1</sup>; Changtong Hao<sup>2</sup>; <sup>1</sup>*Northern Illinois University, DeKalb, IL*; <sup>2</sup>*York University, Toronto, ON*
- ThP 115 **ESI-FTICR Mass Spectrometry and DFT Quantum Calculations of Ionized Aggregates of [Fe(CN)<sub>5</sub>(NO)]<sup>2-</sup> With Bu<sub>4</sub>N<sup>+</sup> And Na<sup>+</sup>;** Gary D. Willett<sup>1</sup>; Stephen B Colbran<sup>1</sup>; Philip A Dean<sup>2</sup>; Keith J Fisher<sup>2</sup>; Ivan F Taylor<sup>1</sup>; <sup>1</sup>*University of New South Wales, Sydney, Australia*; <sup>2</sup>*University of Sydney, Sydney, Australia*; <sup>3</sup>*University of Western Ontario, London, Canada*
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- ION MOLECULE REACTIONS 2, 116 - 129**
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- ThP 116 **Gas Phase Ion Chemistry Relevant to the Interstellar Medium;** Oscar Martinez Jr; Nicholas B. Betts; Stephanie M. Villano; Nicole Eyet; Theodore P. Snow; Veronica M. Bierbaum; *University of Colorado, Boulder, Colorado*
- ThP 117 **Unprecedented Ion-Molecule Reactions of the Sodium Adduct of Benzenedicarboxylates in the Collision Cell of Tandem in Space Mass Spectrometers;** Changching Chan<sup>1</sup>; Mark S. Bolgar<sup>1</sup>; Athula B. Attygalle<sup>2</sup>; <sup>1</sup>*Bristol-Myers Squibb Co., New Brunswick, NJ*; <sup>2</sup>*Stevens Institute of Technology, Hoboken, NJ*
- ThP 118 **Reactivity of a  $\sigma,\sigma$ -Biradical, the 4,5-Didehydroisoquinolinium Ion, and Related Monoradicals Toward Amino Acids and Dipeptides;** Enada F Archibald<sup>1</sup>; Nelson Vinueza<sup>1</sup>; Sen Li<sup>1</sup>; Hilikka Kenttamaa<sup>2</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Chemistry Department, West Lafayette, IN*
- ThP 119 **Cyanodiacetylene in Interstellar Clouds and the Atmosphere of Titan;** Samuel J Edwards; Colin G Freeman; Murray J McEwan; *University of Canterbury, Christchurch, New Zealand*
- ThP 120 **Gas-Phase Reactivity of Aromatic  $s,s$ -Biradicals toward Trinucleoside Diphosphates in an FT-ICR Mass Spectrometer;** Zhicheng Jin; John Nash; Nishi Rochell; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*
- ThP 121 **Gas Phase Ion-Molecule Reactions of N,O-Bis(trimethylsilyl) Acetamide with Different Peptides in the Quadrupole Ion Trap Mass Spectrometer;** Yuriy Pyatkivskyy<sup>1</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>*Northern Illinois University, DeKalb, IL*
- ThP 122 **Structure, Bonding and Reactions within Protonated Acetone-Methanol Cluster Ions;** Chitung Chiang; Brian D. Cunningham; Kristin M. Butterworth; Marek Freindorf; Robert L. DeLeon; Thomas Furlani; James F. Garvey; *University at Buffalo, Buffalo, New York*
- ThP 123 **Distinction of Cyclic, Acyclic, Exocyclic and Spiro Exocyclic Acetals via Structurally Diagnostic Ion/Molecule Reactions with the (CH<sub>3</sub>)<sub>2</sub>N-C=O<sup>+</sup> Acylium Ion;** Mario Benassi Neto<sup>1</sup>; Marcos N Eberlin<sup>1</sup>; <sup>1</sup>*Thomson Lab - UNICAMP, Campinas, Brazil*
- ThP 124 **Comparison of MS-MS Methods to Differentiate C<sub>4</sub>H<sub>6</sub>O Isomers;** Karen S. Wendling; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- ThP 125 **Kinetic Studies and Determination of Proton Affinity Differences with ESI/FT-ICR MS to Investigate the "Reverse Anomeric Effect" in Gas Phase;** Abdullah H. Al-fdeilat; Behrooz Zekavat; Parag Dhake; Andrew Vaino; Touradj Solouki; *University of Maine, Orono, ME*
- ThP 126 **Topological Control of Electronic Spin States in TME-like Diradicals;** Matthew Lenington; Paul G. Wenthold; *Purdue University, West Lafayette, IN*
- ThP 127 **Gas-Phase Reactivity of Carbon-Nitrogen (CN) Ortho-Benzynes in a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer;** Lindsey Kirkpatrick; Mike Yurkovich; Bartlomiej Jankiewicz; Hilikka Kenttamaa; John Nash; *Purdue University, Lafayette, IN*
- ThP 128 **Monitoring Metal Sulfide Cluster Growth in the Gas Phase using FT-ICR MS;** Jeffrey Spraggins; Katherine Mullaugh; George Luther; Douglas Ridge; *University of Delaware, Newark, DE*
- ThP 129 **Reactivity Study on the 4,5,8-Tridehydroisoquinolinium Ion: A  $\sigma,\sigma,\sigma$ -Triradical;** Nelson R. Vinueza; Bartlomiej J. Jankiewicz; John J. Nash; Hilikka I. Kenttamaa; *Purdue University, West Lafayette, IN*

## THURSDAY POSTERS

**ANALYSIS OF PESTICIDES AND HERBICIDES, 130 - 151**

- ThP 130 **Analysis of Water for Pesticides at Low Parts per Trillion (ppt) Levels using Two Dimensional LCMSMS without Any Sample Pre-Treatment;** Stephen J. Lock; *Applied Biosystems, Warrington, UK*
- ThP 131 **Comparing Large Injection Volumes and Online Pre-Concentration for the Analysis of Pesticides in Drinking Water;** Jonathan Beck; Charles Yang; *Thermo Fisher Scientific, San Jose, CA*
- ThP 132 **Comprehensive Two-Dimensional Pesticide Screen for Water and Biological Matrices by On-Line Extraction LC-MS;** Catherine Lafontaine; *Thermo Fisher Scientific, Franklin, MA*
- ThP 133 **High Resolution and High Mass Accuracy: A Perfect Team for Food and Feed Analysis in Complex Matrices;** Markus Kellmann; Lester C. Taylor; Dipankar Ghosh; Andreas Wieghaus; Helmut Muenster; *Thermo Fisher Scientific, Bremen, Germany*
- ThP 134 **Electron Ionization LC-MS of Organochlorine Pesticides: A Novel Approach in Multiresidue Analysis;** Pierangela Palma; Giorgio Famiglini; Helga Truffelli; Elisabetta Pierini; Achille Cappiello; *University of Urbino, Urbino, Italy*
- ThP 135 **Rapid Classification of Perfumes by Neutral Desorption Extractive Electrospray Mass Spectrometry (ND-EESI-MS);** Konstantin Chingini<sup>1</sup>; Gerardo Gamez<sup>1</sup>; Huanwen Chen<sup>2</sup>; Liang Zhu<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>East China Institute of Technology, Fuzhou, China
- ThP 136 **Gas Chromatography/ Mass Spectrometry Analysis of Volatiles from Horses to Discover Candidate Attractants Used by Host-Seeking Mosquitoes;** Ulrich R. Bernier<sup>1</sup>; Brian P. Quinn<sup>1</sup>; Jerome A. Hogsette, Jr.<sup>1</sup>; Daniel L. Kline<sup>1</sup>; Sandra H. TenBroeck<sup>2</sup>; <sup>1</sup>Usda-ars-cmave, Gainesville, FL; <sup>2</sup>University of Florida, Dept. of Animal Science, Gainesville, FL
- ThP 137 **TOF SIMS Analysis of Sulfonylurea Herbicides;** Yanci Liang<sup>1</sup>; Handong Liang<sup>2</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>China University of Mining and Technology, Beijing, China
- ThP 138 **Degradation of Polychlorinated Biphenyls by a Dioxygenase Enzyme Complex and Surfactants;** Nathalie Agar; Justin Powlowski; Catherine Mulligan; David Blank; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 139 **Screening and Trace Level Determination of Emerging Organic Contaminants in Natural and Waste Waters using a LTQ/Orbitrap Mass Spectrometer;** Heinz Singer; Susanne Kern; Sebastian Huntscha; Kathrin Fenner; Hollender Juliane; *Eawag, Duebendorf, Switzerland*
- ThP 140 **High Throughput Analysis of Pesticides in Dietary Supplements by Gas Chromatography Time-of-Flight Mass Spectrometry;** Megan Mcguigan; *LECO Corporation, St. Joseph, MI*
- ThP 141 **The Robustness of Elemental Composition Determination on a Single Quad GC-MS;** James Mullis<sup>1</sup>; Fenghe Qiu<sup>1</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT; <sup>2</sup>Cerno Bioscience, Danbury, CT
- ThP 142 **Accelerated LC-MS-MS for the Quantitation and Confirmation of Pesticides in Food and Water Samples;** Andre Schreiber<sup>1</sup>; Doina Caraiman<sup>2</sup>; Adrian Taylor<sup>2</sup>; Nadia Pace<sup>2</sup>; CJ Baker<sup>3</sup>; <sup>1</sup>Applied Biosystems, Concord, Canada; <sup>2</sup>Mds Analytical Technologies, Concord, ON; <sup>3</sup>University of Calgary, Calgary, Alberta
- ThP 143 **Automated Solid Phase Extraction and Analysis of Sulfonylureas and Related Herbicides in Fortified and Natural Water Samples using LC-ESI/MS-MS;** Josey M Grabuski<sup>1</sup>; Steve J. Cagampan<sup>1</sup>; John Struger<sup>1</sup>; Bernard Rondeau<sup>2</sup>; <sup>1</sup>Environment Canada, Burlington, Canada; <sup>2</sup>Environnement Canada, Montreal, Canada
- ThP 144 **Application of High Resolution Mass Spectrometry to Characterise Photoproducts of Imazamox and the Imazapic Herbicides;** Mourad Harir; Andras Gaspar; Philippe Schmitt-Kopplin; *Helmholtz Zentrum München, Neuherberg, Germany*
- ThP 145 **ICP MS an Emerging Technique for Environmental Analysis;** Marc E. Engel; *FDACS, Tallahassee, FL*
- ThP 146 **Comprehensive Multi-Target Screening of Pesticides in Food Extracts using HPLC-ESI-TOF-MS;** Ben Owens<sup>1</sup>; Petra Decker<sup>2</sup>; Ilmari Krebs<sup>2</sup>; <sup>1</sup>Bruker Daltonics Inc., Raleigh, NC; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany
- ThP 147 **Investigation of Matrix Effects Caused by Dissolved Inorganic Salts in Direct Injection Detection using LC-ESI/MS-MS in Water Analysis;** Wolfram Seitz<sup>1</sup>; Wolfgang Schulz<sup>1</sup>; Detlev Schleuder<sup>2</sup>; Walter H. Weber<sup>1</sup>; <sup>1</sup>Zweckverband Landeswasserversorgung, Langenau, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- ThP 148 **Use of C-13-Labeled Chlorpyrifos to Quantify Oral Bioavailability in the Rat;** Andrea Busby<sup>1</sup>; Jordan Smith<sup>1</sup>; James Campbell<sup>1</sup>; Charles Timchalk<sup>1</sup>; Torika Poet<sup>1</sup>; L. Needham<sup>2</sup>; Dana Barr<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Centers For Disease Control And Prevention, Atlanta, GA
- ThP 149 **Rapid Screening of Adulterated Food Flavorings and Colorings in Solid and Liquid using Electrospray-Assisted Laser Desorption Ionization (ELDI) Mass Spectrometry;** Jingyueh Jeng<sup>1</sup>; Wun-Han Jhan<sup>2</sup>; Jentaie Shiea<sup>2</sup>; <sup>1</sup>Chia Nan University of Pharmacy & Science, tainan, Taiwan; <sup>2</sup>National Sun Yat-sen Univ., Kaohsiung, Taiwan
- ThP 150 **Multi-Residue Analysis of Pesticides in Honey via Cohesive TLX1 System;** Charles T. Yang; *ThermoFisher Scientific, San Jose, CA*
- ThP 151 **High Efficiency Analysis of Pesticides in Environmental Water Samples using Direct Injection and Liquid Chromatography/Quadrupole Time-of-Flight Mass Spectrometry;** Xiaoming Zhao; Chunyan Hao; Paul Yang; *ACS, LaSB/Ministry of the Environment, Etobicoke, Canada*

**NATURAL PRODUCTS, 152 - 179**

- ThP 152 **Analysis of Edible Oils by Combined High Resolution Mass Spectrometry and Statistical Analysis;** Dong Wan Lim; Manhoi Hur; Kyu Hwan Park; Hyun Sik Kim; Jong Shin Yoo; Young Hwan Kim; Sunghwan Kim; *Korea Basic Science Institute, Ochang-myun, Korea*
- ThP 153 **Probing Natural Product Biosynthetic Pathways using Stable Isotopic Labeling by FTMS with Ultra-High Resolution and Accurate Mass;** Xidong Feng; Anokha S Ratnayake; Romila D Charan; Mark Tischler; Frank E Koehn; Guy T Carter; *Chemical & Screening Sciences, Wyeth Research, Pearl River, NY*
- ThP 154 **New Indole and Tetrahydroisoquinoline Alkaloids from Black Cohosh (Actaea racemosa) Identified by Mass Spectrometric Dereplication;** Dejan Nikolic; Tanja Goedecke; Shao-Nong Chen; David Lankin; Guido F Pauli; Richard B van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*



## THURSDAY POSTERS

- ThP 155 **Detection and Characterization of the Secondary Fungal Metabolite Gliotoxin by LC-ESI-MS;** Doyle T. Witt<sup>1</sup>; Kelly M. Thuet<sup>1</sup>; James M. Chapman<sup>1</sup>; Aric Weist<sup>3</sup>; Charles Kenerley<sup>2</sup>; <sup>1</sup>Rockhurst University, Kansas City, MO; <sup>2</sup>Texas A&M University, College Station, TX; <sup>3</sup>University of Missouri, Kansas City, Kansas City, MO
- ThP 156 **FT-ICR-Mass Spectrometric Analysis of Polyketide Biosynthesis: Preliminary Steady-State and Transient Absolute Kinetics of Active-Site Bound Intermediates;** Christopher Rath; David H. Sherman; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- ThP 157 **Identification of Cyclooxygenases Inhibitors (COX) in Cocoa Powders;** Angela Calderon<sup>1</sup>; W. J. Hurst<sup>2</sup>; Hongmei Cao<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>The Hershey Company, Hershey, PA
- ThP 158 **Structure-Based Discovery of Peptide Natural Products;** M. Violet Lee; David F. Iwig; Craig D. Wenger; Neil L. Kelleher; *University of Illinois Urbana Champaign, Urbana, IL*
- ThP 159 **A Post-Column Addition ESI-MS Approach for Simultaneously Analyzing Stilbenoids in Plant Tissues;** Ya-Chin Cheng; Kuo-lung Ku; Lin-Chung Yang; *National Chiayi University, Chiayi City, Taiwan*
- ThP 160 **Distinctive Behaviors of Deuterated Diglycosyl Flavonoids upon Negative ESI FTICR MS;** Sy Liu; *Changchun Inst. Appl. Chem., Changchun, China*
- ThP 161 **Effect of Lycopene on DNA Oxidative Damage in Human Prostate Cancer LNCaP Cells;** Ang Liu; Long Yuan; Richard B. van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- ThP 162 **Metabolic Profiling of Saponins in Medicago Truncatula using UPLC-QToF-MS;** David Huhman<sup>1</sup>; Lloyd W. Sumner<sup>2</sup>; <sup>1</sup>The Samuel Roberts Noble Foundation, Ardmore, OK; <sup>2</sup>The Noble Foundation, Ardmore, OK
- ThP 163 **Separation and Identification of Cis-Monotetrahydrofuran Acetogenins by Chiral Chromatography Coupled to LC-EI-MS;** James M. Chapman<sup>1</sup>; Richard C.D. Brown<sup>2</sup>; Sherif B. Abdel Ghani<sup>2</sup>; Scott Niemann<sup>3</sup>; <sup>1</sup>Rockhurst University, Kansas City, MO; <sup>2</sup>University of Southampton, Southampton, UK; <sup>3</sup>CSS Analytical Company, Inc., Shawnee, KS
- ThP 164 **Determination of Resveratrol in Mediterranean Red Wines by Liquid Chromatography Mass Spectrometry and Isotope Dilution;** Fabio Mazzotti<sup>1</sup>; Leonardo Di Donna<sup>1</sup>; Hicham Benabdelkamel<sup>1</sup>; Giovanni Sindona<sup>1</sup>; Anna Napoli<sup>1</sup>; Bartolo Gabriele<sup>2</sup>; <sup>1</sup>Università della Calabria, Dipartimento di Chimica, Arcavacata di Rende, Italy; <sup>2</sup>Università della Calabria, Dip Scienze farm., Arcavacata di Rende, Italy
- ThP 165 **MALDI-MS Studies of Tubulin-Binding Compounds in Madagascar Periwinkle Extracts;** Paul Hannewald; Benoit Maunit; Jean Francois Muller; *LSMCL, Metz, France*
- ThP 166 **Characterization of Phytoecdysteroid Glycosides in Meadowfoam (Limnanthes alba) Seed Meal by Positive and Negative Ion LC-MS-MS;** Ralph Reed; Fred Stevens; Jeffrey Morre; *Oregon State University, Corvallis, OR*
- ThP 167 **Screening Natural Products for Ligands to Quinone Reductase-2 using Ultrafiltration LC-MS;** Yongsoo Choi<sup>1</sup>; Andrew D Mesecar<sup>1</sup>; Megan Sturdy<sup>1</sup>; John M Pezzuto<sup>2</sup>; Richard B. Van Breemen<sup>3</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>College of Pharmacy, University of Hawaii, Hilo, Hawaii; <sup>3</sup>University of Illinois, Chicago, IL
- ThP 168 **Fingerprint of Herb Product by Matrix-Assisted Laser Desorption Ionization (MALDI);** Fenhong Song; Pei Chen; *USDA, Beltsville, MD*
- ThP 169 **Mechanisms of Chemoprevention by Constituents of the Dietary Supplement Angelica Sinensis;** Dongting Liu; Birgit M. Dietz; Andreas Schinkovitz; Guido F. Pauli; Judy L. Bolton; Richard B. van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- ThP 170 **Quantification and Metabolite Characterization of Xanthohumol and Metabolites in Humans by LC-MS/MC;** John D. Sowell; Ralph L. Reed; Cristobal L. Miranda; Jan F. Stevens; *Oregon State University, Corvallis, OR*
- ThP 171 **Comparison of Caco-2 cell Permeability of Serotonin and N-Methylserotonin;** Soyoun Ahn<sup>1</sup>; Dejan Nikolic<sup>2</sup>; Richard B. Van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois, Chicago, IL; <sup>2</sup>University of Illinois College of Pharmacy, Chicago, IL
- ThP 172 **Fingerprinting Characterization of Copaiba Oils by Electrospray Ionization Mass Spectrometry;** Rogério Cesar Silva<sup>1</sup>; Marcos N Eberlin<sup>2</sup>; <sup>1</sup>Thomson Lab, Campinas, Brazil; <sup>2</sup>Thomson Lab Unicamp, Campinas, Sp, Brazil
- ThP 173 **Structure Elucidation of Clausin A, a Novel Lantibiotic Produced by Bacillus Clausii Probiotic Strain;** Jean-Marie Schmitter<sup>1</sup>; Philippe Bressollier<sup>2</sup>; Benoit Odaert<sup>2</sup>; Maria C Urdaci<sup>2</sup>; <sup>1</sup>IECB, Pessac, France; <sup>2</sup>UMR5248, Pessac, France
- ThP 174 **Natural Product Discovery using an Integrated Nanoelectrospray LC-MS-Microcoil NMR System;** Paul Vouros<sup>1</sup>; Jimmy Orjala<sup>2</sup>; Yiqing Lin<sup>1</sup>; Susan Schiavo<sup>1</sup>; Roger Kautz<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Illinois, Chicago, IL
- ThP 175 **A Fragmentation Study of Isomeric Dihydroxyanthraquinone in Negative Electrospray Ionization by Ion Trap Time of Flight Mass Spectrometry;** Jing Dong<sup>1</sup>; Hong Wang<sup>1</sup>; Leren Wan<sup>2</sup>; Shizhong Chen<sup>1</sup>; Yuki Hashi<sup>2</sup>; <sup>1</sup>School of Pharmaceutical Sciences, Peking Univ., Beijing, China; <sup>2</sup>Shimadzu Beijing Office, Beijing, China
- ThP 176 **Development of a High Throughput LC-MS-MS Method for the Simultaneously Quantification of Multiple Bioactive Polyphenolic Compounds in Various Matrices;** Yan Ling Zhang<sup>1</sup>; James Garcia<sup>2</sup>; Jim Tallman<sup>2</sup>; Richard Staub<sup>2</sup>; Scott Baggett<sup>2</sup>; Isaac Cohen<sup>2</sup>; Uwe Christians<sup>1</sup>; <sup>1</sup>Univ. of Colorado Health Science, Aurora, CO; <sup>2</sup>Bionovo, Aurora, CO
- ThP 177 **Characterization of Commercial Pomegranate Extracts and Determination of Their Anti-Cancer Effects on COLO-357 Pancreatic Cancer Cells;** Carina S. Minardi; Melissa Rowland-Goldsmith; Christina Ly; Matthew Underwood; Nadia Reihanifam; Krista Bledsoe; James Head; Jenna Tong; Marissa Boardman; Autumn Tocchi; Christine A. Hughey; *Chapman University, Orange, CA*
- ThP 178 **Determination of Xanthohumol and its Metabolites in Rat Plasma and Liver after Administration of Xanthohumol and Hops;** Jian Guo; Birgit M. Dietz; Judy L. Bolton; Richard B. van Breemen; *University of Illinois College of Pharmacy, Chicago, IL*
- ThP 179 **Automated Identification of Phenolic Compounds by using Library Search Approach;** María Gómez Romero<sup>1</sup>; Gabriela Zurek<sup>2</sup>; Birgit Schneider<sup>3</sup>; Carsten

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Baessmann<sup>2</sup>; Antonio Segura Carretero<sup>1</sup>; Alberto Fernández Gutiérrez<sup>1</sup>; Félix Salinas<sup>4</sup>; <sup>1</sup>University of Granada, Granada, Spain; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>4</sup>Bruker Daltonics, Inc., Billerica, MA

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- ThP 180 **Electron Ionization Mass Spectra of Derivatives of Substituted Thiophenols**; Anzor Mikaia; Kirill V. Tretyakov; Stephen E. Stein; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 181 **Analysis of Mass Spectra of Silyl Derivatives of Aliphatic Keto- and Hydroxyacids**; Kirill V. Tretyakov; Stephen E. Stein; Anzor Mikaia; Edward White V; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 182 **Information Theoretic Mass Spectral Library Search for Comprehensive Two-Dimensional Gas Chromatography with Mass Spectrometry**; Arvind Visvanathan<sup>1</sup>; Stephen E. Reichenbach; <sup>1</sup>University of Nebraska Lincoln, Lincoln, NE
- ThP 183 **Supercritical Fluid Extraction *in-situ* Derivatization On-Line Solid-Phase Microextraction Combined with Gas Chromatography-Mass Spectrometry for Analysis Preservatives and Antioxidants in Cosmetics**; Tzung-Jie Yang; Feng-Jie Tsai; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- ThP 184 **Purge Assisted Headspace Solid-Phase Microextraction (PA/HS-SPME) Combined with Gas Chromatography-Mass Spectrometry for Determination of Chlorophenols in Aqueous Samples**; Hsin-Pin Ho; Ren-Jye Lee; Jen-Fon Jen; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- ThP 185 **Sensitive Analysis of Amino Acids using Multiple Ion Detection Method**; Tan Guo<sup>1</sup>; Curtis Hedman<sup>1</sup>; Cheng Gu<sup>2</sup>; <sup>1</sup>Wisconsin State Lab of Hygiene, Univ. of Wisconsin, Madison, WI; <sup>2</sup>Department of Crop and Soil Sciences, Michigan State University, MI
- ThP 186 **Metabolic Profiling of Chronic Obstructive Pulmonary Disease by Analysis of Exhaled Breath Volatiles using Gas Chromatography / Time-of-Flight Mass Spectrometry**; Maria Basanta; Roger Jarvis; Roy Goodacre; Dave Singh; Ashley Woodcock; Stephen Fowler; *The University of Manchester, Manchester, UK*
- ThP 187 **Experimental Considerations in the Measurement of Trace Explosives by GC-NCI-MS**; Marcela C Najarro; Bruce Benner; Greg Gillen; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 188 **EI Fragmentation Pathways of N-Acylanilines Bearing a Proximal Halogen Substituent**; Freneil Jariwala; Margaret Figus; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- ThP 189 ***In-situ* Derivatization/Solid-Phase Microextraction Coupled with Gas Chromatography-Negative Chemical Ionization Mass Spectrometry for the Determination of Trichloroethylene Metabolites in Rat Blood**; Yongzhen Liu; Srinivasa Muralidhara; James V. Bruckner; Michael G. Bartlett; *University of Georgia, Athens, GA*
- ThP 190 **Hermeticity Testing and Gas Characterization of MEMS Devices using Mass Spectrometry**; James M. Hochrein; Jason R. Brown; Michael I. White; Steven M. Thornberg; *Sandia National Laboratories, Albuquerque, NM*
- ThP 191 **Evaluation of Microwave Accelerated Derivatization (MAD) for the Comprehensive Analysis of Steroids using Gas Chromatography/Mass Spectrometry**; John Bowden; Dominic Colosi; Timothy Garrett; Richard A. Yost; *University of Florida, Gainesville, FL*
- ThP 192 **The Measurement of Explosives in Several Sample Matrices by Gas Chromatography with Negative Ion Chemical Ionization Mass Spectrometry**; Bruce A. Benner, Jr.; *NIST, Gaithersburg, MD*
- ThP 193 **Development of a new EI/FI Ion Source for a GC-TOF-MS**; Susumu Fujimaki<sup>1</sup>; Kenji Miyamoto<sup>1</sup>; Kazuo Tanaka<sup>1</sup>; Yoshihisa Ueda<sup>1</sup>; Doug Meinhardt<sup>2</sup>; <sup>1</sup>JEOL, Ltd., Tokyo, Japan; <sup>2</sup>JEOL USA Inc., Peabody, MA
- ThP 194 **Automatic Location of Molecular Ions in Mass Spectra for Application to Screening Studies**; Donald C Hilton; Mark Libardoni; *Leco Corporation, Fort Myers, FL*
- ThP 195 **Application of GC-HRMS for the Structural Elucidation of Impurities Observed in 5-chlorovaleryl Chloride (5-CVC)**; Michael Peddicord; Liya Tang; Scott A Miller; Charles Pathirana; Venkatapuram Palaniswamy; *Bristol-Myers Squibb, New Brunswick, NJ*
- ThP 196 **GC-MS with a Fly-Through Ion Source – Fast, Inert, Sensitive, Robust and with Tunable Molecular Ion**; Alexander Gordin; Alexander B. Fialkov; Aviv Amirav; *Tel-Aviv University, Tel-Aviv, Israel*
- ThP 197 **Investigation of Trace Concentrations of Hazardous, Volatile Hydrocarbons in Commercial Beverages**; Sarah J Saylor; Catherine Bentzley; Amos Linenberg; *University of the Sciences in Philadelphia, Philadelphia, PA*
- ThP 198 **Carbon Nanotubes as a Solid-Phase Microextraction Sorbent Coupled to Gas Chromatography-Mass Spectrometry for Determination of Chlorophenols in Aqueous Solution**; Tse-Tsung Ho; Chia-Chun Yao; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- ThP 199 **Bridging the Performance Gap Between GC-MS and GC-MS-MS with Deconvolution Technology**; Terry L. Sheehan<sup>1</sup>; Melissa Churley<sup>1</sup>; Paul Zavitsanos<sup>2</sup>; Mike Szelewski<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Wilmington, DE

## FORENSICS, 200 - 218

- ThP 200 **Efficient Screening Method for Multiple Anabolic Steroids from Various Nutritional Supplements by Liquid Chromatography Tandem Mass Spectrometry**; Caroline Wang; Petra Hartmann-Fischbach; Tim Krueger; Marcia Small; Terry Wells; Anna Telling; *Industrial Laboratories, Wheat Ridge, CO*
- ThP 201 **High-Throughput Screening and Quantification of Doping Agents in Urine using LDTD-APCI-MS-MS**; Patrice Tremblay<sup>1</sup>; Paule Emilie Groleau<sup>2</sup>; Cristiane Ayotte<sup>2</sup>; Pierre Picard<sup>3</sup>; Edith Viel<sup>2</sup>; <sup>1</sup>Phytronix Technologies, Quebec, Canada; <sup>2</sup>Inrs-doping Control, Pointe-claire, QC; <sup>3</sup>Phytronix Technologies, Inc., Quebec, QC
- ThP 202 **LC-MS of Children's Latent Fingerprint Residue**; Kathryn E. O'Brien<sup>1</sup>; Raleigh W. Parrott<sup>1</sup>; Corrie J. Brown<sup>1</sup>; Brian A. Eckenrode<sup>2</sup>; Diane K. Williams<sup>2</sup>; <sup>1</sup>Oak Ridge Institute of Science Education, Oak Ridge, TN; <sup>2</sup>Federal Bureau of Investigation, Quantico, VA
- ThP 203 **Differentiation of Isomeric Compounds and Differentiation of Enantiomeric Compounds with High Resolution LC-MS**; Jaran Jainhuknan<sup>1</sup>; Dungporn

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- Plasen<sup>2</sup>; Theerin Sinchai<sup>3</sup>; <sup>1</sup>*Bruker, Bangkok, Thailand*; <sup>2</sup>*Dept. Pharmacology, Srinakharinwirot Univ., Bangkok, Thailand*; <sup>3</sup>*Department of Toxicology, Inst. Forensic Medicine, Bangkok, Thailand*
- ThP 204 **Equine Anti-doping Pre-Race Screening with Turbulent-Flow LC-MS-MS**; James F Byrd<sup>1</sup>; Scott Stanley<sup>2</sup>; Ben Moeller<sup>2</sup>; Cheah Hun Teong<sup>4</sup>; Shawn Stanley<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, Franklin, CA*; <sup>2</sup>*Uc Davis, Davis, CA*; <sup>3</sup>*Singapore Turf Club, Singapore, Singapore*; <sup>4</sup>*Alpha Analytical, Singapore, Singapore*
- ThP 205 **Multi Target Screening using Scheduled Multiple Reaction Monitoring Acquisition on an LC-MS-MS System and Automatic Library Searching**; Nadia Pace<sup>1</sup>; Sebastian Dresen<sup>2</sup>; Nerea Ferreiros<sup>2</sup>; Andre Schreiber<sup>3</sup>; Houssain El Aribi<sup>1</sup>; Robert Ellis<sup>1</sup>; Wolfgang Weinmann<sup>2</sup>; <sup>1</sup>*MDS Analytical Technologies, Concord, Canada*; <sup>2</sup>*Institute of Legal Medicine, U. Hospital Freiburg, Freiburg, Germany*; <sup>3</sup>*Applied Biosystems, Concord, ON*
- ThP 206 **Toxicological Applications of Ambient Mass Spectrometry: Direct Analysis of Biological Matrices**; Christopher C. Mulligan; Stephen B. Hooser; Jason D. Harper; Nicholas A. Charipar; Christina Wilson; Zheng Ouyang; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- ThP 207 **Automated Platform for Utilization of Sequence Variation in Human Short Tandem Repeats using Electrospray Ionization Mass Spectrometry**; Thomas A. Hall; Sheri Manalili; Kristin A. Sannes-Lowery; Amy S. Schink; Steven A. Hofstadler; *Ibis Biosciences, Inc., Carlsbad, CA*
- ThP 208 **Identification of Benzylpiperazine and Phenylpiperazines in Illicit Forensic Drug Seizures via LC-MS Electrospray Ionization**; Adrian Krawczeniuk; *DOJ/DEA Northeast Laboratory, New York, NY*
- ThP 209 **Detection of Gamma-Hydroxybutyric Acid (GHB) and its Analogs by Liquid Chromatography Mass Spectrometry**; Yuriy Uvaydov; *N/A, New York, NY*
- ThP 210 **Trace Fiber Analysis using Nanomanipulation Coupled to Nanospray Mass Spectrometry**; Nicole Ledbetter; Guido F. Verbeck; *University of North Texas, Colleyville, TX*
- ThP 211 **Application of the Mass-Spectrometry in Forensic Investigation of the Counterfeit Alcohol Products**; Pavel Zinovev; *Republican Forensic Expertise Centre, Tashkent, Uzbekistan*
- ThP 212 **Determination of EDTA in Dried Bloodstains by LC-MS-MS for Forensic Investigations of Possible DNA (Blood) Evidence Tampering**; Samantha J. Richardson<sup>2</sup>; Kevin D. Ballard<sup>1</sup>; <sup>1</sup>*NMS Labs, Willow Grove, PA*; <sup>2</sup>*Celgene, San Diego, CA*
- ThP 213 **Instrumentation Methods for Field Analysis of CW and Human Decomposition VOCs**; Mike E Stevens<sup>1</sup>; Natalie J Mitchell<sup>2</sup>; Brian A Eckenrode<sup>3</sup>; Nishan Dulgerian<sup>3</sup>; Rex A Stockham<sup>3</sup>; <sup>1</sup>*Uniformed Services Univ. of the Health Sciences, Bethesda, MD*; <sup>2</sup>*Oak Ridge Institute for Science and Education, Oak Ridge, TN*; <sup>3</sup>*Federal Bureau of Investigation, Quantico, VA*
- ThP 214 **A Reverse-Energy Ramp Triple Quadrupole MS-MS Library of Food and Environmental Contaminants**; Anna M. Przyborowska; Andre Boegeholz; Raj K.P. Patel; John M. Halket; *King's College London, London, UK*
- ThP 215 **Identification and Quantification of Date Rape Drug Surrogates in Alcohol/Water Matrices using ESI-MS and ESI-MS<sup>n</sup>**; Justin Lygrisse; *Wichita State University, Wichita, KS*
- ThP 216 **Determination of Cocaine and Morphine-Derivatives in Serum using Automated Sample Preparation Coupled with RRLC/Triple Quadrupole Mass Spectrometer**; J. Roehrich<sup>1</sup>; J. Becker<sup>1</sup>; R. Urban<sup>1</sup>; S. Zoermtlein<sup>1</sup>; Juergen Wendt<sup>2</sup>; <sup>1</sup>*Institute of Legal Medicine, Johannes Gutenberg-Un, Mainz, Germany*; <sup>2</sup>*Agilent Technologies, Sales & Service GmbH & Co KG, Waldbronn, Germany*
- ThP 217 **Qualitative and Quantitative Determination of Phencyclidine (PCP) In One-Year-Old Dried Bloodstains in a Forensic Case**; Loan T. Nguyen; Kevin D. Ballard; *NMS Labs, Willow Grove, PA*
- ThP 218 **A Novel and Efficient Screen for Stimulants and Beta-2-Agonists from Various Nutritional Supplements by Liquid Chromatography Tandem Mass Spectrometry**; Caroline Wang; Petra Hartmann-Fischbach; Timothy Krueger; Marcia Small; Terry Wells; Anna Tellingner; *Industrial Laboratories, Wheat Ridge, CO*
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- MICRO-SCALE SEPARATION MS, 219 - 242**
- ThP 219 **Optimization of Column Length and Emitter ID on Peak Capacity, Protein Identification and Dynamic Range in NanoLC-MS**; Mike S. Lee<sup>1</sup>; Jesse Canterbury<sup>2</sup>; Edward J. Hsieh<sup>3</sup>; Gary Valaskovic<sup>4</sup>; Michael J. Maccoss<sup>3</sup>; <sup>1</sup>*Milestone Development Services, Newtown, PA*; <sup>2</sup>*Univ of Washington, Genome S, Seattle, WA*; <sup>3</sup>*University of Washington, Seattle, WA*; <sup>4</sup>*New Objective, Inc., Woburn, MA*
- ThP 220 **Micro-Chromatofocusing (μCF)-Monolithic Liquid Chromatography-Tandem Mass Spectrometry (LC-MS-MS) Combined with Fluorescence Imaging for the Microscale Analysis of Embryonic Stem Cell Proteins**; Katie Hersberger; David M. Lubman; David Misek; *University of Michigan, Ann Arbor, MI*
- ThP 221 **Determining the Presence of Residual Hemoglobin from Bacillus Spores for Forensic Evidence Analysis using HPLC-Chip Cube Ion Trap Mass Spectrometry**; Catherine E Petersen<sup>1</sup>; Helen Kreuzer<sup>1</sup>; Andy Gieschen<sup>2</sup>; Karen Wahl<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Lab, Richland, WA*; <sup>2</sup>*Agilent Technologies, San Diego, CA*
- ThP 222 **Automated 2D LC-MS using a Split-Free Nanoscale LC System**; P. Taylor<sup>1</sup>; A. Podtelejnikov<sup>2</sup>; M.B. Trelle<sup>2</sup>; M.B. Andersen<sup>2</sup>; M. Moran<sup>3</sup>; T. Kislinger<sup>3</sup>; <sup>1</sup>*Hospital for Sick Children, Toronto, Canada*; <sup>2</sup>*Proxeon A/S, Odense, Denmark*; <sup>3</sup>*University of Toronto, Toronto, Canada*
- ThP 223 **Maximizing Performance of Sub-2 μm Packed Nanobore LC Columns: Minimizing Extra-Column Variance**; Carla Marshall-Waggett; Amanda Berg; Gary Valaskovic; *New Objective, Inc., Woburn, MA*
- ThP 224 **OptiPep: A Set of Synthetic Peptide Standards for Optimizing NanoLC-MS-MS**; Andreas Kirschner<sup>1</sup>; Marcus Bantscheff<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technical University Munich, Freising, Germany*; <sup>2</sup>*Cellzome Ag, Heidelberg, Germany*
- ThP 225 **Optimized Two-Dimensional Nano-Liquid chromatography Tandem Mass Spectrometry Protocols for Proteomics Applications: On-Line or Off-Line Coupling?**; Anne-Marie Hesse; Paulo Marcelo; Jean Rossier; Joelle Vinh; *CNRS UMR7637/ESPCI ParisTech, Paris, France*
- ThP 226 **Highly Sensitive Analysis of Pharmaceutically Relevant Analytes, Employing a Novel Ultra High Capacity Chip**; Lukas Trojer; Martin Vollmer; Stephan

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- Buckenmaier; *Agilent Technologies, Waldbronn, Germany*
- ThP 227 **LCMS Strategies for Improved Protein Identification from Complex Mixtures;** Katherine Williams<sup>1</sup>; David Neyer<sup>2</sup>; David Cox<sup>3</sup>; Christie L Hunter<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Foster City, CA*; <sup>2</sup>*Eksigent Technologies, Dublin, CA*; <sup>3</sup>*MDS Analytical Technologies, Concord, ON*
- ThP 228 **Splitless Nano-LC Technology for Biomolecular Research: Proteomics to Fossilomics;** Lisa Freimark<sup>1</sup>; Alexandre Podtelejnikov<sup>2</sup>; John Lindsay<sup>2</sup>; Michael Andersen<sup>2</sup>; Wenxia Zheng<sup>4</sup>; Jeffrey Engelman<sup>3</sup>; Mary Schweitzer<sup>4</sup>; John M Asara<sup>1</sup>; <sup>1</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>2</sup>*Proxeon A/S, Odense, Denmark*; <sup>3</sup>*Massachusetts General Hospital, Boston, MA*; <sup>4</sup>*North Carolina State University, Raleigh, North Carolina*
- ThP 229 **Investigation of Elastomer Core Compression Effect on Minimizing Trapping Column Band Broadening;** Amanda Berg; Carla Marshall-Waggett; Gary Valaskovic; *New Objective, Inc., Woburn, MA*
- ThP 230 **Chip-Based Micellar Electrokinetic Chromatography – Electrospray Ionization Mass Spectrometry Utilized a Low Sheath Flow interface;** Ju-Li Huang; Fu-An Li; Guor-Rong Her; *National Taiwan University, Taipei, Taiwan*
- ThP 231 **Characterization of Single Neurons using Capillary Electrophoresis with Electrospray Ionization Mass Spectrometric Detection;** Theodore E. Lapainis; Stanislav Rubakhin; Jonathan V. Sweedler; *University of Illinois, Urbana, IL*
- ThP 232 **Development of an Integrated High-Pressure Microfluidic Nano-Scale LC Consumable;** Geoff Gerhardt; Christopher Benevides; Bernard Bunner; Dennis DellaRovere; Keith Fadgen; Joseph Michienzi; James Murphy; *Waters Corporation, Milford, MA*
- ThP 233 **Active Spray Control with Electric Field Optimization for Online NanoLC with Polymeric Spray Tips;** Art Fogiel, Jr.; Andris Suna; SAU LAN TANG STAATS; *Phoenix S and T, Inc, Elkton, MD*
- ThP 234 **Capillary Electrophoresis – Mass Spectrometry Based on a PMMA Chip and a Low-Sheath-Flow Interface;** Fu-An Li; Ju-Li Huang; Guor-Rong Her; *National Taiwan University, Taipei, Taiwan*
- ThP 235 **A Zero Dead Volume ESI Coupled Microfluidic Chip for Millisecond Time-resolved Studies by Electrospray Mass Spectrometry;** Derek Wilson; Ethan Tumarkin; *York University, Toronto, Canada*
- ThP 236 **A Novel Microfluidic Chip-Based Column Platform for High Efficiency Separations in an Easy to Use Format;** Don W. Arnold; Nicole Hebert; Patrick Leung; Erika Lin; Remco Van Soest; J. Bryce Young; *Eksigent Technologies, Dublin, CA*
- ThP 237 **High Sensitivity Nanocapillary Chromatography Combined with Active Background Ion Reduction Increases Signal to Noise Ratios, Sensitivity and Overall System Performance;** John M. Neveu<sup>1</sup>; William S. Lane<sup>1</sup>; Bogdan A. Budnik<sup>1</sup>; Gary A. Valaskovic<sup>2</sup>; Ben J. Ngo<sup>2</sup>; <sup>1</sup>*Harvard University, Cambridge, MA*; <sup>2</sup>*New Objective, Inc., Woburn, MA*
- ThP 238 **Optimization of Novel Fused-Core Silica Particle Nanobore Columns Using a Pump Switching Motif for Mass Spectrometry;** Robert Moody<sup>1</sup>; Gary Valaskovic<sup>2</sup>; Mike S. Lee<sup>3</sup>; <sup>1</sup>*MAC-MOD Analytical, Chadds Ford, PA*; <sup>2</sup>*New Objective, Inc., Woburn, MA*; <sup>3</sup>*Milestone Development Services, Newtown, PA*
- ThP 239 **Complementarities of MALDI and ESI for 2DLC-MS-MS: Expanding Proteome Coverage of Complex Samples with Multiple Dimensions of Analysis;** Sega Ndiaye; Anne-Marie Hesse; Jean Rossier; Joelle Vinh; *CNRS UMR7637/ESPCI ParisTech, Paris, France*
- ThP 240 **Microfluidic Chip Electrophoresis/Mass Spectrometry Interface Designed to Function with Low Electroosmotic Flow for the Analysis of Proteins;** Xiuli Mao; Brent R. Reschke; Kathleen C. Kelly; Aaron T. Timperman; *Department of Chemistry, West Virginia University, Morgantown, WV*
- ThP 241 **Improvement of Sequence Coverage and Sensibility in Two-Dimensional Nano-Liquid Chromatography Tandem-Mass Spectrometry Thanks to Contaminants' Removal;** Anne-Marie Hesse; Paulo Marcelo; Jean Rossier; Joelle Vinh; *CNRS UMR 7637/ESPCI ParisTech, Paris, France*
- ThP 242 **Enhanced Chromatographic Resolution using Polymeric Based Reversed Phase Materials for Online Electrospray LC-MS of Intact Proteins;** Robert N. O'meally; Marjan Gucek; Robert N. Cole; *Johns Hopkins School of Medicine, Baltimore, MD*
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- CARBOHYDRATES/OLIGOSACCHARIDES – BIOMARKER DISCOVERY, 243 - 250**
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- ThP 243 **Coupling of Fully Automated Chip-Based Electrospray Ionization to High Capacity Ion Trap Mass Spectrometer for High Throughput Ganglioside Analysis;** Cristina Mosoarca<sup>1</sup>; Marius Chirita<sup>1</sup>; Reinaldo Almeida<sup>2</sup>; Mark Allen<sup>2</sup>; Alina D. Zamfir<sup>1</sup>; <sup>1</sup>*National Institute for R&D in Electrochemistry, Timisoara, Romania*; <sup>2</sup>*Advion BioSciences, Norfolk, UK*
- ThP 244 **Changes in the Glycosylation Pattern of Total Serum IgG in Patients with Rheumatoid Arthritis Analyzed by MALDI-TOF MS;** Katrin Spärbier<sup>1</sup>; Hassan Dihazi<sup>2</sup>; Sabine Blaschke<sup>2</sup>; Gary Krupp<sup>3</sup>; Gerd-Anton Mueller<sup>2</sup>; Flad Thomas<sup>4</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Leipzig, Germany*; <sup>2</sup>*University Hospital Goettingen, Goettingen, Germany*; <sup>3</sup>*Bruker Daltonics Inc, Fremont, CA*; <sup>4</sup>*Panatecs GmbH, Tuebingen, Germany*
- ThP 245 **Derivatization of N-linked Glycans for Sensitive Detection by MALDI-TOF MS toward Glyco-Biomarker Discovery;** Osamu Tani<sup>2</sup>; Hisashi Narimatsu<sup>1</sup>; Akihiko Kameyama<sup>1</sup>; <sup>1</sup>*Research Center for Medical Glycoscience, AIST, Tsukuba, Japan*; <sup>2</sup>*shimadzu Corporation, Kyoto, Japan*
- ThP 246 **Digging Deep into the Human Serum Glycome;** Caroline Chu<sup>1</sup>; Milady Ninonuevo<sup>1</sup>; Brian H. Clowers<sup>1</sup>; Patrick D. Perkins<sup>2</sup>; Kevin Killeen<sup>2</sup>; Suzanne Miyamoto<sup>3</sup>; Rudolf Grimm<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*; <sup>3</sup>*UC Davis Cancer Center, Sacramento, CA*
- ThP 247 **Quantitative Derivatization of  $\alpha$ 2,3- and  $\alpha$ 2,6-Sialoglycans for the Detection Glyco-Biomarkers by MALDI-TOF MS;** Masaaki Toyoda; Hiromi Ito; Yu-ki Matsuno; Hisashi Narimatsu; Akihiko Kameyama; *Research Center for Medical Glycoscience, AIST, Tsukuba, Japan*
- ThP 248 **Glycan Markers for Ovarian Cancer with High Sensitivity and High Specificity;** Hyun Joo An<sup>1</sup>; Scott Kronewitter<sup>1</sup>; Jaehan Kim<sup>1</sup>; Maria Lorna De Leoz<sup>1</sup>; Sean Beecroft<sup>1</sup>; Gary Leiserowitz<sup>2</sup>; Suzanne Miyamoto<sup>2</sup>; Kit Lam<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*UC Davis Cancer Center, Sacramento, CA*

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- ThP 249 **Analysis of O-linked Glycans Derived from Normal and Diseased EOC Plasma by Nano LC-ESI-FTICR Mass Spectrometry**; Michael S. Bereman; Taufika Islam Williams; Adam Hawkridge; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- ThP 250 **Changes of Glycosylation in Cancer: The Case of AGP**; Timea Imre<sup>1</sup>; Tibor Kremmer<sup>1</sup>; Krisztina Ludanyi<sup>1</sup>; Laszlo Drahos<sup>1</sup>; Karoly Heberger<sup>1</sup>; Gabriella Pocsfalvi<sup>2</sup>; Karoly Vekey<sup>1</sup>; <sup>1</sup>*Hungarian Academy of Sci. Chemical Research Center, Budapest, Hungary*; <sup>2</sup>*Inst. Sci. dell' Alimentazione, CNR, Avellino, Italy*
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- LIPIDS: BIOCHEMISTRY & STEROIDS 2, 251 - 267**
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- ThP 251 **Comparison of LC-MS-MS and Radioimmunoassay for DHEAS Determinations in Chimpanzees (*Pan troglodytes*)**; Sarah Pruett; M. Kyle Cannon; James G. Herndon; Mark Wilson; *Yerkes Natl. Primate Res. Ctr., Emory University, Atlanta, GA*
- ThP 252 **Comparison of Combined Isoprostane Metabolites with the Single Isomer 2,3-dinor-iPF2a-III in Human Urine as a Biomarker of Oxidative Stress**; Weiyang Yan<sup>1</sup>; Gary D. Byrd<sup>2</sup>; <sup>1</sup>*Wake Forest University, Winston-Salem, NC*; <sup>2</sup>*R.J. Reynolds Tobacco Co., Winston-salem, NC*
- ThP 253 **A Sphingosine Kinase Activity Assay using Direct Infusion Electrospray Ionization Tandem Mass Spectrometry**; YouXun Jin<sup>1</sup>; Hwan-Soo Yoo<sup>1</sup>; Yong-Moon Lee<sup>1</sup>; Akio Kihara<sup>3</sup>; Yasuyuki Igarashi<sup>3</sup>; Hun-Young So<sup>2</sup>; Hyong-Ha Kim<sup>2</sup>; Yong-Hyeon Yim<sup>2</sup>; <sup>1</sup>*Chungbuk National University, Chongju, South Korea*; <sup>2</sup>*KRISS, Daejeon, south korea*; <sup>3</sup>*Hokkaido University, Sapporo, Japan*
- ThP 254 **Analysis of Lipid Storage Myopathy (ETFHD Mutant or PNPLA2 Mutant) by Direct Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry**; Nobuhiro Zaima<sup>1</sup>; Yuki Sugiura<sup>3</sup>; Aya Ohkuma<sup>2</sup>; Satomi Okahashi<sup>2</sup>; Satoru Noguchi<sup>2</sup>; ichizo nishino<sup>2</sup>; Tohru Ibi<sup>5</sup>; Fumiko Ozawa<sup>4</sup>; Ko Sahashi<sup>4</sup>; Mitsutoshi Setou<sup>6</sup>; *Mitils, Tokyo, Japan*; <sup>2</sup>*National Center of Neurology and Psychiatry, Tokyo, Japan*; <sup>3</sup>*Tokyo Institute of Technology, Tokyo, Japan*; <sup>4</sup>*Aichi Medical University, Aichi, Japan*; <sup>5</sup>*Aichi Medical University College of Nursing, Aichi, Japan*; <sup>6</sup>*Hamamatsu University School of Medicine, Hamamatsu, Japan*
- ThP 255 **LC-MS Analysis of Diacylglycerol Lipase-Mediated Lipid Metabolism in Neural Cells**; Giuseppe Astarita; Daniele Piomelli; *Univ. California Irvine, Irvine, CA*
- ThP 256 **Optimization of Triacylglyceride Production from Diatoms as Potential Feedstock For Biodiesel Production**; Pamela Lane<sup>1</sup>; Frank Zendejas<sup>1</sup>; Eizadora T. Yu<sup>1</sup>; Sara P. Gaucher<sup>2</sup>; Kenneth Sale<sup>1</sup>; Blake Simmons<sup>1</sup>; Todd W. Lane<sup>1</sup>; <sup>1</sup>*Sandia National Laboratories, Livermore, CA*; <sup>2</sup>*Amyris Biotechnologies, Emeryville, CA*
- ThP 257 **Lc-MS Analysis of 2 Day Old Rat Pup Brain Gangliosides from Mothers Supplemented during Pregnancy with Dairy Derived Complex Lipids**; Bertram Fong<sup>3</sup>; Edwin Lowe<sup>1</sup>; Mark Vickers<sup>2</sup>; Paul McJarrow<sup>3</sup>; Carmen Norris<sup>3</sup>; <sup>1</sup>*University of Tasmania, Hobart, Australia*; <sup>2</sup>*Liggins Institute, Auckland, New Zealand*; <sup>3</sup>*Fonterra Reseach Centre, Palmerston North, New Zealand*
- ThP 258 **Direct Analysis of Intact and Oxidized Phospholipids and Sphingolipids in Tissue Samples by Desorption Electrospray Ionization Mass Spectrometry**; Marcela Nefliu; Nicholas Manicke; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- ThP 259 **A Highly Sensitive Metabolic Profiling of Human Serum and Prostatic Androgens by Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry**; Kouwa Yamashita; Madoka Takahashi; Kanae Sukegawa; Mitsuteru Numazawa; *Tohoku Pharmaceutical University, Sendai, Japan*
- ThP 260 **Mass Spectrometric Analysis of Changes in Phospholipid Levels in JAR Cells upon Estrogen Stimulation**; Mallikharjuna Reddy Bogala<sup>1</sup>; Subhrangsu S. Mandal<sup>1</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>*The University of Texas at Arlington, Arlington, TX*
- ThP 261 **Desferal Selectively Normalizes Levels of Membrane Raft Lipids in Liver of Rabbits Challenged with High Cholesterol Diet**; Guangzhou Shu; Andrew Jenner; Robin Chan; Xueli Guan; Ning Pan; Benny Kwong-Huat Tan; Markus R Wenk; Barry Halliwell; *National University of Singapore, Singapore*
- ThP 262 **Diels-Alder Derivatization with 4-substituted 1,2,4-triazole-3,5-diones for Analysis of Vitamin D Metabolites and Other Lipids using UPLC-ESI-MS-MS**; Pavel aronov<sup>1</sup>; Katrin Georgi<sup>1</sup>; Sung Hee Hwang<sup>1</sup>; Katja Dettmer<sup>2</sup>; Bruce D Hammock<sup>1</sup>; <sup>1</sup>*UC Davis, Davis, CA*; <sup>2</sup>*University of Regensburg, Regensburg, Germany*
- ThP 263 **GC-MS Characterization of Antioxidant Pregnane Type Steroidal Saponin from Aegle Marmelos Leaves**; Nilesh Kumar Sharma; Ramasre Prasad; *Indian Institute of Technology, Roorkee, INDIA*
- ThP 264 **Strategies for Bioassay-Directed UPLC-MS Discovery of Variant CAR Ligands using Multiplexed CID and Mass Defect Filtering**; Michael C. Stagliano<sup>2</sup>; Joshua G. DeKeyser<sup>2</sup>; Curtis J. Omiecinski<sup>2</sup>; A. Daniel Jones<sup>1</sup>; <sup>1</sup>*Michigan State University, East Lansing, MI*; <sup>2</sup>*Pennsylvania State University, University Park, PA*
- ThP 265 **Lipidomic and Metabolic Study by Mass Spectrometry in Correlation with Aging in C. Elegans**; Johann Rivière; María Eugenia Soria Diaz; Emmanuel Varesio; Gerard Hopfgartner; *University of Geneva, Geneva, Switzerland*
- ThP 266 **LC-MS Analysis of 80 Day Old Rat Brain Phospholipids from Rats Supplemented from Ten Days Old with Complex Lipids**; Carmen Norris<sup>1</sup>; Edwin Lowe<sup>2</sup>; Mark Vickers<sup>3</sup>; Paul McJarrow<sup>1</sup>; Bertram Fong<sup>1</sup>; <sup>1</sup>*Fonterra Research Centre, Palmerston North, New Zealand*; <sup>2</sup>*University of Tasmania, Hobart, Australia*; <sup>3</sup>*Liggins Institute, Auckland, New Zealand*
- ThP 267 **Ozone Induced Oxidation of Plasmalogen Glycerophospholipids**; Kelly Wynalda; Robert C. Murphy; *University of Colorado Health Sciences Center, Aurora, CO*
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- LC-MS, 268 - 297**
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- ThP 268 **Ultrafiltration Tandem Mass Spectrometry Based Screening Assay for the Discovery of Bcl-2 Family Antiapoptotic Protein Inhibitors**; Suma Ramagiri; Fei Ma; Eldon Geisert; Duane Miller; Charles Ryan Yates; *University of Tennessee Health Science Center, Memphis, TN*
- ThP 269 **High Performance Liquid Chromatography Separation Followed by Tandem Mass Spectrometry Analysis of Hydroxyatrazine in Drinking Water and Urine**; Do-Gyun Kim<sup>1</sup>; Parinya Panuwet<sup>1</sup>; Larry L. Needham<sup>1</sup>; Dana B. Barr<sup>1</sup>; <sup>1</sup>*ORISE Fellow, CDC/NCEH/DLS/OAT, Atlanta, GA*

## THURSDAY POSTERS

- ThP 270 **LC-HRMS Profile of Plasma Samples of High Fat and Fructose Diet Rats to Study Insulin Resistance in Diabetes;** Claudio Medana; Claudio Baiocchi; Francesco Carbone; Valeria Giancotti; Manuela Aragno; Ilenia Vercellinato; *University of Turin, Torino, Italy*
- ThP 271 **Analysis of HPLC Loading Conditions for Maximal Mass Spectrometry Peptide Identifications;** Amelia Peterson<sup>2</sup>; Laura Hohmann<sup>1</sup>; Li Huang<sup>1</sup>; Bong Kim<sup>1</sup>; Jimmy K Eng<sup>3</sup>; Daniel B Martin<sup>1</sup>; <sup>1</sup>*Institute for Systems Biology, Seattle, WA*; <sup>2</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>3</sup>*University of Washington, Seattle, WA*
- ThP 272 **A Low Flow – Liquid Junction Capillary Electrophoresis/Mass Spectrometry Interface for Nonvolatile Buffer;** Fu-An Li; Ju-Li Huang; Guor-Rong Her; *National Taiwan University, Taipei, Taiwan*
- ThP 273 **Development of a High Throughput Antibacterial Assay using Selective Biomimetic Target Complexation and ESI-MS Detection;** Sijia Shen; Manishkumar D. Joshi; Laura D. Mydlarz; Kevin A. Schug; *University of Texas, Arlington, TX*
- ThP 274 **Rapid Determination of the Applicability of Hydrophilic Interaction Chromatography Utilizing ACD Labs Log D Suite: A Bioanalytical Application;** Eugene P. Kadar; Chad E. Wujcik; David P. Wolford; Olga Kavetskaia; *Pfizer Inc., Groton, CT*
- ThP 275 **In vitro and in vivo Multiplexed Detection of Matrix Metalloproteinases using Microdialysis Sampling and LC-MS-MS;** Ying Wang<sup>1</sup>; Daniel Loegering<sup>2</sup>; Dmitri Zagorevski<sup>1</sup>; Michelle Lennartz<sup>2</sup>; Julie Stenken<sup>3</sup>; <sup>1</sup>*Rensselaer Polytechnic Institute, Troy, NY*; <sup>2</sup>*Albany Medical College, Albany, NY*; <sup>3</sup>*University of Arkansas, Fayetteville, AR*
- ThP 276 **A Comparison of LC-MS Mass Analyzers for Screening, Confirmation and Quantification of Drugs in Blood;** John M. Hughes<sup>1</sup>; Greg Kilby<sup>1</sup>; Michael C. Zumwalt<sup>1</sup>; Jeri D. Roper-Miller<sup>2</sup>; Peter R. Stout<sup>2</sup>; H. Chip Walls<sup>3</sup>; <sup>1</sup>*Agilent Technologies, Pleasanton, CA*; <sup>2</sup>*RTI International, Research Triangle Park, NC*; <sup>3</sup>*U. of Miami Medical School, Miami, FL*
- ThP 277 **Extraction of Corticosteroids using 96-Well Supported Liquid Extraction (SLE) and LC-MS-MS Analysis;** Lee Williams; Steve Jordan; Helen Lodder; Matthew Cleeve; Richard Calverley; Joanna Smith; *Biotage GB Limited, Hengoed, UK*
- ThP 278 **LC-MS Top-Down Analysis and Intact Mass Analysis of Recombinant Immunoglobulin Gamma Antibodies on Orbitrap;** Pavel V. Bondarenko<sup>3</sup>; Vlad Zabrouskov<sup>1</sup>; Alexander Makarov<sup>2</sup>; Zhongqi Zhang<sup>3</sup>; <sup>1</sup>*ThermoFisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; <sup>3</sup>*Amgen, Inc., Thousand Oaks, CA*
- ThP 279 **A Novel Analytical Approach for OATPs Hepatic Uptake Transport Assays using LC-MS-MS;** Limin He; Ilaria Badagnani; Adrian Fretland; William Fitch; Mario Monshouwer; *Roche Palo Alto, Palo Alto, CA*
- ThP 280 **Development of a LC-MS-MS Method for Measuring Deuterium Incorporation into DNA;** Randall Purves; Denis Normandin; Simon Wong; Yves Boie; Karen Ng; Kevin Bateman; *Merck Frosst Canada Ltd., Kirkland, Canada*
- ThP 281 **Mapping Post Translational Modifications using Single Aliquot/Dual Scanning Method;** Valerie Cavett<sup>1</sup>; Stephanie M. Prater<sup>1</sup>; Simon J. Prosser<sup>2</sup>; John L. Cleveland<sup>1</sup>; Silvia Coenen<sup>1</sup>; Frank C. Dorsey<sup>1</sup>; Thomas N. Corso<sup>2</sup>; Jennifer Busby<sup>1</sup>; <sup>1</sup>*TSRI-Scripps Florida, Jupiter, FL*; <sup>2</sup>*Advion Biosciences, Inc., Ithaca, NY*
- ThP 282 **Causes of Dynamic Range Limitations in Proteomics Experiments;** Chris Lock; David Cox; Stephen A Tate; *MDS Sciex, Concord, Canada*
- ThP 283 **Sample Injection is the Main Thing Limiting Chromatographic Performance: A Multi-Stage Approach toward Achieving “Ultra Performance” using Ordinary Hardware;** QingPing Han; Mark J. Hayward; *Lundbeck Research USA, Stockton, NJ*
- ThP 284 **Identification of Oxygen Functionalities in Analytes by Mass Spectrometry;** Jennifer N Reece; Mingkun Fu; Steven C Habicht; Nelson R Vinueza; Hilkka I Kenttamaa; *Purdue University, West Lafayette, IN*
- ThP 285 **Simultaneous Analytical Method for 44 Illegal Compounds in Foods by LC-ESI-MS-MS;** Taehyung Yoon; Eunju Kim; Hyungwook Chung; Sujung Hu; Sung-Kug Park; Jangduck Choi; Gun-Jo Woo; Dongmi Choi; *Korea Food & Drug Administration, Seoul, South Korea*
- ThP 286 **Peptide Retention Prediction for Reversed-Phase Sorbents with Alternative Selectivity: Application in Proteomics;** Chris Kuusselka<sup>1</sup>; Vic Spicer<sup>2</sup>; Kenneth G. Standing<sup>2</sup>; Werner Ens<sup>2</sup>; John A. Wilkins<sup>2</sup>; Oleg V. Krokhin<sup>2</sup>; <sup>1</sup>*Manitoba Centre for Proteomics and Systems Biology, Winnipeg, Canada*; <sup>2</sup>*University of Manitoba, Winnipeg, Canada*
- ThP 287 **Application of LC-MS-MS with APCI Source for the Analysis of a Liquid Crystal Mixture;** Sung-Chan Jo; Weonsik Oh; *Samsung Electronics Co., Ltd., Yongin, South Korea*
- ThP 288 **Polar Small Molecule Analysis in Serum by Pretreatment and Multi-Mode HPLC Columns;** Ken Tseng<sup>1</sup>; Kei Oide<sup>2</sup>; Kazunori Iwata<sup>2</sup>; <sup>1</sup>*Shodex, New York, NY*; <sup>2</sup>*Showa Denko, KK, Kawasaki, Japan*
- ThP 289 **Determination of the Cyclic Dipeptide FK228 in Human and Mouse Plasma by LC-MS;** Xiaohong Chen<sup>1</sup>; Erin Gardner<sup>2</sup>; William Figg<sup>1</sup>; <sup>1</sup>*National Institute of Health, Bethesda, MD*; <sup>2</sup>*SAIC-Frederick, NCI-Frederick, Frederick, MD*
- ThP 290 **Methodology of Accelerating Bioanalysis Method Development in Drug Discovery with LC-MS-MS;** Ling Morgan<sup>1</sup>; Xin Zhang<sup>2</sup>; Lily Li<sup>3</sup>; <sup>1</sup>*Tandem Labs, Woburn, MA*; <sup>2</sup>*Tandem Labs New England, Woburn, MA*; <sup>3</sup>*Tandemlabs, Woburn, MA*
- ThP 291 **Evaluation of High Sensitive Analysis of Hydrophilic Compounds using LC-MS-MS with Ion-Suppressor Device;** Seiji Ito; Fumiya Nakata; Yuji Sawada; *Tosoh Corporation, Ayase, Japan*
- ThP 292 **Indirect Analysis of a Wet Strength Resin in Cellulose Containing Materials by LC-MS;** Teresa E. Peterson; *Kimberly-Clark, Roswell, GA*
- ThP 293 **Quantitative LC-MS-MS Methods Development for a Very Polar Aminoglycoside Compound: Gentamicin;** Deqing Xiao; *Pfizer, Groton, CT*
- ThP 294 **Determination of Plasma Epinephrine, Norepinephrine and Dopamine by LC-MS-MS using Isobaric Amine Reactive Tags;** Michal Weinstock<sup>1</sup>; Brian Williamson<sup>2</sup>; Scott B. Daniels<sup>1</sup>; Subodh Nimkar<sup>1</sup>; Jolaine Twentyman<sup>3</sup>; Ravinder J. Singh<sup>3</sup>; Babu Purkayastha<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*; <sup>2</sup>*Ab, Framingham, MA*; <sup>3</sup>*Mayo Clinic, Rochester, MN*
- ThP 295 **Assessing the Effect of Ethylene Oxide Sterilization on a Therapeutic Protein in Pre-Filled Devices;** Oleg Borisov; Galahad U. Deperalta; Victor Ling; *Genentech, South San Francisco, CA*

## THURSDAY POSTERS

- ThP 296 **C18 Ceramide Analysis in Mammalian Cells Employing Reversed-Phase High Performance Liquid Chromatography Tandem Mass Spectrometry**; Teka-Ann S. Haynes; Penelope J. Duerksen-Hughes; Maria Filippova; Valery Filippov; Kangling Zhang; *Loma Linda University, Mentone, CA*
- ThP 297 **Improved Overall Mass Spectral Acquisition Rates using a Novel HPLC Storage Loop**; Charlene Bierl<sup>1</sup>; Simon J Prosser<sup>2</sup>; Stephen R Master<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Advion BioSystems, Ithaca, NY*
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- CLINICAL CHEMISTRY – LARGE MOLECULE, 298 - 308**
- ThP 298 **Demonstration by Tandem Mass Spectrometry of Leukocyte Cell-Derived Cheomtaxin 2(LECT2) Composition of Renal Amyloid**; Charles Murphy; Shuching Wang; Alan Solomon; *Univ. of Tennessee Graduate School of Medicine, Knoxville, TN*
- ThP 299 **Clinical Protein Analysis: Quantitation of Urinary Albumin by LC-MS-MS using a Recombinant 15N Labeled Albumin Internal Standard and Tryptic Digestion**; Jesse C. Seegmiller; David R. Barnidge; Bradley E. Burns; Timothy S. Larson; Aisha Shaikh; Ward H. Lutz; Rajiv Kumar; John C. Lieske; *Mayo Clinic, Rochester, MN*
- ThP 300 **Rapid Reagentless Detection of *M. tuberculosis* H37Ra in Respiratory Effluents**; Kristl Adams<sup>1</sup>; Paul T. Steele<sup>1</sup>; Mike Bogan<sup>1</sup>; Nicole M. Sadler<sup>2</sup>; Sue Martin<sup>1</sup>; Audrey Martin<sup>3</sup>; Matthias Frank<sup>1</sup>; <sup>1</sup>*Lawrence Livermore National Laboratory, Livermore, CA*; <sup>2</sup>*University of California, Davis, CA*; <sup>3</sup>*Michigan State University, East Lansing, MI*
- ThP 301 **Affinity Capture and MALDI MS Analysis of Vancomycin-Resistant Enterococci**; Ya-Shiuan Lin<sup>1</sup>; Pei-Jane Tsai<sup>2</sup>; yu-chie chen<sup>1</sup>; <sup>1</sup>*National Chiao Tung Univ., Hsinchu, Taiwan*; <sup>2</sup>*National Applied Research Laboratories, Taipei, Taiwan*
- ThP 302 **Ceruloplasmin Quantitation in Dried Blood Spots by LC-MS-MS for Newborn Screening of Wilson Disease**; Katerina Sadilkova<sup>1</sup>; Amy R. de Wilde<sup>2</sup>; Martin Sadilek<sup>3</sup>; Valeria Vasta<sup>1</sup>; Sihoun Hahn<sup>2</sup>; <sup>1</sup>*Seattle Children's Research Institute, Seattle, WA*; <sup>2</sup>*University of Washington School of Medicine, Seattle, WA*; <sup>3</sup>*University of Washington, Seattle, WA*
- ThP 303 **Lipoprotein Compositional Changes Due to Storage: An Important Factor to Consider in Biomarker Discovery**; Haihong Zhou; Laura Swift; Ekaterina G. Deyanova; Kai Zhou; Matthew Mazur; Fanyu Meng; Robert Settlege; Yudong He; Xuemei Zhao; Nathan Yates; Ronald Hendrickson; *Merck Research Laboratories, Rahway, NJ*
- ThP 304 **Multiplexed Screening of the Cellular Uptake of Gold Nanoparticles using Laser Desorption/Ionization Mass Spectrometry (LDI-MS)**; Zhengjiang Zhu; Partha Ghosh; Oscar R. Miranda; Vincent M. Rotello; Richard W. Vachet; *University of Massachusetts Amherst, Amherst, MA*
- ThP 305 **Discovering Glycomic Markers for Prostate Cancer by Analyzing Serum Before and After Prostatectomy**; Maria Lorna De Leoz<sup>1</sup>; Hyun Joo An<sup>1</sup>; Scott Kronewitter<sup>1</sup>; Sean Beecroft<sup>1</sup>; Jaehan Kim<sup>1</sup>; Ruth Vinall<sup>2</sup>; Suzanne Miyamoto<sup>2</sup>; Ralph deVere White<sup>2</sup>; Kit S. Lam<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, CA*; <sup>2</sup>*UC Davis Cancer Center, Sacramento, CA*
- ThP 306 **Mass Spectrometric Quantification of Cardiolipin in Human Serum by MALDI-TOF with HPLC/ESI-MS Validation**; Elizabeth Ogbonna<sup>2</sup>; Kai Hamazaki<sup>1</sup>; Alfred L. Yerger<sup>2</sup>; Hee-yong Kim<sup>1</sup>; <sup>1</sup>*NIAAA, NIH, Bethesda, MD*; <sup>2</sup>*NICHD, NIH, Bethesda, MD*
- ThP 307 **Leukotriene E4 in Human Urine: Comparison of On-Line Purification and Liquid Chromatography-Tandem Mass Spectrometry with Enzyme Immunoassay**; Michael Armstrong; Nichole Reisdorph; Weiming Shen; Andy Liu; Ron Harbeck; *National Jewish Medical and Research Center, Denver, CO*
- ThP 308 **Rapid Multidrug-Resistance Profiling and Characterization of Mycobacterium Tuberculosis**; Christian Massire<sup>1</sup>; Cristina Ivy<sup>1</sup>; Natalia E. Kurepina<sup>2</sup>; Dorothy Fallows<sup>2</sup>; Barry N. Kreiswirth<sup>2</sup>; Gilla Kaplan<sup>2</sup>; Lawrence B. Blyn<sup>1</sup>; Ranga Sampath<sup>1</sup>; Steven A. Hofstadler<sup>1</sup>; David J. Ecker<sup>1</sup>; <sup>1</sup>*Ibis Biosciences, Inc., Carlsbad, CA*; <sup>2</sup>*Public Health Research Institute, Newark, NJ*
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- SMALL MOLECULE ANALYSIS FOOD: RELATED AND OTHER, 309 - 328**
- ThP 309 **Electrospray Ionization FT-ICR/MS Analysis of Iron and Ruthenium Complexes: Study of Oxidation and Solvent Effects**; Jeremie Ponthus; Christophe Roulet; Claudine Rangheard; Cecilia Citadelle; *Institut Francais du Petrole, Vernaison, France*
- ThP 310 **Polyphenol Analysis in Tea Extracts and Wines by LC-MS-MS**; Ruiqing Qiu; Johnie Brown; Stephen J. Lock; *Applied Biosystems, Framingham, MA*
- ThP 311 **Determination of Fatty Acid Composition of Triglycerides and Edible Oils with Graphite-Assisted Laser Desorption/Ionization (GALDI) Mass Spectrometry**; Jiangwei Li<sup>1</sup>; Hui Zhang<sup>2</sup>; Haitao Guo<sup>1</sup>; Edward S. Yeung<sup>1</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Pfizer Inc., Groton, CT*
- ThP 312 **Differentiation of Some Cyclic and Bicyclic  $\beta$ -Amino Acid Diastereomers Studied by Kinetic Method**; Anna R. M. Hyyryläinen<sup>1</sup>; Jaana M. H. Pakarinen<sup>1</sup>; Ferenc Fülöp<sup>2</sup>; Pirjo Vainiotalo<sup>1</sup>; <sup>1</sup>*University of Joensuu, Joensuu, Finland*; <sup>2</sup>*University of Szeged, Szeged, Hungary*
- ThP 313 **Enantioselective Determination of Acebutolol Enantiomers in Human Plasma by Liquid Chromatography with Tandem Mass Spectrometry using Cellobiohydrolase Chiral Stationary Phase**; Hongliang Jiang; Xiang-yu Jiang; Qin Ji; *Covance Laboratories Inc., Madison, WI*
- ThP 314 **Liquid Chromatography/Tandem Mass Spectrometric Method for the Quantification of Trans, Trans-2,4-Decadienal in Restaurant Kitchen**; Chiyang Wang; Hui Ling Lee; Dennis Paul Hsientang Hsieh; Kuen-Yuh Wu; *National Health Research Institutes, Miaoli, Taiwan*
- ThP 315 **Effects of Matrix Constituents and Ion Source Conditions on Electrospray Ionization Behavior of Byproducts Formed During Lignocellulosic Biomass Pretreatment Processes**; Ramin Vismeh; Shishir P. S. Chundawat; Venkatesh Balan; Bruce E. Dale; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- ThP 316 **Liquid Chromatography/Multi-Stage Mass Spectrometry for the Determination of Bisphenol Diglycidyl Ethers and its Derivatives in Canned Foods**; Maria Teresa Galceran; Hector Gallart-Ayala; Encarnacion Moyano; *University of Barcelona, Barcelona, SPAIN*
- ThP 317 **Mass Spectra of Cyclic Phosphonates and Phosphothionates Related to Chemical Weapon Convention**; Meehir Palit; Gary Mallard; *Org. for the*



## THURSDAY POSTERS

- Prohibition of Chemical Weapon (OPCW), The Hague, Netherlands*
- ThP 318 **Easy Ambient Sonic-Spray Ionization Mass Spectrometry (EASI-MS) for Quality Control and Typification of Biodiesel**; Renato Haddad; Rodrigo R. Catharino; Marcos N Eberlin; *Thomson Lab Unicamp, Campinas, Sp, Brazil*
- ThP 319 **Determination of Pesticide Residues in Foods using LTQ Orbitrap Mass Spectrometer**; CheongTae Kim<sup>1</sup>; Jongsoo Park<sup>2</sup>; *<sup>1</sup>NongShim Co., Ltd., Seoul, South Korea; <sup>2</sup>Euro Science Co., Ltd., Seoul, South Korea*
- ThP 320 **Identification of Impurities in the CCQM Sample by Ion Trap Time-of-Flight Mass Spectrometry**; Kang Ma<sup>1</sup>; Leren Wan<sup>2</sup>; Ting Huang<sup>1</sup>; Jingsong Wu<sup>2</sup>; Yuki Hashi<sup>2</sup>; *<sup>1</sup>National Institute of Metrology of China, Beijing, China; <sup>2</sup>Shimadzu Beijing Office, Beijing, China*
- ThP 321 **HPLC-ESI-MS Analysis of Laccase-Catalyzed Decolourization of Malachite Green**; Kumarasamy Murugesan; In-Hee Yang; Young-Mo Kim; Jong-Rok Jeon; Yoon-Seok Chang; *POSTECH, Pohang, South Korea*
- ThP 322 **Identification of Additives and Pesticides in Food and Water using Accurate Mass, Isotopic Mass Defects, and the “Rule-of-Three”**; Earl Michael Thurman; Imma Ferrer; *CEMS, University of Colorado, Boulder, CO*
- ThP 323 **Trimeric Cluster Formation – Important Step in Chiral Discrimination using Cooks’ Kinetic Method**; Karel Lemr<sup>1</sup>; Vaclav Ranc<sup>1</sup>; Petr Bednar<sup>1</sup>; Vladimír Havlicek<sup>2</sup>; *<sup>1</sup>Palacky University, Olomouc, Czech Republic; <sup>2</sup>Institute of Microbiology, Prague 4, Czech Republic*
- ThP 324 **Study for Measuring Accurate Composition of Insoluble Phthalocyanine Pigments by Mass Spectrometry**; Shuji Kagawa; *Mitsubishi Chemical Group, Yokohama, Japan*
- ThP 325 **Enantiomeric Discrimination between D- and L-Amino Acids using Optically Pure (+) / (-) Na<sub>2</sub>[Sb<sub>2</sub>(L-, D-tart)2] as Chiral-Selectors by ESI-MS**; Aruna B. Wijeratne; Sandra E. Spencer; Daniel W. Armstrong; Kevin A. Schug; *University of Texas, Arlington, TX*
- ThP 326 **Unique Fragmentation Pattern of EDTA-Fe(III) by Ion Trap Time of Flight Mass Spectrometry with Negative Electrospray Ion Source**; Leren Wan<sup>1</sup>; Fan Xiang<sup>2</sup>; Hashi Yuki<sup>1</sup>; *<sup>1</sup>Shimadzu Beijing Office, Beijing, China; <sup>2</sup>Shimadzu Biotech, Pleasanton, CA*
- ThP 327 **Identification and Quantitation of Sorbitol-Based Nuclear Clarifying Agents Extracted From Common Polypropylene-Derived Laboratory and Consumer Plasticware**; Jeffrey G. McDonald<sup>1</sup>; Carolyn L. Cummins<sup>1</sup>; Robert M. Barkley<sup>2</sup>; Bonne M. Thompson<sup>1</sup>; Holly A. Lincoln<sup>1</sup>; *<sup>1</sup>UT Southwestern Medical Center, Dallas, TX; <sup>2</sup>Univ. of Colorado Denver, Aurora, CO*
- ThP 328 **Two-Dimensional SFC/SFC/MS for the Analysis of Chiral Compounds**; Lu Zeng; Rongda Xu; Derek B. Laskar; Daniel B. Kassel; *Takeda San Diego, Inc., San Diego, CA*
- ThP 331 **Case Studies of Accurate Measurement of Small Molecules Drugs in Various Tissues: Knowledge Versus Assumption**; Marcele I. Barroso; Kris King; Chris Tran; Xin Zhang; *Tandem Labs, Woburn, MA*
- ThP 332 **Determination of 2-Pyrrolidinone in Swine Liver and Muscle by LC-MS-MS**; Yuhui Yang; Louis Crouch; Farhad Sayyarpour; *Schering-Plough Research Institute, Lafayette, NJ*
- ThP 333 **LC-MS-MS Bioanalysis of Acidic and Basic Compounds Utilizing a Double Liquid-Liquid Extraction with a pH Change in between**; Rachel Sun; Gary Overdorf; *Bioanalytical Systems, Inc., West Lafayette, IN*
- ThP 334 **Subchronic Carcinogen Dosing and Native Metabolic DNA Adduct Formation Monitored by LC-MS**; James Glick; Paul Vouros; *Northeastern University, Boston, MA*
- ThP 335 **Quantification of Etheno DNA Adduct by Isotope Dilution Capillary Liquid Chromatography Nanospray Ionization Tandem Mass Spectrometry**; Hauh-Jyun Candy Chen; Chia-Yen Wu; *National Chung Cheng Univers, Chia-Yi, Taiwan*
- ThP 336 **LC-MS-MS Quantification of Neurotransmitter Biomarkers for Efficacy Measurements**; David P. Budac; Mark J. Hayward; *Lundbeck Research US, Paramus, NJ*
- ThP 337 **Evaluation of Precision, Accuracy and Dilution Reliability in Upper Portions of Quadratic Calibration Curves in LC-MS and LC-MS-MS Bioanalytical Methods**; Alexandre Cadieux; Troy Bradley; Fabio Garofolo; *Algorithme Pharma Inc., Laval (Montreal), QC, Canada*
- ThP 338 **A Sensitive and High Throughput Assay for the Quantitation of Volatile Amines in Bio-fluids using Aqueous Normal Phase LC-MS-MS**; Michael Ma; Wechao Chen; Yong Q. Tang; *Arena Pharmaceuticals, San Diego, CA*
- ThP 339 **Measurement of Testosterone in Human Urine by Direct Injection using Nano-Pump Switching with Nanospray Tandem Mass Spectrometry(ESI-MS-MS)**; Daniel Magiera<sup>1</sup>; Mike S. Lee<sup>2</sup>; Gary Valaskovic<sup>3</sup>; *<sup>1</sup>Molecular MS Diagnostics, Cranston, RI; <sup>2</sup>Milestone Development Services, Newtown, PA; <sup>3</sup>New Objective, Inc., Woburn, MA*
- ThP 340 **Detection and Quantification of Sirtuin Metabolite O-Acetyl-ADP-Ribose (OAAADPr) in Mouse Liver Extracts using <sup>13</sup>C-OAAADPr and LC-MS-MS**; Susan Lee; Lei Tong; John M Denu; *UW Madison, Madison, WI*
- ThP 341 **Assessing Receptor Occupancy at the D2 Receptor: Quantitation of Cold Raclopride after Blocking with Haloperidol by LC-MS-MS**; James P. Bulgarelli<sup>1</sup>; Norman C. Ledonne, Jr.<sup>1</sup>; Paul Altiero<sup>1</sup>; Donna L. Maier<sup>2</sup>; Dan Widzowski<sup>2</sup>; Teng Peng<sup>2</sup>; My Linh T. Do<sup>2</sup>; *<sup>1</sup>Discovery DMPK, AstraZeneca Pharmaceuticals, Wilmington, DE; <sup>2</sup>Neuroscience Biology, AstraZeneca Pharmaceuticals, Wilmington, DE*
- ThP 342 **Serum Retinoid Levels are Decreased While Lysophosphatidic Acid Levels are Increased in Response to Liver Injury (Fibrosis) in Rats**; hideji fujiwara; Maria A Payne; Jon A Klover; Marek M Nagiec; W. Rodney Mathews; *Pfizer Global R&D, Chesterfield, MO*
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- QUANTITATION OF SMALL MOLECULES/BIOANALYSIS, 329 - 348**
- ThP 329 **Method Validation for Application of Artificial Cerebrospinal Fluid in Bioanalysis**; Yongkai Sun; Qingguo Tian; Voon Ong; *Memory Pharmaceuticals, Montvale, NJ*
- ThP 330 **Determination of Zolendronic Acid in Human and Dog Saliva using High-Performance Liquid Chromatography and Tandem Mass Spectrometry**;



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- ThP 343 **A Sensitive and Rugged Method to Measure Endogenous Levels of Homocysteine, S-adenosylmethionine(SAM) and S-adenosylhomocysteine(SAH) in Biological Samples using LC-MS-MS;** Suzie Yeh; Na Sang; Bart Emary; Rena Zhang; *Merck & Co., Inc, West Point, PA*
- ThP 344 **Comparison of Atmospheric Pressure Ionization Techniques for Quantitative Tandem Mass Spectrometry of Seven Androgens of Interest in Prostate Cancer Research;** Fred Bjorn Lih<sup>1</sup>; Mark A. Titus<sup>2</sup>; James L. Mohler<sup>2</sup>; Kenneth B. Tomer<sup>1</sup>; <sup>1</sup>*NIEHS/NIH, RTP, NC*; <sup>2</sup>*Roswell Park Cancer Institute, Buffalo, NY*
- ThP 345 **Comparison of Laser Diode Thermal Desorption (LDTD) Source vs LC-MS for the Analysis of a Therapeutic Drug in Biological Extracts;** Tony Edge<sup>1</sup>; Christopher Smith<sup>1</sup>; Steve Hill<sup>1</sup>; Pierre Picard<sup>3</sup>; Sylvain Letarte<sup>2</sup>; Ian D. Wilson<sup>1</sup>; Peter Vince<sup>1</sup>; <sup>1</sup>*AstraZeneca, Macclesfield, UK*; <sup>2</sup>*Phytronix Technologies, Blainville, QC*; <sup>3</sup>*Phytronix Technologies, Inc., Quebec, QC*
- ThP 346 **Accelerating High Quality Bioanalytical LC-MS Assays in a Regulated Environment;** Ethan R. Badman; Zhenmin Liang; Surendra Bansal; *Hoffmann-La Roche, Inc., Nutley, NJ*
- ThP 347 **Development of a Multiplexed Bioanalytical Method to Support Simultaneous LC-MS-MS Analysis of Phosphate Ester Prodrug and Parent Pharmaceutical Compounds;** Marc Browning; Daniel G. Morgan; Timothy Olah; *Bristol-Myers Squibb Company, Wallingford, CT*
- ThP 348 **A Novel LC-MS-MS Bioanalytical Method for the Accurate Measurement of Anandamide Level in Rat Brain Samples;** Min Wan; Siwei Ding; Sophia Yap; Jerry Miller; *Renovis, South San Francisco, CA*
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- METABOLOMICS 3 - METHODS, 349 - 379**
- ThP 349 **Dual Post-Column Addition for Enhanced Plant Metabolomics by (-)ESI-LC/FTICR-MS;** Jun Han<sup>1</sup>; Dustin Lippert<sup>2</sup>; Darryl Hardie<sup>1</sup>; Monica H. Elliott<sup>1</sup>; Ryan M. Danell<sup>3</sup>; Joerg Bohlmann<sup>2</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Center, Victoria, BC, Canada*; <sup>2</sup>*University of British Columbia, Vancouver, BC, Canada*; <sup>3</sup>*Danell Consulting, Greenville, NC*
- ThP 350 **Mass Spectrometry Protocols to Differentiate Target and/or Unknown Metabolites from Breakdown Products;** Ill Yang<sup>1</sup>; Shengmin Sang<sup>2</sup>; Lisa M. Domico<sup>3</sup>; Gail D. Zeevalk<sup>4</sup>; Chung S. Yang<sup>2</sup>; Brian T. Buckley<sup>1</sup>; <sup>1</sup>*Bionomics Research & Technology Center, EOHSI, Piscataway, NJ*; <sup>2</sup>*Ernest Mario School of Pharmacy, Rutgers, Piscataway, NJ*; <sup>3</sup>*Children's Hospital of Philadelphia, Philadelphia, PA*; <sup>4</sup>*University of Medicine and Dentistry of New Jersey, Piscataway, NJ*
- ThP 351 **Determination of Differentiating Skin Lipids for Phenotypic Murine Variations using Statistical Analysis Software to Process HPLC-MS Data;** Johnie Brown<sup>1</sup>; Yoshikazu Uchida<sup>2</sup>; Walter Holleran<sup>2</sup>; Susan C. Leonard<sup>1</sup>; Ruiqing Qiu<sup>1</sup>; Jeffrey Miller<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*; <sup>2</sup>*School of Medicine, UCSF, San Francisco, CA*
- ThP 352 **MassBank : Mass Spectral Database for Metabolome Analysis;** Hisayuki Horai<sup>1</sup>; Masanori Arita<sup>2</sup>; Takaaki Nishioka<sup>1</sup>; <sup>1</sup>*Keio University, Tsuruoka, Japan*; <sup>2</sup>*University of Tokyo, Kashiwa, Japan*
- ThP 353 **A Data Analysis Algorithm for Automated Relative Quantification of Stable Isotope-Labeled Metabolites;** Michael R. Shortreed; Ju Shin Lee; Brian L. Frey; Lloyd M. Smith; *University of Wisconsin, Madison, WI*
- ThP 354 **Endogenous Profiling of Sebum Lipid Components for Metabonomics Applications;** Joelle Onorato; Petia Shipkova; Michael D. Reily; *Bristol-Myers Squibb, Princeton, NJ*
- ThP 355 **Probing Drug Mechanism of Action via Cellular Metabolomics and Fluxomics: An Unexpected Effect of the Dihydrofolate Reductase Inhibitor Trimethoprim;** Yun Kyung (Sophia) Kwon; Wenyun Lu; Joshua D. Rabinowitz; *Princeton University, Princeton, NJ*
- ThP 356 **Resolving Ionic Metabolites with Ion Pair/Reverse Phase LC-MS;** Baichen Zhang<sup>1</sup>; Leslie M. Hicks<sup>2</sup>; <sup>1</sup>*Donald Danforth Center, St Louis, MO*; <sup>2</sup>*Danforth Center, St. Louis, MO*
- ThP 357 **Discerning Isomeric Metabolites using High Resolution Mass Spectral Trees;** Piotr T. Kasper<sup>1</sup>; Miguel Rojas<sup>1</sup>; Agnieszka Kraj<sup>2</sup>; Theo Reijmers<sup>2</sup>; Rob van der Heijden<sup>2</sup>; Thomas Hankemeier<sup>1</sup>; <sup>1</sup>*Netherlands Metabolomics Centre, Leiden University, Leiden, Netherlands*; <sup>2</sup>*Leiden University, Leiden, Netherlands*
- ThP 358 **Eicosanoids by LC-MS-MS: Sensitive Multi-Target-Profiling Combined with Structural Verification for Evaluation of Potential Biomarkers;** Uta Ceglarek<sup>2</sup>; Axel Besa<sup>3</sup>; Roland Geyer<sup>1</sup>; <sup>1</sup>*Applera Europe B.V., Rotkreuz, Switzerland*; <sup>2</sup>*ILM, University Hospital Leipzig, 04103 Leipzig, Germany*; <sup>3</sup>*Applied Biosystems, Darmstadt, Germany*
- ThP 359 **Mapping of Chemical and Biochemical Relationships of Mass Spectrometry-Based Metabolomics Data;** Dinesh Kumar; Tobias Kind; Oliver Fiehn; *UC Davis, Davis, CA*
- ThP 360 **Metabolite Identification using a Novel Nanoelectrospray LC-EC-array-MS Integrated System;** Susan Schiavo<sup>1</sup>; Erika Ebbel<sup>2</sup>; Swati Sharma<sup>3</sup>; Wayne Matson<sup>3</sup>; Bruce Kristal<sup>4</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Boston U School of Medicine, Boston, MA*; <sup>3</sup>*Bedford VA Hospital, Bedford, MA*; <sup>4</sup>*Brigham + Women's Hospital, Boston, MA*
- ThP 361 **Automated On-Line Sample Cleanup and LC-MS-MS Determination of Catecholamines and Related Compounds in Rat Brain Striatum;** Ge Zu<sup>2</sup>; Li Zhang<sup>1</sup>; Monika Wrona<sup>2</sup>; Glenn Dryhurst<sup>2</sup>; <sup>1</sup>*Penn State University, University Park, PA*; <sup>2</sup>*University of Oklahoma, Norman, OK*
- ThP 362 **Application of the Accurate Mass and Time Tag Approach in Lipidomics Studies of Type 1 Diabetes Mellitus;** Christina Sorensen<sup>1</sup>; Jie Ding<sup>1</sup>; Qibin Zhang<sup>1</sup>; Patricia W. Mueller<sup>2</sup>; Richard D. Smith<sup>1</sup>; Tom Metz<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*United States Centers for Disease Control, Atlanta, GA*
- ThP 363 **Profiling of Cationic Metabolites in Human CSF by LC-MS;** Khin Than Myint<sup>2</sup>; Ken Aoshima<sup>1</sup>; Satoshi Tanaka<sup>2</sup>; Tatsuji Nakamura<sup>1</sup>; Yoshiya Oda<sup>1</sup>; <sup>1</sup>*Laboratory of Core Technology, Eisai Co., Ltd., Tsukuba, Ibaraki 300-2635, Japan*; <sup>2</sup>*CREST, Japan Science and Technology, Saitama 332-0012, Japan*
- ThP 364 **Paired Stable Isotope Metabolic Tracers (PSIMT): A Novel Approach for Elucidation and Discovery of Drug Metabolites;** Nicolas A. Stewart<sup>1</sup>; Jennifer N. Sutton<sup>2</sup>; Raman Venkataraman<sup>1</sup>; Michael Athanas<sup>3</sup>; Robert A. Branch<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>*University of Pittsburgh, Pittsburgh, PA*; <sup>2</sup>*Thermo Fisher Scientific, Cambridge, MA*; <sup>3</sup>*Vast Scientific, Cambridge, MA*

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- ThP 365 **Identification of Metabolomic Components from Urine using Retention Time, Accurate Mass Database and a Molecular Formula Generator;** Theodore R. Sana; Keith Waddell; Steven M. Fischer; *Agilent Technologies, Santa Clara, CA*
- ThP 366 **Sniper Metabolomics of Biofluids for Disease State Biomarker Discovery;** Bridgit O. Crews; Sunia Trauger; Gary Siuzdak; *The Scripps Research Institute, La Jolla, CA*
- ThP 367 **A Quick Mass Spectrometry Based Tissue Metabolomics Method: Multi-Fraction Preparation using Automated Homogenizer and Liquid-Liquid Extraction;** Xiang He; *PPD Biomarker Discovery Sciences, LLC, Menlo Park, CA*
- ThP 368 **Automated and Quantitative Extraction of Metabolites from Bacteria;** Munehiro Teshima; Norma Pawley; John Dunbar; Clifford Unkefer; Pat Unkefer; *Los Alamos National Laboratory, Los Alamos, NM*
- ThP 369 **Development of an HPLC-TOF-MS Screening-Platform to Assess ppHypSys-Dependent Metabolic Changes in Nicotiana Attenuata during Insect Herbivory;** Matthias Schoettner<sup>1</sup>; Eva Rothe<sup>1</sup>; Emmanuel Gaquerel<sup>1</sup>; Beatrice Berger<sup>1</sup>; Birgit Schneider<sup>2</sup>; Robert Fazette<sup>3</sup>; Gabriela Zurek<sup>2</sup>; Ian T. Baldwin<sup>1</sup>; <sup>1</sup>*Max Plack Institute for Chemical Ecology, Jena, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Bruker Daltonics, Billerica, MA*
- ThP 370 **<sup>13</sup>C-/<sup>12</sup>C-Stable Isotope Labeling for ESI Signal Enhancement and Absolute Quantitation of Metabolomes;** Kun Guo; Liang Li; *University of Alberta, Chemistry Dept., Edmonton, Canada*
- ThP 371 **Nanostructure Initiator Mass Spectrometry (NIMS): Profiling of Xenobiotic and Endogenous Metabolites in Biological Tissues and Biofluids;** Oscar Yanes<sup>1</sup>; Trent Northen<sup>1</sup>; Mayra N. Estrada<sup>1</sup>; Wilasinee Uritboonthai<sup>1</sup>; Paul H Benton<sup>1</sup>; Michael J Potchoiba<sup>2</sup>; Marianne Manchester<sup>1</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*Pfizer Global Research and Development, Groton, Connecticut*
- ThP 372 **Metabolomics using LCMS Data Represented by Single Spectra;** Gordana Ivosev; Ron Bonner; Lyle Burton; *MDS Sciex, Concord, Canada*
- ThP 373 **A Software Suite for Comprehensive Detection, Annotation and Comparison of Peaks Detected by LC-FTICR-MS;** Nozomu Sakurai<sup>1</sup>; Yukiko Nakamura<sup>1</sup>; Yoko Iijima<sup>1</sup>; Takeshi Ara<sup>1</sup>; Yoshiyuki Ogata<sup>1</sup>; Ken-ichi Tanaka<sup>2</sup>; Koh Aoki<sup>1</sup>; Koei Okazaki<sup>1</sup>; Hideyuki Suzuki<sup>1</sup>; Daisaku Ohta<sup>3</sup>; Shigehiko Kanaya<sup>2</sup>; Kazuki Saito<sup>4</sup>; Daisuke Shibata<sup>1</sup>; <sup>1</sup>*Kazusa DNA Research Institute, Kisarazu, Japan*; <sup>2</sup>*Nara Inst. Sci. Technol, Ikoma, Japan*; <sup>3</sup>*Osaka Prefecture Univ., Sakai, Japan*; <sup>4</sup>*Chiba Univ., Chiba, Japan*
- ThP 374 **Targeted Metabolomics – Simultaneous and Quantitative LC-MS-MS Analysis of Energy Metabolism Intermediates in Biological Samples;** Therese Koal; Doreen Kirchberg; Cornelia Röhring; Sascha Dammeyer; Hans-Peter Deigner; Klaus Weinberger; *BIOCRATES Life Sciences AG, Innrain 66, A-6020, Innsbruck, Austria*
- ThP 375 **Automated Mass Spectra Interpretation Approach to Data Reduction for LC-MS Metabonomics Analysis;** Serhiy Hnatyshyn<sup>13</sup>; Mark Sanders<sup>2</sup>; Petia Shipkova<sup>13</sup>; Emily Luk<sup>13</sup>; Bethanne Warrack<sup>13</sup>; Michael Reily<sup>13</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Bristol-Myers Squibb, Hopewell, NJ*
- ThP 376 **The Characterization of a Novel Endogenous Metabolite and its Protein Interactions through Untargeted Metabolomics and Proteomics;** Sunia A. Trauger; Jaroslaw Kalisiak; Ewa Kalisiak; Gary Siuzdak; *The Scripps Research Institute, La Jolla, CA*
- ThP 377 **Utility of Stable Labels for Metabonomics: Metabolites of Bromoethylamine, a Potent Nephrotoxicant;** Petia Shipkova<sup>1</sup>; Mark Sanders<sup>2</sup>; Serhiy Hnatyshyn<sup>1</sup>; Haiying Zhang<sup>1</sup>; Bethanne Warrack<sup>1</sup>; Nelly Aranibar<sup>1</sup>; Jeff Vassallo<sup>1</sup>; Lois Lehman-McKeeman<sup>1</sup>; <sup>1</sup>*Bristol Myers Squibb, Princeton, NJ*; <sup>2</sup>*Thermo Fisher Scientific, Somerset, NJ*
- ThP 378 **Chemical Reference Libraries are Essential for Structural Elucidation in Metabolomics;** John Lennon; Anne Evans; Eric Milgram; *Metabolon, Inc., Durham, NC*
- ThP 379 **Evaluation of Columns and Gradients for LC-MS-Based Non-Targeted Metabonomics;** Chiuwa Emily Luk<sup>1</sup>; Serhiy Hnatyshyn<sup>1</sup>; Mark Sanders<sup>2</sup>; Petia Shipkova<sup>1</sup>; Bethanne Warrack<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb Co, Princeton, NJ*; <sup>2</sup>*Thermo Fisher Scientific, Somerset, NJ*
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- PEPTIDES: GLYCOPEPTIDES, 380 - 390**
- ThP 380 **Improved Site-Specific Glycopeptide Profiling of Pharmaceutical Compounds by Novel Enrichment Strategies and Online Capillary LC-ESI and MALDI-MS-MS Analysis;** Paige Weis<sup>1</sup>; Jessica Wohlgemuth<sup>2</sup>; Thomas Eichhorn<sup>2</sup>; Christian Hunzinger<sup>2</sup>; Robertus Hendriks<sup>2</sup>; Sven Andrecht<sup>2</sup>; <sup>1</sup>*EMD Biosciences, Inc., Madison, WI*; <sup>2</sup>*Merck KGaA, Darmstadt, Germany*
- ThP 381 **Exploiting the Differential Fragmentation of O-linked Glycopeptide Ions for the Elucidation of Protein Glycosylation;** Richard Seipert; Eric D. Dodds; Carlito Lebrilla; *University of California Davis, Davis, CA*
- ThP 382 **On-Target Digestion using Ionic Liquid Matrixes for Glycopeptide Analysis;** Yuko Fukuyama; Atsuhiko Toyama; Koichi Tanaka; *Shimadzu corporation, Kyoto, Japan*
- ThP 383 **Identification of an IgG Degradants Detected by Size Exclusion Chromatography and Electrophoretic Techniques using Electrospray Ionization and MALDI Mass Spectrometry;** Li Zhang; Andy Blum; Hans Fajardo; Damian Houde; Richard Strong; Zoran Sosic; Rohin Mhatre; Yelena Lyubarskaya; *Analytical Development Dept., BiogenIdec Inc., Cambridge, MA*
- ThP 384 **Characterisation of Mucin-Like Glycopeptide Linker Domains;** Pia H. Jensen<sup>1</sup>; Daniel Kolarich<sup>1</sup>; Helena Nevalainen<sup>1</sup>; Hans J. Wirth<sup>2</sup>; Nicolle H. Packer<sup>1</sup>; <sup>1</sup>*Macquarie University, North Ryde, Australia*; <sup>2</sup>*SGE Analytical Science, Ringwood, Australia*
- ThP 385 **Functionalized MALDI Surface for Specific Detection of Glycopeptides;** Mohammed Kajjout; Caroline Tokarski; Séverine Le Gac; Christian Rolando; *Univ. des Science/Tech de Lille, Villeneuve d'Ascq, France*
- ThP 386 **Mapping Tissue-Specific Expression of Extracellular Proteomes;** Yuan Tian; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
- ThP 387 **A Combination Strategy to Analyze the N-Linked Sialylated Glycoproteins Based on Protein Separation by 2DE;** Piliang Hao; Yan Ren; Siqi Liu; *Beijing Genomics Institute, CAS, Beijing, China*
- ThP 388 **Combined X!Tandem Identification of N – Glycosylated and Unmodified Peptide CID MS2**

## THURSDAY POSTERS

- Spectra with Prior Glycan Related Peak Filtering;** Sakari Joenväärä<sup>1</sup>; Hannu Peltoniemi<sup>1</sup>; Ilja Ritamo<sup>2</sup>; Risto Renkonen<sup>3</sup>; <sup>1</sup>MediCel Ltd, Helsinki, Finland; <sup>2</sup>Finnish Red Cross Blood Service, Helsinki, Finland; <sup>3</sup>Haartman Institute, Helsinki University, Helsinki, Finland
- ThP 389 **Determination of the Glycopeptide Structure of Insulin and IGF-I Receptors;** Sergei Ilchenko<sup>1</sup>; Mark R. Chance<sup>1</sup>; Linda J. Whittaker<sup>2</sup>; Jonathan Whittaker<sup>2</sup>; <sup>1</sup>Center for Proteomics, Case Western Reserve Univer, Cleveland, OH; <sup>2</sup>Depart. of Nutrition, Case Western Reserve Univer, Cleveland, OH
- ThP 390 **De Novo Glycan Structure Search with Protonated CID MS-MS Spectra of Native N-glycopeptides;** Hannu Peltoniemi<sup>1</sup>; Sakari Joenväärä<sup>1</sup>; Ilja Ritamo<sup>3</sup>; Risto Renkonen<sup>2</sup>; <sup>1</sup>MediCel Ltd, Helsinki, Finland; <sup>2</sup>Haarman Institute, Helsinki University, Helsinki, Finland; <sup>3</sup>Finnish Red Cross Blood Service, Helsinki, Finland
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- LCMS SAMPLE PREPARATION, 391 - 412**
- ThP 391 **Improved Throughput and Reproducibility Utilizing Turbulent Flow Online Sample Preparation in Quantitative SRM Analyses of Furosemide in Equine Plasma;** Heidi M Snapp<sup>2</sup>; Jeffrey Rudy<sup>1</sup>; Joseph DiBussolo<sup>3</sup>; Hidehiko Hazumaya<sup>2</sup>; Cornelius Uboh<sup>4</sup>; <sup>1</sup>PA Equine Toxicology, West Chester, PA; <sup>2</sup>University of Pennsylvania, Kennett Square, PA; <sup>3</sup>Thermo Fisher, Franklin, MA; <sup>4</sup>West Chester Univ., West Chester, PA
- ThP 392 **Novel Automated Sample Preparation Procedures for LC-MS-MS using Hamilton Microlab AT Plus 2 Robot and 96-Well Protein Precipitation Plates;** Jie Zhang; Shimin Wei; Tom Smith; Francis Tse; *Novartis Pharmaceuticals Corp, East Hanover, NJ*
- ThP 393 **Method Development and Validation of an APCI LC-MS-MS Method for Midazolam and 1'-Hydroxy-Midazolam in Human Plasma;** Stacey L. Zeman; Sarah M. Burke; Rachel Antico; Sara L. Jones; George P. Hade III; *Advion BioSciences, INC, Ithaca, NY*
- ThP 394 **A New Online SPE/LC-MS-MS Method for Screening 128 Relevant Pesticides in Fruit and Vegetables;** Meike Baden<sup>1</sup>; Norbet Helle<sup>1</sup>; Fredrick D. Forster<sup>2</sup>; Juergen Wendt<sup>3</sup>; <sup>1</sup>TeLA GmbH Bremerhaven, Bremerhaven, Germany; <sup>2</sup>Gerstel GmbH & Co KG, Muelheim an der Ruhr, Germany; <sup>3</sup>Agilent Technologies, Waldbronn, Germany
- ThP 395 **Determination of Roxithromycin in Human Plasma by LC-MS-MS;** Bipin Vanmalibhai Patel<sup>1</sup>; Mandev Patel<sup>2</sup>; <sup>1</sup>Cadila Pharmaceuticals Ltd, Ahmedabad, India; <sup>2</sup>Visnagar College of Pharmacy, Visnagar, India
- ThP 396 **Matrix Blind Generic On-Line Method for Biological Fluids;** Francois Espourteille; Chris Esposito; *Thermo Fisher Scientific, Franklin, MA*
- ThP 397 **Extraction of Propranolol and 4-hydroxy Propranolol Metabolite from Rat Plasma using Biocompatible Solid Phase Micro Extraction (SPME);** Janusz Pawliszyn<sup>2</sup>; Dajana Vucokovic<sup>2</sup>; Craig Aurand<sup>1</sup>; Katherine Stenerson<sup>1</sup>; Robert Shirey<sup>1</sup>; Leonard Sidisky<sup>1</sup>; Yong Chen<sup>1</sup>; <sup>1</sup>Supelco/ Sigma Aldrich, Bellefonte, PA; <sup>2</sup>University of Waterloo, Waterloo, ON, Canada
- ThP 398 **Evaluating the Matrix Effect of Esterase Inhibitors as Analyte Stabilizers on Bioanalysis by LC-MS-MS;** Naiyu Zheng<sup>1</sup>; Jianing Zeng<sup>1</sup>; Eliza N. Fung<sup>1</sup>; Adela Buzescu<sup>1</sup>; Paul Crane<sup>2</sup>; Mark E. Arnold<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Research & Development, Princeton, NJ;
- <sup>2</sup>Bristol-Myers Squibb Medical Imaging Group, Billerica, MA
- ThP 399 **Determination of Sedative-Hypnotic Drugs in Urine by using LC-MS-MS;** Ren-Jye Lee; Chiou-Shu Lin; Chung-Yu Chen; Maw-Rong Lee; *National Chung-Hsing University, Taichung, Taiwan*
- ThP 400 **The Development of a Two-Leveled Orthogonal Interface for On-Line Coupling Solid Phase Extraction and Capillary Electrophoresis-Mass Spectrometry;** Wei-Han Li; Guor-Rong Her; *National Taiwan University, Taipei, Taiwan*
- ThP 401 **LC-MS-MS Method for the Rapid Determination of Melamine and Cyanuric Acid in Pet Food Samples;** Adrian Taylor; Sylvie Beudet; Mauro Aiello; Takeo Sakuma; *MDS Analytical Technologies, Concord, Canada*
- ThP 402 **Method Development and Validation of EC0225, a Novel Folate Receptor-Specific Anti-Tumor Agent in Human Plasma by LC-MS-MS; Overcoming Stability Challenges;** Dale Campbell<sup>1</sup>; Jeff Nicoson<sup>2</sup>; Nikki Parker<sup>2</sup>; Chris Leamon<sup>2</sup>; Daniel Mulvana<sup>1</sup>; <sup>1</sup>Advion BioServices, Ithaca, NY; <sup>2</sup>Endocyte, Inc., West Lafayette, IN
- ThP 403 **Evaluation of Plasma Extract Cleanliness using Various Commercially Available Mixed-Mode Resin-Based Cation Exchange Spe Sorbents;** Lee Williams; Matthew Cleeve; Scott Merriman; Steve Plant; Steve Jordan; Joanna Smith; Richard Calverley; *Biotage GB Limited, Hengoed, UK*
- ThP 404 **Analysis of Resveratrol in Balb/c Mice Serum using UPLC-Tandem Mass Spectrometry;** Nathan C. Twaddle<sup>1</sup>; Martin S. Hoagland<sup>2</sup>; Joseph S. Sandhorst<sup>2</sup>; William G. Helferich<sup>2</sup>; Daniel R. Doerge<sup>1</sup>; <sup>1</sup>NCTR/FDA, Jefferson, AR; <sup>2</sup>University of Illinois, Champaign, IL
- ThP 405 **Determination of Florfenicol Amine in Swine Tissues by Hydrophilic Interaction LC-MS-MS;** Yuhui Yang; Louis Crouch; Farhad Sayyarpour; *Schering-Plough Research Institute, Lafayette, NJ*
- ThP 406 **Sensitive Assays using HILIC-SPE and HILIC-LC-MS-MS for Quantification of Hydrophilic Anti-Influenza Drugs;** Niklas Lindegardh; Warunee Hanpithakpong; *MORU, Bangkok, Thailand*
- ThP 407 **Faster, More Reliable Automated Analysis by Polymeric Mixed Mode SPE with Narrow Particle Size Distribution";** William Hudson; Paul A Boguszewski; *Varian, Inc., Lake Forest, CA*
- ThP 408 **Determination of Bisphenol A Diglycidyl Ether and its Derivatives in Canned Foods using Liquid Chromatography/Electrospray Ionization Tandem Mass Spectrometry;** Jungju Seo; Mi-Jin Lee; *Korea Basic Science Institute, Seoul, South Korea*
- ThP 409 **Automated SPE Method Development and Bioanalysis of 2,3-dinor-iPF2 $\alpha$ -III in Urine;** Kenneth C. Lewis<sup>1</sup>; John D. Lennon<sup>1</sup>; Kim Gamble<sup>2</sup>; <sup>1</sup>OpAns, LLC, Durham, NC; <sup>2</sup>Microliter Analytical Supplies, Suwanee, GA
- ThP 410 **LC-MS Determination of Tiopronin and Metabolites in Biological Matrix after Stabilization with Isobutyl Acrylate;** Alexandre Pimenov; Jeffry Plomley; Timothy Samuels; *Charles River Laboratories, Senneville (Montréal), Canada*
- ThP 411 **Sample Preparation and Protein Removal:- A Comparison of Serum Protein Removal with Various Sample Preparation Techniques using Gel Electrophoresis;** Lee Williams<sup>1</sup>; Steve Jordan<sup>1</sup>; Matthew Cleeve<sup>1</sup>; Richard Calverley<sup>1</sup>; Joanna Smith<sup>1</sup>;

## THURSDAY POSTERS

- Richard Jones<sup>2</sup>; Jason T. Taylor<sup>2</sup>; Rick Edmondson<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Hengoed, UK; <sup>2</sup>Fda/nctr, Jefferson, AR
- ThP 412 **Quantification of Letrozole and Genistein in Mouse Serum using UPLC-ES/MS-MS;** Kellie Woodling; Mona I. Churchwell; Daniel R. Doerge; *Natl. Cen. Tox. Res., Jefferson, AR*
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- PHOSPHOPEPTIDE ENRICHMENT, 413 - 430**
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- ThP 413 **Identification of Phosphorylation Site of an Arabidopsis CNGC by a Calcium-Dependent Protein Kinase with TiO<sub>2</sub> Column Enrichment and Mass Spectrometry;** Ing-Feng Chang<sup>1</sup>; David Quilicy<sup>2</sup>; Yoshimi Barron<sup>2</sup>; Jeffrey Harper<sup>2</sup>; <sup>1</sup>Institute of plant Biology/National Taiwan U, Taipei, Taiwan; <sup>2</sup>University of Nevada, Reno, Reno, NV
- ThP 414 **Dynamics of Protein Phosphorylation Induced by Oxidative Stress in Mammalian Cells using a New On-Line Enrichment Strategy for Phosphopeptide Analysis;** Yelena Margolin<sup>1</sup>; Emily A. Freeman<sup>1</sup>; Karl Mechtler<sup>2</sup>; William S. Lane<sup>3</sup>; Bogdan A. Budnik<sup>3</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Harvard University, Hsph, Boston, MA; <sup>2</sup>Imp Research Institute of Mo, Vienna, Austria; <sup>3</sup>Harvard University, Cambridge, MA
- ThP 415 **Modified Surface Metal Oxide for Enrichment of Phosphopeptides;** Ashok K. Shukla<sup>1</sup>; Mukta M. Shukla<sup>1</sup>; Diane Rutkowski<sup>1</sup>; Appavu K. Sundaram<sup>2</sup>; Vladimir M. Doroshenko<sup>2</sup>; <sup>1</sup>Glygen Corp., Columbia, MD; <sup>2</sup>MassTech, Inc., Columbia, MD
- ThP 416 **Phosphopeptide Enrichment and Characterization using TiO<sub>2</sub> Coated Magnetic Beads Combined with MALDI MS-MS and ESI MS-MS;** Lei Cheng<sup>1</sup>; Martin R. Larsen<sup>1</sup>; Sven Andrecht<sup>2</sup>; Jörg von Hagen<sup>2</sup>; Ole N. Jensen<sup>1</sup>; <sup>1</sup>Univ. Southern Denmark, Odense, Denmark; <sup>2</sup>Merck KGaA, Darmstadt, Germany
- ThP 417 **Evaluation and Optimization of Phosphoproteomic Approaches Combining Selective Metal Oxide-Based Enrichment with Peptide Fractionation Methods;** Hye Kyong Kweon; Peter Ulintz; Philip Andrews; *University of Michigan, Ann Arbor, MI*
- ThP 418 **Optimization of Metal Oxide Resins for Enrichment of Phosphorylated Peptides Prior to Mass Spectrometric Analyses: Application to the CD34 Antigen;** Matthew B. Gates; Jason G. Williams; Carol S. Trempus; Sung-Jen Wei; Maggie M. Humble; Robert M. Petrovich; Raymond W. Tennant; Kenneth B. Tomer; Leesa J. Deterding; *NIEHS, Raleigh, NC*
- ThP 419 **Characterization and Development of Zirconia Functionalized MALDI Surfaces Used for *in situ* Phosphopeptide Enrichment;** Grady Blacken<sup>1</sup>; Michael Volny<sup>2</sup>; Matthew Diener<sup>3</sup>; Karl E. Jackson<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Purdue University, Lafayette, IN; <sup>3</sup>Department of Chemistry, Uni, Seattle, WA
- ThP 420 **Optimization of Elution Conditions for Phosphopeptides Captured by Aliphatic Hydroxy Acid-Modified Metal Oxide Chromatography (HAMMOC);** Yutaka Kyono<sup>1</sup>; Naoyuki Sugiyama<sup>2</sup>; Koshi Imami<sup>1</sup>; Masaru Tomita<sup>1</sup>; Yasushi Ishihama<sup>1</sup>; <sup>1</sup>Keio Univ. IAB, Tsuruoka, Japan; <sup>2</sup>Human Metabolome Technologies, Inc., Tsuruoka, Japan
- ThP 421 **Immobilized Metal Affinity Chromatography Revisited: pH/acid Control toward Full Recovery and Selectivity in Phosphoproteomics;** Chia-Feng Tsai<sup>1</sup>; Yi Ting Wang<sup>1</sup>; Pei-Yi Lin<sup>1</sup>; Kuan-Ting Pan<sup>2</sup>; Kay-hooi Khoo<sup>3</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Nrpgm Core Facilities For Proteomics, Taipei, Taiwan; <sup>3</sup>Ibc, Academia Sinica, Taiwan, Taipei, Taiwan
- ThP 422 **Enrichment of Phosphopeptides using Porous Tin Dioxide Microspheres as Affinity Material;** Alexander Leitner<sup>1</sup>; Martin Sturm<sup>1</sup>; Wolfgang Lindner<sup>1</sup>; Jan-Henrik Småt<sup>2</sup>; Mika Lindén<sup>2</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Åbo Akademi University, Turku, Finland
- ThP 423 **Improved Phosphopeptide Enrichment on Titanium- and Zirconium- Dioxide Columns for the Analysis of Phosphorylation Sites of Protein Complexes;** Michael Mazanek<sup>2</sup>; Goran Mitulovic<sup>1</sup>; Christoph Stingl<sup>2</sup>; Otto Hudecz<sup>2</sup>; James Hutchins<sup>2</sup>; Thomas Köcher<sup>2</sup>; Jan-Michael Peters<sup>1</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>Imba Inst. of Mol. Biotech., Vienna, Austria; <sup>2</sup>Imp Research Institute of Mo, Vienna, Austria
- ThP 424 **Optimization of Phosphopeptide Enrichment by Magnetite Nanoparticles;** Yi Huang<sup>1</sup>; Qihui Shi<sup>2</sup>; Chia-Kuang Tsung<sup>2</sup>; Yanbao Yu<sup>1</sup>; Ruyun Du<sup>3</sup>; Pengyuan Yang<sup>3</sup>; Carol E. Parker<sup>1</sup>; Stuckey Galen D. <sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>University of California, Santa Barbara, CA; <sup>3</sup>Fudan University, Shanghai, China
- ThP 425 **Selective Extraction and Enrichment of Multi-Phosphorylated Peptides Prior to MALDI MS Analysis;** Chih-Che Wu; *Department of Applied Chemistry, National Chi Nan, Puli, Taiwan*
- ThP 426 **Zirconium Phosphonate-Based Phosphopeptide Enrichment on a MALDI Chip;** Udo Roth; Karen Kowalewski; Christoph Menzel; Christopher Belisle; Kerstin Steinert; *Qiagen GmbH, Hilden, Germany*
- ThP 427 **Electrostatic Repulsion-Hydrophilic Interaction Chromatography (ERLIC) for Specific Enrichment and Identification of Phosphopeptides;** Goran Mitulovic<sup>1</sup>; Andrew Alpert<sup>2</sup>; Karl Mechtler<sup>3</sup>; <sup>1</sup>IMBA Inst. of Molecular Biotechnology, Vienna, Austria; <sup>2</sup>Polylc Inc., Columbia, MD; <sup>3</sup>Imp Research Institute of Mo, Vienna, Austria
- ThP 428 **Phosphopeptide Enrichment Enabled by Free Flow Electrophoresis;** David Craft<sup>1</sup>; Sabine Kronbauer<sup>2</sup>; Chae Kim<sup>1</sup>; Craig A Gelfand<sup>1</sup>; Christoph Eckerskorn<sup>2</sup>; Gerhard Weber<sup>2</sup>; Mikkel Nissum<sup>2</sup>; <sup>1</sup>BD Diagnostics PAS, Franklin Lakes, NJ; <sup>2</sup>BD Diagnostics, Martinsried, Germany
- ThP 429 **Enrichment of Phosphopeptides by Fe3+-Immobilized Magnetic Affinity Nano-Particles for Phosphoproteome Analysis of Plasma Membrane of Mouse Liver;** Yanguan Zhang; Feng Tan; Wei Mi; Jinglan Wang; Junying Wei; Yun Cai; Xiaohong Qian; *Beijing Institute of Radiation Medicine, Beijing, China*
- ThP 430 **Optimization of Immobilized Gallium (III) Ion Affinity Chromatography for Highly Selective Enrichment of Phosphopeptides;** Uma K. Aryal; Douglas JH Olson; Andrew RS Ross; *National Research Council, Plant Biotechnology Ins, Saskatoon, Canada*
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- PTMs – DEAMINATION, DISULFIDES, 431 - 449**
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- ThP 431 **Characterization of Novel Oxidation Products of Cysteine in an Active Site Motif Of PTP1B;** Vivekananda Shetty<sup>1</sup>; Thomas Neubert<sup>2</sup>; <sup>1</sup>Immunotope, Inc., Doylestown, PA; <sup>2</sup>Skirball Institute, Nyumc, New York, NY
- ThP 432 **Determination of Disulfide Bond Arrangement of the Oligomeric HIV Envelope Protein CON-S gp140 & Delta;CFI by LC/ESI-FTICR Mass Spectrometry;** Ying Zhang<sup>1</sup>; Eden P. Go<sup>1</sup>; Feng Gao<sup>2</sup>; Sushma Menon<sup>1</sup>; Hua-Xin Liao<sup>2</sup>; Laura L. Sutherland<sup>2</sup>; S. Munir Alam<sup>2</sup>; Barton F. Haynes<sup>2</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>University of

## THURSDAY POSTERS

- ThP 433 **Posttranslational Modifications of  $\alpha$ - and  $\beta$ -tubulin in *Toxoplasma Gondii***; Hui Xiao; Berta Burd; Hongshan Zhang; Kami kim; Louis Weiss; Ruth Hogue Angeletti; Pascal Verdier-Pinard; *Albert Einstein College of Medicine, Bronx, NY*
- ThP 434 **Asn Deamidation and Asp Isomerization in Calmodulin: Influence of Calcium and pH**; Chunxiang Yao<sup>1</sup>; Jason J Courmoyer<sup>1</sup>; Xiaojuan Li<sup>1</sup>; Nadezda Sargaeva<sup>1</sup>; Cheng Lin<sup>1</sup>; Raman Mathur<sup>2</sup>; Peter B. O'connor<sup>1</sup>; <sup>1</sup>*Boston University Medical School, Boston, MA*; <sup>2</sup>*Boston University, Boston, MA*
- ThP 435 **Integrating Two Affinity Pull-Down Strategies with Mass Spectrometry to Characterize a Novel PTM in the Escherichia Coli Ribosomal Protein S12**; Michael Brad Strader<sup>1</sup>; Suwako Fujigaki<sup>1</sup>; Cai Yun Chen<sup>1</sup>; Nina Costantino<sup>3</sup>; W. Judson Hervey IV<sup>2</sup>; Anthony J. Makusky<sup>1</sup>; Donald L. Court<sup>3</sup>; Sanford P. Markey<sup>1</sup>; Jeffrey A. Kowalak<sup>1</sup>; <sup>1</sup>*National Institute of Mental Health, Bethesda, MD*; <sup>2</sup>*University of TN/Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>3</sup>*National Cancer Institute, Fredrick, MD*
- ThP 436 **Analysis of Levuglandin-Peptide Adducts by LC-MS-MS: Towards Mapping of Lipid-Protein Modifications**; Almary Chacon; Valery Yermalitsky; Amy Ham; Irene Zagol-Ikapitte; Richard M. Caprioli; Olivier Boutaud; John A. Oates; *Vanderbilt University, Nashville, TN*
- ThP 437 **A Simple Method for the Comprehensive Assignment of Disulfide Pairs in Complex Proteins using ECD on an LTQ-FT**; Benjamin J. Madden; Gennett M. Myhre; Christopher J Mason; Federspiel J. Mark; H. Robert Bergen, Iii; *Mayo Clinic, Rochester, MN*
- ThP 438 **Mass Spectrometry-Based Identification and Quantitative Analysis of Post-Translational Cysteine Modification**; Kuanting Pan<sup>1</sup>; Chi-Chi Chou<sup>1</sup>; Yi-Yun Chen<sup>3</sup>; Shu-Yu Lin<sup>1</sup>; Kay-Hooi Khoo<sup>2</sup>; <sup>1</sup>*NRPGM Core Facilities for Proteomics, Taipei, Taiwan*; <sup>2</sup>*Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*; <sup>3</sup>*National Taiwan University, Taipei, Taiwan*
- ThP 439 **CE-MS as a Detection Scheme for Disulfide-Linked Peptides**; Brad J. Williams; William K. Russell; David H. Russell; *Texas A&M University, College Station, TX*
- ThP 440 **A Bead Based Approach for Highly Specific Enrichment of Citrulline Containing Peptides**; Astrid EV Tuttoren<sup>1</sup>; Anders Holm<sup>1</sup>; Marit Jørgensen<sup>2</sup>; Burkhard Fleckenstein<sup>1</sup>; <sup>1</sup>*Univ. of Oslo, Oslo, Norway*; <sup>2</sup>*Rikshospitalet University Hospital, Oslo, Norway*
- ThP 441 **An Improved Method for the Identification of 4-hydroxy-2-nonenal (HNE) Schiff Base Adducts using Data-Dependent and Neutral Loss-Driven MS3 Acquisition**; Navin Rauniyar; Stanley M. Stevens, Jr.; Laszlo Prokai; *University of North Texas Health Science Center, Fort Worth, TX*
- ThP 442 **Assessing the Reaction Profile and Cross-Linking Ability of Acrolein Reacted with Peptides Containing Varying Nucleophilic Side Chains**; Lewis C Jackson; Marc Knecht; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- ThP 443 **MS-MS Analysis of Non-tryptic Palmitoylated Peptides Show Complex Fragmentation Pathways**; Bernd O. Keller<sup>1</sup>; Morris A. Kostiuik<sup>2</sup>; Luc G. Berthiaume<sup>2</sup>; <sup>1</sup>*University of British Columbia, Vancouver, Canada*; <sup>2</sup>*University of Alberta, Edmonton, Canada*
- ThP 444 **Mass Spectrometric Characterization of Covalent Modification of Human Serum Albumin by  $\alpha,\beta$ -Unsaturated Aldehydes**; Qingyuan Liu; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- ThP 445 **ECD and IRMPD of Amyloid Beta Protein Fragment 1-40 and Synthetic Beta-linked Peptides**; Nadezda P. Sargaeva; Jason J. Courmoyer; Chunxiang Yao; Cheng Lin; Peter B. O'Connor; *Boston University School of Medicine, Boston, MA*
- ThP 446 **A Comprehensive Mass Spectrometry Based Platform using Hydrazide-Functionalized Reagents for Mapping Sites of Protein Carbonylation**; Mikel R. Roe; Ladora V. Thompson; Edgar Arriaga; Timothy J. Griffin; *University of MN, Minneapolis, MN*
- ThP 447 **Determination of Citrullinated Sites of Alpha-Fibrinogen in Rheumatoid Arthritis Synovial Fluid using Immunocapture and Two Dimensional Liquid Chromatography Mass Spectrometry**; Khue Truong<sup>1</sup>; Yunan Miao<sup>1</sup>; Roger Moore<sup>1</sup>; Terry Lee<sup>2</sup>; <sup>1</sup>*City of hope, Duarte, CA*; <sup>2</sup>*Beckman Research Institute, Duarte, CA*
- ThP 448 **Isoaspartomics of Anthrax Vaccine Stability and Other Applications**; Jason J Courmoyer<sup>1</sup>; Cheng Lin<sup>2</sup>; Peter B. O'connor<sup>2</sup>; <sup>1</sup>*Boston University Medical School, Boston, MA*; <sup>2</sup>*Boston University, Boston, MA*
- ThP 449 **Affinity Labeling and Mass Spectrometric Detection of  $\alpha$ -Aminoacidic and  $\gamma$ -Glutamic Semialdehydes**; Juan Chavez; Claudia Maier; *Oregon State University, Corvallis, OR*
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- PROTEINS – GENERAL 2, 450 - 465**
- ThP 450 **Mass Spectrometric Identification of Transcobalamin, a Cobalamin-Binding Protein in Crude Mitochondrial Fibroblasts from Patients with Inborn Errors of B12 Metabolism**; Lama Yamani; Angela Hosack; Brian M. Gilfix; David Watkins; David S. Rosenblatt; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 451 **A Proteomics Approach to Understanding Nuclear Autoantigenic Sperm Protein (Nasp)'s Role in a Nuclear Receptor Regulatory Complex**; Richard T. Richardson<sup>1</sup>; Nedyalka N. Dicheva<sup>2</sup>; Viorel Mocanu<sup>2</sup>; Carol E. Parker<sup>2</sup>; Oleg M. Alekseev<sup>1</sup>; Xian Chen<sup>2</sup>; Michael G. O'Rand<sup>1</sup>; <sup>1</sup>*Dept. of Cell & Development Biology, UNC, Chapel Hill, NC*; <sup>2</sup>*UNC-Duke Proteomics Center, UNC, Chapel Hill, NC*
- ThP 452 **Interaction of Platinum Anti-Cancer Drugs with Copper Transport Proteins**; Chak M. Sze<sup>2</sup>; Zhiguang Xiao<sup>2</sup>; Paul S. Donnelly<sup>2</sup>; George N. Khairallah<sup>2</sup>; Richard A. J. O'hair<sup>1</sup>; Anthony G. Wedd<sup>2</sup>; <sup>1</sup>*University of Melbourne, Melbourne, Australia*; <sup>2</sup>*Bio21 Institute, the University of Melbourne, Melbourne, Australia*
- ThP 453 **High Charge-State Data-Dependent Sequencing of Peptides Allows Selective Identification of Disulfide Bridges**; Scott A. Shaffer; Alexander Scherl; Pragya Singh; Kayte Zumberge; Byron Gallis; Yihuan S. Tsai; David R. Goodlett; *Univ. of Washington, Seattle, WA*
- ThP 454 **Identification of Transcription Factor Effectors using FAC-MS**; Ricardo Marti-Arbona; Munehiro Teshima; Penelopev Anderson; Pat Unkefer; Clifford NM Unkefer; *Los Alamos National Laboratory, Los Alamos, NM*
- ThP 455 **New Approaches for Investigating Ribosomal Readthrough Control of Gene Expression in Moloney Murine Leukemia Virus using High Resolution Mass Spectrometry**; Arie Hawkins; Daniele Fabris; *U. Maryland Baltimore County, Baltimore, MD*
- ThP 456 **Structural Characterization of Helicobacter Pylori KDO8P Synthase by Electrospray Mass**

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- Spectrometry**; Zhili Li; *Chinese Academy of Medical Sciences, Beijing, China*
- ThP 457 **Comprehensive Proteomic Characterization of S.Aureus Phages 80alpha and SaPII**; Anton Poliakov<sup>1</sup>; Jenny Chang<sup>1</sup>; Michael Spilman<sup>1</sup>; Terje Dokland<sup>1</sup>; Gail Christie<sup>2</sup>; James Mobley<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*Virginia Commonwealth University, Richmond, Virginia*
- ThP 458 **Identification of Novel Protein Interactions in the eIF4B-RNA Complex by Tandem Affinity Purification using a Chimeric Construct of His-eIF4B-Flag**; David Shahbazian; David Blank; Nahum Sonenberg; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 459 **Aging, Disease and the Insolubleome: Identification of SDS-Insoluble Proteins in Disease and Aging Models from Multiple Organisms by Mass Spectrometry**; Emily A. Gaman; Pedro Rodrigues; Aaron W. Miller; Silvestre Alavez; John P. Miller; Birgit Schilling; Lisa M. Ellerby; Gordon J. Lithgow; Robert E. Hughes; Bradford W. Gibson; *Buck Institute for Age Research, Novato, CA*
- ThP 460 **Development of Mass Spectrometry Protein Standards using Sequence-Validated Human Open Reading Frames**; Thomas Beardslee<sup>2</sup>; Mahbod R. Hajivandi<sup>1</sup>; Thomas Chappell<sup>1</sup>; Gavin Meredith<sup>1</sup>; R. Marshall Pope<sup>1</sup>; Paul Predki<sup>1</sup>; Alexander Bell<sup>3</sup>; <sup>1</sup>*Invitrogen, Carlsbad, CA*; <sup>2</sup>*Invitrogen Corporation, Carlsbad, CA*; <sup>3</sup>*McGill University, Toronto, Canada*
- ThP 461 **Identification of Differentially Expressed Proteins in Dendritic Cells Pulsed by Chlamydia Trachomatis by Two-Dimensional Differential Gel Electrophoresis**; Dongxia Wang<sup>1</sup>; Yiming Ye<sup>1</sup>; Carolyn Black<sup>1</sup>; Joseph Igietsme<sup>1</sup>; Qing He<sup>2</sup>; <sup>1</sup>*Centers of Disease Control and Prevention (CDC), Atlanta, GA*; <sup>2</sup>*Morehouse School of Medicine, Atlanta, GA*
- ThP 462 **Complete Characterization of Complex Proteins on Chips**; Catherine Mulligan; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 463 **Peptide Mapping Suggests that the Biological Activity of Celastrol, a Natural Quinone Methide Triterpene, is Thiol-Specific**; Anna-Karin Svensson<sup>1</sup>; Lada Klaić<sup>1</sup>; Christopher D'Angelo<sup>1</sup>; Adam Lucas<sup>2</sup>; Richard B. Silverman<sup>1</sup>; Richard I. Morimoto<sup>1</sup>; <sup>1</sup>*Northwestern University, Chicago, IL*; <sup>2</sup>*The Chicago Biomedical Consortium/Northwestern Uni, Evanston, IL*
- ThP 464 **Characterization of 5-hydroxyeicosanoid Dehydrogenase in the Regulation of 5-oxo-6,8,11,14-icosatetraenoic Synthesis**; Gail Grant; David Blank; William S. Powell; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 465 **Top-Down Sequence Analysis of Antibody LC and Fc Fragments by an Ion-mobility Time-of-Flight Mass Spectrometer**; Weibin Chen<sup>1</sup>; Carola W.N. Dame<sup>2</sup>; Asish Chakraborty<sup>1</sup>; Siqun Huang<sup>1</sup>; John Gebler<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Department of Pharmacy & Pharmacology, The Netherlands Cancer In, The Netherlands*
- 
- PROTEINS: RECOMBINANT, 466 - 490**
- ThP 466 **Detailed Annotation of Qualitative Differences in Recombinant Protein Samples by Top-Down LC-MALDI-reISD – A QC Exercise**; Anja Resemann; Cole Zimmerman; Detlev Suckau; *Bruker Daltonics, Bremen, Germany*
- ThP 467 **Analysis of Low-Abundant Sequence Variants using LC-MS-MS Peptide Mapping and Mascot Error Tolerant Search**; Yi Yang<sup>1</sup>; Viswanatham Katta<sup>2</sup>; Boyan Zhang<sup>3</sup>; <sup>1</sup>*Genentech, Inc, South San Francisco, CA*; <sup>2</sup>*Genentech Inc., S. San Francisco, CA*; <sup>3</sup>*Genentech, Inc., South San Francisco, CA*
- ThP 468 **Performance of an Affinity Mass Spectrometric Method for Characterizing Antibody Drug Conjugates in Plasma**; Luna Liu; Keyang Xu; Helga Raab; Jagath R. Junutula; Surinder Kaur; *Genentech, Inc., South San Francisco, CA*
- ThP 469 **Use of Mass Spectrometry to Help Drive the Design of a Biopharmaceutical Drug Candidate from Inception into Early Development**; Jennifer F. Nemeth; Catherine Gress; Tracy Spinka-Doms; Chichi Huang; Vedrana Stojanovic-Susulic; *Centocor R&D, Radnor, PA*
- ThP 470 **Optimizing the On-Line Mass Spectrometric Analysis of Immunoconjugates**; Galahad U. Deperalta<sup>1</sup>; Chien Lee<sup>2</sup>; Charity Bechtel<sup>2</sup>; Victor Ling<sup>2</sup>; <sup>1</sup>*Genentech, S. San Francisco, CA*; <sup>2</sup>*Genentech, Inc., S. San Francisco, CA*
- ThP 471 **LC-MS Methods for the Analysis of Glycation in IgG Molecules**; Nicole L Stackhouse; David Hambly; Bruce A Kerwin; Michael J Treuheit; Himanshu S Gadgil; *Amgen, Seattle, WA*
- ThP 472 **Software Tools for Screening Protein Sequence Variants in Monoclonal Antibodies**; Louissette Basa<sup>1</sup>; Darren Brown<sup>2</sup>; Bao-jen Shyong<sup>1</sup>; Rodney Keck<sup>1</sup>; <sup>1</sup>*Genentech, Inc., So. San Francisco, CA*; <sup>2</sup>*Genentech, Inc., Oceanside, CA*
- ThP 473 **Mass Spectrometric Determination of Disulfide Linkages in Recombinant Proteins Using On-line LC-MS with Electron Transfer Dissociation**; Shiaw-Lin Wu; Haitao Jiang; Qiaozhen Lu; Shujia Dai; William Hancock; Barry L. Karger; *Northeastern University, Boston, MA*
- ThP 474 **Pharmacokinetic Study of Protein Drugs in Human Serum using an Optimized Sample Handling Procedure with LC-MS Approach**; Qiaozhen (Cheryl) Lu; Shiaw-Lin Wu; William S. Hancock; *Northeastern University, Boston, MA*
- ThP 475 **Isomerization at the Hinge Aspartate is a Major Degradant in IgG1 Antibodies under Accelerated Stress Conditions**; David Hambly; Joanna Scavezze; Christine Siska; Douglas Banks; Bruce Kerwin; Himanshu Gadgil; *Amgen Inc., Seattle, WA*
- ThP 476 **Growth Time Dependent Proteomic Profiling of Corynebacterium Glutamicum Performed in Different Growth Media Allows Optimizing an Alternative Protein Expression System**; Eberhard Durr; Julie Zorman; Susanne Secore; Loren Schultz; Joseph Joyce; Annaliesa Anderson; Michael Caulfield; *Merck & Co; MRL Vaccines Basic Research, West Point, PA*
- ThP 477 **Middle-Down LC-MS Characterizations of Monoclonal IgG Antibodies**; Jason L. Richardson; Robert Hong; Tamer Eris; Zhongqi Zhang; *Amgen, inc., Thousand Oaks, CA*
- ThP 478 **LC-MS-MS Peptide Map Optimization for a Conjugated Antibody**; Timothy K. Slattery; Ola M. Saad; Jakub Baudys; Surinder Kaur; *Genentech, Inc., South San Francisco, CA*
- ThP 479 **Characterizing Glycosylation Patterns in Recombinant IgG2/4 Monoclonal Antibodies through a Directed Approach Combining Fluorescence HPLC, MALDI-ToF-MS, and LC-MS and MS-MS**; Adam W. Lucka; Rekha Patel; Christine Nowak; Bruce Andrien; *Alexion Pharmaceuticals, Cheshire, CT*

## THURSDAY POSTERS

- ThP 480 **MALDI/TOF MS Analysis of PEG and PEGylated Proteins;** Yunping Huang; Anulfo Valdez; Barbara Twarowska; Reb Russell; Michael Grace; Mei Lin; *Bristol-Myers Squibb Company, Pennington, NJ*
- ThP 481 **In vivo and in vitro Expression of Stable-Isotope Labeled Clinical Proteins for Application as Mass Spectral-Based Reference Method Internal Standards;** Johanna E. Camara; Faith A. Hays; Nathan G. Dodder; Prasad T. Reddy; Illarion V. Turko; David M. Bunk; *NIST, Gaithersburg, MD*
- ThP 482 **Ligand Binding-Mass Spectrometry Methods for Understanding Macromolecular Drug Biotransformation and Impact on Immunoassay Quantification;** Michael Hall<sup>1</sup>; Jean W Lee<sup>2</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*; <sup>2</sup>*Amgen, Inc, Thousand Oaks, CA*
- ThP 483 **Deamidation of the Fc Portion of a Recombinant Monoclonal Antibody;** Sandipan Sinha<sup>1</sup>; Lei Zhang<sup>1</sup>; Todd D. Williams<sup>2</sup>; Josef Vlasak<sup>3</sup>; Roxana Ionescu<sup>3</sup>; Elizabeth M. Topp<sup>1</sup>; <sup>1</sup>*University of Kansas, Lawrence, KS*; <sup>2</sup>*Mass Spectrometry Laboratory, Lawrence, KS*; <sup>3</sup>*Merck Research Laboratories, Inc., West Point, PA*
- ThP 484 **Pepsin Digestion for LC-MS-MS Peptide Mapping of a Trypsin Resistant Antibody;** Timothy K. Slattery; Ola M. Saad; Surinder Kaur; *Genentech, Inc., South San Francisco, CA*
- ThP 485 **Profiling Cell Culture Media via LC-MS and Multivariate Statistical Analysis;** Catalin Doneanu; Weibin Chen; Ignatius Kass; John Gebler; *Waters Corporation, Milford, MA*
- ThP 486 **Rapid Characterization of Intact Therapeutic Proteins by Top-down Mass Spectrometry;** Jennifer Zhang; Viswanatham Katta; *Genentech Inc., South San Francisco, CA*
- ThP 487 **Targeted LC-MS-MS Characterizes a Recombinant Fusion-Protein Therapeutic: Confirmation and Quantification of Sequence Heterogeneity and Low-Frequency Post-Translational Modifications;** Matthew Champion<sup>1</sup>; Leah Luna<sup>2</sup>; <sup>1</sup>*Applied Biosystems, Foster City, CA*; <sup>2</sup>*Centers for Disease Control, Atlanta, GA*
- ThP 488 **Investigation of Decreased Antigen Binding Observed in the Cell Culture Development of a Monoclonal Antibody;** Ping Hu; Aston Liu; Leonard Olszewski; *GlaxoSmithKline, King of Prussia, PA*
- ThP 489 **Comparison of Glycosylation Profiles across Host Cells and Cell Lines for Multiple IgG-Based Therapeutic Proteins using High Resolution Mass Spectrometry;** Steven C. Pomerantz; Jennifer F. Nemeth; *Centocor Research and Development, Radnor, PA*
- ThP 490 **Structural Elucidation of the MBP (Maltose Binding Protein) C-termini from Fusion Proteins in *Pichia pastoris* Expression System;** Zhiguo Li<sup>1</sup>; Wilson Leung<sup>2</sup>; Joan Lin-Cereghino<sup>2</sup>; Geoffrey Lin-Cereghino<sup>2</sup>; Andreas Franz<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of The Pacific, Stockton, CA*; <sup>2</sup>*Depart of Bio Sci, University of the Pacific, Stockton, CA*
- ThP 491 **Hydrogen/Deuterium Exchange: Electrospray Ionization Mass Spectrometry for Probing Structural Changes in Proteins upon Microwave Irradiation;** Urooj A. Mirza; Birendra N. Pramanik; Ajay K. Bose; *Schering Plough Institute, Kenilworth, NJ*
- ThP 492 **HD Desktop: A Web Based Software Application for Rapid Analysis and Visualization of Hydrogen Exchange Mass Spectra;** Bruce D. Pascal; Michael J. Chalmers; Scott A. Busby; Patrick R. Griffin; *The Scripps Research Institute, Jupiter, FL*
- ThP 493 **Recent Advances in UPLC for Hydrogen Exchange Mass Spectrometry: High-Speed & High-Resolution Separations at Zero Degrees Celsius;** Thomas E. Wales<sup>1</sup>; Keith Faden<sup>2</sup>; Geoff Gerhardt<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- ThP 494 **Extension of a SUPREX with Protease Digestion Protocol to Multimeric Proteins;** Ying Xu<sup>1</sup>; Michael C. Fitzgerald<sup>2</sup>; <sup>1</sup>*Department of Chemistry, Duke University, Durham, NC*; <sup>2</sup>*Duke University, Durham, NC*
- ThP 495 **Control of Back Exchange and Experimental Reproducibility for the Detection of Protein Conformational Changes by Hydrogen Exchange Mass Spectrometry;** William I Burkitt; Gavin O'Connor; *LGC, London, UK*
- ThP 496 **Mass Spectrometric Method to Determine pKa Values of Individual Histidine Residues in Proteins;** Masaru Miyagi<sup>1</sup>; Takashi Nakazawa<sup>2</sup>; <sup>1</sup>*Case Western Reserve Univ, Cleveland, OH*; <sup>2</sup>*Nara Women's University, Nara, Japan*
- ThP 497 **Reduced Labeling and its Benefits for HDX-MS Protocols;** Andrew J. Percy; Gordon W. Slysz; David C. Schriemer; *University of Calgary, Calgary, Canada*
- ThP 498 **Conformer Structures of Gaseous Protein Ions from Deuteration Effects on Infrared Photodissociation Spectra;** Xianglei Kong<sup>1</sup>; Giuseppe Infusini<sup>2</sup>; Cheng Lin<sup>2</sup>; Honghai Jiang<sup>1</sup>; Kathrin Breuker<sup>3</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>*Cornell University, Ithaca, NY*; <sup>2</sup>*Boston U School of Medicine, Boston, MA*; <sup>3</sup>*University of Innsbruck, Innsbruck, Austria*
- ThP 499 **Gas Phase H/D Exchange of Hemoglobin Monomers, Dimers and Tetramers;** P. John Wright; Donald J. Douglas; *University of British Columbia, Vancouver, BC*
- ThP 500 **Comparing Peloruside and Laulimalide Induced Microtubule Stabilization using HDX and Data-Directed Ligand Docking;** Torin Huzil<sup>2</sup>; Jack Tuszynski<sup>2</sup>; Melissa Bennett<sup>1</sup>; David Schriemer<sup>1</sup>; <sup>1</sup>*University of Calgary, Calgary, Canada*; <sup>2</sup>*University of Alberta, Edmonton, Canada*
- ThP 501 **Effects of RPLC Separation Conditions on Back-Exchange in Solution-Phase Hydrogen/Deuterium Exchange Mass Spectrometry;** George M. Bou-Assaf<sup>1</sup>; Mark R. Emmett<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL*; <sup>2</sup>*Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL*
- ThP 502 **Can ETD Accurately Measure the H/D Exchange of Individual Residues in Proteins? – A Study of the Amyloidogenic Protein  $\beta$ -2-microglobulin;** Kasper D. Rand; Martin Zehl; Ole N. Jensen; Thomas J.D. Jørgensen; *University of Southern Denmark, Odense, Denmark*
- ThP 503 **Software for the Semi-Automated Analysis of MALDI-TOF-Generated Hydrogen Deuterium Exchange (HDX) Data;** Pornpat Nikamanon; Elroy Pun; Wayne Chou; Marek Daniel Koter; Paul David Gershon; *University of California, Irvine, CA*
- ThP 504 **HYDRA: A Flexible Software Package for 'One-Click' HDX-MS Data Analysis;** Gordon W. Slysz; CJ Baker; Benjamin M. Bozsa; Anthony Dang; David C. Schriemer; *University of Calgary, Calgary, Canada*
- ThP 505 **Measurement of Protein Structure and Folding Differences Associated with Systematic Mutations of the Protein Staphylococcal Nuclease using HX-HPLC-ESI-MS;** Rohana Liyanage; Nagarjuna

## PROTEIN CONFORMATION HD EXCHANGE 2, 491 - 508



## THURSDAY POSTERS

- Devarapalli; Latisha M. Puckett; Jennifer Gidden; Wesely E. Stites; Jackson O. Lay, Jr.; *University of Arkansas, Department of Chemistry, Fayetteville, AR*
- ThP 506 **Dual Protease On-line Digestion for High Density Protein Mapping of Large Proteins in Hydrogen/Deuterium Exchange Mass Spectrometry;** Susan L. Chen<sup>1</sup>; Virgil Woods, Jr.<sup>2</sup>; Roland S. Annan<sup>1</sup>; <sup>1</sup>*GlaxoSmithKline, King of Prussia, PA*; <sup>2</sup>*University of California, La Jolla, CA*
- ThP 507 **Implementing HDX-MS Data in Directed Docking Applications: Rationalizing Amplitude with MD Simulations;** Evan Kelly; Melissa Bennett; Gordon Slysz; Andrew Percy; Hiroaki Ishida; Hans Vogel; David Schriemer; *University of Calgary, Calgary, Canada*
- ThP 508 **Using IM-MS and HDX-MS to Study Native Protein Conformations;** Hannah Florance<sup>1</sup>; Peter Faull<sup>1</sup>; Jason Kalapothakis<sup>1</sup>; Bryan J. McCullough<sup>2</sup>; Ted R. Hupp<sup>1</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>*The University of Edinburgh, Edinburgh, UK*; <sup>2</sup>*The University of Manchester, Manchester, UK*
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- PROTEOMICS – GENERAL, METHODS, 509 - 516**
- ThP 509 **A New Polyacrylamide Gel System Based on an Alternative Crosslinker for Proteomic Research;** Sandra Bornemann; Michael Karas; *Johann Wolfgang Goethe-University, Frankfurt, Germany*
- ThP 510 **The Specificity of Pepsin for Proteolytic Digestion and MS Applications;** Melissa H. Palashoff<sup>1</sup>; Martha Stapels<sup>2</sup>; Keith Fadgen<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Brighton, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- ThP 511 **Capillary Gradient Chromatofocusing-Mass Spectrometry using Low Buffer Concentrations in the Analysis of Proteins;** James A Hribar; Xiang Zhou; David Anderson; *Cleveland State Univ., Cleveland, OH*
- ThP 512 **Assessing Free Cysteines and Open Disulfides in an Albumin Fusion Protein by Ellman's Reaction with Mass Spectrometry;** Andrea Meeler; *Human Genome Sciences, Inc., Rockville, MD*
- ThP 513 **Characterization of Covalently Bound Agonists of Kappa-Opioid Receptors By Mass Spectrometric Analysis;** Feng Yan<sup>1</sup>; Viorel Mocanu<sup>3</sup>; Ruslan V. Bikbulatov<sup>2</sup>; Jordan K. Zjawiony<sup>2</sup>; Xian Chen<sup>3</sup>; Bryan Roth<sup>3</sup>; <sup>1</sup>*Case Western Reserve University, Cleveland, OH*; <sup>2</sup>*University of Mississippi, University, MS*; <sup>3</sup>*University of North Carolina, Chapel Hill, NC*
- ThP 514 **High Pressure Trypsin Digestion of Proteins for Proteomic Analysis;** Shane A. Wyatt; Timothy R. Croley; *Commonwealth of Virginia, Richmond, VA*
- ThP 515 **An Approach for Quantifying the Digestion Efficiency of Hemoglobin by LC-MS;** Adrienne K. Barry; Maria Ospina; Hubert Vesper; *Centers for Disease Control and Prevention, Atlanta, GA*
- ThP 516 **Analysis of Efficiency of Microwave-Assisted Enzymatic Digestion of Proteins;** Anton Karnoup; Krishnamoorthy Kuppannan; Scott Young; *The Dow Chemical Company, Midland, MI*
- 
- PROTEOMICS: BIOMARKER ASSAYS 2, 517 - 532**
- ThP 517 **Discovery of Biomarkers in Cutaneous Leishmaniasis Patients;** Momar Ndao; Manfred Fussi; Christine Straccini; Brian . Ward; Bernard Gibbs; *McGill University, Montreal, Canada*
- ThP 518 **Finding the Needle: Accurate Inclusion Mass Screening for Biomarker Triage and Assay Development;** Jacob D. Jaffe; Hasmik Keshishian; Terri Addona; Michael Gillette; Steven A. Carr; *Broad Institute, Cambridge, MA*
- ThP 519 **High Sensitivity Nano-LC-MS-MS Analysis of Urinary Hydroxylslypyridinoline and Lysylpyridinoline as Measurement of Collagen Turnover;** Michel Boutin<sup>1</sup>; Marjo Jauhiainen<sup>1</sup>; Bateman Kevin<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*IRIC, University of Montreal, Montreal, Canada*; <sup>2</sup>*Merck Frosst Center for Therapeutic Research, Kirkland, Canada*
- ThP 520 **Targeted Protein Expression Profiling using MRM: Genetic vs. Environmental Variation of Plasma Protein Levels using a Twin Cohort;** Christie L Hunter<sup>1</sup>; Veronica Saenz-Vash<sup>3</sup>; Marjorie Minkoff<sup>1</sup>; Steven A Carr<sup>3</sup>; Leigh Anderson<sup>2</sup>; <sup>1</sup>*Applied Biosystems, Foster City, CA*; <sup>2</sup>*the Plasma Proteome Institute, Washington, DC*; <sup>3</sup>*Broad Institute, Cambridge, MA*
- ThP 521 **Single Reaction Monitoring (SRM) of Pro-Alpha (2) I Collagen: Validation of a Novel Biomarker of Urogenital Complications from Diabetes;** Kathleen C Lundberg<sup>1</sup>; George Christ<sup>2</sup>; Janna Kiselar<sup>1</sup>; Daniela Schlatter<sup>1</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>*Case Western Reserve University, Cleveland, OH*; <sup>2</sup>*Wake Forest University School of Medicine, Winston-Salem, NC*
- ThP 522 **Differential Proteomic Profiling of Serum Samples from Rheumatoid Arthritis Patients by Two-Step Abundant Protein Depletion;** Shanhua Lin; Hua Lin; Melissa Chen; Jing Wang; Erika Price; Jaya Kothule; Sophia Chen; Chris Becker; *Ppd Biomarker Discovery Sciences, Menlo Park, CA*
- ThP 523 **Biological Reference Materials for Proteomics: Tandem Mass Tag-Labeled Reference Materials and Their Utility for Mass Spectrometry-Based Multipoint Calibration and Quantification;** Peter Schulz-Knappe<sup>1</sup>; Christian Baumann<sup>1</sup>; Josef Schwarz<sup>1</sup>; Jürgen Schäfer<sup>1</sup>; Ian Pike<sup>3</sup>; Malcolm Ward<sup>3</sup>; Karsten Kuhn<sup>1</sup>; Frank Vitzthum<sup>2</sup>; <sup>1</sup>*Proteome Sciences R&D GmbH Co.KG, Frankfurt, Germany*; <sup>2</sup>*Dade Behring Marburg GmbH, Marburg, Germany*; <sup>3</sup>*Proteome Sciences Plc., Cobham, UK*
- ThP 524 **Reproducibility of MRM-Based Assays for Quantitative Verification of Candidate Protein Biomarkers in Plasma: an Interlaboratory Study;** Terri Addona<sup>1</sup>; Stephen Hall<sup>2</sup>; Steven J. Skates<sup>3</sup>; David Bunk<sup>4</sup>; CPTAC Verification Work Group<sup>5</sup>; <sup>1</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*University of California San Francisco, San Francisco, CA*; <sup>3</sup>*Massachusetts General Hospital, Boston, MA*; <sup>4</sup>*Nist, Gaithersburg, MD*; <sup>5</sup>*National Cancer Institute, Bethesda, MD*
- ThP 525 **Developing SISCAPA-MRM-MS Biomarker Verification Technology Including a Comparison between Rabbit Polyclonal, Mouse Monoclonal, and Rabbit Monoclonal Antibodies;** Regine M. Schoenherr; Li-Chia Feng; Lei Zhao; Jeffrey R. Whiteaker; Amanda G. Paulovich; *Fred Hutchinson Cancer Research Center, Seattle, WA*
- ThP 526 **Improving the Sensitivity of LC-MS-MS Assays for Low Abundance Protein Biomarkers: Bridging the Gap with ELISA;** Lee W. Ott<sup>1</sup>; Michael J. Berna<sup>1</sup>; Gary A. Valaskovic<sup>3</sup>; Bradley L. Ackermann<sup>2</sup>; <sup>1</sup>*Eli Lilly and Company, Greenfield, IN*; <sup>2</sup>*Eli Lilly & Company, Greenfield, IN*; <sup>3</sup>*New Objective, Inc., Woburn, MA*
- ThP 527 **Global MRM MS-Based Assays for FFPE Cancer Tissues using In-Sample Internal Standards;** Toshihide Nishimura<sup>2</sup>; Masaharu Nomura<sup>5</sup>; Hiroko Endo<sup>1</sup>; Sumie Ando<sup>2</sup>; Kiyonaga Fujii<sup>4</sup>; Yasuhiko



## THURSDAY POSTERS

- Bando<sup>1</sup>; Hiromasa Tojo<sup>3</sup>; Ryutaro Nishiyama<sup>6</sup>; Takashi Hirano<sup>5</sup>; Kouichi Yoshida<sup>5</sup>; David Krizman<sup>7</sup>; Harubumi Kato<sup>5</sup>; <sup>1</sup>Biosys Technologies, Tokyo, Japan; <sup>2</sup>Applied Biosystems Japan, Tokyo, Japan; <sup>3</sup>Osaka University, Osaka, Japan; <sup>4</sup>Hokkaido University, Sapporo, Japan; <sup>5</sup>Tokyo Medical University, Tokyo, Japan; <sup>6</sup>Leica Microsystems Japan, Tokyo, Japan; <sup>7</sup>Expression Pathology, Gaithersburg, MD
- ThP 528 **Signal Amplifications of Biological Events on Biosurfaces with Am-Tag**; Jung Rok Lee<sup>1</sup>; Ju Hee Lee<sup>2</sup>; Kwang Pyo Kim<sup>1</sup>; Hyung Soon Park<sup>3</sup>; Woon Seok Yeo<sup>2</sup>; <sup>1</sup>Molecular Biotechnology, Konkuk University, Seoul, South Korea; <sup>2</sup>Bioscience and Biotechnology, Konkuk University, Seoul, South Korea; <sup>3</sup>ProbiOND, Seoul, South Korea
- ThP 529 **Protein Expression Identifies Pseudallescheria Boydii Fungal Infection**; Michaela Therova-Smetkova<sup>2</sup>; Jan Nedved<sup>1</sup>; David Vydra<sup>2</sup>; Dalibor Dolezal<sup>2</sup>; Marta Dziechciarkova<sup>2</sup>; Vladimir Havlicek<sup>1</sup>; Marian Hajduch<sup>2</sup>; <sup>1</sup>MBU AV CR, Praha, Czech Republic; <sup>2</sup>Laboratory of Experimental Medicine, Olomouc, Czech Republic
- ThP 530 **Urinary Proteome in Kidney Disease and Transplant Rejection**; Gary Nelsestuen; Stephen Harvey; Matthew Stone; Yan Zhang; Sanjeev Akkina; Hassan Ibrahim; William Oetting; *University of Minnesota, Minneapolis, MN*
- ThP 531 **Evaluation of Strategies for High Sensitivity Protein Monitoring in Human Plasma using Liquid Chromatography-Multiple Reaction Monitoring/Mass Spectrometry (LC-MRM/MS)**; Richard C. Jones<sup>1</sup>; David L. Allen<sup>1</sup>; Sandy Schultz<sup>1</sup>; Isabel Riba Garcia<sup>2</sup>; Simon J. Gaskell<sup>2</sup>; Michael R. Pisano<sup>1</sup>; <sup>1</sup>NextGen Sciences, Ann Arbor, MI; <sup>2</sup>University of Manchester, Manchester, UK
- ThP 532 **Antibody Characterization for the Development of a Standardized Immunoassay for Human Cardiac Troponin I**; Mark S. Lowenthal; Nathan G. Dodder; Hua-Jun He; Kenneth D. Cole; David M. Bunk; Lili Wang; *National Institute of Standards and Technology, Gaithersburg, MD*
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- PROTEOMICS: APPLICATIONS, 549 - 587**
- ThP 549 **Investigation of Interaction between CDK Inhibitor ZK243919 and Human Pyridoxal Kinase (PDXK) by Chemical Proteomics and Further *in vitro* Experiments**; Enrico Missner; Inke Bahr; Volker Badock; Peter Donner; *Bayer HealthCare Pharmaceuticals, Berlin, Germany*
- ThP 550 **Evaluating the Molecular Architecture of the Rpd3-Sin3 Histone Deacetylase Complex using Complex Based Proteomic Data**; Joshua M. Gilmore<sup>1</sup>; Mihaela E Sardu<sup>1</sup>; Michael J. Carrozza<sup>2</sup>; Bing Li<sup>1</sup>; Jerry L. Workman<sup>1</sup>; Amber L. Mosley<sup>1</sup>; Laurence Florens<sup>1</sup>; Michael P. Washburn<sup>1</sup>; <sup>1</sup>Stowers Institute for Medical Research, Kansas City, MO; <sup>2</sup>NIH, Reasech Triangle Park, NC
- ThP 551 **Stable Isotope Labeling and LC-MS Analysis of Proteins Secreted by Activated Pancreatic Stellate Cells**; Angela Y Wehr<sup>1</sup>; Kenneth Yu<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Univ. of Penn/Center For Can, Philadelphia, PA
- ThP 552 **Top-Down Analysis of Histones using FFE and RP-HPLC on Monolithic Capillary Columns and FT-ICR MS**; Evert-Jan Sneekes<sup>1</sup>; Jun Han<sup>3</sup>; Monica Elliot<sup>3</sup>; Juan Ausio<sup>3</sup>; Remco Swart<sup>1</sup>; Albert J.R. Heck<sup>2</sup>; Christoph Borchers<sup>3</sup>; <sup>1</sup>Dionex Corporation Amsterdam, Amsterdam, Netherlands; <sup>2</sup>Utrecht University/Netherlands Proteomics Centre, Utrecht, Netherlands; <sup>3</sup>Uvic-gbc Proteomics Centre, Victoria, BC
- ThP 553 **Oxygen Isotope Substitution of Pre-Existing Peptidyl Phosphates for Analysis of Phosphotyrosinyl Proteomes**; Yu Shi; Bekim Bajrami; Selina A. Osei; Xudong Yao; *Chemistry Department, University of Connecticut, Storrs, CT*
- ThP 554 **Non-Tagged Peptidomics Combined with Systems Biology Yields Novel Insights into the World of Cystic Fibrosis**; Senait G. Asmellash<sup>1</sup>; Jennifer S. Guimbellot<sup>1</sup>; Gregory J. Bowersock<sup>2</sup>; Carol A. Ballinger<sup>1</sup>; Edward M. Postlethwait<sup>1</sup>; Eric J. Sorscher<sup>1</sup>; Hector Ramos<sup>2</sup>; Rong J. Qi<sup>3</sup>; Joseph D. Shambaugh<sup>3</sup>; James A. Mobley<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>Institute of Systems Biology, Seattle, WA; <sup>3</sup>Genedata Inc., Waltham, MA
- ThP 555 **The Proteome of Arabidopsis Thaliana Analyzed by Electron Transfer Dissociation**; Kai Scheffler<sup>1</sup>; Martin Hornshaw<sup>2</sup>; Bernd Mueller<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Dreieich, Germany; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, UK; <sup>3</sup>Dept. of Biology, Ludwig-Maximilians-University, Munich, Germany
- ThP 556 **Measuring Protein Synthesis as Part of Proteomics Study on Pancreas Cancer Cell Proliferation**; Yingchun Zhao<sup>1</sup>; Wai-Nang Paul Lee<sup>2</sup>; Shu Lim<sup>2</sup>; Jing Xiao<sup>1</sup>; Robert R. Recker<sup>1</sup>; Gary Guishan Xiao<sup>1</sup>; <sup>1</sup>Creighton University, Omaha, NE; <sup>2</sup>Mass Spectrometry Core Facility, Pediatrics, Torrance, CA
- ThP 557 **Investigating the Effect of Oxidative Stress on the Human 26S Proteasome Complex using LTQ-Orbitrap Mass Spectrometer**; Xiaorong Wang; Nelson Jen; Lan Huang; *Departments of Physiology & Biophysics and Develo, Irvine, CA*
- ThP 558 **Analytical Strategies for Characterisation and Quantitation of Zinc-Binding Proteins by 2D-LC coupled to ICP-MS, ESI-Q-TOF-MS and MALDI-TOF-TOF-MS**; Lidia K. Siemieniako<sup>1</sup>; Josephine Bunch<sup>1</sup>; Alison Graham<sup>1</sup>; Cameron W. Mcleod<sup>1</sup>; Robert Poole<sup>1</sup>; Donna Potts<sup>2</sup>; <sup>1</sup>The University of Sheffield, Sheffield, UK; <sup>2</sup>Applied Biosystems, Warrington, UK
- ThP 559 **Proteomic Analysis of Activin-Dependent Follistatin Transcription in Gonadotrope-Derived aT3-1 Cells**; Karsten Schmidt; Amy L. Blount; Wylie W. Vale; Wolfgang H. Fischer; Louise M. Bilezikjian; *The Salk Institute, La Jolla, CA*
- ThP 560 **Application of LTQ-Orbitrap Top-Down Analysis of Small Plasma Proteins: A Model Study with Transthyretin**; Roger Theberge; Mark E. McComb; Weiwei Tong; Giuseppe Infusini; Catherine E. Costello; *Boston U School of Med, Boston, MA*
- ThP 561 **Label-Free Relative Quantitation of Developmentally Expressed Soluble Proteins in the Ripening Fruit of Citrus Sinensis**; Richard A. Eigenheer; Mario Fon; Ehud Katz; Eduardo Blumwald; Brett S. Phinney; *UC Davis, Davis, CA*
- ThP 562 **A High-Coverage Approach for Human Urine Proteome: Touching Phosphorylation in Urine**; Qing-Run Li; Ke-Xin Fan; Jie Dai; Rong-Xia Li; Rong Zeng; *Shanghai Institutes for Biological Sciences, Shanghai, China*
- ThP 563 ***In vivo* Proteomics in Drosophila Melanogaster by Tandem Affinity Purification of Protein Complexes and Analysis by Protein Center & Trade Software**; Johanna S Rees<sup>1</sup>; Svenja Hester<sup>1</sup>; Julie A Howard<sup>1</sup>; Daniel J St. Johnston<sup>1</sup>; Morten Bern<sup>2</sup>; Kathryn S Lilley<sup>1</sup>;

## THURSDAY POSTERS

- ThP 564 <sup>1</sup>University of Cambridge, Cambridge, UK; <sup>2</sup>Proxeon, Odense M, Denmark  
**Characterization of VGLUT-1 and VGAT Specific Subpopulations of Synaptic Vesicles by Stable Isotope Labeling;** Mads Gronborg<sup>1</sup>; Dietmar Riedel<sup>2</sup>; Henning Urlaub<sup>3</sup>; Reinhard Jahn<sup>1</sup>; <sup>1</sup>Department of Neurobiology, MPI bpc, Göttingen, Germany; <sup>2</sup>Laboratory of Electron Microscopy, MPI bpc, Göttingen, Germany; <sup>3</sup>Bioanalytical Mass Spectrometry Group, MPI bpc, Göttingen, Germany
- ThP 565 **Absolute Quantification of Plasma Glycoproteins by Multiple Reaction Monitoring Mass Spectrometry of Proteotypic Peptides for Breast Cancer Biomarker Discovery;** Simon Letarte<sup>1</sup>; Jingchun Chen<sup>1</sup>; Mi-youn Brusniak<sup>1</sup>; Emma Nimeus<sup>2</sup>; Hamid Mirzaei<sup>1</sup>; Vinzenz Lange<sup>3</sup>; John Didion<sup>1</sup>; Nichole King<sup>1</sup>; Carey Sheu<sup>1</sup>; Bruno Domon<sup>3</sup>; Julian D Watts<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>University hospital, Lund, Sweden; <sup>3</sup>ETH, Zurich, Switzerland
- ThP 566 **Proteomics Characterization of Bacillus Ralstonia Pickettii from Endothelial Cell Line by 2D Protein SEC-RP HPLC and Mass Spectrometry;** Wantao Ying; Claire Dauly; Nicolas Clavreul; David H. Perlman; Richard A. Cohen; Catherine E. Costello; Mark E. McComb; Boston University School of Medicine, Boston, MA
- ThP 567 **Amplification of Pathological Differences of Diseases using Biochemical and Bioinformatical Approaches;** Gregory Czerwieniec; Carla Guimaraes; Yiannis Ioannou; Rong Wang; Mount Sinai School of Med, New York, NY
- ThP 568 **Proteome Analysis of Yeast using Gel Eluted Liquid Fraction Entrapment Electrophoresis – A Solution-Phase Method for Mass Separation and Analysis;** John C. Tran; Alan A. Doucette; Dalhousie University, Halifax, NS
- ThP 569 **Optimizing the Characterization of Extracellular Matrix Proteins using Ultrasonic Assisted In-Solution Tryptic Digestion;** Lauren A. Kiemele<sup>1</sup>; Aarthi Shankar<sup>1</sup>; Pepper Schedin<sup>1</sup>; Kirk Hansen<sup>2</sup>; <sup>1</sup>UCHSC, Aurora, CO; <sup>2</sup>Univ. of Colorado HSC, Aurora, CO
- ThP 570 **Mass Spectral Analysis of Influenza Vaccine Formulations: Hemagglutinin Quantitation;** Terry D. Cyr; Marybeth Cameron; Jeremy Brazeau; Health Canada, Ottawa, Canada
- ThP 571 **Analysis of Viral Capsid HK97 via Cryodetection MALDI TOF in the MegaDalton Mass Range;** David M. Sipe<sup>1</sup>; Abdil Ozdemir<sup>2</sup>; Brian Firek<sup>2</sup>; Roger Hendrix<sup>2</sup>; Mark E. Bier<sup>1</sup>; <sup>1</sup>Carnegie Mellon University, Pittsburgh, PA; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Sakarya University, Sakarya, Turkey
- ThP 572 **The Yeast Nuclear Proteome: Composition and Complexes;** Sharon Gauci Versteeg<sup>1</sup>; Liesbeth M Veenhoff<sup>2</sup>; Albert J. R. Heck<sup>1</sup>; Jeroen Krijgsveld<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>University of Groningen, Groningen, Netherlands
- ThP 573 **SILAC-labeling of Human Embryonic Stem Cells for Quantitative Proteomics;** Tatyana A. Prokhorova; Kristoffer T. G. Rigbolt; Pia T. Johansen; Irina Kratchmarova; Moustapha Kassem; Blagoy Blagoev; University of Southern Denmark, Odense, Denmark
- ThP 574 **Iterative Exclusion (IE)-MS Analysis: Uncovering the Hidden Proteome;** Sean C Bendall<sup>1</sup>; Chris Hughes<sup>1</sup>; Mick Bhatia<sup>2</sup>; Gilles Lajoie<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, ON; <sup>2</sup>McMaster University, Hamilton, Canada
- ThP 575 **Using Label-Free Quantification to Assess Sample Preparation: Application to Protein Expression Dynamics of Marek's Disease Viral Infection;** Mialy F. Ramaroson; Kevin Blackburn; Hsiao-Ching S. Liu; Michael B. Goshe; NC State University, Raleigh, NC
- ThP 576 **A Novel Cytomegalovirus Protein Interacts with the Histone Deacetylase-Containing NuRD Complex to Alter Cellular Gene Expression and Promote Virus Replication;** Ileana M. Cristea<sup>1</sup>; Scott S. Terhune<sup>2</sup>; Nathaniel J. Moorman<sup>1</sup>; Michael P. Rout<sup>3</sup>; Thomas Shenk<sup>1</sup>; Brian T. Chait<sup>3</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>3</sup>Rockefeller University, New York, NY
- ThP 577 **Quantitating CNS-derived Apolipoprotein E Isoforms using Bottom-Up Proteomics;** Kristin R Wildsmith; Karen R Browning; Kwasi G Mawuenyega; Alan E Davis; R. Reid Townsend; Randall J Bateman; Washington Univ. School of Medicine, Saint Louis, MO
- ThP 578 **A Two-Phased Targeted Proteomic Approach Allowing Testing of Thousands of Biomarker Candidates;** Liming Hou<sup>1</sup>; ChenWei Lin<sup>1</sup>; Alexei Krasnoselsky<sup>1</sup>; Mary Trute<sup>1</sup>; Jeffrey R. Whiteaker<sup>1</sup>; Regine M. Schoenherr<sup>1</sup>; Li-Chia Feng<sup>1</sup>; Karen S. Kelly-Spratt<sup>1</sup>; Sharon Pitteri<sup>1</sup>; Ted Holzman<sup>1</sup>; Philip Gafken<sup>1</sup>; Lisa A. Jones<sup>1</sup>; Jason M. Hogan<sup>1</sup>; Samir Hanash<sup>1</sup>; Martin McIntosh<sup>1</sup>; Christopher J. Kemp<sup>1</sup>; Dan Martin<sup>2</sup>; Peter Nelson<sup>1</sup>; Amanda Paulovich<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>Institute for Systems Biology, Seattle, WA
- ThP 579 **Use of Peptide Analog Diversity Library Beads for Increased Depth of Proteomic Analysis; Application to Cerebrospinal Fluid;** Kevin S. Shores<sup>2</sup>; D. Gomika Udugamasooriya<sup>3</sup>; Thomas Kodadek<sup>3</sup>; Daniel R. Knapp<sup>1</sup>; <sup>1</sup>Medical University of SC, Charleston, SC; <sup>2</sup>University of Texas, Austin, TX; <sup>3</sup>University of Texas Southwestern Med. Ctr., Dallas, Tx
- ThP 580 **Identification of Tranilast-Binding Proteins from Mouse Xenograft Model with Human and Mouse Genome Sequence Information;** Masayuki Haramura; Noriyuki Inomata; Takashi Shinkawa; Kohji Nagano; Chugai Pharmaceutical, Kamakura, Japan
- ThP 581 **Depletion Effect of High-Abundance Urine Proteins for Detecting Markers of Bladder Cancer in Urine by Quantitative Mass Spectrometry;** Yi-Ting Chen<sup>1</sup>; Meng-Chieh Chen<sup>1</sup>; Chi-De Chen<sup>1</sup>; Yulun Chiu<sup>1</sup>; Chien-Lun Chen<sup>2</sup>; <sup>1</sup>Chang Gung University, Taoyuan, Taiwan; <sup>2</sup>Chang Gung Memorial Hospital, Taoyuan, Taiwan
- ThP 582 **Revealing the HIV-1-Host Interactome;** Yang Luo<sup>1</sup>; Ileana M. Cristea<sup>2</sup>; Michael Rout<sup>1</sup>; Brian Chait<sup>1</sup>; Mark Muesing<sup>3</sup>; <sup>1</sup>The Rockefeller University, New York, NY; <sup>2</sup>Princeton University, Princeton, NJ; <sup>3</sup>Aaron Diamond AIDS Research Center, New York, NY
- ThP 583 **Identification of Thioredoxin Targets using a Quantitative Proteomics Approach Based on Isotope-Coded Affinity Tags and LC-MS-MS;** Per M Hagglund<sup>1</sup>; Jakob Bunkenborg<sup>2</sup>; Kenji Maeda<sup>1</sup>; Christine Finnie<sup>1</sup>; Birte Svensson<sup>1</sup>; <sup>1</sup>Technical University of Denmark, Kgs Lyngby, Denmark; <sup>2</sup>Cebi, University of Southern Denmark, Odense, Denmark
- ThP 584 **Efficient Profiling of Nuclear Proteins in Mouse Embryonic Stem Cell;** Lu Yu; Mercedes Pardo; Sajani Swamy; Peri Tate; Jyoti Choudhary; Wellcome Trust Sanger Institute, Cambridge, UK
- ThP 585 **Proteome Alteration Induced by hTERT Transfection of Human Fibroblast Cells;** Gabriel Mazzucchelli<sup>1</sup>; Valerie Gabelica<sup>2</sup>; Nicolas Smargiasso<sup>1</sup>;

## THURSDAY POSTERS

- Maximilien Fléron<sup>1</sup>; Wilson Ashimwe<sup>1</sup>; Frederic Rosu<sup>1</sup>; Marie-claire Gillet<sup>1</sup>; Jean-François Riou<sup>2</sup>; Edwin De Pauw<sup>3</sup>; <sup>1</sup>University of Liege, Liege, Belgium; <sup>2</sup>Museum National d'Histoire Naturelle, Paris, FR; <sup>3</sup>Liege University, Liege, Belgium
- ThP 586 **Identifying Cell Surface Glycoproteins using Hydrazone Chemistry in Combination with 2D-LC/ESI-MS-MS**; Claudia A. McDonald; Jane Y. Yang; Arthur Arcinas; Ten-Yang Yen; Bruce A. Macher; *San Francisco State University, San Francisco, CA*
- ThP 587 **Characterization of Glia using Direct Single-Cell MALDI-TOF MS Analysis**; Ann Knolhoff; Ping Yin; Larry Millet; Martha Gillette; Jonathan Sweedler; *University of Illinois, Urbana, IL*
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- PROTEOMICS: BIOMARKER DISCOVERY 4, 588 - 606**
- ThP 588 **Plasma Proteome Profiling of a Mouse Model of Breast Cancer Identifies a Panel of Candidate Markers Potentially Applicable to Human**; Sharon Pitteri; Vitor M Faca; Karen S. Kelly-Spratt; A. Erik Kasarda; Hong Wang; Qing Zhang; Lisa Newcomb; Sophie Paczesny; Sandra Pereira Faca; Gina Choi; Alexei Krasnoselsky; Matthew Fitzgibbon; Martin Mcintosh; Christopher J. Kemp; Samir Hanash; *Fred Hutchinson Cancer Research Center, Seattle, WA*
- ThP 589 **Discovery and Independent Validation of Plasma Biomarkers for Renal Carcinoma**; Chuck Hannum<sup>1</sup>; Cedric L. Wiesner<sup>1</sup>; Robert Dubridge<sup>1</sup>; John C. Cheville<sup>2</sup>; Robert Figlin<sup>3</sup>; Karen Reckamp<sup>3</sup>; Chris Becker<sup>4</sup>; Sushmita Roy<sup>4</sup>; Jordan Hiller<sup>1</sup>; Keith Wilson<sup>1</sup>; <sup>1</sup>PDL BioPharma, Fremont, CA; <sup>2</sup>Mayo Clinic, Rochester, MN; <sup>3</sup>City of Hope National Medical Center, Duarte, CA; <sup>4</sup>PPD Biomarker Discovery Sciences, LLC, Menlo Park, CA
- ThP 590 **Utility of Depletion in MRM Assays**; Mahbod R. Hajivandi; Xiquan Liang; Paul Predki; R. Marshall Pope; *Invitrogen, Carlsbad, CA*
- ThP 591 **Proteomic Analysis of Sjögren's Syndrome and MALT Lymphoma**; Jiang Jiang; Shen Hu; David T. Wong; *University of California Los Angeles, Los Angeles, CA*
- ThP 592 **LC/ESIMS Analysis of Desmosine and Isodesmosine - Biomarkers for Chronic Obstructive Pulmonary Disease (COPD)**; Shuren Ma<sup>2</sup>; Jiangtao He<sup>3</sup>; Seymour Lieberman<sup>1</sup>; Gerard M Turino<sup>1</sup>; Yong Lin<sup>1</sup>; <sup>1</sup>St.Luke/Roosevelt Hospital Center, New York, NY; <sup>2</sup>Roosevelt Hospital, New York, NY; <sup>3</sup>Columbia University, New York, NY
- ThP 593 **Sensitization of B-CLL Lymphocytes – Quest for a Protein Marker. Which Mass Spectrometry Quantitative Technique Will Give the Answer?**; David Potesil<sup>1</sup>; Sona Cejkova<sup>2</sup>; Ludmila Rocnova<sup>2</sup>; Martin Trbusek<sup>2</sup>; Zbynek Zdrahal<sup>1</sup>; Jan Havlis<sup>1</sup>; <sup>1</sup>Faculty of Science, Masaryk University, Brno, Czech Republic; <sup>2</sup>University Hospital Brno, Brno, Czech Republic
- ThP 594 **Profiling Mouse Brain Protein Abundance and Oxidative Modification Changes in a Neurotoxin-Induced Parkinson's Disease Model**; Xu Zhang<sup>1</sup>; Mark H Chin<sup>2</sup>; Athena A Schepmoes<sup>1</sup>; Vladislav A Petyuk<sup>1</sup>; Dave J. Anderson<sup>1</sup>; David G Camp<sup>1</sup>; Desmond J. Smith<sup>2</sup>; Richard D. Smith<sup>1</sup>; Weijun Qian<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>UCLA, Los Angeles, CA
- ThP 595 **Evaluation of Urine as a Source Material for Biomarker Discovery and Verification**; Eric Thomas; Wei Guan; Rebecca Sutphen; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- ThP 596 **Characterization of *in vitro* Lung Cancer Secretome and a Comparison with Differentially Expressed Plasma Proteins from Lung Cancer Patients**; Dan Huang<sup>12</sup>; Timothy Britt Langston<sup>3</sup>; Willie J. McKinney<sup>3</sup>; Gaurav S.J.B. Rana<sup>3</sup>; Jason W. Flora<sup>3</sup>; <sup>1</sup>Clearpoint, Richmond, Virginia; <sup>2</sup>Clearpoint, Richmond, v; <sup>3</sup>Philip Morris USA, Richmond, Virginia
- ThP 597 **Identification of Platelet Factor-4 as an Indicator of Blood Count Recovery in Acute Myeloid Leukemia Patients in Complete Remission**; Jin Young Kim<sup>1</sup>; Hoi-Jeong Lim<sup>2</sup>; Ho-Jun Song<sup>3</sup>; Jae Seong Kim<sup>4</sup>; Hyeoung-Joon Kim<sup>4</sup>; Myung-Geun Shin<sup>4</sup>; Jong Shin Yoo<sup>2</sup>; John Yates<sup>1</sup>; Seung-won Lee<sup>4</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Korea Basic Science Institute, Ochang, Korea; <sup>3</sup>Chonnam National University School of Dentistry, Gwangju, Korea; <sup>4</sup>Chonnam National University Medical School, Gwangju, Korea
- ThP 598 **Altered Membrane Proteomic Signature in Human Colorectal Cancer Revealed by Label-free Quantitation Strategy**; Chien-Peng Wu<sup>1</sup>; Pei-Yi Lin<sup>2</sup>; Chih-Wei Chien<sup>2</sup>; Chia-Li Han<sup>2</sup>; Chih-Chiang Tsou<sup>3</sup>; Ting-Yi Sung<sup>3</sup>; Wen-Lian Hsu<sup>2</sup>; Yu-Ju Chen<sup>2</sup>; <sup>1</sup>National Taiwan Ocean University, Keelung, Taiwan; <sup>2</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>3</sup>Institute of Information Science, Academia Sinica, Taipei, Taiwan
- ThP 599 **A Comparison of Normalization Models for Spectral Counting Data**; Ann L. Oberg; Douglas W. Mahoney; Patrick S. Quint; Jeanette E. Eckel-Passow; Garth D. Nelson; Jonathan J. Harrington; Terry M. Therneau; David A. Ahlquist; H. Robert Bergen, III; *Mayo Clinic, Rochester, MN*
- ThP 600 **Discovery of Protein Disease Biomarkers for Schizophrenia in Serum using Label-Free NanoLC-MSE Validated using ELISA**; Yishai Levin<sup>1</sup>; Lan Wang<sup>1</sup>; Emanuel Schwarz<sup>1</sup>; F. Markus Leweke<sup>2</sup>; Sabine Bahn<sup>1</sup>; <sup>1</sup>Institute of Biotechnology University of Cambridge, Cambridge, UK; <sup>2</sup>University of Cologne, Cologne, Germany
- ThP 601 **Unraveling Secrets of the Secretome: Approaches to Identifying Secreted Lung Cancer Proteins during Epithelial to Mesenchymal Transition (EMT)**; Pratik Jagtap; Jayson A. Falkner; George Michailidis; Angela Walker; Eric Simon; Gilbert Omenn; Venkateshwar Keshamouni; Philip Andrews; *University of Michigan, Ann Arbor, MI*
- ThP 602 **Performance and Optimization of LC-MS-MS Platforms for Proteomic Analyses: An Interlaboratory Study**; Daniel C. Liebler<sup>1</sup>; Amanda Paulovich<sup>2</sup>; Amy-joan L. Ham<sup>1</sup>; David Tabb<sup>3</sup>; Lisa Zimmerman<sup>3</sup>; Dean Billheimer<sup>4</sup>; David Bunk<sup>5</sup>; Stephen Stein<sup>5</sup>; Paul Rudnick<sup>3</sup>; Cliff Speigelman<sup>6</sup>; Karl R. Clauser<sup>7</sup>; Ron Blackman<sup>7</sup>; Chris Kinsinger<sup>8</sup>; CPTAC Discovery Work Group<sup>8</sup>; <sup>1</sup>Vanderbilt Univ. School of Medicine, Nashville, TN; <sup>2</sup>Fred Hutchinson Cancer Resea, Seattle, WA; <sup>3</sup>Vanderbilt University, Nashville, TN; <sup>4</sup>University of Utah, Salt Lake City, UT; <sup>5</sup>NIST, Gaithersburg, MD; <sup>6</sup>Texas A&M University, College Station, TX; <sup>7</sup>Broad Institute of Mit And Harvard, Boston, MA; <sup>8</sup>National Cancer Institute, Bethesda, MD
- ThP 603 **Proteomic Analysis of Mouse Plasma Proteins in Huntington's Disease by Multidimensional Chromatography Coupled with Mass Spectrometry**; Xiaoyun Liu; Benjamin R. Miller; George V. Rebec; David E. Clemmer; *Indiana University, Bloomington, IN*
- ThP 604 **Two-Dimensional Protein and Peptide Separation of Serum by Preparative Monolith Chromatography for**

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- Biomarker Research;** Linda IJsselstijn; Deborah Kronenberg; Peter J Koudstaal; Monique M B Breteler; Peter A E Sillevius Smit; Theo M Luider; *Erasmus Medical Center, Rotterdam, Netherlands*
- ThP 605 **Serum Protein Biomarker Discovery in Genetically Engineered Mouse Models of Pancreatic Cancer via HTP MD-Fractionation and LC-MS(MS)<sup>2</sup>;** Kyoko Kojima; Gregory J. Bowersock; John D. Christein; Christopher A. Klug; James A. Mobley; *University of Alabama At Birmingham, Birmingham, AL*
- ThP 606 **Secreted Proteins of Malignant Breast Cells Coordinate Angiogenesis through ECM Degradation;** Xiquan Liang; Jarkko Huuskonen; Mahbod R. Hajivandi; Paul Predki; R. Marshall Pope; *Invitrogen, Carlsbad, CA*
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- PROTEOMICS - TISSUE, 607 - 628**
- ThP 607 **Application of Difference In-Gel Electrophoresis and MALDI-ToF/ToF Mass Spectrometry to Assess Hypoxia-Induced Changes in the Zebrafish Skeletal Muscle Proteome;** Kan Chen; Richard B. Cole; Bernard B. Rees; *University of New Orleans, New Orleans, LA*
- ThP 608 **Large-Scale Quantitative Proteomic Analysis of Skin Biopsy Samples to Assess the Effects of SDS-Induced Erythema;** Erika P Parkinson<sup>1</sup>; Paul J Skipp<sup>1</sup>; Andrew Garrow<sup>2</sup>; Maja Aleksic<sup>2</sup>; Daniel J. Scott<sup>2</sup>; Geraldine Clough<sup>1</sup>; C. David O'Connor<sup>1</sup>; <sup>1</sup>*Univ. of Southampton, Southampton, UK*; <sup>2</sup>*Unilever, Bedford, UK*
- ThP 609 **A Comparison of Multi-Dimensional Approaches for Enhanced Proteomic Analyses of FFPE Tissues;** Paul L Auger JR; Wen Yu; Dan Fitzpatrick; Mike Davis; Scott D. Patterson; *Amgen, Thousand Oaks, CA*
- ThP 610 **Proteomics and Phosphoproteomics of Human Skeletal Muscle Mitochondria using Phosphopeptide Enrichment and Tandem Mass Spectrometry;** Xiaolu Zhao<sup>1</sup>; Kurt Højlund<sup>3</sup>; Martin Mogensen<sup>2</sup>; Ole Nørregaard Jensen<sup>1</sup>; <sup>1</sup>*Uni. of Southern Denmark, Dept. of BMB, Odense, Denmark*; <sup>2</sup>*Uni. of Southern Denmark, Inst. Sport Science, Odense, Denmark*; <sup>3</sup>*Odense Uni. Hospital, Diabetes Research Centre, Odense, Denmark*
- ThP 611 **A Comprehensive Look at the Proteome Profile of Zebrafish (*Danio rerio*) Gill;** Andrea G. De Souza; Tyson J. MacCormack; Greg G. Goss; Liang Li; *University of Alberta, Edmonton, Canada*
- ThP 612 **Application of Laser Capture Microdissection Analysis for CNS Circadian Studies: A Powerful Tool for Proteomic Research;** Ronald A. Miller; *Merck, West Point, PA*
- ThP 613 **Proteomic Characterization of the Gut Microbiomes of Gnotobiotic Mice after Colonization with Single or Dual Bacterial Strains;** Alison Russell<sup>1</sup>; Nathan C. Verberkmoes<sup>1</sup>; Manesh Shah<sup>1</sup>; Michael Mahowald<sup>2</sup>; Jeffrey Gordon<sup>2</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*Center for Genome Sciences, Washington University, St. Louis, MO*
- ThP 614 **MALDI-MS Analysis of Whole Collagens and Their Cyanogen Bromide-Peptides to Study the Network of Fibrillar-Forming Collagens I, III, and V;** Werner Henkel; Klaus Dreisewerd; Andreas Rohlfing; *University of Muenster, Muenster, Germany*
- ThP 615 **Characterization of Matrix Effects in Complex Human Cardiac Tissue using Multiple Reaction Monitoring;** Kelli Kline<sup>1</sup>; Henrick Horita<sup>1</sup>; Michael J. Maccoss<sup>2</sup>; Christine Wu<sup>1</sup>; <sup>1</sup>*University of Colorado, Aurora, CO*; <sup>2</sup>*University of Washington, Seattle, WA*
- ThP 616 **Complete 2D Gel Mapping of Human Brain Samples from Vanishing White Matter (VWM) Patients;** Bhushan Kulkarni; Adeline Vanderver; Yetrib Hathout; Kristy J. Brown; Asako Takanohashi; *Children's National Medical Center, Washington, DC*
- ThP 617 **Tandem Mass Spectrometry Analysis of Fibrils from Tissue Deposits in a Patient with Primary Amyloid Disease;** Zhenning Hong; Giuseppe Infusini; Roger Theberge; Amareth Lim; Tatiana Prokaeva; Lawreen H Connors; Martha Skinner; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- ThP 618 **Comprehensive Proteome Mapping of Escherichia Coli by LC-ESI MS-MS Combined with Sequential Protein Precipitation and Solubilization;** Xiaoxia Ye; Nan Wang; Joel Weiner; Liang Li; *Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*
- ThP 619 **The Peptidomics of Pancreas;** Karl Skold<sup>1</sup>; Mats G Borén<sup>1</sup>; Marcus Svensson<sup>1</sup>; Celiné Fernandes<sup>3</sup>; Mikhail Savitski<sup>2</sup>; Roman Zubarev<sup>2</sup>; Per E. Andren<sup>2</sup>; Peter James<sup>3</sup>; <sup>1</sup>*Denator AB, R&D, Uppsala, Sweden*; <sup>2</sup>*Uppsala University, Uppsala, Sweden*; <sup>3</sup>*Lund University, Lund, Sweden*
- ThP 620 **Time Dependent Proteomic Variations in Tissue Specimens by Matrix-Assisted Desorption Ionization Mass Spectrometry;** Pierre Chaurand; Joey C. Latham; Kirk B. Lane; Shannon Cornett; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- ThP 621 **Proteome Measurements towards Understanding Parkinson's Disease Utilizing Drosophila Models;** Zhiyin Xun; Thomas C. Kaufman; David E. Clemmer; *Indiana University, Bloomington, IN*
- ThP 622 **On Tissue Fractionation: Unmasking Difficult Proteins for MALDI Profiling;** David Bonnel; Julien Franck; Mohamed El Ayed; Maxence Wisztorski; Michel Salzet; Isabelle Fournier; *MALDI Imaging Team, University of Lille, Villeneuve d'Ascq, France*
- ThP 623 **Analysis of Corneal Proteins from the Epithelium and Endothelium of Mature Rabbit Cornea using Shotgun Proteomics;** Mitchell Meade; Pavel Shiyanov; John J Schlager; *AFRL, Wright Patterson AFB, OH*
- ThP 624 **Identification and Quantification of Post-Synaptic Density Proteins in Human Postmortem Tissue;** Matthew L Macdonald<sup>1</sup>; Anamika Banerjee<sup>1</sup>; Zi-Ping Nie<sup>1</sup>; Colin G. Barry<sup>2</sup>; Chang-Gyu Hahn<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Univ. of Penn/Center for Can, Philadelphia, PA*
- ThP 625 **Proteomics Analysis Identified Molecular Signatures for Diabetes Mellitus Associated Erectile Dysfunction;** Elizabeth H Yohannes<sup>1</sup>; Jinsook Chang<sup>1</sup>; Kelvin P Davies<sup>2</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>*Case Western Reserve University, Cleveland, OH*; <sup>2</sup>*Albert Einstein College of Medicine, Bronx, NY*
- ThP 626 **Quantitative Proteomics of Stem Cells by SILAC and Label-Free Methods;** Johannes Graumann<sup>1</sup>; Nina Hubner<sup>1</sup>; Jeong Beom Kim<sup>2</sup>; Kinarm Ko<sup>2</sup>; Chanchal Kumar<sup>1</sup>; Markus Moser<sup>1</sup>; Juergen Cox<sup>1</sup>; Hans Schoeler<sup>2</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>*Max Planck Institute For Biochemistry, Martinsried, Germany*; <sup>2</sup>*Max Planck Institute for Molecular Biomedicine, Muenster, Germany*
- ThP 627 **Statistically Quantitative Survey of Human Serum Proteome Associated with Type 2 Diabetes;** Rong-Xia Li<sup>1</sup>; Hai-Bing Chen<sup>2</sup>; Jie Dai<sup>1</sup>; Wei-Ping Jia<sup>2</sup>; Jia-Rui Wu<sup>1</sup>; RONG ZENG<sup>1</sup>; <sup>1</sup>*Shanghai Institutes for Biological Sciences, Shanghai, China*; <sup>2</sup>*Shanghai Diabetes Institute, Shanghai, China*
- ThP 628 **Protein Profiling of Intestinal Tumors in ApcMin/+ Mouse;** Wenhong Zhu; Changming Fang; Yoshinobu

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Igarashi; Jeffrey W. Smith; *The Burnham Institute, La Jolla, CA*

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- ThP 629 **An Automation Tool for Building NIST Library of Peptide Ion Fragmentation Spectra;** Qian Dong; Jeri Roth; Yuri Mirokhin; Paul Rudnick; Stephen Stein; *NIST, Gaithersburg, MD*
- ThP 630 **GelKeys-2D: Web-Based LIMS for 2D Gel Image Storage, Markup, and Sharing;** Kip L Bodi<sup>1</sup>; James West<sup>2</sup>; David H. Perlman<sup>2</sup>; Mark E. McComb<sup>2</sup>; Catherine E. Costello<sup>2</sup>; David C. Seldin<sup>1</sup>; <sup>1</sup>*Amyloid Treatment and Research Program, Boston, MA*; <sup>2</sup>*Cardiovascular Proteomics Center, BUSM, Boston, MA*
- ThP 631 **De Novo Sequencing of Cyclic Peptides;** Pavel Pevzner<sup>1</sup>; Nuno Bandeira<sup>2</sup>; Julio Ng<sup>1</sup>; Dario Meluzzi<sup>1</sup>; Roger Linington<sup>3</sup>; Pieter Dorrestein<sup>4</sup>; <sup>1</sup>*UCSD, La Jolla, CA*; <sup>2</sup>*University of California, La Jolla, CA*; <sup>3</sup>*UCSC, Santa Cruz, CA*; <sup>4</sup>*Scaggs School of Pharmacy, UCSD, La Jolla, CA*
- ThP 632 **Colander: A Probability-Based Support Vector Machine-Learning Algorithm for Automatic Screening of CID Phosphospectra Prior to Database Search;** Bingwen Lu; Cristian I. Ruse; John R. Yates; *The Scripps Research Inst, La Jolla, CA*
- ThP 633 **Identifying Phenotype Relevant Protein Structural Variations by Mass Spectrometry using Statistical Learning Approaches;** Zheng Li<sup>1</sup>; Catherine E. Costello<sup>2</sup>; Mark E. McComb<sup>2</sup>; <sup>1</sup>*Boston University, Biomedical Engineering, Boston, MA*; <sup>2</sup>*Boston University Med. School, CPC, Boston, MA*
- ThP 634 **Census: A Tool for Quantitative Analysis of Complex Peptide Mixtures via Stable Isotope Labeling or Differential LC-MS;** Sung Kyu Park<sup>1</sup>; John Venable<sup>2</sup>; Tao Xu<sup>1</sup>; John Yates<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*Genomics Institute For The Novartis Research Found, San Diego, CA*
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