

## ASMS CALENDAR

- October 20 - 24, 2006** **Asilomar Conference on Mass Spectrometry**  
Asilomar Conference Center, Pacific Grove,  
California  
*"Fundamentals of Gas Phase Ion Chemistry:  
Experiment and Theory"*  
Program Chairs: Frantisek Turecek and Thomas Morton
- November 9 - 10, 2006** **Fall Workshop**  
Catamaran Resort, San Diego, California  
*"The Present and Future of Quadrupole Ion Trap  
Mass Spectrometry"*  
Program Chairs: Victor Ryzhov and Richard Vachet
- January 19 - 22, 2007** **Sanibel Conference**  
Sundial Beach Resort, Sanibel Island, Florida  
**Imaging Mass Spectrometry**  
Program Chairs: Richard Caprioli, Ron Heeren,  
and Markus Stoeckli

## ANNUAL CONFERENCES

- June 3 - 7, 2007** **55<sup>th</sup> ASMS Conference on Mass Spectrometry**  
Indianapolis, IN
- June 1 - 5, 2008** **56<sup>th</sup> ASMS Conference on Mass Spectrometry**  
Denver, CO
- May 31 - June 4, 2009** **57<sup>th</sup> ASMS Conference on Mass Spectrometry**  
Philadelphia, PA
- May 23 - 27, 2010** **58<sup>th</sup> ASMS Conference on Mass Spectrometry**  
Salt Lake City, UT
- June 5 - 9, 2011** **59<sup>th</sup> ASMS Conference on Mass Spectrometry**  
Denver, CO



ASMS  
2019 Galisteo Street, Building I-1, Santa Fe, NM 87505  
Telephone: (505) 989-4517 | Fax: (505) 989-1073  
E-mail: [office@asms.org](mailto:office@asms.org)  
Web page: <http://www.asms.org>

54th ASMS Conference on Mass Spectrometry and Allied Topics May 28 - June 1, 2006



## 54th ASMS Conference on Mass Spectrometry and Allied Topics

May 28 - June 1, 2006  
Seattle, Washington



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*Title information in the following sections appears as provided by authors.*

*The complete abstract database is available through the ASMS web page: <http://www.asms.org>*

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## GENERAL INFORMATION

Welcome to the 54<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Washington State Convention & Trade Center. Corporate Member hospitality suites are in the convention center during the daytime hours. Evening suites are located in the Westin Hotel, 1900 5<sup>th</sup> Avenue, Seattle, WA.

- **PLENARY SESSIONS.** There will be coffee and pastries provided 7:30 – 8:00 am. Lectures begin at 8:00 am.
- **ORAL SESSIONS**
  - Session A (MOA, TOA, WOA, ThOA)
  - Session B (MOB, TOB, WOB, ThOB)
  - Session C (MOC, TOC, WOC, ThOC)
  - Session D (MOD, TOD, WOD, ThOD)
  - Session E (MOE, TOE, WOE, ThOE)
  - Session F (MOF, TOF, WOF, ThOF)
  - Session G (MOG, TOG, WOG, ThOG)
- **POSTERS AND EXHIBIT BOOTHS** are in the Exhibit Hall
- **REGISTRATION** is open as follows: 10:00 am – 8:00 pm on Sunday, 7:30 am – 5:00 pm on Monday through Thursday.
- **CORPORATE HOSPITALITY SUITES.** See page 10-14.
  - Daytime suites are on level 2 and 3 of the convention center.
  - Evening Suites are the Westin Hotel. Shuttle service will be provided to the Westin in the evenings.

**SUNDAY TUTORIAL LECTURES.** The tutorial session begins at 5:00 pm, Sunday.

- *The Fundamentals of Peptide Ion Fragmentation - What We Should Know and Why We Should Care*  
**Simon Gaskell**, University of Manchester
- *EIMS and CIMS from A to Z*  
**Burnaby Munson**, University of Delaware

**BROADCASTING OF SESSIONS.** Tutorial lectures, plenary sessions, and oral sessions will be web cast. Your last name and the User ID on the back of your name badge must be entered to view presentations. Presentations will be available until July 1, after which the files will be destroyed. Web casting of presentations does not constitute publication and in no way jeopardizes the rights of authors to publish material that has been presented. To access the presentations, go to [www.asms.org](http://www.asms.org). There are computers in the Exhibit Hall to view presentations. Complimentary headsets for use with your personal laptop are available in the registration area.

**INTERNET ACCESS.** Free wireless access is provided in the Exhibit Hall.

**ORAL PRESENTATIONS.** Only LCD computer projectors will be used for oral sessions. The ASMS session computers will be running Windows XP and the most recent version of PowerPoint. **Presenters must go to the speaker room at least one day prior to their talks** to load presentations on the ASMS computers. The speaker room is Room 601. The room is open with a technician present:

**Sunday:** 1:00 – 7:00 pm

**Monday through Wednesday:** 8:00 am – 1:00 pm

**POSTER PRESENTATIONS.** Posters must be in place by 8:00 am on the day scheduled and removed at 7:30 pm. Thursday posters must be removed at 2:30 pm. **Refer to the poster numbers in this final program for board assignments.** Authors are expected to supply pushpins to mount their posters. Poster titles begin on page 52.

### POSTER ATTENDANCE

- **ODD-NUMBERED POSTERS:** Authors must be present 8:45 - 10:15 am on the day scheduled.
- **EVEN-NUMBERED POSTERS:** Authors must be present 1:30 - 3:00 pm on the day scheduled. **The Thursday afternoon session is 1:00 – 2:30 pm.**

All poster authors are encouraged to be present during the lunch break on the day of their posters.

**INTEREST GROUP MEETINGS.** Interest Group meetings are scheduled during the lunch break, 12:15 – 1:30 pm. Anyone interested in the topics is encouraged to buy a lunch in the Exhibit Hall and take it to the meeting. Schedule is on page 18.

**WORKSHOPS.** Workshops are scheduled 5:30 – 7:00 pm on Monday and Tuesday. See page 18 for schedule.

**CONFERENCE PROCEEDINGS.** The conference proceedings will be published on DVD after the conference. Manuscripts or pdf of PowerPoint files must be submitted through the ASMS web site prior to the conference.

**WELCOME MIXER SUNDAY, 7:00 - 9:00 PM, Exhibit Hall.**

**CONFERENCE FINALE, 6:00 PM, THURSDAY.** The conference will conclude on Thursday evening, June 1, with a buffet at the Museum of Flight, the original location of the Boeing plant. The museum chronicles the history of flight with actual displays of aircraft from every era of aviation. Buses will begin departing at 5:45 pm from the convention center bus entrance. Cost: \$20 for each conference registrant and registered guest. Ticket sales close at 12 noon on Monday.

**GUEST REGISTRATION.** Guest registration includes:

- Continental breakfast on 9:00 – 10:00 am on Monday in Room 620
  - Monday afternoon motor coach tour to Chateau St. Michelle Winery and boat cruise of Lake Union. Tour buses will depart promptly at 12:15 pm on Monday.
- Cost for guest registration: \$40.

**LUNCHES.** Lunches may be purchased in the Exhibit Hall.

## GENERAL INFORMATION

**EMPLOYMENT CENTER.** The Employment Center is located in the Exhibit Hall. Candidates and employers may register with the center beginning at 5:00 pm on Sunday. You must supply at least 20 copies of your resumé. The center is open Monday through Wednesday, 8:30 am to 5:00 pm, and Thursday, 8:30 am to 1:00 pm. Employers and candidates may come to the room to search the database of candidates and positions. There are a limited number of spaces available for conducting interviews. Interview spaces must be reserved one day in advance. **Participants in the Employment Center must be registered for the conference.**

### CONFERENCE HOTELS

| HOTEL        | LOCATION                    | PHONE        |
|--------------|-----------------------------|--------------|
| Crowne Plaza | 1113 6 <sup>th</sup> Avenue | 206.464.1980 |
| Hilton       | 1301 6 <sup>th</sup> Avenue | 206.624.0500 |
| Grand Hyatt  | 721 Pine Street             | 206.774.1234 |
| Mayflower    | 405 Olive Way               | 206.623.8700 |
| Red Lion     | 1415 5 <sup>th</sup> Avenue | 206.971.8000 |
| Renaissance  | 515 Madison Street          | 206.583.0300 |
| Sheraton     | 1400 6 <sup>th</sup> Avenue | 206.621.9000 |
| Westin       | 1900 5 <sup>th</sup> Avenue | 206.728.1000 |

**SHUTTLE BUS SERVICE** is provided during the following hours:

- Sunday: 3:00 pm to 10:00 pm between hotels and convention center
- Monday – Thursday: 7:00 am to 8:00 pm between hotels and convention center
- Monday – Wednesday, 8:00 – 11:00 pm between Westin hotel hospitality suites and other hotels

### CONFERENCE REGULATIONS

- **Name badges** are required for all conference sessions, including the exhibit hall and the employment center.
- **No smoking** is permitted in the convention center.
- **Cell phones** must be **turned off** in oral sessions.
- **No photography or recording** in any session, including posters.
- **The placement of advertising** in the meeting area is strictly limited to Corporate Members. There are poster boards and tables in the Exhibit Hall for corporate member notices and literature. No signs on easels are permitted except at doors to hospitality suite rooms.
- **No hardware, terminals, accessories, or any items** for sale may be displayed in any area of the conference, except in corporate exhibit booths and hospitality suites.
- There may be **no organized activities** (even off-site) other than those approved by ASMS during the conference week (5:00 pm on Sunday through 9:00 pm on Thursday).
- **Corporate or institutional logos** may appear only in the title of posters in technical sessions. Logos appearing anywhere else in a poster will be removed or covered by ASMS.

### ASMS

ASMS  
2019 Galisteo Street, Building I-1  
Santa Fe, NM 87505  
Phone: (505) 989-4517 Fax: (505) 989-1073  
E-mail: [office@asms.org](mailto:office@asms.org)

### MEDIA EVENTS

Corporate media events are scheduled in Room 615. Members of the press and financial institutions are welcome.

#### Monday

|                  |                    |          |
|------------------|--------------------|----------|
| Thermo Electron  | 11:00 – 12:00 noon | Room 615 |
| Shimadzu Biotech | 8:30-9:30 am       | Room 615 |
| Waters           | 4:30 - 5:30 pm     | Room 615 |

#### Tuesday

|                      |                    |          |
|----------------------|--------------------|----------|
| Agilent Technologies | 11:00 – 12:00 noon | Room 615 |
| Bruker Daltonics     | 2:15 – 3:15 pm     | Room 615 |

## ASMS BOARD OF DIRECTORS

*President* **Alan G. Marshall**  
NHMFL, Florida State University  
Tallahassee, FL

*Vice President  
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The Dupont Company  
Wilmington, DE

*Vice President  
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San Diego, CA

*Secretary* **Frantisek Turecek**  
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Seattle, WA

*Treasurer* **Richard J. Van Berkel**  
Oak Ridge National Laboratory  
Oak Ridge, TN

*Member at Large  
Publications* **Carlito B. Lebrilla**  
University of California  
Davis, CA

*Member at Large  
Education* **O. David Sparkman**  
University of the Pacific  
Stockton, CA

*Member at Large  
Measurements  
& Standards* **Philip C. Price**  
The Dow Chemical Company  
South Charleston, WV

*Past President* **Catherine E. Costello**  
Boston University School of Medicine  
Boston, MA

*Executive  
Director* **Judith A. Sjoberg**  
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Santa Fe, NM 87505  
505-989-4517  
E-mail: [judith@asms.org](mailto:judith@asms.org)

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**Miquela Ortiz**, [miquela@asms.org](mailto:miquela@asms.org)  
**Brent Watson**, [brent@asms.org](mailto:brent@asms.org)  
**Carol Ann Short**, [carolann@asms.org](mailto:carolann@asms.org)

## ASMS

announces the election of these members to the  
Board of Directors

Vice President for Programs



**Gary Glish**  
University of North Carolina

Treasurer



**Julia Laskin**  
Pacific Northwest Natl Laboratory

Member at Large for Education



**Orval A. Mamer**  
McGill University

Member at Large for Measurements & Standards



**David N. Heller**  
US FDA

## INTEREST GROUP COORDINATORS

|                                                  |                                                                                                                   |
|--------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <i>Analytical Lab Managers</i>                   | Amy Harms<br>University of Wisconsin                                                                              |
| <i>Biological Macromolecules</i>                 | Viswanatham Katta<br>Genentech, Inc.                                                                              |
| <i>Clinical Chemistry</i>                        | Donald H. Chace<br>Pediatrix Analytical                                                                           |
| <i>Computer Applications</i>                     | Jeffrey L. Whitney, Novatia LLC.                                                                                  |
| <i>Drug Metabolism &amp; Pharmacokinetics</i>    | Walter Korfmacher,<br>Schering Plough<br>Ajai Chaudhary, Eli Lilly<br>Jonathan L. Josephs<br>Bristol-Myers Squibb |
| <i>Environmental Applications</i>                | Alaee Mehran                                                                                                      |
| <i>Flavor, Fragrance and Foodstuff</i>           | Dennis Swijter<br>IFF                                                                                             |
| <i>Forensics</i>                                 | Brian Eckenrode, FBI Academy<br>John Reynolds, LLNL                                                               |
| <i>FTMS</i>                                      | Michael A. Freitas<br>Ohio State University                                                                       |
| <i>Fundamentals</i>                              | Kelly Sullivan, Pacific Northwest Laboratory                                                                      |
| <i>History</i>                                   | O. David Sparkman<br>University of the Pacific                                                                    |
| <i>Hydrocarbon and Chemical Process</i>          | Ryan P. Rodgers<br>Florida State University                                                                       |
| <i>Hydrogen Exchange &amp; Covalent Labeling</i> | John Engen<br>University of New Mexico                                                                            |
| <i>Ion Mobility MS</i>                           | Richard Yost<br>University of Florida                                                                             |
| <i>Ion Trap MS</i>                               | Richard Vachet<br>University of Massachusetts                                                                     |
| <i>LC/MS Related Topics</i>                      | Gérard Hopfgartner<br>University of Geneva                                                                        |
| <i>Metabolomics</i>                              | Grace Tong<br>Scripps Research Institute                                                                          |
| <i>Metal Ion Coordination Chemistry</i>          | Mary T. Rodgers<br>Wayne State University                                                                         |
| <i>Pharmaceuticals</i>                           | David Peake<br>Eli Lilly Company                                                                                  |
| <i>Polymeric Materials</i>                       | Patricia Peacock, The Dupont Co.                                                                                  |
| <i>TOF-MS</i>                                    | Matt Lasater<br>Thermo Electron Corp.                                                                             |
| <i>Young Mass Spectrometrists</i>                | Kristina Håkansson<br>University of Michigan                                                                      |

## COMMITTEES

|                                     |                                                                                                                                                       |
|-------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>Awards</i>                       | Richard Caprioli<br>Veronica Bierbaum<br>Fred McLafferty<br>Robert Murphy<br>Catherine Fenselau                                                       |
| <i>Asilomar Conference</i>          | Brad Gibson, Chair<br>Hillka Kentämaa<br>Stephen Hofstadler<br>Catherine Costello                                                                     |
| <i>Corporate Liaison</i>            | Catherine Costello, Chair<br>Daniel Kassel<br>Michael Sabatino<br>Lauri Caviston<br>Ted Thomson<br>Arthur E. Simms<br>Lance Nicolaysen<br>Wendy Weise |
| <i>Education</i>                    | David Sparkman, Chair<br>Victor Ryzhov<br>Chrys Wesdemiotis<br>J. Throck Watson<br>Cecilia Basic                                                      |
| <i>Archivist</i>                    | Michael Grayson                                                                                                                                       |
| <i>Measurements &amp; Standards</i> | Phil Price, Chair<br>William E. Wallace<br>David Heller<br>Dwight Matthews<br>Jody Shoemaker                                                          |
| <i>Nominating</i>                   | David Burinsky<br>Richard Caprioli<br>Veronica Bierbaum                                                                                               |
| <i>Publications</i>                 | Kermit Murray, Chair<br>Carol Nilsson<br>Susan Weintraub<br>Neil Kelleher<br>Michael Gross (Ex Officio)                                               |
| <i>Sanibel</i>                      | Vicki Wysocki, Chair<br>Charles McEwen<br>Peter O'Connor<br>Philip Price                                                                              |

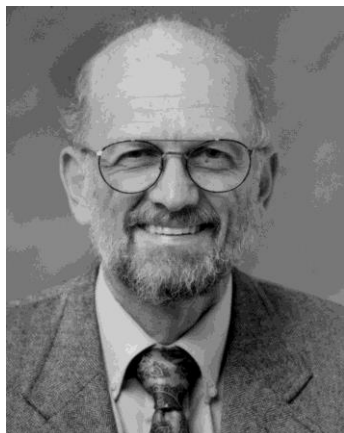


## AWARDS

### AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

**Award Lecture: 8:00 am, Tuesday**

**2006 Recipient: R. Graham Cooks**



This Award recognizes achievement in or contribution to fundamental or applied mass spectrometry. The 2006 Award is presented to **Professor R. Graham Cooks** of the Purdue University for his development of the “kinetic method” as a tool for ion/molecule studies. In 1977, he and Terry Kruger sent a Communications to the Editor of JACS titled “Intrinsic Basicity Determination Using Metastable Ions.” This introductory work described the measurement of proton affinities based on the competition for a proton by two gas-phase bases. The idea of setting up a competition for charge to determine relative affinity for the charged species could be accomplished using a variety of instruments and ionization modes. Many new spectrometer designs were driven by the value of the kinetic method-related measurements they could provide. A unique contribution of the method was its applicability to organic, organometallic, and inorganic systems inaccessible by other techniques. During the 1980s and 1990s, the kinetic method was applied to gas-phase acidity and basicity; electron, metal ion, and halogen cation affinities; proton affinities of free radicals; and cluster ion structures. In the last five years, the method has seen new biological applications such as the quantitation of chiral drugs. It is notable that Professor Cooks prefaced a recent review

article with the Lorenz quote: “...the epidemic delusion that only numerical and measurable reality has validity must be confronted and contradicted.” The increasingly broad applications of this tool to problems ranging from physical chemistry to drug design is a testament to the value of Professor Cooks’ contribution, and his perspective on the balance of measurement and results.

### THE BIEMANN MEDAL

**Award Lecture: 8:00 am, Wednesday**

**2006 Recipient: David E. Clemmer**



The Biemann Medal recognizes a significant achievement in basic or applied mass spectrometry made by an individual early in his or her career. The award is presented in honor of Professor Klaus Biemann and is endowed by contributions from his students, postdoctoral associates, and friends. The 2006 Medal is presented to **David E. Clemmer** of Indiana University for his achievements and contributions integrating ion mobility separations with a variety of MS technologies. His initial high-impact IMS/MS paper published seven years ago has been cited 78 times. In 2002, he was featured in a Popular Science article, illustrating the breadth of his influence and enthusiasm. His group has built new instruments, and then applied these new tools to the important problems of protein folding, analysis of complex biological mixtures, proteome mapping, and polypeptide sequencing. A single LC-IMS-CID-MS experiment on human plasma has generated 600,000 fragment peaks, 20,000 precursor peaks, and identified 280 proteins. A similar investigation of fruit fly tissue has yielded over one thousand proteins. By consistently applying a multi-disciplinary approach (engineering,

chemistry, software, biology) to problem solving, he is often generating unexpected results. Professor Clemmer feels that “We are moving toward an era when surgery will be the last treatment of choice for patients with cancer. We’ll treat cancer and many other diseases at the molecular level.”

### CALL FOR NOMINATIONS FOR 2007

**Award for a Distinguished Contribution in Mass Spectrometry.** The person nominated should have made a contribution that has had a significant impact on the fundamental understanding and/or practice of mass spectrometry. Eligibility is not restricted to members of ASMS. The award is announced at the ASMS Annual Conference with the presentation of a \$10,000 cash award and a recognition plaque..

Name of person nominated \_\_\_\_\_

Affiliation \_\_\_\_\_

Address \_\_\_\_\_

Nominee’s email: \_\_\_\_\_

Your Name & email: \_\_\_\_\_

Supporting letters (one page) will be provided by: \_\_\_\_\_

**The Biemann Medal** recognizes a significant achievement in basic or applied mass spectrometry made by an individual early in his or her career. The award is conferred at the ASMS Annual Conference with the presentation of the Biemann Medal and a cash award.

The above individual is nominated for:

- ☐ Distinguished Contribution in Mass Spectrometry  
☐ Biemann Medal

Please enclose the following:

1. **Short description of the achievement** (1-2 paragraphs);
2. **A list of the nominee’s publications** pertaining to this award and;
3. **A copy of no more than two of the nominee’s publications** relevant to the subject.

Send completed nomination form and enclosures for receipt by November 30 to:

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

## 2006 RESEARCH AWARDS

*Sponsored by*  
**Thermo Electron Corporation**



**Weiguo Andy Tao**  
*Purdue University*

*Sponsored by*  
**Applied Biosystems/MDS Sciex**



**Heather Desaire**  
*University of Kansas*

*Sponsored by*  
**Waters Corporation**



**Ryan Julian**  
*University of California, Riverside*

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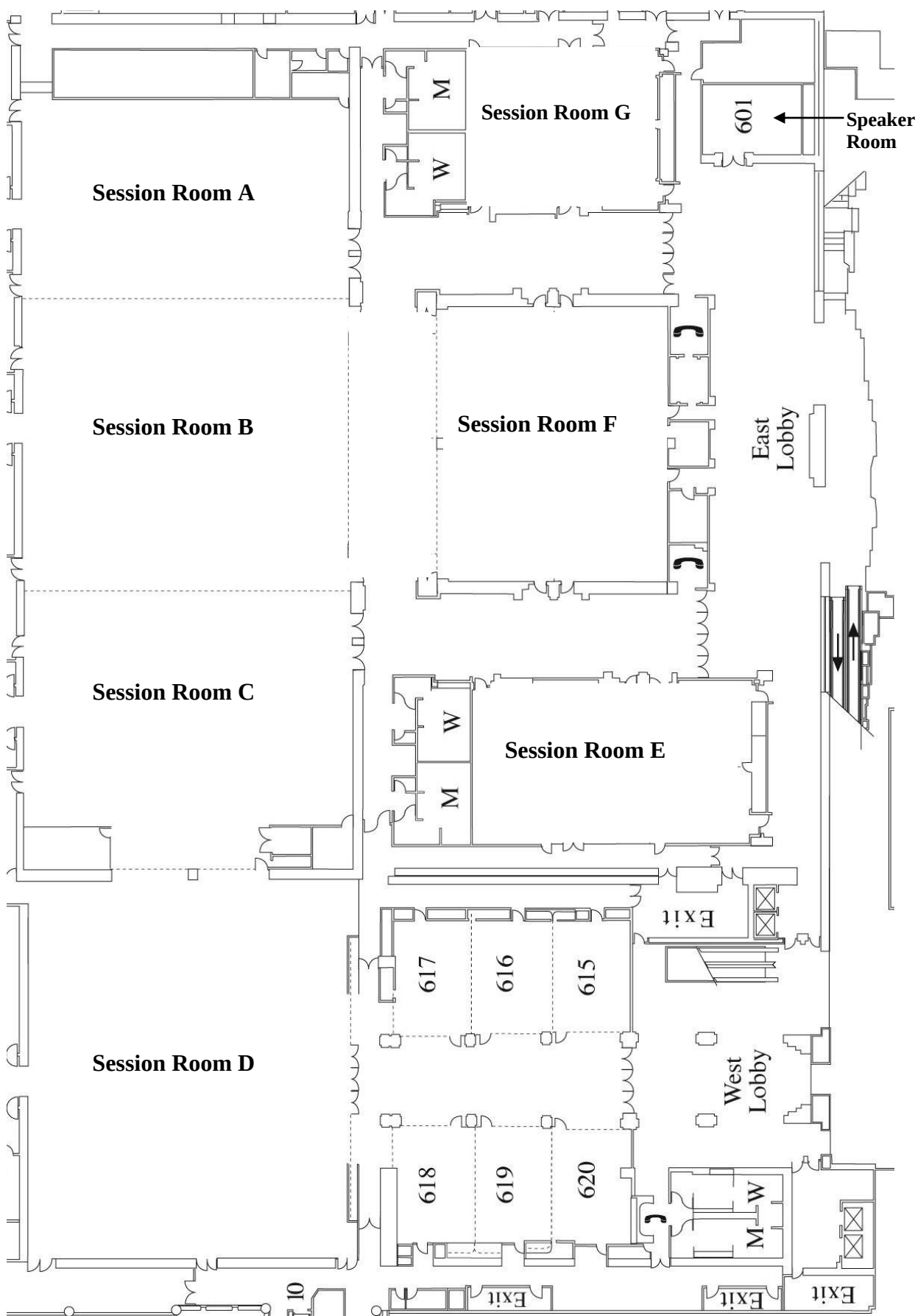
### CALL FOR 2007 RESEARCH AWARD PROPOSALS

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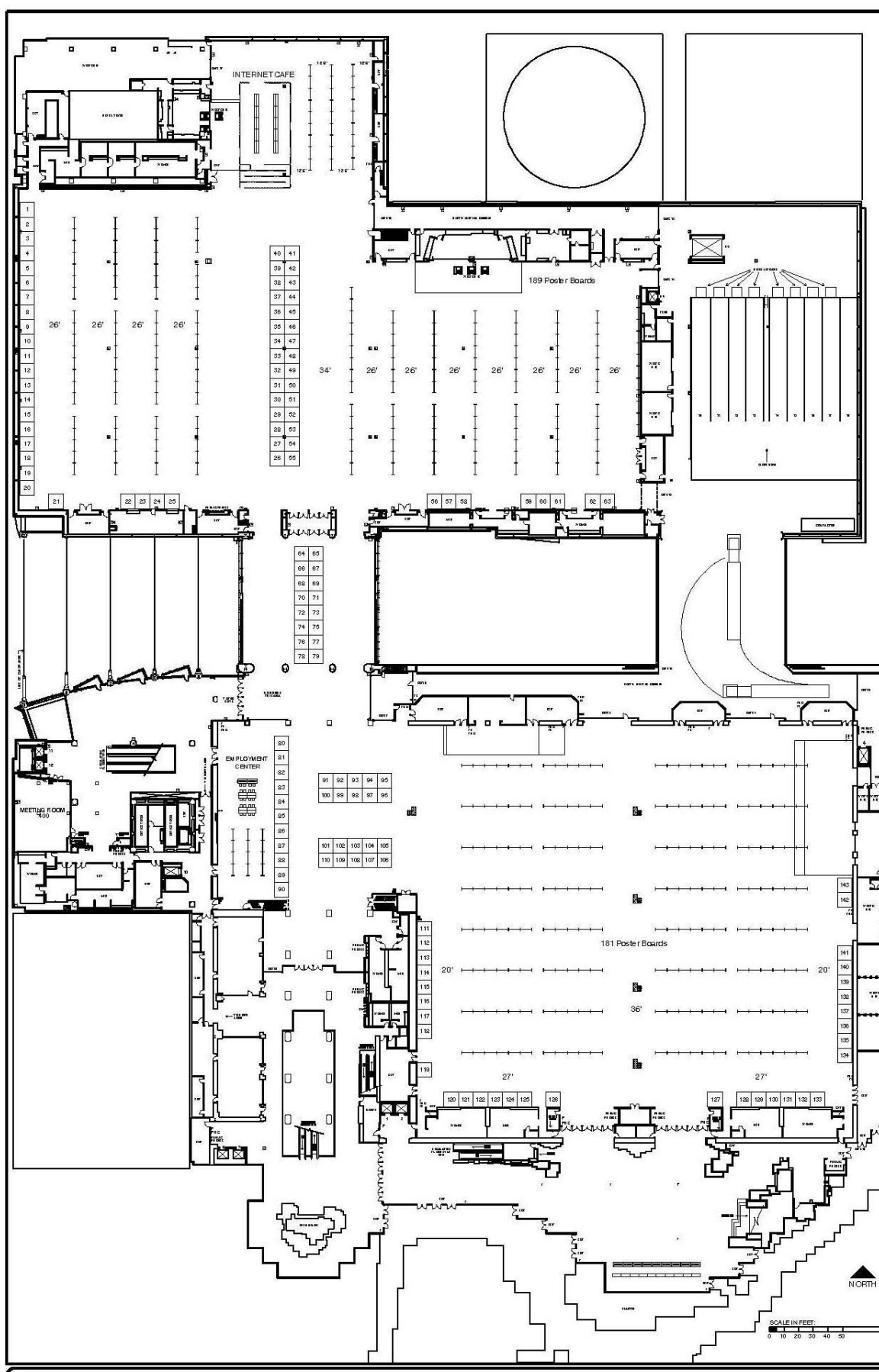
- OBJECTIVE** To promote academic research by young scientists in mass spectrometry.
- ELIGIBILITY** Open to academic scientists within four years of joining the tenure track faculty or equivalent in a North American university. Applicants may not have previously received an award under this program.
- APPLICATION** Applicants should submit **SEVEN** collated sets of the following
1. One-page fiscal proposal and justification
  2. List of current research support
  3. Three-page proposal, including references, figures, etc.
  4. *Curriculum vitae*
  5. Two letters of recommendation (may be sent directly to ASMS)
- DEADLINE** Application materials, including letters of recommendation, must be received in the ASMS office by November 30. Send to:  
ASMS, 2019 Galisteo Street, Building I-1, Santa Fe, NM 87505
- FISCAL** The awards of \$25,000 each will be made to a university in the name of the selected individual and for the researcher's exclusive use. In accepting this award, the institution will agree not to charge overhead on the funds.
- INFORMATION** Contact ASMS. Telephone: (505) 989-4517 • Fax: (505) 989-1073 • [office@asms.org](mailto:office@asms.org)



CONVENTION CENTER FLOOR PLAN, 6<sup>TH</sup> LEVEL



# FLOOR PLAN - POSTERS AND EXHIBITS

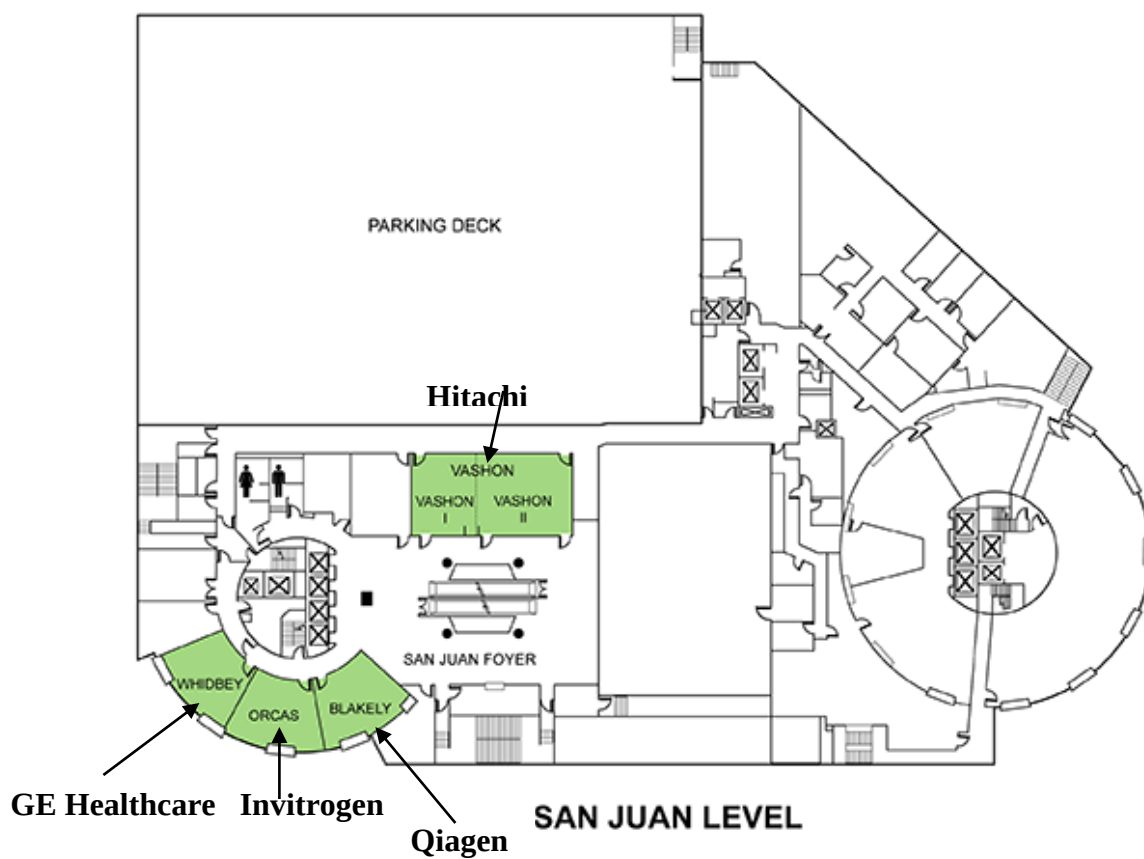
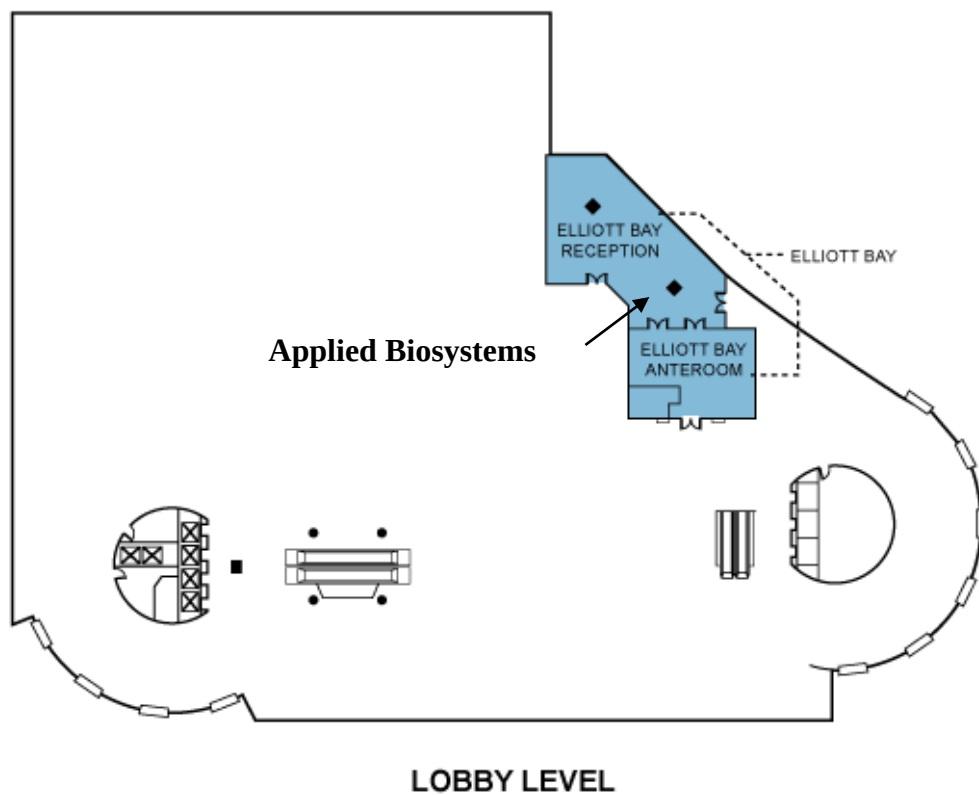


| ASMS CORPORATE MEMBERS                  |                      |                    |               |
|-----------------------------------------|----------------------|--------------------|---------------|
| Company                                 | Booth/Poster/Library | Conv. Ctr. Suite   | Westin Suite  |
| Accium BioSciences .....                | 130/Poster           |                    |               |
| Adaptive Bioinformatics, LLC .....      | Poster               |                    |               |
| Advanced Chemistry Development .....    | 74/Poster.....       |                    | Olympic       |
| Advion BioSciences.....                 | 26.....              | Room 212           |               |
| Agilent Technologies .....              | 65/Poster.....       | Room 206 .....     | Fifth Avenue  |
| AIM Research Co. ....                   | 107/Poster           |                    |               |
| Alcatel Vacuum Products, Inc. ....      | 85                   |                    |               |
| Alcott Chromatography, Inc. ....        | 68/Poster            |                    |               |
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| Dupont Analytical Solutions.....        | 17                   |                    |               |
| Eksigent Technologies .....             | 110/Poster.....      |                    | Adams & Baker |
| Elsevier .....                          | 24                   |                    |               |
| EMD Biosciences .....                   | 12/Poster            |                    |               |
| Entech Instruments .....                | 135/Poster           |                    |               |
| ESA, Inc.....                           | 128                  |                    |               |
| ETP Electron Multipliers .....          | Poster               |                    |               |
| Extrel CMS .....                        | Poster               |                    |               |
| FLUOROTECHNICS Pty Ltd.....             | 60                   |                    |               |

| ASMS CORPORATE MEMBERS                |                      |                  |               |
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| Flux Instruments AG .....             | 51                   |                  |               |
| GB Scientific.....                    | 53/Poster            |                  |               |
| GE Healthcare.....                    | 9                    |                  | Whidbey       |
| Genebio SA.....                       | 79/Poster            |                  |               |
| Genedata AG.....                      | 137                  |                  |               |
| Gen Next Technologies, Inc. ....      | Poster               |                  |               |
| Genomics Life Sci. Software .....     | 95/Poster            | Room 205         |               |
| Genome Alberta                        |                      |                  |               |
| Genome Web, LLC.....                  | Library              |                  |               |
| Genomic Solutions Inc.....            | 67/Poster            | Room 309         |               |
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| Gerstel, Inc.....                     | 61                   |                  |               |
| GL Sciences.....                      | 45                   |                  |               |
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| Griffin Analytical Technologies ..... | 56                   |                  |               |
| Hamamatsu Corporation .....           | 142/Poster           |                  |               |
| Harvard Apparatus.....                | 102/Poster           |                  |               |
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| Indigo Biosystems, Inc.....           | 138                  |                  |               |
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| Intl Equipment Trading Ltd. ....      | 69/Poster            |                  |               |
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| IonSpec Corporation .....             | 78                   |                  |               |
| Isotec.....                           | Poster               |                  |               |
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| Konik Instruments, Inc.....           | 136                  |                  |               |
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| LabKey Software, LLC.....             | Poster               |                  |               |
| LEAP Technologies.....                | 72/Poster            |                  | Cascade I-C   |
| LECO Corporation.....                 | 83/Poster            |                  |               |
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| Novatia, LLC .....                    | 106/Poster           |                  |               |
| Omni Enclosures.....                  | 116                  |                  |               |
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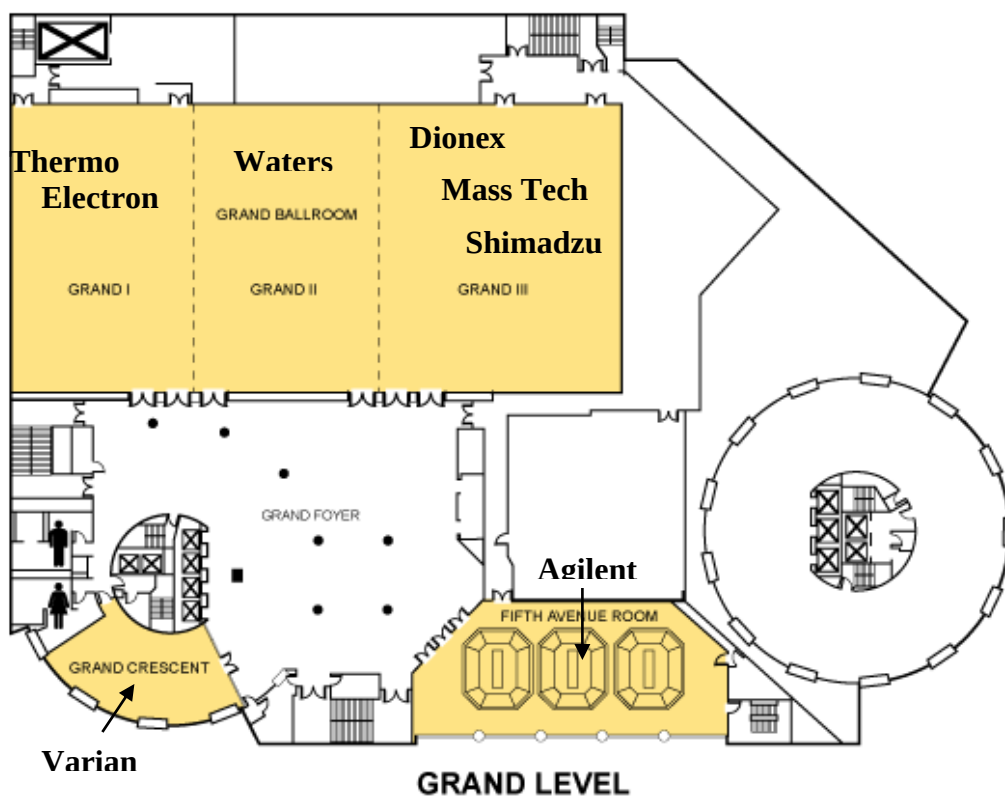
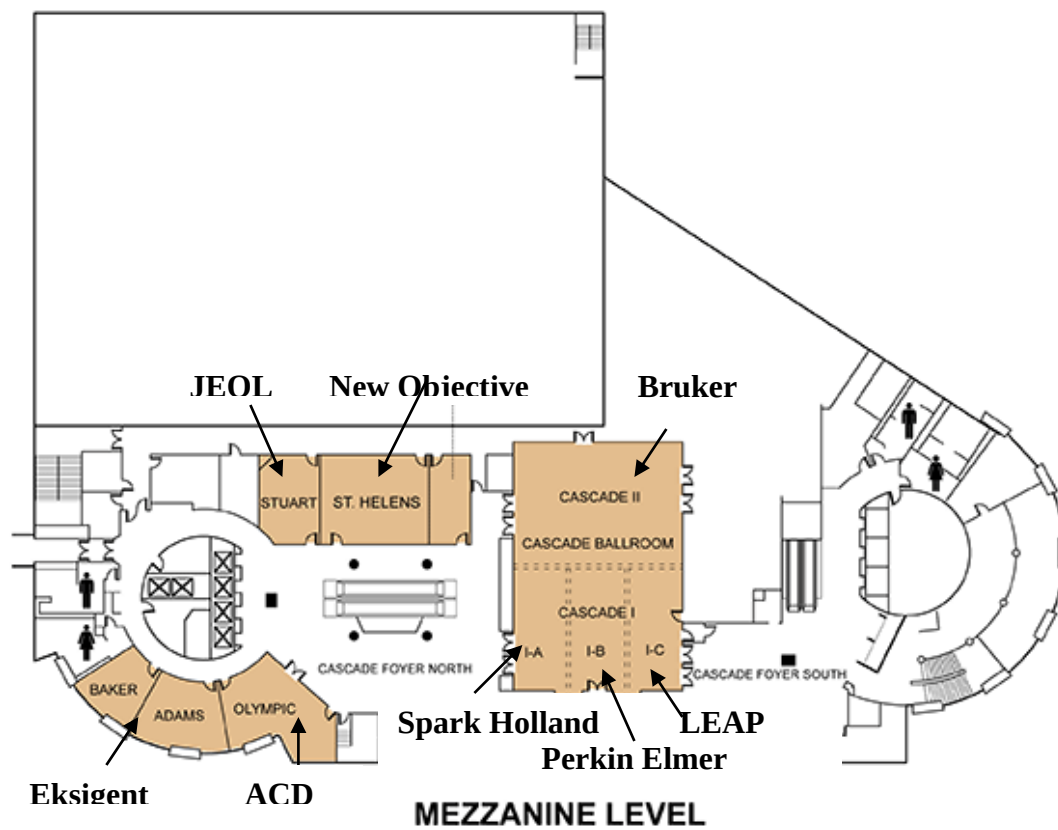
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| Rosetta Biosoftware .....                    | 64                   | Room 203         |                |
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## WESTIN HOTEL HOSPITALITY SUITES





# WESTIN HOTEL HOSPITALITY SUITES



## PROGRAM ACKNOWLEDGEMENTS

**Barbara S. Larsen**, *Vice President for Programs*

### STUDENT ASSISTANTS

Graduate students are assisting with all aspects of the conference, including registration, oral and poster sessions, and the employment center. The students each receive a stipend to assist with their conference expenses. Elsevier Science has generously underwritten the stipends.

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Kelly Sullivan  
Dennis F. Swijter  
Richard Vachet  
Jeffrey Whitney

## CONFERENCE PROGRAM OVERVIEW

|                |                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|----------------|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>SUNDAY</b>  | 9:00 am - 4:30 pm   | <b>SHORT COURSES</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|                | 10:00 am – 8:00 pm  | <b>Registration</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|                | 5:00 - 6:30 pm      | <b>TUTORIAL LECTURES</b> <ul style="list-style-type: none"> <li><i>The Fundamentals of Peptide Ion Fragmentation - What We Should Know and Why We Should Care;</i> <b>Simon Gaskell</b>, University of Manchester</li> <li><i>EIMS and CIMS from A to Z</i> <b>Burnaby Munson</b>, University of Delaware</li> </ul>                                                                                                                                                                               |
|                | 7:00 - 9:00 pm      | <b>RECEPTION IN THE EXHIBIT HALL</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>MONDAY</b>  | 7:30 am             | <b>WAKE-UP COFFEE</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|                | 8:00 – 8:45 am      | <b>PLENARY LECTURE:</b> <b>Lisa Randall</b> , Harvard University<br><i>Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions</i>                                                                                                                                                                                                                                                                                                                                           |
|                | 8:45 - 10:15 am     | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|                |                     | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>MOA: Endogenous Metabolite Profiling</li> <li>MOB: Peptides and Proteins as Biomarkers</li> <li>MOC: Membrane Proteins and Hydrophobic Peptides</li> <li>MOD: Distributing the Future: Enabling High Throughput Analysis</li> <li>MOE: Forensic Science and Detection</li> <li>MOF: Ion Mobility</li> <li>MOG: Quantitation of Polymers</li> </ul>                                                                                     |
|                | 10:15 am – 12:15 pm |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|                | 12:15 - 1:30 pm     | <b>LUNCH BREAK AND INTEREST GROUP MEETINGS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|                | 1:30 - 3:00 pm      | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|                |                     | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>MOA: Biomarker Evaluation</li> <li>MOB: Posttranslational Modifications Beyond Phosphorylation</li> <li>MOC: Time-of-Flight Instrumentation</li> <li>MOD: Protein Ligand Complexes</li> <li>MOE: Forensics and Clinical Investigations of Microorganisms</li> <li>MOF: FTMS: Instrumentation</li> <li>MOG: Analysis of Polymer Mixtures</li> </ul>                                                                                     |
|                | 3:00 - 5:00 pm      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|                | 5:30 - 7:00 pm      | <b>WORKSHOPS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| <b>TUESDAY</b> | 7:30 am             | <b>WAKE-UP COFFEE</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|                | 8:00 – 8:45 am      | <b>AWARD LECTURE: Recipient of the Award for a Distinguished Contribution in Mass Spectrometry</b>                                                                                                                                                                                                                                                                                                                                                                                                 |
|                | 8:45 - 10:15 am     | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|                |                     | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>TOA: Metabolite Identification Using Hyphenated MS Techniques</li> <li>TOB: New Ion Trapping Technologies</li> <li>TOC: Challenge of Dynamic Range in Proteomics: Novel Approaches in Separation, High Mass Accuracy and Quantification</li> <li>TOD: Glycomics</li> <li>TOE: Detection and Decontamination of Indoor Environments</li> <li>TOF: Intact Protein Separation and MS</li> <li>TOG: Organic Reaction Mechanisms</li> </ul> |
|                | 10:15 am – 12:15 pm |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|                | 12:15 - 1:30 pm     | <b>LUNCH BREAK AND INTEREST GROUP MEETINGS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|                | 1:30 - 3:00 pm      | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|                |                     | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>TOA: Metabolite Profiling</li> <li>TOB: MS Contribution to the Immunology of Disease</li> <li>TOC: Clinical Mass Spectrometry Assays</li> <li>TOD: Carbohydrates</li> <li>TOE: New and Emerging Contaminants</li> <li>TOF: Hydrocarbons to Petroleum</li> <li>TOG: Elemental and Isotopic MS in Biology</li> </ul>                                                                                                                     |
|                | 3:00 - 5:00 pm      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|                | 5:30 - 7:00 pm      | <b>WORKSHOPS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

# CONFERENCE PROGRAM OVERVIEW, CONTINUED

|           |                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|-----------|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| WEDNESDAY | 7:30 am             | <b>WAKE-UP COFFEE</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|           | 8:00 - 8:45 am      | <b>AWARD LECTURE: Recipient of the Biemann Medal</b>                                                                                                                                                                                                                                                                                                                                                                                                                     |
|           | 8:45 - 10:15 am     | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|           | 10:15 am - 12:15 pm | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• WOA: Direct Ionization Techniques</li> <li>• WOB: Instrumentation and Methods for Quadrupole and Linear Ion Traps</li> <li>• WOC: Detection of Cellular Pathways by a Proteomics Approach</li> <li>• WOD: Bioinformatics</li> <li>• WOE: Fluorinated Organics in the Environment</li> <li>• WOF: From Nucleic Acids to DNA / RNA Complexes</li> <li>• WOG: Ion Solvation</li> </ul>                        |
|           | 12:15 - 1:30 pm     | <b>LUNCH BREAK AND INTEREST GROUP MEETING</b>                                                                                                                                                                                                                                                                                                                                                                                                                            |
|           | 1:30 - 3:00 pm      | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|           | 3:00 - 5:00 pm      | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• WOA: Quantitative Protein Profiling</li> <li>• WOB: Phosphorylation of Proteins</li> <li>• WOC: Methods to Increase Throughput for PK Analysis</li> <li>• WOD: Impurity / Degradation in Drug Products and Packaging</li> <li>• WOE: Instrumentation and Methodology for Imaging MS</li> <li>• WOF: On-Line Analysis of Organic Aerosols</li> <li>• WOG: Fundamentals of Ion Molecule Reactions</li> </ul> |
|           | 5:15 - 6:00 pm      | <b>ASMS BUSINESS MEETING</b>                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|           | 6:30 - midnight     | <b>CORPORATE HOSPITALITY SUITES</b>                                                                                                                                                                                                                                                                                                                                                                                                                                      |

|          |                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|----------|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| THURSDAY |                     | <b>Late start this morning! Go straight to the exhibit hall.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|          | 8:45 - 10:15 am     | <b>POSTER SESSION AND EXHIBITS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|          | 10:15 am - 12:15 pm | <b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA: Biomarkers for Drug Safety and Efficacy</li> <li>• ThOB: Protein Networks and Their Regulation</li> <li>• ThOC: MS Imaging of Small Molecules</li> <li>• ThOD: Lipidomics</li> <li>• ThOE: Nanospray LC/MS of Small Molecules</li> <li>• ThOF: Spectroscopy of Ions</li> <li>• ThOG: Atmospheric Chemistry</li> </ul>                                                                                                                    |
|          | 12:15 - 1:00 pm     | <b>LUNCH BREAK</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|          | 1:00 - 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>• ThOA: Reactive Metabolites and Toxicological Links</li> <li>• ThOB: Novel MS Instrumentation</li> <li>• ThOC: Methods for Probing Protein Conformation</li> <li>• ThOD: Atmospheric Pressure Ionization Techniques</li> <li>• ThOE: Mechanisms of Peptide Fragmentation</li> <li>• ThOF: Flavors and Fragrances</li> <li>• ThOG: Mass Spectrometry (and Theoretical) Methods for Probing the Conformations of Ions in the Gas Phase</li> </ul> |
|          | 4:45 - 5:30 pm      | <b>PLENARY LECTURE: Diane L. Evans, NASA; Exploring Earth</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|          | 6:00 pm             | <b>CLOSING EVENT: Museum of Flight</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |

### INTEREST GROUP MEETINGS, 12:15 – 1:30 pm

Interest Group meetings are open to all interested persons.

Participants may purchase a box lunch in the exhibit hall and take it to the meeting room.

| <b>MONDAY</b><br><b>12:30 - 1:30 pm</b>                                                                                                                                     | <b>TUESDAY</b><br><b>12:30 - 1:30 pm</b>                                                                            | <b>WEDNESDAY</b><br><b>12:30 - 1:30 pm</b>                                              |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
| <b>Young Mass Spectrometrists Interest Group Meeting: The Early Days of Biological MS: What Happened Before ESI and MALDI?</b><br>Kristina Hakansson, presiding<br>Room 617 | <b>Flavors, Fragrances and Foodstuffs Interest Group Meeting</b><br>Dennis F. Swijter, presiding<br>Room 617        | <b>Clinical Chemistry Interest Group Meeting</b><br>Donald Chace, presiding<br>Room 620 |
| <b>Ion Traps Interest Group Meeting</b><br>Richard Vachet, presiding<br>Room 618                                                                                            | <b>Forensics Interest Group Meeting</b><br>John Reynolds, presiding<br>Room 618                                     |                                                                                         |
| <b>Fundamentals Interest Group Meeting</b><br>Kelly Sullivan and JC Poutsma, presiding<br>Room 619                                                                          | <b>Polymeric Materials Interest Group Meeting</b> Patricia Peacock, presiding<br>Room 619                           |                                                                                         |
| <b>Hydrocarbon Interest Group Meeting</b><br>Ryan Rodgers, presiding<br>Room 620                                                                                            | <b>Analytical Lab Managers Interest Group Meeting</b><br>Amy Harms, presiding<br>Room 620                           |                                                                                         |
|                                                                                                                                                                             | <b>Metal Ion Interest Group Meeting</b><br>Mary T. Rodgers, presiding<br>Session Room E                             |                                                                                         |
|                                                                                                                                                                             | <b>Hydrogen Exchange and Covalent Labeling Interest Group Meeting</b><br>John R. Engen, presiding<br>Session Room G |                                                                                         |

### WORKSHOPS, 5:30 – 7:00 pm

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.

| <b>MONDAY</b><br><b>5:30 – 7:00 pm</b>                                                                                                                                                                    | <b>TUESDAY</b><br><b>5:30 – 7:00 pm</b>                                                                                                                                                        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Hyphenation of Separation Science with MS: Current Practice and Future Perspective</b> Arranged by LC/MS Interest Group.<br>G rard Hopfgartner, presiding<br>Session Room A                            | <b>MS Instrument Leasing-Exploring the Options and Avoiding the Pitfalls</b> Arranged by Pharmaceuticals Interest Group. David Peake and Brad Ackermann, presiding<br>Session Room A           |
| <b>Where Is Metabolite Profiling Being Used?</b><br>Arranged by Metabolomics Interest Group<br>Grace O'Maille and Ben Bolanos, presiding<br>Session Room B                                                | <b>Top Down Protein Sequencing on 2D and 3D Ion Traps</b><br>Arranged by Ion Traps Interest Group<br>Richard Vachet, presiding<br>Session Room B                                               |
| <b>New Instrumentation for Metabolite Identification</b> Arranged by Drug Metabolism & Pharmacokinetics Int Group<br>Walter Korfmacher, Ajai Chaudhary, and Jonathan Josephs, presiding<br>Session Room C | <b>Bridging the Gap between Biomarker Discovery and Clinical Chemistry Procedures</b> Arranged by Clinical Chemistry Interest Group; Donald Chace and Jack Henion, presiding<br>Session Room C |
| <b>Critical Role of Mass Accuracy</b><br>Arranged by FTMS Interest Group<br>Michael A. Freitas and Christopher L. Hendrickson, presiding<br>Session Room D                                                | <b>Open Source Software for MS: More than Just Free Stuff</b><br>Arranged by Computer Applications Interest group<br>Jeffrey Whitney, presiding<br>Session Room D                              |
| <b>Novel Ionization Techniques</b> Arranged by Fundamentals Interest Group. Kelly Sullivan and JC Poutsma, presiding<br>Session Room E                                                                    | <b>LC/MS Applications in Environmental Analysis</b> Arranged by Environmental Interest Group<br>Alaee Mehran, presiding<br>Session Room E                                                      |
| <b>Forensics.</b> Arranged by Forensics Interest Group<br>John Reynolds, presiding<br>Session Room F                                                                                                      | <b>What Can Ion Mobility Do for your Mass Spectrometry?</b><br>Arranged by Ion Mobility Interest Group<br>Herb Hill, presiding<br>Session Room F                                               |
| <b>NIH Electronic Submission of Grant Applications: Are you ready?</b> Douglas Sheeley, presiding<br>Session Room G                                                                                       | <b>Protein Aggregation and Mass Spectrometry.</b> Arranged by Biological Macromolecules Interest Group<br>Viswanatham Katta, presiding<br>Session Room G                                       |

## POSTER OVERVIEW

### MONDAY POSTER TOPICS

These posters should be set up at 7:30 am and removed at 7:30 pm on Monday. See list on page 52.

#### *Poster Numbers*

|                                                                |         |
|----------------------------------------------------------------|---------|
| Quantitative Analysis of Drugs and Metabolites I .....         | 9-30    |
| Quantitative Analysis of Drugs: Method Development .....       | 31-55   |
| Quantitation of Endogenous Compounds and Natural Products..... | 56-82   |
| Clinical Chemistry I .....                                     | 83-96   |
| Sample Preparation for LC/MS I .....                           | 97-120  |
| Homeland Security and Forensics.....                           | 121-135 |
| Detection of Compounds of Forensic Interest.....               | 136-153 |
| Ion Mobility I .....                                           | 154-170 |
| Instrumentation – TOFMS .....                                  | 171-197 |
| Instrumentation – FTMS .....                                   | 198-220 |
| Synthetic Polymers.....                                        | 221-233 |
| Microbial Analysis - Methods and Characterization..            | 234-254 |
| Undergraduate Posters .....                                    | 269-290 |
| High Throughput Analysis .....                                 | 291-321 |
| Bioinformatics I .....                                         | 322-351 |
| Non-Covalent Interactions I .....                              | 352-374 |
| Peptides: Fragmentation and Sequencing I .....                 | 375-397 |
| Modified Proteins I .....                                      | 398-416 |
| Proteins General I.....                                        | 417-430 |
| Proteins – Membrane .....                                      | 431-454 |
| Carbohydrates/Oligosaccharides I.....                          | 455-468 |
| Proteomics: New Methods I.....                                 | 469-497 |
| Proteomics: Lower Organisms .....                              | 498-528 |
| Proteomics: Sample Preparation and Methodologies I....         | 529-551 |
| Proteomics: Quantitative Techniques I .....                    | 552-584 |
| Proteomics: Mammalian .....                                    | 585-608 |
| Proteomics: Cancer Biomarkers.....                             | 609-642 |
| Proteomics: Methods for Phospho Proteins .....                 | 643-661 |

### TUESDAY POSTER TOPICS

These posters should be set up at 7:30 am and removed at 7:30 pm on Tuesday. See list on page 80.

#### *Poster Numbers*

|                                                             |         |
|-------------------------------------------------------------|---------|
| Isotope Ratio MS .....                                      | 9-12    |
| Particle Analysis .....                                     | 13-16   |
| Hydrocarbons and Petrochemicals by FTMS .....               | 17-23   |
| Metabolite Profiling and Identification: Applications ..    | 24-45   |
| Metabolite Profiling and Identification: Methods.....       | 46-60   |
| Metabolism Xenobiotics .....                                | 61-75   |
| Quantitative Analysis of Drugs and Metabolites II.....      | 76-98   |
| Quantitative Analysis of Drugs:<br>Method Development ..... | 99-122  |
| Reaction Intermediates.....                                 | 123-130 |
| Ion Structures and Energetics .....                         | 131-159 |
| Environmental Analysis: Water .....                         | 160-181 |
| Environmental Analysis: Air .....                           | 182-195 |
| Sample Preparation for LC/MS II.....                        | 196-220 |
| Clinical Chemistry II .....                                 | 221-247 |
| Immunology.....                                             | 248-264 |
| Natural Products .....                                      | 265-270 |
| MALDI Tandem MS.....                                        | 271-277 |
| Metal Ions in Biology .....                                 | 278-319 |
| Glycoproteins I .....                                       | 320-340 |
| Modified Proteins II.....                                   | 341-354 |
| Neuropeptides .....                                         | 355-368 |
| Protein Conformation I: Hydrogen Exchange.....              | 369-394 |
| Peptides: Fragmentation and Sequencing II.....              | 395-418 |
| Peptides: Quantitation.....                                 | 419-437 |
| Peptides: Post-Translational Modifications I.....           | 438-457 |
| Phosphopeptide Enrichment .....                             | 458-474 |
| Proteomics: Fundamental Studies.....                        | 475-490 |
| Proteomics: New Methods II .....                            | 491-534 |
| Proteomics: Sample Preparation and Fractionation II..       | 535-551 |
| Proteomics: Quantitative Techniques II.....                 | 552-579 |
| Proteomics: Biochemistry - Non-Mammalian .....              | 580-600 |
| Proteomics: Biomarkers in Tissue and Serum .....            | 601-637 |
| Bioinformatics II.....                                      | 638-662 |
| Recombinant Proteins .....                                  | 663-673 |

## POSTER OVERVIEW

### WEDNESDAY POSTER TOPICS

These posters should be set up at 7:30 am and removed at 7:30 pm on Wednesday. See list on page 108.

|                                                                  | <i>Poster Numbers</i> |
|------------------------------------------------------------------|-----------------------|
| Ion Molecule Reactions.....                                      | 9-23                  |
| Ionization Mechanisms .....                                      | 24-36                 |
| Direct Ionization Techniques .....                               | 37-51                 |
| Computer Applications .....                                      | 52-82                 |
| Environmental Analysis: Food and Pesticides .....                | 83-106                |
| Agriculture and Pesticide Analysis .....                         | 107-118               |
| LC/MS.....                                                       | 119-137               |
| GC/MS .....                                                      | 139-147               |
| Methods for Small Molecule Analysis .....                        | 148-178               |
| Drug Metabolism: High Throughput.....                            | 179-198               |
| Quantitative Analysis of Drugs and Metabolites III...            | 199-219               |
| Pharmaco Kinetics: Methods and Applications .....                | 220-241               |
| MALDI Sample Preparation I.....                                  | 242-260               |
| Instrumentation: New Concepts I.....                             | 261-281               |
| Instrumentation: Mass Analyzers (Quadrupoles and Traps)<br>..... | 291-315               |
| Imaging MS.....                                                  | 316-337               |
| Surface Analysis.....                                            | 338-345               |
| Non-Covalent Complexes .....                                     | 346-353               |
| Carbohydrates and Oligosaccharides II .....                      | 354-373               |
| Glycoproteins II .....                                           | 374-394               |
| Nucleic Acids .....                                              | 395-424               |
| Peptides: Fragmentation and Sequencing III.....                  | 425-441               |
| Peptides: General .....                                          | 450-461               |
| Peptides: Post-Translational Modifications II .....              | 462-477               |
| Phosphorylated Proteins.....                                     | 478-499               |
| Protein Conformation II .....                                    | 500-516               |
| Bioinformatics III.....                                          | 517-548               |
| Proteomics: Biomarkers .....                                     | 549-577               |
| Proteomics: Technique Comparisons.....                           | 579-606               |
| Proteomics: Sample Preparation III .....                         | 607-630               |
| Proteomics: 2D Electrophoresis .....                             | 636-644               |
| Proteomics: Quantitation Techniques III .....                    | 645-668               |

### THURSDAY POSTERS

These posters should be set up at 7:30 am and removed at 2:30 pm on Thursday. See list on page 135.

|                                                              | <i>Poster Numbers</i> |
|--------------------------------------------------------------|-----------------------|
| Atmospheric Chemistry .....                                  | 9-13                  |
| Atmospheric Pressure Photo Ionization .....                  | 14-31                 |
| Direct Ionization Techniques II .....                        | 32-39                 |
| Instrumentation: Ion Sources .....                           | 40-61                 |
| Ion Mobility II .....                                        | 62-77                 |
| ESI/Nanospray Sample Preparation .....                       | 78-89                 |
| Micro and Nano Scale Separations .....                       | 90-114                |
| MALDI Sample Preparation II .....                            | 115-136               |
| Instrumentation: New Concepts II .....                       | 137-150               |
| Portable Instrumentation .....                               | 151-160               |
| Flavors and Fragrances .....                                 | 161-165               |
| Drug Metabolism: Reactive Intermediates and Adducts<br>..... | 166-175               |
| Chiral Analysis .....                                        | 176-183               |
| Small Molecule Analysis .....                                | 184-217               |
| Toxicology .....                                             | 218-250               |
| Ion Activation and Dissociation.....                         | 251-267               |
| Carbohydrates and Oligosaccharides III .....                 | 291-311               |
| Imaging MS II.....                                           | 312-335               |
| Lipids: Structural Analysis and Profiling.....               | 336-357               |
| Lipids: Biochemistry and Signaling.....                      | 358-371               |
| Lipids: Oxidized Lipids and Sterols.....                     | 372-384               |
| Bioinformatics IV .....                                      | 385-411               |
| Metabolomics and Biomarker Discovery.....                    | 412-447               |
| Metabolomic and Biomarker Applications .....                 | 450-467               |
| Non-Covalent Interactions II .....                           | 468-486               |
| Proteins General II .....                                    | 487-500               |
| Modified Proteins: Oxidation .....                           | 501-516               |
| Protein Conformation III.....                                | 517-533               |
| Proteins: Folding.....                                       | 534-546               |
| Proteomics: Labeling and Affinity Methods.....               | 547-564               |
| Proteomics: Detection of Biomolecules .....                  | 565-589               |
| Proteomics: Medical Applications .....                       | 590-615               |
| Proteomics: Quantitation Techniques IV .....                 | 616-647               |
| Proteomics: Phosphorylated Applications .....                | 648-669               |

## MONDAY ORAL SESSIONS

### MONDAY MORNING, MAY 29

#### 8:00 – 8:45 am: PLENARY LECTURE

**Lisa Randall**, Harvard University  
*Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions*

#### 8:45 – 10:15 am: POSTER SESSION AND EXHIBITS

Monday posters. Authors of odd-numbered posters present.  
See list beginning on page 53.

#### 10:15 am – 12:15 pm: PARALLEL SESSIONS

#### Session Room A: 10:15 am – 12:15 pm ENDOGENOUS METABOLITE PROFILING

Mark Sanders, presiding

- MOA am 10:15 **Comprehensive Dynamics of the E. coli Metabolome**; Joshua D. Rabinowitz<sup>1</sup>; Jie Yuan<sup>1</sup>; Elizabeth Kimball<sup>1</sup>; Sunil Bajad<sup>1</sup>; Matthew Brauer<sup>1</sup>; Wenyun Lu<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ
- MOA am 10:35 **Validating Endogenous Biochemical Molecules To Be Used for Biomarker Discovery**; Lily Li<sup>1</sup>; Amy Deik<sup>1</sup>; Kojo Abdul-Hadi<sup>1</sup>; David Ho<sup>1</sup>; Yulin Huang<sup>1</sup>; Keith Ohm<sup>1</sup>; <sup>1</sup>PharmaKD Inc., Woburn, MA
- MOA am 10:55 **Investigation of a Potential Marker for Phospholipidosis: Normalization Strategies for Metabonomic Analysis of Urine Samples**; Bethanne M. Warrack<sup>1</sup>; Serhiy Hnatyshyn<sup>1</sup>; Petia Shipkova<sup>2</sup>; Haiying Zhang<sup>1</sup>; Mark Sanders<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb, Hopewell, NJ
- MOA am 11:15 **Development and Validation of a Protein Precipitation LC-MS Method for the Metabonomic Analysis of Rat Plasma**; Mark Jairaj<sup>1</sup>; K. Magnus Åberg<sup>1</sup>; Henrik Toft Pedersen<sup>2</sup>; Dorrit Baunsgaard<sup>2</sup>; <sup>1</sup>Novo Nordisk A/S, MolPAGE, Måløv, Denmark; <sup>2</sup>Novo Nordisk A/S, Protein Structure and Biophysics, Måløv, Denmark
- MOA am 11:35 **Integration of UPLC-MS with Other Analytical Methods by Correlation of Data Sets**; Derek J. Crockford<sup>1</sup>; Jeremy K. Nicholson<sup>1</sup>; <sup>1</sup>Imperial College, London, United Kingdom
- MOA am 11:55 **Integrated Approach for Structural Profiling of Endogenous Metabolites**; Robert Mistrik<sup>1</sup>; Juraj Lutisan<sup>1</sup>; Milos Suchy<sup>1</sup>; <sup>1</sup>HighChem, Bratislava, Slovakia

#### Session Room B: 10:15 am – 12:15 pm PEPTIDES AND PROTEINS AS BIOMARKERS

H. Robert Bergen, presiding

- MOB am 10:15 **Novel Approach to Identify Low Abundance Biomarkers in Serum**; Hoo-Keun Lee<sup>1</sup>; Paola Picotti<sup>1</sup>; Bruno Domon<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>IMSB ETH Zurich, Zurich, Switzerland
- MOB am 10:35 **Quantitative Proteomic Analysis of Brain Striata from Neurotoxin-Induced Mouse Models of Parkinson's Disease**; Wei-Jun Qian<sup>1</sup>; Haixing Wang<sup>1</sup>; Mark H. Chin<sup>2</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>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>UCLA School of Medicine, Los Angeles, CA
- MOB am 10:55 **Development of a Method for Quantification of HER-2 in Formalin-Fixed Paraffin Embedded Breast Cancer Tissue and Serum**; Timothy D. Veenstra<sup>1</sup>; Brian L. Hood<sup>1</sup>; David B. Krizman<sup>2</sup>; Marlene M. Darfler<sup>2</sup>; Thomas G. Guile<sup>2</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>Expression Pathology Incorporated, Gaithersburg, MD
- MOB am 11:15 **Discovery and Validation of Glioblastoma Multiform Biomarkers Using Microdissected Tissue Specimens Coupled with Targeted and MS-Based Proteomic Studies**; Weijie Wang<sup>1</sup>; Tong Guo<sup>2</sup>; Cheng S. Lee<sup>2</sup>; Paul A. Rudnick<sup>1</sup>; Zhengping Zhuang<sup>3</sup>; Robert Weil<sup>4</sup>; Brian M. Balgley<sup>1</sup>; <sup>1</sup>Calibrant Biosystems, Gaithersburg, MD; <sup>2</sup>University of Maryland, College Park, MD; <sup>3</sup>NINDS, Bethesda, MD; <sup>4</sup>Cleveland Clinic Foundation, Cleveland, OH
- MOB am 11:35 **False Discovery Rates in Protein Identification**; Richard C. Jones<sup>1</sup>; Sheeno Thyparambil<sup>1</sup>; Jason T. Taylor<sup>1</sup>; Ricky D. Edmondson<sup>1</sup>; <sup>1</sup>National Center for Toxicological Research, Jefferson, AR
- MOB am 11:55 **Candidate Protein Biomarker Verification in Plasma: Improved Limits of Detection and Quantitation**; Hasmik Keshishian<sup>1</sup>; Eric Kuhn<sup>1</sup>; Michael Burgess<sup>1</sup>; Terri Addona<sup>1</sup>; Steven A Carr<sup>1</sup>; <sup>1</sup>Broad Institute of Harvard and MIT, Cambridge, MA



## MONDAY ORAL SESSIONS

**Session Room C: 10:15 am – 12:15 pm**  
**MEMBRANE PROTEINS AND**  
**HYDROPHOBIC PEPTIDES**  
 Christine Wu, presiding

- MOC am 10:15 **Membrane Proteomics of Model Organisms and Formalin-Fixed and Paraffin-Embedded Tissues Using Capillary Isoelectric Focusing-Based Multidimensional Separations Coupled with ESI-Tandem MS**; Weijie Wang<sup>1</sup>; Tong Guo<sup>1</sup>; Paul A. Rudnick<sup>2</sup>; Brian M. Balgley<sup>2</sup>; Clive R. Taylor<sup>3</sup>; Shan-Rong Shi<sup>3</sup>; Cheng S. Lee<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>Calibrant Biosystems, Gaithersburg, MD; <sup>3</sup>University of Southern California, Los Angeles, CA
- MOC am 10:35 **Increasing Coverage in the Transmembrane Domain with Activated Ion Electron-Capture Dissociation for Top-Down Mass Spectrometry of Integral Membrane Proteins**; Julian P. Whitelegge<sup>1</sup>; Vlad Zabrouskov<sup>2</sup>; Jennifer Zhang<sup>2</sup>; Thomas C. McClure<sup>2</sup>; <sup>1</sup>University of California, Los Angeles, CA; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- MOC am 10:55 **Chemical strategies for the Molecular Characterization of Membrane Proteins Using Mass Spectrometry**; Anna E. Speers<sup>1</sup>; Christine C Wu<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Aurora, CO
- MOC am 11:15 **Comparison of Multidimensional Separation Strategies for Studying Membrane Proteomes**; Hongbin Liu<sup>1</sup>; Jim Martosella<sup>1</sup>; Nina Zolotarjova<sup>1</sup>; Susanne Moyer<sup>1</sup>; Peter Mrozinski<sup>1</sup>; Rhonda Taylor<sup>1</sup>; Jerome Bailey<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Wilmington, DE
- MOC am 11:35 **Quantitative Profiling of the Lipid Raft Proteome from Wild-type and Mutant Gag-Expressing Cells**; Josip Blonder<sup>1</sup>; Akira Ono<sup>2</sup>; King C. Chan<sup>1</sup>; David A. Lucas<sup>1</sup>; Haleem J. Issaq<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; Eric O. Freed<sup>3</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>University of Michigan Medical School, Ann Arbor, MI; <sup>3</sup>National Cancer Institute at Frederick, Frederick, MD
- MOC am 11:55 **Profiling the HeLa Cell Membrane Proteome with Novel Compounds, Mass Spectrometry and Immunofluorescence**; Wei Yi<sup>1</sup>; Xiaoting Tang<sup>1</sup>; Gerhard R. Munske<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

**Session Room D: 10:15 am – 12:15 pm**  
**DISTRIBUTING THE FUTURE:**  
**ENABLING HIGH THROUGHPUT ANALYSIS**  
 Mark Cole, presiding

- MOD am 10:15 **Novel Sample Handling and Introduction Technology Decouples Throughput and Carryover by Utilizing Autonomous Syringes**; Thomas Londo<sup>1</sup>; Paul Grippo<sup>1</sup>; Daniel Bantz<sup>1</sup>; Paul Horvat<sup>1</sup>; Frank Sylva<sup>1</sup>; Angela Tseng<sup>1</sup>; Maxwell MacLean<sup>1</sup>; Chuck Schelberg<sup>1</sup>; Eric Willet<sup>1</sup>; Byron Kieser<sup>2</sup>; Peter Kovarik<sup>3</sup>; Mauro Aiello<sup>3</sup>; Thomas Covey<sup>3</sup>; <sup>1</sup>Parker Life Sciences, Hollis, NH; <sup>2</sup>Applied Biosystems / MDS Sciex, Toronto, Canada; <sup>3</sup>MDS Sciex, Toronto, Canada
- MOD am 10:35 **Ultra-Rapid Separation and Quantitation of Peptides via a Nanoelectrospray-Differential Mobility Spectrometry-Mass Spectrometer System**; Daren S. Levin<sup>1</sup>; Paul Vouros<sup>1</sup>; Raanan Miller<sup>2</sup>; Erkinjon Nazarov<sup>2</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Sionex Corporation, Bedford, MA
- MOD am 10:55 **Heat and Serve: Rapid Pharmacokinetics Using a Laser Diode Thermal Desorption (LDTD) Ion Source for Mass Spectrometry**; Kevin P. Bateman<sup>1</sup>; Pierre Picard<sup>2</sup>; Christophe Mellon<sup>1</sup>; Sylvain Letarte<sup>2</sup>; <sup>1</sup>Merck Frosst, Montreal, Canada; <sup>2</sup>Phytronix, Quebec, Canada
- MOD am 11:15 **Evaluation of a Dual-Spray Electrospray Ionization Source for High-Throughput Bioanalytical Mass Spectrometry**; John S. Janiszewski<sup>1</sup>; Walter E. Mitchell<sup>1</sup>; Lisa Cousins<sup>2</sup>; Reza Javahery<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>Ionics Mass Spectrometry Group, Concord, Ontario, Canada
- MOD am 11:35 **Factors Limiting Throughput for MALDI Quantitation by MRM**; Bradley B. Schneider<sup>1</sup>; Jay J. Corr<sup>1</sup>; Thomas R. Covey<sup>1</sup>; <sup>1</sup>MDS SCIEX, Concord, Canada
- MOD am 11:55 **Evaluation of Desorption Electrospray Ionization (DESI) in Support of High Throughput Screening Assays**; Michael J. Ford<sup>1</sup>; Colleen Mcnaney<sup>1</sup>; Dieter Drexler<sup>1</sup>; Mark Sanders<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Wallingford, CT

# MONDAY ORAL SESSIONS

| <b>Session Room E: 10:15 am – 12:15 pm</b><br><b>FORENSIC SCIENCE AND DETECTION</b><br>John G. Reynolds, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Session Room F: 10:15 am – 12:15 pm</b><br><b>ION MOBILITY</b><br>David Clemmer, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| <p>MOE am 10:15 <b>Applications of Mass Spectrometry in Forensic Science;</b> <u>Fred L. Fricke</u><sup>1</sup>; <sup>1</sup>U.S. FDA, Cincinnati, OH</p> <p>MOE am 10:35 <b>Rapid Analysis of Drugs of Abuse in Oral Fluids by LC/MS/MS;</b> <u>Michael Zumwalt</u><sup>1</sup>; Christine Moore<sup>2</sup>; <sup>1</sup>Agilent Technologies, Englewood, CO; <sup>2</sup>Immunalysis, Corp., Pomona, CA</p> <p>MOE am 10:55 <b>High-throughput Quantitative Analysis of Aflatoxin Exposure by LC/MS/MS;</b> <u>Robert A. Everley</u><sup>2</sup>; Frederic L. Ciner<sup>1</sup>; Dongliang Zhang<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</p> <p>MOE am 11:15 <b>Permeation of Organophosphates in Polymeric Materials;</b> <u>Gary S. Groenewold</u><sup>1</sup>; Garold L. Gresham<sup>1</sup>; Anita K. Gianotto<sup>1</sup>; Marnie M. Cortez<sup>1</sup>; Anthony D. Appelhans<sup>1</sup>; Mark L. Stone<sup>1</sup>; Eric S. Peterson<sup>1</sup>; Chris J. Orme<sup>1</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID</p> <p>MOE am 11:35 <b>Desorption Electrospray Tandem Mass Spectrometry (DESI-MS/MS) of Chemical Warfare Agents from Solid Phase Microextraction (SPME) Fibers;</b> <u>Paul A. D'Agostino</u><sup>1</sup>; Claude L. Chenier<sup>1</sup>; James R. Hancock<sup>1</sup>; Carmela R. Jackson Lepage<sup>1</sup>; <sup>1</sup>DRDC Suffield, Medicine Hat, Canada</p> <p>MOE am 11:55 <b>A Survey Of Surface Sampling Mass Spectrometric Methods For Chemical Weapons Forensic Analysis;</b> <u>Peter T.A. Reilly</u><sup>1</sup>; Bruce A. Tomkins<sup>1</sup>; Rob R. Smith<sup>1</sup>; Wayne H. Griest<sup>1</sup>; Gary J. Van Berkel<sup>1</sup>; Douglas C. Duckworth<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN</p> | <p>MOF am 10:15 <b>Mobilities and Melting;</b> Colleen M. Neal<sup>1</sup>; Anne K. Starace<sup>1</sup>; <u>Martin F. Jarrold</u><sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN</p> <p>MOF am 10:35 <b>Using Ion Mobility Mass Spectrometry to Measure Oligomer-Size Distributions and Structures for the Early Stages of Assembly of A<math>\beta</math>;</b> <u>Summer L. Bernstein</u><sup>1</sup>; Nicholas Dupuis<sup>1</sup>; Thomas Wyttienbach<sup>1</sup>; Noel Lazo<sup>2</sup>; Gal Bitan<sup>2</sup>; David B. Teplow<sup>2</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara, Ca; <sup>2</sup>University of California, Los Angeles, Ca</p> <p>MOF am 10:55 <b>Characterising a Travelling Wave-Based Ion Mobility Separator;</b> <u>Kevin Giles</u><sup>1</sup>; Steven D. Pringle<sup>1</sup>; Jason L. Wildgoose<sup>1</sup>; Robert H. Bateman<sup>1</sup>; <sup>1</sup>Waters MS Technologies Centre, Manchester, UK</p> <p>MOF am 11:15 <b>Ion Mobility-Mass Spectrometry Analysis of Large Protein-Protein Complexes: An Approach for Heterogeneous Systems;</b> <u>Brandon T. Ruotolo</u><sup>1</sup>; Justin L. P. Benesch<sup>1</sup>; Suk Hyung<sup>1</sup>; Kevin Giles<sup>2</sup>; Robert H. Bateman<sup>2</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, UK; <sup>2</sup>Waters MS Technologies Center, Manchester, UK</p> <p>MOF am 11:35 <b>IMS-IMS and IMS-IMS-IMS/MS for Separating Peptide and Protein Fragment Ions;</b> <u>Samuel I. Merenbloom</u><sup>1</sup>; Stormy L. Koeniger<sup>1</sup>; Stephen J. Valentine<sup>2</sup>; Manolo D. Plasencia<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Predictive Physiology and Medicine, Bloomington, IN</p> <p>MOF am 11:55 <b>High-Resolution FAIMS Using New Planar Geometry Analyzers;</b> <u>Keqi Tang</u><sup>1</sup>; Alexandre A. Shvartsburg<sup>1</sup>; Fumin Li<sup>1</sup>; David C. Prior<sup>1</sup>; Michael A. Buschbach<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA</p> |

## MONDAY ORAL SESSIONS

### Session Room G: 10:15 am – 12:15 pm QUANTITATION OF POLYMERS

Tony Jackson, presiding

- MOG am 10:15 **Development of NIST SRM 2881, an Absolute Molecular Mass Distribution Polymer Standard;** William E. Wallace<sup>1</sup>; Charles M Guttman<sup>1</sup>; Kathleen M Flynn<sup>1</sup>; Anthony J Kearsley<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- MOG am 10:35 **Quantitative Analysis of Polymer End Group Distributions;** Alyison M. Leigh<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH, USA*
- MOG am 10:55 **Mass Spectral Analysis of Polystyrene-Based Polymers Generated by RAFT Polymerization;** Dmitri Zagorevski<sup>1</sup>; Mohammed J. Nasrullah<sup>1</sup>; Vajjula Raghunadh<sup>1</sup>; Brian C. Benicewicz<sup>1</sup>; <sup>1</sup>*Rensselaer Polytechnic Institute, Troy, NY*
- MOG am 11:15 **The Study of Salt/Analyte Ratios for Four Matrices in MALDI TOFMS;** William J. Erb<sup>1</sup>; Kevin G. Owens<sup>1</sup>; Andrew J. Hotelling<sup>2</sup>; <sup>1</sup>*Drexel University, Philadelphia, PA*; <sup>2</sup>*Eastman Kodak, Rochester, NY*
- MOG am 11:35 **Investigating Solvent-Free MALDI Sample Preparation with MS and Microscopy;** Scott D. Hanton<sup>1</sup>; Jim R. Stets<sup>1</sup>; Todd M. McEvoy<sup>1</sup>; <sup>1</sup>*Air Products and Chemicals, Inc., Allentown, PA*
- MOG am 11:55 **Proposed Modifications to MALDI-CID Fragmentation Mechanisms of Silver Ionized Polystyrene Oligomers;** Michael J. Polce<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH*

### MONDAY AFTERNOON, MAY 29

#### 12:30 – 1:30 pm: INTEREST GROUP MEETINGS

##### **Young Mass Spectrometrists Interest Group Meeting. The Early Days of Biological MS: What Happened Before ESI and MALDI?**

Kristina Hakansson, presiding. Room 617

##### **Ion Traps Interest Group Meeting**

Richard Vachet, presiding. Room 618

##### **Fundamentals Interest Group Meeting**

Kelly Sullivan and JC Poutsma, presiding. Room 619

##### **Hydrocarbon Interest Group Meeting**

Ryan Rodgers, presiding. Room 620

#### 1:30 – 3:00 pm: POSTER SESSION AND EXHIBITS

Monday posters. Authors of even-numbered posters present.  
See list beginning on page 53.

#### 3:00 – 5:00 pm: PARALLEL SESSIONS

### Session Room A: 3:00 – 5:00 pm BIOMARKER EVALUATION

Kevin I. Duffin, presiding

- MOA pm 03:00 **Biomarkers for Affective Disorders;** Chris W. Turck<sup>1</sup>; Rainer Landgraf<sup>1</sup>; Giuseppina Maccarrone<sup>1</sup>; Claudia Ditzén<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Psychiatry, Munich, Germany*
- MOA pm 03:20 **Multiple Proteomics Approaches for the Discovery of New Biomarkers of Alzheimer's Disease;** Malcolm A Ward<sup>1</sup>; Abdul Hye<sup>2</sup>; Steve Lynham<sup>2</sup>; James Campbell<sup>1</sup>; Helen L Byers<sup>1</sup>; Jules A Westbrook<sup>1</sup>; Karsten Kuhn<sup>1</sup>; Pat Sham<sup>2</sup>; Brian Anderton<sup>2</sup>; Simon Lovestone<sup>2</sup>; <sup>1</sup>*Proteome Sciences plc, London, United Kingdom*; <sup>2</sup>*Institute of Psychiatry, London, United Kingdom*
- MOA pm 03:40 **Using LC-SRM with Stable Isotope Dilution to Expedite Evaluation of Novel Peptide and Protein Biomarkers;** Brad Ackermann<sup>1</sup>; Mike Berna<sup>1</sup>; Yuejun Zhen<sup>1</sup>; Tomoyuki Oe<sup>1</sup>; Chris Schmalz<sup>1</sup>; <sup>1</sup>*Eli Lilly and Company, Greenfield, IN*
- MOA pm 04:00 **Quantitative Verification of Cardiac Markers in Human Plasma by Isotope Dilution Mass Spectrometry and High-resolution SRM (hSRM);** Tori Richmond<sup>1</sup>; Mark Harrison<sup>1</sup>; Leo Bonilla<sup>1</sup>; <sup>1</sup>*Thermo BRIMS Center, Cambridge, MA*
- MOA pm 04:20 **Histones as Biomarkers in Chronic Lymphocytic Leukemia;** Xiaodan Su<sup>1</sup>; David E. Lucas<sup>1</sup>; Liwen Zhang<sup>1</sup>; Melanie E. Davis<sup>1</sup>; Amy R. Knapp<sup>1</sup>; Mark R. Parthun<sup>1</sup>; Guido Marcucci<sup>1</sup>; Michael R. Grever<sup>1</sup>; John C. Byrd<sup>1</sup>; Michael A. Freitas<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*
- MOA pm 04:40 **The Search for Biomarkers of Mammary Tumors: New Insights from the Proteomics of Infiltrating Ductal Carcinoma;** Lambert C Ngoka<sup>1</sup>; <sup>1</sup>*Virginia Commonwealth University, Richmond, VA*

## MONDAY ORAL SESSIONS

| <b>Session Room B: 3:00 – 5:00 pm</b><br><b>POSTTRANSLATIONAL MODIFICATIONS BEYOND PHOSPHORYLATION</b><br>Roman Zubarev, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | <b>Session Room C: 3:00 – 5:00 pm</b><br><b>TIME-OF-FLIGHT INSTRUMENTATION</b><br>John B. Hoyes, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
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| <p>MOB pm 03:00 <b>Selective Detection and Quantitation of Protein Arginine and Lysine Methylation by NanoLC-MS/MS;</b> <u>Manuel Tzouros</u><sup>1</sup>; Albert J. R. Heck<sup>1</sup>; Jeroen Krijgsveld<sup>1</sup>; <sup>1</sup><i>Utrecht University, Utrecht, The Netherlands</i></p> <p>MOB pm 03:20 <b>Top-Down MS Characterization of GlnK, GlnB Protein Uridylylation in Response to Nitrogen Availability for <i>Rhodopseudomonas palustris</i>;</b> <u>Robert L Hettich</u><sup>1</sup>; Heather Connelly<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; Tse Yuan<sup>1</sup>; Patricia Lankford<sup>1</sup>; Dale Pelletier<sup>1</sup>; <sup>1</sup><i>Oak Ridge National Lab, Oak Ridge, TN</i></p> <p>MOB pm 03:40 <b>Characterization of Glycosylation of Membrane Receptors at Low Levels Using Extended Range Proteomic Analysis (ERPA);</b> <u>Tomas Rejtar</u><sup>1</sup>; Lingyun Li<sup>1</sup>; Shujia Dai<sup>1</sup>; Jeongkwon Kim<sup>1</sup>; Jian Min Ren<sup>1</sup>; Victor Andreev<sup>1</sup>; Shiaw-Lin Wu<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup><i>Northeastern University, Boston, MA</i></p> <p>MOB pm 04:00 <b>Breaking the Histone Code: Analyzing the Interdependence of Acetylation and Methylation on Histone H3 Using Electron Transfer Dissociation (ETD);</b> <u>Beatrix M Ueberheide</u><sup>1</sup>; Sean D Taverna<sup>1</sup>; C David Allis<sup>1</sup>; Jeffrey Shabanowitz<sup>2</sup>; Donald F Hunt<sup>2</sup>; <sup>1</sup><i>Rockefeller University, New York, NY</i>; <sup>2</sup><i>University of Virginia, Charlottesville, VA</i></p> <p>MOB pm 04:20 <b>Discovery of Novel and Unexpected Modifications by ModifiComb: the Case of Glu-Methylation in Human Cells;</b> <u>Michael L. Nielsen</u><sup>1</sup>; Mikhail M. Savitski<sup>1</sup>; Roman A. Zubarev<sup>1</sup>; <sup>1</sup><i>Biological and Medical Mass Spectrometry, Uppsala, Sweden</i></p> <p>MOB pm 04:40 <b>Comparative Analysis of Post-Translational Modifications in Young and Aged Lens: Does Deamidation Contribute to Crystallin Insolubility?;</b> <u>Phillip A. Wilmarth</u><sup>1</sup>; Stephen Tanner<sup>2</sup>; Surendra Dasari<sup>1</sup>; Michael A. Riviere<sup>1</sup>; Vineet Bafna<sup>2</sup>; Pavel A. Pevzner<sup>2</sup>; Larry L. David<sup>1</sup>; <sup>1</sup><i>Oregon Health &amp; Science University, Portland, OR</i>; <sup>2</sup><i>University of California, San Diego, La Jolla, CA</i></p> | <p>MOC pm 03:00 <b>A Method to Increase the Duty Cycle of an Orthogonal Acceleration Time-of-Flight Mass Spectrometer;</b> <u>Robert H Bateman</u><sup>1</sup>; Kevin Giles<sup>1</sup>; Steven D Pringle<sup>1</sup>; Jason L Wildgoose<sup>1</sup>; <sup>1</sup><i>Waters MS Technologies Centre, Manchester, UK</i></p> <p>MOC pm 03:20 <b>Distance-of-Flight MS – Exploratory Implementation in a Q/oTOF Mass Spectrometer;</b> <u>Christie Enke</u><sup>1</sup>; Gareth Dobson<sup>1</sup>; <sup>1</sup><i>University of New Mexico, Albuquerque, NM</i></p> <p>MOC pm 03:40 <b>Space Charge Effects in Multireflecting Time-of-Flight Mass Spectrometer;</b> <u>Boris Kozlov</u><sup>1</sup>; Michail Gavrik<sup>1</sup>; Yurii Hasin<sup>1</sup>; Sergei Kirillov<sup>1</sup>; Andrei Monakhov<sup>1</sup>; Andrei Trufanov<sup>1</sup>; Michail Yavor<sup>1</sup>; Anatolii Verentchikov<sup>1</sup>; <sup>1</sup><i>Institute for Analytical Instrumentation, St. Petersburg, Russia</i></p> <p>MOC pm 04:00 <b>Multiplex Data Acquisition in Multiple Time-Dispersive Separation Dimensions;</b> <u>John A. McLean</u><sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup><i>Texas A&amp;M University, College Station, TX</i></p> <p>MOC pm 04:20 <b>Development of a Novel High-Performance MALDI-TOF Mass Spectrometer with Spiral Ion Trajectory;</b> Takaya Satoh<sup>1</sup>; Takafumi Sato<sup>1</sup>; Susumu Fujimaki<sup>1</sup>; Junichi Osuga<sup>1</sup>; Akihiko Kusai<sup>1</sup>; J. Douglas Meinhardt<sup>2</sup>; <u>Jun Tamura</u><sup>1</sup>; <sup>1</sup><i>JEOL Ltd., Akishima, Tokyo, Japan</i>; <sup>2</sup><i>JEOL USA, Inc., Peabody, MA</i></p> <p>MOC pm 04:40 <b>A New Class of Robust Sub-Nanosecond TOF Detectors with High Dynamic Range;</b> <u>Dick Stresau</u><sup>1</sup>; Kevin Hunter<sup>1</sup>; Wayne Sheils<sup>1</sup>; Peter Raffin<sup>1</sup>; Yair Benari<sup>1</sup>; <sup>1</sup><i>ETP Electron Multipliers, Ermington, Australia</i></p> |

## MONDAY ORAL SESSIONS

### Session Room D: 3:00 – 5:00 pm PROTEIN LIGAND COMPLEXES

Amina S. Woods, presiding

- MOD pm 03:00 **Assembling Protein Specificity through Peptidic Contacts by ESI-MS: Integrins and the RGD Motif;** Kevin A Schug<sup>1</sup>; Misjudeen Raji<sup>1</sup>; Jung-Mo Ahn<sup>2</sup>; <sup>1</sup>U.T.-Arlington, Arlington, TX; <sup>2</sup>U.T.-Dallas, Richardson, TX
- MOD pm 03:20 **Mass Spectrometry and ECD of Noncovalent Alpha-Synuclein Ligand Complexes;** Yongming Xie<sup>1</sup>; Sheng Yin<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California-Los Angeles, Los Angeles, CA
- MOD pm 03:40 **Phosphate and the Stabilization of Receptor-Receptor and Receptor-Ligand Interactions;** Shelley N Jackson<sup>1</sup>; Hay-Yan J Wang<sup>1</sup>; Amina S Woods<sup>1</sup>; Alfred Yergey<sup>2</sup>; <sup>1</sup>NIDA IRP, NIH, Baltimore, MD; <sup>2</sup>LCMB, NICHD, NIH, Bethesda, MD
- MOD pm 04:00 **Protein-Carbohydrate Complexes: Effects of Protein Dimerization upon Carbohydrate Ligand Binding;** Julie A. Leary<sup>1</sup>; Yonhao Yu<sup>1</sup>; Matthew Schenauer<sup>1</sup>; Matthew Sweeney<sup>1</sup>; <sup>1</sup>University of California, Davis, CA
- MOD pm 04:20 **An Accurate Mass Measurement Approach for Heterogeneous Protein Assemblies – Application to Intact Bacterial Ribosomes;** Adam R.C. McKay<sup>1</sup>; Brandon T. Ruotolo<sup>1</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, UK
- MOD pm 04:40 **Study of Non-Covalent Interaction between Odorant Binding Protein and Ligands by Nano-Electrospray Mass Spectrometry;** Sandra Alves<sup>1</sup>; Arul Marie<sup>2</sup>; Lionel Tcatchoff<sup>3</sup>; Jean Claude Pernollet<sup>3</sup>; Jean Claude Tabet<sup>1</sup>; <sup>1</sup>Université Pierre et Marie Curie, Paris, France; <sup>2</sup>Museum National d'Histoire Naturelle, Paris, France; <sup>3</sup>Biochimie et Structure des Protéines, INRA 477, Jouy-en-Josas, France

### Session Room E: 3:00 – 5:00 pm FORENSICS AND CLINICAL INVESTIGATIONS OF MICROORGANISMS

Danielle Dickinson, presiding

- MOE pm 03:00 **Non-Traditional Signatures in Biological Forensics;** Karen L. Wahl<sup>1</sup>; Kristin H. Jarman<sup>1</sup>; John B. Cliff<sup>1</sup>; Nancy B. Valentine<sup>1</sup>; David S. Wunschel<sup>1</sup>; Joel Forrester<sup>1</sup>; Timothy J. Johnson<sup>1</sup>; Helen Kreuzer<sup>1</sup>; Catherine E. Petersen<sup>1</sup>; Heather C. Edberg<sup>1</sup>; Scott Lea<sup>1</sup>; Orville T. Farmer<sup>1</sup>; May-Lin Thomas<sup>1</sup>; Dan Gaspar<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- MOE pm 03:20 **Intact Protein Analysis of Bacterial Extracts as a Means of Achieving Strain Level Typing;** Tracie L Williams<sup>1</sup>; Denis Andrzejewski<sup>1</sup>; Rebecca L Bell<sup>1</sup>; Steven M Musser<sup>1</sup>; <sup>1</sup>Center for Food Safety and Applied Nutrition, FDA, College Park, MD
- MOE pm 03:40 **Multiplexed Analysis of Genetic Biomarkers for Forensic Analysis and Pathogen Fingerprinting: Deployment of Mass Spectrometry-Based Signature Detection;** Steven A. Hofstadler<sup>1</sup>; James C. Hannis<sup>1</sup>; Jared J. Drader<sup>1</sup>; Jose Gutierrez<sup>1</sup>; Jose Gutierrez<sup>1</sup>; Abel Gutierrez<sup>1</sup>; Amy Schink<sup>1</sup>; Matthew Van Ert<sup>2</sup>; David M. Wagner<sup>2</sup>; Joseph Busch<sup>2</sup>; James Schupp<sup>2</sup>; Paul Keim<sup>2</sup>; Kristin A. Sannes-Lowery<sup>1</sup>; David Ecker<sup>1</sup>; Ranga Sampath<sup>1</sup>; Mark W. Eshoo<sup>1</sup>; <sup>1</sup>Ibis Division of Isis Pharmaceuticals, Carlsbad, CA; <sup>2</sup>Northern Arizona University, Flagstaff, AZ
- MOE pm 04:00 **Classification and Identification of Microbial Agents Based on Proteogenomic Similarities Revealed by Mining of Proteomics Data;** Jacek P. Dworzanski<sup>1</sup>; Danielle N. Dickinson<sup>2</sup>; Samir V. Deshpande<sup>3</sup>; Brian A. Eckenrode<sup>4</sup>; Charles H. Wick<sup>5</sup>; <sup>1</sup>SAIC, Aberdeen Proving Ground, MD; <sup>2</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>3</sup>Science and Technology Corporation, Edgewood, MD; <sup>4</sup>FBI Counterterrorism and Forensic Science Research, Quantico, VA; <sup>5</sup>U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD
- MOE pm 04:20 **Following the Metabolic and Morphological Changes of Individual Bacillus Atrophaeus Cells during the Sporulation Process Using Bioaerosol Mass Spectrometry;** Herbert J. Tobias<sup>1</sup>; Maurice Pitesky<sup>1</sup>; David P. Fergenson<sup>1</sup>; Paul T. Steele<sup>1</sup>; Joanne Horn<sup>1</sup>; Matthias Frank<sup>1</sup>; Eric E. Gard<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Lab, Livermore, CA

## MONDAY ORAL SESSIONS

MOE pm 04:40 **Development and Validation of MS Methods for Diagnosis of Anthrax Infection and the Quantification of Anthrax Toxins;** John R. Barr<sup>1</sup>; Anne E. Boyer<sup>1</sup>; James L. Pirkle<sup>1</sup>; Conrad P. Quinn<sup>1</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, GA*

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| <b>Session Room F: 3:00 – 5:00 pm</b><br><b>FTMS: INSTRUMENTATION</b><br>Julia Laskin, presiding |
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MOF pm 03:00 **High-Field Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Ultrahigh Mass Resolving Power, Mass Accuracy, Speed, and Dynamic Range;** Christopher L. Hendrickson<sup>1</sup>; Greg T. Blakney<sup>1</sup>; John P. Quinn<sup>1</sup>; Tanner M. Schaub<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*

MOF pm 03:20 **It's All About the Fields;** James E. Bruce<sup>1</sup>; Saiful Chowdhury<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Xiaoting Tang<sup>1</sup>; Si Wu<sup>1</sup>; Wei Yi<sup>1</sup>; Kai Zhang<sup>1</sup>; <sup>1</sup>*Washington State University, Pullman, WA*

MOF pm 03:40 **Theory and Practice of the Orbitrap Mass Analyzer;** Alexander A. Makarov<sup>1</sup>; <sup>1</sup>*Thermo Electron (Bremen) GmbH, Bremen, Germany*

MOF pm 04:00 **Development of a Novel Laser-Induced Acoustic Desorption (LIAD) "Fiberless" Probe Coupled with a Fourier-Transform Ion Cyclotron Resonance Mass Spectrometer;** Ryan C. Shea<sup>1</sup>; Putuma Gqamana<sup>1</sup>; Linan Yang<sup>1</sup>; Hilkka I. Kenttämä<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*

MOF pm 04:20 **Current Progress in Supercomputer Modeling of Ion Clouds Behavior in FT ICR Cells;** Eugene N. Nikolaev<sup>1</sup>; Ron M.A. Heeren<sup>2</sup>; Alexander M. Popov<sup>3</sup>; Alexander V. Pozdnev<sup>3</sup>; Konstantin S. Chingin<sup>1</sup>; Marija S. Sharova<sup>3</sup>; Wojciech Burakiewicz<sup>2</sup>; <sup>1</sup>*The Institute for Energy Problems of Chem. Physics, Moscow, Russia*; <sup>2</sup>*FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands*; <sup>3</sup>*Moscow State University, Moscow, Russia*

MOF pm 04:40 **Estimating Relative Isoaspartyl/Aspartyl Abundances Using ECD;** Jason Cournoyer<sup>1</sup>; Peter O'Connor<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*

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| <b>Session Room G: 3:00 – 5:00 pm</b><br><b>ANALYSIS OF POLYMER MIXTURES</b><br>Chrys Wesdemiotis, presiding |
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MOG pm 03:00 **Desorption Electrospray Ionisation (DESI) Mass Spectrometry and Tandem Mass Spectrometry of Low Molecular Weight Synthetic Polymers;** Anthony T. Jackson<sup>1</sup>; Jonathan P. Williams<sup>2</sup>; James H. Scrivens<sup>2</sup>; <sup>1</sup>*ICI Measurement Science Group, Redcar, UK*; <sup>2</sup>*University of Warwick, Coventry, UK*

MOG pm 03:20 **MALDI-TOF MS Analysis of Ballistic Materials;** Anthony P. Gies<sup>1</sup>; David M. Hercules<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*

MOG pm 03:40 **MALDI-ToF MS and GPC Analysis of an Ammonium Functionalized Polyester;** Mark A. Arnould<sup>1</sup>; Robin L. Sheppard<sup>1</sup>; <sup>1</sup>*Xerox Corporation, Webster, NY*

MOG pm 04:00 **A Simultaneous Multi-Sample On-Target Parallel Homogenization/Transfer Method for Solvent-Free MALDI-MS Analysis of Synthetic Polymers;** Sarah Trimpin<sup>1</sup>; Charles N. McEwen<sup>2</sup>; <sup>1</sup>*Oregon Health & Science University, CROET, Portland, OR*; <sup>2</sup>*DuPont Corporate Center for Analytical Sciences, Wilmington, DE*

MOG pm 04:20 **Disilyloxane-Containing Silsesquioxanes Revealed by ESI-FTMS;** Huiping Chen<sup>1</sup>; Bizhong Zhu<sup>1</sup>; <sup>1</sup>*Dow Corning Corporation, Midland, MI*

MOG pm 04:40 **MALDI- and ESI-TOF Mass Spectrometry for Two-Dimensional Polymer Characterization;** Steffen M. Weidner<sup>1</sup>; Jana Falkenhagen<sup>1</sup>; Ralph-Peter Krueger<sup>1</sup>; Ulrich Just<sup>1</sup>; <sup>1</sup>*Federal Inst. for Materials Research and Testing, Berlin, Germany*

## MONDAY ORAL SESSIONS

### 5:30 – 7:00 pm: WORKSHOPS

#### **Hyphenation of Separation Science with MS: Current Practice and Future Perspective.**

Arranged by LC/MS  
Interest Group. Gérard Hopfgartner, presiding  
Session Room A

#### **Where Is Metabolite Profiling Being Used?**

Arranged by Metabolomics Interest Group  
Grace O'Maille and Ben Bolanos, presiding  
Session Room B

#### **New Instrumentation for Metabolite Identification.**

Arranged by Drug Metabolism & Pharmacokinetics Int Grp  
Walter Korfmacher, Ajai Chaudhary, and  
Jonathan Josephs, presiding  
Session Room C

#### **Critical Role of Mass Accuracy**

Arranged by FTMS Interest Group  
Michael A. Freitas and Christopher L. Hendrickson, presiding  
Session Room D

#### **Novel Ionization Techniques.**

Arranged by Fundamentals  
Interest Group. Kelly Sullivan and JC Poutsma, presiding  
Session Room E

#### **Forensics.**

Arranged by Forensics Interest Group  
John Reynolds, presiding  
Session Room F

#### **NIH Electronic Submission of Grant Applications: Are You Ready?**

Douglas Sheeley, presiding  
Session Room G

## TUESDAY ORAL SESSIONS

### TUESDAY MORNING, MAY 30

**8:00 – 8:45 am: PLENARY LECTURE**  
**R. Graham Cooks: Recipient of the Award for a Distinguished Contribution in Mass Spectrometry**

**8:45 – 10:15am: POSTER SESSION AND EXHIBITS**  
 Tuesday posters. Authors of odd-numbered posters present.  
 See list beginning on page 80.

### 10:15 am – 12:15 pm: PARALLEL SESSIONS

#### Session Room A: 10:15 am – 12:15 pm METABOLITE IDENTIFICATION USING HYPHENATED MS TECHNIQUES

James A. Yergey, presiding

- TOA am 10:15 **Data Independent Acquisition for Metabolite Identification Using Alternating High and Low Energy Scans with a QqTof Instrument;** Russell Mortishire-Smith<sup>1</sup>; Mark Wrona<sup>2</sup>; Desmond O'Connor<sup>1</sup>; Kevin P. Bateman<sup>2</sup>; <sup>1</sup>Merck Sharp and Dohme, Harlow, United Kingdom; <sup>2</sup>Merck Frosst, Montreal, Canada
- TOA am 10:35 **Towards Comprehensive Detection of Metabolites Using Polarity Switching Data Collection and Post-Acquisition Data Mining Strategies;** Carmal Seto<sup>1</sup>; Gary Impey<sup>1</sup>; <sup>1</sup>Applied Biosystems/MDS Sciex, Concord, Canada
- TOA am 10:55 **Characterization of *in vivo* and *in vitro* Metabolites of a PDE4 Inhibitor By LC-MS/MS and 1H NMR;** Chandra Prakash<sup>1</sup>; Miao Zhuang<sup>1</sup>; <sup>1</sup>Pfizer Global Reserach & Development, Groton, CT
- TOA am 11:15 **Cross Correlation Algorithms Combined with MS/MS Spectral Libraries of Structural Analogues for the Automated Regional Assignment of Metabolic Modification;** Jonathan Josephs<sup>1</sup>; Stephen Johnson<sup>1</sup>; Brian Claus<sup>1</sup>; Robert Langish<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Hopewell, NJ
- TOA am 11:35 **Metabolite Prediction and a Two-Step Metabolite Identification Approach in Early Drug Discovery;** Peter L Jacobs<sup>1</sup>; Harrie AM Peters<sup>1</sup>; Lars Ridder<sup>1</sup>; Markus Wagener<sup>1</sup>; <sup>1</sup>NV Organon, Oss, The Netherlands
- TOA am 11:55 **What and How Much Information Can We Really Extract in an Automated Manner from LC/MS Data?** Robyn A. Rourick<sup>1</sup>; John P. Walsh<sup>1</sup>; Bayliss Mark<sup>23</sup>; Vitaly Lashin<sup>23</sup>; <sup>1</sup>Kalypsys, Inc., San Diego, CA; <sup>2</sup>Advanced Chemistry Development, Toronto, Canada; <sup>3</sup>Advanced Chemistry Development, Moscow, Russia

#### Session Room B: 10:15 am – 12:15 pm NEW ION TRAPPING TECHNOLOGIES

Chris Hendrickson, presiding

- TOB am 10:15 **Driving Ion Axial Motion in the Orbitrap Mass Analyzer;** Robert J. Noll<sup>1</sup>; Qizhi Hu<sup>1</sup>; Richard H. Perry<sup>1</sup>; Guangxiang Wu<sup>1</sup>; Wolfgang R. Plass<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Justus-Liebig-Universität, Giessen, Germany
- TOB am 10:35 **Squeezing a Camel through the Eye of a Needle: a Curved Linear Trap for Pulsed Ion Injection into Orbitrap Analyzer;** Alexander Kholomeev<sup>1</sup>; Alexander Makarov<sup>1</sup>; Eduard Denisov<sup>1</sup>; Oliver Lange<sup>1</sup>; Wilko Balschun<sup>1</sup>; Stevan Horning<sup>1</sup>; <sup>1</sup>Thermo Electron (Bremen) GmbH, Bremen, Germany
- TOB am 10:55 **Hybrid Linear Iontrap-Orbitrap Mass Spectrometer for On- and Offline Top-Down Characterization;** Leonie F. Waanders<sup>1</sup>; Boris Macek<sup>1</sup>; Tiziana Bonaldi<sup>1</sup>; Michiel Vermeulen<sup>1</sup>; Jesper V. Olsen<sup>1</sup>; Reinaldo Almeida<sup>2</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max-Planck Institute for Biochemistry, Martinsried, Germany; <sup>2</sup>Advion Biosciences, Norwich, UK
- TOB am 11:15 **Neutral Loss Triggered ETD for Characterization of Post Translational Modifications;** Ralf Hartmer<sup>1</sup>; Markus Lubeck<sup>1</sup>; Carsten Baessmann<sup>1</sup>; Andreas Brekenfeld<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany
- TOB am 11:35 **Improvement of ETD Efficiency for Low Charge States via an Automated Supplemental Activation Tool;** Danielle L. Swaney<sup>1</sup>; Graeme C. McAlister<sup>1</sup>; Jae C. Schwartz<sup>2</sup>; John E.P. Syka<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin at Madison, Madison, WI; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- TOB am 11:55 **A Novel 3D Linear Ion Trap for a High Efficiency Linked Scan Mass Spectrometer;** Andrew N. Krutchinsky<sup>1</sup>; Herbert Cohen<sup>2</sup>; Brian T. Chait<sup>2</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>Rockefeller University, New York, NY



## TUESDAY ORAL SESSIONS

| <b>Session Room C: 10:15 am – 12:15 pm</b><br><b>CHALLENGE OF DYNAMIC RANGE IN</b><br><b>PROTEOMICS: NOVEL APPROACHES IN</b><br><b>SEPARATION, HIGH MASS ACCURACY AND</b><br><b>QUANTIFICATION</b><br>David Han, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b>Session Room D: 10:15 am – 12:15 pm</b><br><b>GLYCOMICS</b><br>Heather Desaire, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
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| <p>TOC am 10:15 <b>Challenges of Dynamic Range in Shotgun Proteomics</b>; <u>John R. Yates</u><sup>1</sup>; <sup>1</sup><i>The Scripps Research Institute, LaJolla, CA</i></p> <p>TOC am 10:35 <b>Strategies to Overcome the Dynamic Range Problem in Proteomics: Repeated Identification, Subcellular Fractionation, and Enrichment Approaches for Higher Proteome Coverage</b>; <u>Linfeng Wu</u><sup>1</sup>; Sun-IL Hwang<sup>1</sup>; Debbie Lundgren<sup>1</sup>; Karim Rezaul<sup>1</sup>; Viveka Mayya<sup>1</sup>; Long J. Lu<sup>2</sup>; Mark Gerstein<sup>2</sup>; David Han<sup>1</sup>; <sup>1</sup><i>University of Connecticut Health Center, Farmington, CT</i>; <sup>2</sup><i>Yale University, New Haven, CT</i></p> <p>TOC am 10:55 <b>Substoichiometric Posttranslational Modifications: Unexpected Challenge for Dynamic Range in Proteomics</b>; <u>Roman A. Zubarev</u><sup>1</sup>; Michael L. Nielsen<sup>1</sup>; Mikhail M. Savitski<sup>1</sup>; <sup>1</sup><i>Uppsala University, Uppsala, Sweden</i></p> <p>TOC am 11:15 <b>High Throughput Quantitative Proteomics with High Mass Accuracy: Novel Software for Assessing the Role of Dynamic Range in Quantitation</b>; <u>Corey E. Bakalarski</u><sup>1</sup>; Joshua E. Elias<sup>1</sup>; Scott A. Gerber<sup>2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup><i>Harvard Medical School, Boston, MA</i>; <sup>2</sup><i>Dartmouth Medical School, Hanover, NH</i></p> <p>TOC am 11:35 <b>Novel Strategy for Rapid Screening and Quantification of Biomarkers in Serum</b>; <u>Bruno Domon</u><sup>1</sup>; Jianru Zeng-Stahl<sup>2</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup><i>IMSB - ETH Zurich, Zurich, Switzerland</i>; <sup>2</sup><i>Applied Biosystems, Darmstadt, Germany</i></p> <p>TOC am 11:55 <b>XMudPIT – A Novel Approach for Multidimensional Separation of Peptides with Liquid Chromatography/Mass Spectrometry</b>; <u>Johannes A. Hewel</u><sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup><i>The Scripps Research Institute, La Jolla, CA</i></p> | <p>TOD am 10:15 <b>Specificity of Glycosaminoglycan Binding to CCR2 Chemokines: Significance of Sulfation Binding sites</b>; <u>Julie A. Leary</u><sup>1</sup>; Matthew D. Sweeney<sup>1</sup>; <sup>1</sup><i>University of California, Davis, CA</i></p> <p>TOD am 10:35 <b>Comparative Glycoproteomics of the <i>Trypanosoma Cruzi</i> Lifecycle</b>; <u>Ron Orlando</u><sup>1</sup>; James Atwood<sup>1</sup>; Art Nuccio<sup>1</sup>; Fernanda Ludolf<sup>1</sup>; Brent Weatherly<sup>2</sup>; Rick Tarleton<sup>2</sup>; <sup>1</sup><i>CCRC/UGA, Athens, GA</i>; <sup>2</sup><i>Department of Cellular Biology, UGA, Athens, GA</i></p> <p>TOD am 10:55 <b>Comparative Glycomic Profiling through Solid-phase Deuteromethylation and Permethylolation</b>; <u>Yehia Mechref</u><sup>1</sup>; Pilsoo Kang<sup>2</sup>; Milos V. Novotny<sup>2</sup>; <sup>1</sup><i>METACyt Biochemical Analysis Center, Bloomington, IN 47405</i>; <sup>2</sup><i>Department of Chemistry, Indiana University, Bloomington, IN</i></p> <p>TOD am 11:15 <b>Novel Tags for the Stable Isotopic Labeling of Carbohydrates and Quantitative Analysis by Mass Spectrometry</b>; <u>Michael J. Bowman</u><sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup><i>Boston University School of Medicine, Boston, MA</i></p> <p>TOD am 11:35 <b>Using Ion-Pairing for Acidic Glycopeptide Analysis</b>; <u>Ying Zhang</u><sup>1</sup>; Hui Jiang<sup>1</sup>; Eden P. Go<sup>1</sup>; Janet Irungu<sup>1</sup>; Dilusha S. Dalpathado<sup>1</sup>; George R. Bousfield<sup>2</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup><i>Department of Chemistry, University of Kansas, Lawrence, KS</i>; <sup>2</sup><i>Department of Biology, Wichita State University, Wichita, KS</i></p> <p>TOD am 11:55 <b>Quantification, Isobar Resolution and High Throughput Analysis of Carbohydrate Glycans</b>; <u>Vernon N. Reinhold</u><sup>1</sup>; David J. Ashline<sup>1</sup>; Anthony J. Lapadula<sup>1</sup>; Hailong Zhang<sup>1</sup>; Justin M. Prien<sup>1</sup>; <sup>1</sup><i>Center for Structural Biology, UNH, Durham, NH</i></p> |

## TUESDAY ORAL SESSIONS

### Session Room E: 10:15 am – 12:15 pm DETECTION AND DECONTAMINATION OF INDOOR ENVIRONMENTS

Gary Groenewold, presiding

- TOE am 10:15 **Addressing Physio-chemical Controls on Indoor Detection and Decontamination of Chemical Warfare Agents;** Adam H Love<sup>1</sup>; Carolyn J Koester<sup>1</sup>; William J Smith<sup>1</sup>; Bradley R Hart<sup>1</sup>; M. Lee Davisson<sup>1</sup>; Sharon J Shields<sup>1</sup>; Armando Alcaraz<sup>1</sup>; John G Reynolds<sup>1</sup>; <sup>1</sup>*Lawrence Livermore National Laboratory, Livermore, CA*
- TOE am 10:35 **Analysis and Detection of Chemical Warfare Agent Surrogates on Polyurethane Foams and Fabrics by Thermal Desorption with Mass Spectrometry Detection;** Theodore T. Borek<sup>1</sup>; Deborah Hunka<sup>1</sup>; <sup>1</sup>*Sandia National Laboratories, Albuquerque, NM*
- TOE am 10:55 **Modification of Metal Contaminants on Oxide Surfaces by Laser Irradiation;** Anita K. Gianotto<sup>1</sup>; Recep Avci<sup>2</sup>; Muhammedin Deliorman<sup>2</sup>; Eric Williams<sup>2</sup>; Marnie M. Cortez<sup>1</sup>; Robert V. Fox<sup>1</sup>; Gary S. Groenewold<sup>1</sup>; <sup>1</sup>*Idaho National Laboratory, Idaho Falls, ID*; <sup>2</sup>*Montana State University, Bozeman, MT*
- TOE am 11:15 **Rapid Separation and Identification of CBW Agents in Food and Consumer Matrices using FAIMS-MS Technology;** Beata M. Kolakowski<sup>1</sup>; Margaret A. McCooye<sup>1</sup>; Zoltan Mester<sup>1</sup>; Paul A. D'Agostino<sup>2</sup>; <sup>1</sup>*NRC Institute for National Measurement Standards, Ottawa, Canada*; <sup>2</sup>*Defence Research and Development Canada, Suffield, Canada*
- TOE am 11:35 **Detection of Ricin in Food Matrices by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry;** Frederick J. Cox<sup>1</sup>; Lindy Dejarme<sup>2</sup>; Edward R. Richter<sup>3</sup>; <sup>1</sup>*Battelle Eastern Science & Tech Center, Aberdeen, MD*; <sup>2</sup>*Battelle, Columbus, OH*; <sup>3</sup>*Richter International, Columbus, OH*
- TOE am 11:55 **Rapid Identification and Area Delineation of Dispersed Chemicals using a Surface-Sampling TOFMS, Ion Correlation Program, and Inexpensive Autosampler;** Andrew H. Grange<sup>1</sup>; Robert J. Cody, Jr.<sup>2</sup>; G. Wayne Sovocool<sup>1</sup>; <sup>1</sup>*U.S. EPA, ORD, NERL, ESD, Las Vegas, NV*; <sup>2</sup>*JEOL USA, Inc., Peabody, MA*

### Session Room F: 10:15 am – 12:15 pm INTACT PROTEIN SEPARATIONS AND MS

Martha M. Vestling, presiding

- TOF am 10:15 **Analysis of Human Esophagus Tissue Proteins through Automated Integration of Monolithic-LC with On-Plate Digestion for MALDI-MS and Intact MW Analysis;** David M. Lubman<sup>1</sup>; Chul Yoo<sup>1</sup>; Suping Zheng<sup>1</sup>; Jia Zhao<sup>1</sup>; Manoj Pal<sup>1</sup>; Katie Hersberger<sup>1</sup>; Christian G. Huber<sup>2</sup>; David G. Beer<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Saarland University, Saarbrücken, Germany*
- TOF am 10:35 **When Mass Spectrometry “Gels”;** Rachel R Ogorzalek Loo<sup>1</sup>; Yanan Yang<sup>1</sup>; Ivory Peng<sup>1</sup>; Jason Dunsmore<sup>1</sup>; Jentiae Shiea<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>*University of California, Los Angeles, CA*; <sup>2</sup>*National Sun Yat-Sen University, Kaohsiung, Taiwan*
- TOF am 10:55 **High-throughput Identification of Intact Proteins and Comparative Analysis of *Saccharomyces Cerevisiae* using <sup>14</sup>N/<sup>15</sup>N Metabolic Labeling and Top-Down Proteomics;** Bryan A. Parks<sup>1</sup>; Jon T. Ferguson<sup>1</sup>; Yi Du<sup>1</sup>; Patricia Burke<sup>1</sup>; Kurt Kwast<sup>1</sup>; Allen Marshall<sup>2</sup>; Chris Hendrickson<sup>2</sup>; Tanner Schaub<sup>2</sup>; Neil Kelleher<sup>1</sup>; <sup>1</sup>*Univ. of Illinois, Champaign, Illinois*; <sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee, Florida*
- TOF am 11:15 **Reversed-Phase LC/UV/MS for Characterizing Heterogeneity of Intact Monoclonal Antibodies;** Thomas M. Dillon<sup>1</sup>; Douglas S. Rehder<sup>1</sup>; Gary D. Pipes<sup>1</sup>; Margaret Ricci<sup>1</sup>; Himanshu S. Gadgil<sup>1</sup>; Dirk Chelius<sup>1</sup>; Da Ren<sup>1</sup>; Pavel V. Bondarenko<sup>1</sup>; <sup>1</sup>*Amgen, Department of Pharmaceuticals, Thousand Oaks, California*
- TOF am 11:35 **MALDI Proteomics Chip;** Harrison K. Musyimi<sup>1</sup>; Hamed Shadpour<sup>1</sup>; Steven A. Soper<sup>2</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>*Louisiana State University, Baton Rouge, LA*; <sup>2</sup>*Center for BioModular Multi-Scale Systems (CBM2), Baton Rouge, LA*
- TOF am 11:55 **Rapid, Comprehensive and High-Resolution Intact Protein Separation for Proteomics;** Andrew R Pitt<sup>1</sup>; Karl E V Burgess<sup>1</sup>; Ken Cook<sup>2</sup>; Remco Swart<sup>3</sup>; <sup>1</sup>*University of Glasgow, Glasgow, UK*; <sup>2</sup>*Dionex UK, Camberley, UK*; <sup>3</sup>*Dionex, Amsterdam, Netherlands*

## TUESDAY ORAL SESSIONS

### Session Room G: 10:15 am – 12:15 pm ORGANIC REACTION MECHANISMS

Douglas P. Ridge, presiding

- TOG am 10:15 **Organic Reaction Mechanisms in Mass Spectrometry;** Hilkka I. Kenttamaa<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- TOG am 10:35 **Gas Phase Studies of Nucleophilic Substitution and Elimination Reactions Utilizing Deuterium Kinetic Isotope Effects;** Veronica M. Bierbaum<sup>1</sup>; Stephanie M. Villano<sup>1</sup>; Nicole Eyet<sup>1</sup>; Shuji Kato<sup>1</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*
- TOG am 10:55 **Gas Phase Reactivity of Adenine and Derivatives: How Damaged Bases Differ from Natural Nucleobases and Unusual C-H Acidities;** Seema Sharma<sup>1</sup>; Xiaofeng Shi<sup>1</sup>; Meng Xu<sup>1</sup>; Jeehiun K. Lee<sup>1</sup>; <sup>1</sup>*Rutgers University, Piscataway, NJ*
- TOG am 11:15 **H/D Exchange of Deprotonated Amino Acids;** Zhixin Tian<sup>1</sup>; Dana Reed<sup>1</sup>; Steven R Kass<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*
- TOG am 11:35 **Reactions of Distonic Radical Anions with Molecular Oxygen: Trapping Peroxyl Radicals in the Gas Phase;** David G. Harman<sup>1</sup>; Stephen J. Blanksby<sup>1</sup>; <sup>1</sup>*University of Wollongong, Wollongong, Australia*
- TOG am 11:55 **Investigation of Aromatic s,s-Biradicals' Reactions with Nucleosides and Oligonucleotides in an FT-ICR Mass Spectrometer;** Linan Yang<sup>1</sup>; Ryan C. Shea<sup>1</sup>; Hilkka I. Kenttamaa<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*

### TUESDAY AFTERNOON, MAY 30

#### 12:30 – 1:30 pm: INTEREST GROUP MEETINGS

##### Flavors, Fragrances and Foodstuffs Interest Group Meeting

Dennis F. Swijter, presiding  
Room 617

##### Forensics Interest Group Meeting

John Reynolds, presiding  
Room 618

##### Polymeric Materials Interest Group Meeting

Patricia Peacock, presiding  
Room 619

##### Analytical Lab Managers Interest Group Meeting

Amy Harms, presiding  
Room 620

##### Metal Ion Interest Group Meeting

Mary T. Rodgers, presiding  
Session Room E

##### Hydrogen Exchange and Covalent Labeling

Interest Group Meeting  
John R. Engen, presiding  
Session Room G

#### 1:30 – 3:00 pm: POSTER SESSION AND EXHIBITS

Tuesday posters. Authors of even-numbered posters present.  
See list beginning on page 80.

#### 3:00 – 5:00 pm: PARALLEL SESSIONS

### Session Room A: 3:00 – 5:00 pm METABOLITE PROFILING

Oliver Fiehn, presiding

- TOA pm 03:00 **Metabolomics by Chip Based Nanospray Infusion and its Application in Drug Development;** Olaf Boernsen<sup>1</sup>; Stephan Gatzek<sup>1</sup>; <sup>1</sup>*Novartis Pharma AG, Basel, Switzerland*
- TOA pm 03:20 **Investigation of Analytical Variation in Metabonomic Analysis Using LC-MS;** Tim Sangster<sup>1</sup>; Toby Athersuch<sup>2</sup>; Ian Wilson<sup>3</sup>; Lyle Burton<sup>4</sup>; Julie Wingate<sup>4</sup>; <sup>1</sup>*Huntingdon Life Sciences, East Millstone, NJ*; <sup>2</sup>*Imperial College London, London, UK*; <sup>3</sup>*AstraZeneca, Macclesfield, UK*; <sup>4</sup>*Applied Biosystems / MDS Sciex, Toronto, Canada*
- TOA pm 03:40 **The Use of Isotope Ratio Measurements to Reduce the Number of Candidate Elemental Compositions from Accurate Mass Determination;** Kirsten Hobby<sup>1</sup>; Robert Bateman<sup>1</sup>; <sup>1</sup>*Water Corporation, Micromass MS Technologies, Manchester, UK*
- TOA pm 04:00 **Ionizable Isotopic Labeling Reagents for Relative Quantification and Structural Elucidation of Metabolites;** Michael R. Shortreed<sup>1</sup>; Shane M. Lamos<sup>1</sup>; Brian L. Frey<sup>1</sup>; Margaret F. Philips<sup>1</sup>; Peter J. Belshaw<sup>1</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*
- TOA pm 04:20 **Metabolomic Profiling of Brain Tissue Extracts from Alcohol Preferring and Non-Preferring Rats; Toward Identification of Alcoholism Biomarkers;** Yehia Mechref<sup>2</sup>; Jason Starkey<sup>1</sup>; Tatiana Rojkovicova<sup>1</sup>; Ali Kettani<sup>3</sup>; Catherine Stacey<sup>3</sup>; William J. McBride<sup>4</sup>; Milos V. Novotny<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Indiana University, Bloomington, IN*; <sup>2</sup>*METACyt Biochemical Analysis Center, Bloomington, IN*; <sup>3</sup>*Bruker Daltonics, Billerica, MA*; <sup>4</sup>*Department of Psychiatry, Indiana University, Indianapolis, IN*
- TOA pm 04:40 **Differential Amino Acid Flux Analyses of E. coli by On-Line Sample Preconcentration with Capillary Electrophoresis-Ion Trap Mass Spectrometry;** Richard Lee<sup>1</sup>; Philip Britz-McKibbin<sup>1</sup>; <sup>1</sup>*McMaster University, Hamilton, Canada*

## TUESDAY ORAL SESSIONS

| <b>Session Room B: 3:00 – 5:00 pm</b><br><b>MS CONTRIBUTION TO THE</b><br><b>IMMUNOLOGY OF DISEASE</b><br>Anthony W. Purcell, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>Session Room C: 3:00 – 5:00 pm</b><br><b>CLINICAL MASS SPECTROMETRY ASSAYS</b><br>Donald H. Chace, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
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| <p>TOB pm 03:00 <b>Characterization of Immune Responses to Pathogen Challenge by MS Based Epitope Excision;</b> <u>Kenneth B. Tomer</u><sup>1</sup>; Christine Hager-Braun<sup>1</sup>; Roxana Iacob<sup>1</sup>; Jason Williams<sup>1</sup>; Jeffery F. Kuhn<sup>1</sup>; <sup>1</sup>NIEHS/NIH, Research Triangle Park, NC</p> <p>TOB pm 03:20 <b>Proteomics in Islet Diabetes Research Using Surface Enhanced Laser Desorption/Ionization Time-of-Flight Mass Spectrometry;</b> <u>Peter Bergsten</u><sup>1</sup>; Jian-Man Lin<sup>1</sup>; Henrik Ortsäter<sup>1</sup>; Tea Sundsten<sup>1</sup>; <sup>1</sup>Uppsala university, Uppsala, Sweden</p> <p>TOB pm 03:40 <b>Direct Discovery of Class I HLA Antigens that Distinguish Virus-Infected and Cancerous Cells;</b> <u>William H. Hildebrand</u><sup>1</sup>; Angela Wahl<sup>1</sup>; Wilfried Bardet<sup>1</sup>; Melva Gonzalez<sup>1</sup>; Ken W. Jackson<sup>1</sup>; Jon Weidanz<sup>2</sup>; Fredda Schafer<sup>1</sup>; <sup>1</sup>University of Oklahoma HSC, Oklahoma City, OK; <sup>2</sup>Texas Tech University, Amarillo, TX</p> <p>TOB pm 04:00 <b>Mass Spectrometry Contributions to Immunology of Disease;</b> <u>Nina Hillen</u><sup>1</sup>; <sup>1</sup>Institute for Cell Biology, Tuebingen, Germany</p> <p>TOB pm 04:20 <b>Assessing the Diversity of the Immunoepitome;</b> <u>Frank R Rooney</u><sup>1</sup>; Nicholas A Williamson<sup>2</sup>; <sup>1</sup>Applied Biosystems, Melbourne, Australia; <sup>2</sup>Bio21, University of Melbourne, Victoria, Australia</p> <p>TOB pm 04:40 <b>Identification of Modified MHC Class II Self Peptides from Spleen of <i>Listeria</i> Infected Mice;</b> <u>James J Walters</u><sup>1</sup>; Anish Suri<sup>1</sup>; Jamie Ireland<sup>1</sup>; Shirley Petzold<sup>1</sup>; Emil R Unanue<sup>1</sup>; Michael L Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO</p> | <p>TOC pm 03:00 <b>The Growing Acceptance of Mass Spectrometry in Routine Clinical Analysis;</b> <u>Michael Morris</u><sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK</p> <p>TOC pm 03:20 <b>Analysis of Variance-Principal Component Analysis: A Soft Tool for Proteomic Discovery of MALDI-MS Biomarkers from Amniotic Fluids;</b> <u>Alfred L Yergey</u><sup>1</sup>; Peter de B Harrington<sup>2</sup>; Nancy E Vieira<sup>1</sup>; Roberto Romero<sup>1</sup>; <sup>1</sup>NICHD, NIH, Bethesda, MD; <sup>2</sup>Chemistry &amp; Biochemistry, Ohio University, Athens, OH</p> <p>TOC pm 03:40 <b>MS-Based High Throughput Identification and Strain Typing of Clinically Relevant Bacteria: <i>Acinetobacter baumannii</i> and Other Drug Resistant Pathogens;</b> <u>Steven A. Hofstadler</u><sup>1</sup>; Mark Eshoo<sup>1</sup>; Ranga Sampath<sup>1</sup>; Christian Massire<sup>1</sup>; Joseph Ecker<sup>1</sup>; Larry Blyn<sup>1</sup>; Tom Hall<sup>1</sup>; Ray Ranken<sup>1</sup>; Thuy Panella<sup>1</sup>; Cristina Ivy<sup>1</sup>; Yun Jiang<sup>1</sup>; Amy Schink<sup>1</sup>; Jared Drader<sup>1</sup>; Dave Ecker<sup>1</sup>; <sup>1</sup>Ibis Division of Isis Pharmaceuticals, Carlsbad, CA</p> <p>TOC pm 04:00 <b>Clinical Mass Spectrometry Based Immunoassays;</b> <u>Urban A. Kiernan</u><sup>1</sup>; Kemmons A. Tubbs<sup>1</sup>; Eric E. Niederkofler<sup>1</sup>; Dobrin Nedelkov<sup>1</sup>; Allan L. Bieber<sup>1</sup>; Randall W. Nelson<sup>1</sup>; <sup>1</sup>Intrinsic Bioprobes, Inc, Tempe, AZ</p> <p>TOC pm 04:20 <b>Profiling Oligosaccharides Shed By Cells for Disease Marker Discovery;</b> <u>Crystal Kirmiz</u><sup>1</sup>; Bensheng Li<sup>1</sup>; Caroline Chu<sup>1</sup>; Brian Clowers<sup>1</sup>; Hyunjo An<sup>1</sup>; Suzanne Miyamoto<sup>1</sup>; Ralph DeVere White<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA</p> <p>TOC pm 04:40 <b>Selective Profiling of Proteins in Cancer Cells from Fine Needle Aspirates by MALDI-TOF Mass Spectrometry;</b> <u>Pierre Chaurand</u><sup>1</sup>; Joseph M Amann<sup>1</sup>; Adriana Gonzalez<sup>1</sup>; James A. Mobley<sup>1</sup>; Pierre P. Massion<sup>1</sup>; David P. Carbone<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN</p> |

## TUESDAY ORAL SESSIONS

| <b>Session Room D: 3:00 – 5:00 pm</b><br><b>CARBOHYDRATES</b><br>Jane Thomas-Oates, presiding                                                                                                                                                                                                                                                                                                              | <b>Session Room E: 3:00 – 5:00 pm</b><br><b>NEW AND EMERGING CONTAMINANTS</b><br>Enrico Davoli, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
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| TOD pm 03:00 <b>IRMPD of Potential Glycan Markers for Diseases;</b> <u>Carlito B. Lebrilla</u> <sup>1</sup> ; <sup>1</sup> <i>University of California, Davis, Davis, CA</i>                                                                                                                                                                                                                               | TOE pm 03:00 <b>Emerging Environmental Contaminants and Current Issues;</b> <u>Susan D. Richardson</u> <sup>1</sup> ; <sup>1</sup> <i>U.S. EPA, National Exposure Research Laboratory, Athens, GA</i>                                                                                                                                                                                                                                                                                                                                                                                             |
| TOD pm 03:20 <b>Online Normal-phase Capillary Liquid Chromatography – MALDI-TOF/TOF Tandem Mass Spectrometry for the Detailed Structure Elucidation of Oligosaccharides;</b> <u>Elaine Stephens</u> <sup>1</sup> ; Sarah L. Maslen <sup>1</sup> ; Alex Adam <sup>2</sup> ; <sup>1</sup> <i>Chemistry Department, Cambridge University, Cambridge, UK;</i> <sup>2</sup> <i>Dionex UK Ltd, Camberley, UK</i> | TOE pm 03:40 <b>Illicit Drugs as Emerging Contaminants: Residues in Surface Waters Allow Monitoring of Community Drug Abuse;</b> <u>Roberto Fanelli</u> <sup>1</sup> ; Sara Castiglioni <sup>2</sup> ; Chiara Chiabrando <sup>1</sup> ; Renzo Bagnati <sup>1</sup> ; Ettore Zuccato <sup>1</sup> ; <sup>1</sup> <i>Istituto Mario Negri, Milano, Italy;</i> <sup>2</sup> <i>University of Insubria, Varese, Italy</i>                                                                                                                                                                             |
| TOD pm 03:40 <b>Structural Glycomics of the Human Parasite <i>Schistosoma mansoni</i>;</b> <u>Manfred Wuhrer</u> <sup>1</sup> ; Cornelis H. Hokke <sup>1</sup> ; André M. Deelder <sup>1</sup> ; <sup>1</sup> <i>Leiden University Medical Center, Leiden, the Netherlands</i>                                                                                                                             | TOE pm 04:00 <b>Mass Spectrometric Study of Environmental Contamination Related to Military Training;</b> <u>Denise K. MacMillan</u> <sup>1</sup> ; Randy D. Laubscher <sup>2</sup> ; Sally L. Yost <sup>2</sup> ; Judy C. Pennington <sup>3</sup> ; <sup>1</sup> <i>Engineer Research and Development Center, Omaha, NE;</i> <sup>2</sup> <i>SpecPro Incorporated, Huntsville, AL;</i> <sup>3</sup> <i>Engineer Research and Development Center, Vicksburg, MS</i>                                                                                                                               |
| TOD pm 04:00 <b>Structural Characterization of Lipooligosaccharides from Gram Negative Bacteria Using Multiple-Stage MS on a vMALDI Linear Ion Trap Mass Spectrometer;</b> <u>Simon Allen</u> <sup>1</sup> ; Deborah M. Post <sup>1</sup> ; Bradford W. Gibson <sup>1</sup> ; <sup>1</sup> <i>Buck Institute for Age Research, Novato, CA</i>                                                              | TOE pm 04:20 <b>Real-Time Measurement of Woodsmoke and Hydrocarbon Tracer Species in Urban Airshed Transects by Mobile Membrane Introduction Tandem Mass Spectrometry (MIMS-MS/MS);</b> Alexander J. Thompson <sup>1</sup> ; Charles W. LeBlanc <sup>2</sup> ; Chris D. Simpson <sup>3</sup> ; Erik T. Krogh <sup>1</sup> ; <u>Chris G. Gill</u> <sup>1</sup> ; <sup>1</sup> <i>Applied Environmental Research Labs, Malaspina, Nanaimo, BC, Canada;</i> <sup>2</sup> <i>Environmental Division, Cantest Ltd., Burnaby, BC, Canada;</i> <sup>3</sup> <i>University of Washington, Seattle, WA</i> |
| TOD pm 04:20 <b>Structure Studies of Sulfated Carbohydrates Using ECD and EDD;</b> Jeremy J. Wolff <sup>1</sup> ; <u>I. Jonathan Amster</u> <sup>1</sup> ; <sup>1</sup> <i>University of Georgia, Athens, GA</i>                                                                                                                                                                                           | TOE pm 04:40 <b>Proteomics Methods for the Detection and Quantification of Toxins and Allergens in Foods;</b> <u>John H. Callahan</u> <sup>1</sup> ; Kevin J. Shefcheck <sup>1</sup> ; Steven M. Musser <sup>1</sup> ; <sup>1</sup> <i>FDA/CFSAN, College Park, MD</i>                                                                                                                                                                                                                                                                                                                            |
| TOD pm 04:40 <b>Comparison of Methods for the Simultaneous Detection of O-GlcNAc Modified and Phosphopeptides;</b> <u>Lauren E. Ball</u> <sup>1</sup> ; Maria G. Buse <sup>1</sup> ; <sup>1</sup> <i>Medical University of South Carolina, Charleston, SC</i>                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

## TUESDAY ORAL SESSIONS

| <b>Session Room F: 3:00 – 5:00 pm</b><br><b>HYDROCARBONS TO PETROLEUM</b><br>William J. Simonsick, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                          | <b>Session Room G: 3:00 – 5:00 pm</b><br><b>ELEMENTAL AND ISOTOPIC MS IN BIOLOGY</b><br>David W. Koppenaal, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
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| TOF pm 03:00 <b>Soft Photon Ionization TOFMS Coupled to Gas Chromatography: Novel GCxMS Approach for Comprehensive Characterization of Complex Hydrocarbon Samples;</b> <u>Ralf Zimmermann</u> <sup>1</sup> ;                                                                                                                                                                                                                                                                                                                                                         | TOG pm 03:00 <b>Determination of Intramolecular &amp;delta; <sup>13</sup>C From Fragments of Incomplete Pyrolysis in the Lactic Acid Analogue Propylene Glycol;</b> <u>Christopher J. Wolyniak</u> <sup>1</sup> ;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| Werner Welthagen <sup>1</sup> ; Marc Gonin <sup>2</sup> ; Katrin Fuhrer <sup>2</sup> ; Fabian Mühlberger <sup>1</sup> ; <sup>1</sup> GSF Research Centre and University Augsburg, Oberschleissheim, Germany; <sup>2</sup> TOFWERK, Thun, Switzerland                                                                                                                                                                                                                                                                                                                  | Gavin L. Sacks <sup>1</sup> ; J. Thomas Brenna <sup>1</sup> ; <sup>1</sup> Cornell University, Ithaca, NY                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| TOF pm 03:20 <b>Molecular Profiling of Petroleum and Petrochemicals by GC-FIMS;</b> <u>Chang Hsu</u> <sup>1</sup> ; Charles Yarbrough <sup>2</sup> ; Ricky Pujol <sup>1</sup> ; Haven Aldrich <sup>1</sup> ; <sup>1</sup> ExxonMobil Process Research Laboratories, Baton Rouge, LA; <sup>2</sup> ExxonMobil Chemical Co., Baton Rouge, LA                                                                                                                                                                                                                            | TOG pm 03:20 <b>New Tools for Elemental and Isotopic MS in Biology;</b> <u>Gary Hieftje</u> <sup>1</sup> ; Francisco Andrade <sup>1</sup> ; Gerardo Gamez <sup>1</sup> ; Steven Ray <sup>1</sup> ; Duane Rogers <sup>1</sup> ; Gregory Schilling <sup>1</sup> ; Michael Webb <sup>1</sup> ; William Wetzel <sup>1</sup> ; <sup>1</sup> Indiana University, Bloomington, IN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| TOF pm 03:40 <b>Detailed Characterization of GPC Fractionated Athabaskan Asphaltenes by FT-ICR Mass Spectrometry;</b> <u>Brandie M. Craven</u> <sup>2</sup> ; Tanner M. Schaub <sup>1</sup> ; Ryan P. Rodgers <sup>1</sup> ; Heather D. Dettman <sup>3</sup> ; Sara L. Salmon <sup>3</sup> ; Alan G. Marshall <sup>2</sup> ; <sup>1</sup> National High Magnetic Field Laboratory, FSU, Tallahassee, Florida; <sup>2</sup> Department of Chemistry and Biochemistry, FSU, Tallahassee, Florida; <sup>3</sup> National Centre for Upgrading Technology, Devon, Alberta | TOG pm 03:40 <b>Whole Gel Elution - µLC Coupled to ICP-MS, MALDI and Electrospray MS for the Characterisation of Metalloproteins in Biological Samples;</b> <u>Sarah L. Stokes</u> <sup>1</sup> ; Josephine Bunch <sup>1</sup> ; Alison Graham <sup>1</sup> ; Robert K Poole <sup>1</sup> ; Cameron W McLeod <sup>1</sup> ; <sup>1</sup> The University of Sheffield, Sheffield, United Kingdom<br><br>TOG pm 04:00 <b>Novel Mass Spectrometry Based Flow Cytometer;</b> <u>Vladimir I. Baranov</u> <sup>1</sup> ; Dmitry R. Bandura <sup>1</sup> ; Scott D. Tanner <sup>1</sup> ; Olga I. Ornatsky <sup>1</sup> ; <sup>1</sup> University of Toronto, Toronto, Canada<br><br>TOG pm 04:20 <b>Parallel Elemental and Molecular Mass Spectrometry (PEMMS) for Comprehensive Speciation of Metals;</b> <u>Gavin L. Sacks</u> <sup>1</sup> ; Louis A. Derry <sup>1</sup> ; J. Thomas Brenna <sup>1</sup> ; <sup>1</sup> Cornell University, Ithaca, NY |
| TOF pm 04:00 <b>Self-Association of Polar Organics in Petroleum Derived Materials Determined by Mass Spectrometry;</b> <u>Ryan P. Rodgers</u> <sup>1</sup> ; Tanner M. Schaub <sup>1</sup> ; Donald F. Smith <sup>2</sup> ; Parviz Rahimi <sup>3</sup> ; Alan G. Marshall <sup>2</sup> ; <sup>1</sup> National High Magnetic Field Laboratory, FSU, Tallahassee, Florida; <sup>2</sup> Department of Chemistry and Biochemistry, FSU, Tallahassee, Florida; <sup>3</sup> National Centre for Upgrading Technology, Devon, Alberta                                     | TOG pm 04:40 <b>A New Approach for Tagging and Quantitative Determination of Proteins and Peptides Based on Lanthanide Complexes and LC/Sector Field ICP-MS;</b> <u>Michael W. Linscheid</u> <sup>1</sup> ; Stefan Pieper <sup>1</sup> ; Robert Ahrends <sup>1</sup> ; Meike Hamester <sup>3</sup> ; Torsten Lindemann <sup>3</sup> ; Christian Scheler <sup>2</sup> ; <sup>1</sup> Humboldt-Universitaet, Berlin, Germany; <sup>2</sup> Proteome Factory AG, Berlin, Germany; <sup>3</sup> Thermo, Bremen, Germany                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| TOF pm 04:20 <b>Positive and Negative Mode ESI Analysis on Heavy Crude Oils;</b> <u>Katianna A. Pihakari</u> <sup>1</sup> ; Anding Fan <sup>1</sup> ; Robert T. McIver <sup>1</sup> ; <sup>1</sup> IonSpec corporation, Lake Forest, CA                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| TOF pm 04:40 <b>Molecular Characterization and Reactivity of Marine Humic Acids by High Resolution Electrospray Fourier Transform-Ion Cyclotron Resonance Mass Spectrometry;</b> Sarah A.L. Caccamise <sup>2</sup> ; Rachel L. Sleighter <sup>1</sup> ; Susan A. Hatcher <sup>1</sup> ; <u>Patrick G. Hatcher</u> <sup>1</sup> ; <sup>1</sup> Old Dominion University, Norfolk, VA; <sup>2</sup> Ohio State University, Columbus, OH                                                                                                                                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

## TUESDAY ORAL SESSIONS

### 5:30 – 7:00 pm: WORKSHOPS

**MS Instrument Leasing-Exploring the Options and Avoiding the Pitfalls.** Arranged by Pharmaceuticals Interest Group.  
David Peake and Brad Ackermann, presiding  
Session Room A

**Top Down Protein Sequencing on 2D and 3D Ion Traps.**  
Arranged by Ion Traps Interest Group  
Richard Vachet, presiding  
Session Room B

**Bridging the Gap between Biomarker Discovery and Clinical Chemistry Procedures.** Arranged by Clinical Chemistry Interest Group; Donald Chace and Jack Henion, presiding  
Session Room C

**Open Source Software for MS: More than Just Free Stuff.**  
Arranged by Computer Applications Interest group  
Jeffrey Whitney, presiding  
Session Room D

**LC/MS Applications in Environmental Analysis.**  
Arranged by Environmental Interest Group.  
Alaee Mehran, presiding  
Session Room E

**What Can Ion Mobility Do for your Mass Spectrometry?**  
Arranged by Ion Mobility Interest Group.  
Herb Hill, presiding  
Session Room F

**Protein Aggregation and Mass Spectrometry.**  
Arranged by Biological Macromolecules Interest Group.  
Viswanatham Katta, presiding  
Session Room G

## WEDNESDAY ORAL SESSIONS

### WEDNESDAY MORNING, MAY 31

**8:00 – 8:45 am: PLENARY LECTURE**  
**David E. Clemmer: Recipient of the Biemann Medal**

### 8:45 – 10:15am: POSTER SESSION AND EXHIBITS

Wednesday posters.  
 Authors of odd-numbered posters present.  
 See list beginning on page 108.

### 10:15 am – 12:15 pm: PARALLEL SESSIONS

**Session Room A: 10:15 am – 12:15 pm**  
**DIRECT IONIZATION TECHNIQUES**  
 Bradley L. Ackermann, presiding

- WOA am 10:15 **Desorption Electrospray Ionization (DESI)- Direct Ionization under Ambient Pressures and Temperatures**; R. Graham Cooks<sup>1</sup>; Huanwen Chen<sup>1</sup>; Ismael Cotte-Rodriguez<sup>1</sup>; Demian R. Ifa<sup>1</sup>; Marcela Nefliu<sup>1</sup>; Qingyu Song<sup>1</sup>; Nari Talaty<sup>1</sup>; Zoltan Takats<sup>1</sup>; Andre Venter<sup>1</sup>; Justin M. Wiseman<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- WOA am 10:35 **Evaluation of DART (Direct Analysis in Real Time) in Chemical Reaction Monitoring**; Melissa Gomez<sup>1</sup>; Robert L. Johnson<sup>1</sup>; Jon D. Williams<sup>1</sup>; <sup>1</sup>*GlaxoSmithKline, Research Triangle Park, NC*
- WOA am 10:55 **Bioanalysis without Sample Cleanup or Chromatography: Is It Still a Dream?**; Jing-Tao Wu<sup>1</sup>; Doug Simmons<sup>2</sup>; Brian Musselman<sup>2</sup>; <sup>1</sup>*Millennium Pharmaceuticals, Inc, Cambridge, MA*; <sup>2</sup>*IonSense, Danverse, MA*
- WOA am 11:15 **Routine Quantitative Analysis of Drugs Using MALDI – MS/MS**; Richard King<sup>1</sup>; Emily Adarayan<sup>1</sup>; Deborah Dooney<sup>1</sup>; <sup>1</sup>*Merck & Co. Inc., West Point, PA*
- WOA am 11:35 **High Sensitivity Analysis of Volatile and Semi-volatile Compounds by Direct Ionization ASAP-MS on an Orbitrap Mass Spectrometer**; Charles N McEwen<sup>1</sup>; <sup>1</sup>*DuPont Corporate Center for Analytical Sciences, Wilmington, DE*
- WOA am 11:55 **Reactive Desorption Electrospray Ionization (DESI) and Direct Analysis in Real Time (DART) for High-Throughput Screening of Counterfeit Antimalarials by MS**; Leonard Nyadong<sup>1</sup>; Christina Hampton<sup>1</sup>; Horace Leung<sup>1</sup>; Paul Newton<sup>2</sup>; Michael Green<sup>3</sup>; Victor de Jesus<sup>4</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Inst of Technology, Atlanta, GA*; <sup>2</sup>*Wellcome Trust-Mahosot Hospital-Oxford University, Vientianne, Lao PDR*; <sup>3</sup>*Center for Disease Control and Prevention, Atlanta, GA*; <sup>4</sup>*Georgia Tech Research Institute, Atlanta, GA*

**Session Room B: 10:15 am – 12:15 pm**  
**INSTRUMENTATION AND METHODS FOR QUADRUPOLE AND LINEAR ION TRAPS**

John E. P. Syka, presiding

- WOB am 10:15 **Evolution or Intelligent Design? Events in the Creation of the Ion Trap Mass Spectrometer**; John F J Todd<sup>1</sup>; <sup>1</sup>*University of Kent, Canterbury, UK*
- WOB am 10:55 **Ion/Ion Reactions in a Quadrupole Time-of-Flight Mass Spectrometer: Instrumentation and Application**; Yu Xia<sup>1</sup>; Paul Chrisman<sup>1</sup>; David Erickson<sup>1</sup>; Xiaorong Liang<sup>1</sup>; Jian Liu<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; Frank A. Londry<sup>2</sup>; Min Yang<sup>2</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*MDS SCIEX, Concord, ON, Canada*
- WOB am 11:15 **Linear Radio-Frequency-Quadrupole Ion Trap for Electron Capture Dissociation Coupled to a Liquid Chromatograph**; Takashi Baba<sup>1</sup>; Hiroyuki Satake<sup>1</sup>; Hideki Hasegawa<sup>1</sup>; Naomi Manri<sup>1</sup>; Yuichiro Hashimoto<sup>1</sup>; Atsumu Hirabayashi<sup>1</sup>; Izumi Waki<sup>1</sup>; Toshiyuki Yokosuka<sup>2</sup>; Kiyomi Yoshinari<sup>2</sup>; Kinya Kobayashi<sup>2</sup>; <sup>1</sup>*Central Research Laboratory, Tokyo, Japan*; <sup>2</sup>*Hitachi Research Laboratory, Hitachi, Japan*
- WOB am 11:35 **Ion Attachment Reactions with Implications for Gas-Phase Enzymology**; Graeme C. McAlister<sup>1</sup>; Jae C. Schwartz<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Thermo Electron, San Jose, CA*
- WOB am 11:55 **Photoactive Chemical Crosslinker for Identification of Protein Interactions by Infrared Multiphoton Dissociation – Mass Spectrometry**; Myles W. Gardner<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>*The University of Texas at Austin, Austin, TX*



# WEDNESDAY ORAL SESSIONS

## Session Room C: 10:15 am – 12:15 pm DETECTION OF CELLULAR PATHWAYS BY A PROTEOMICS APPROACH

Markus Kalkum, presiding

- WOC am 10:15 **Proteomic Approaches for Dissecting Complex Biological Systems;** Brian T. Chait<sup>1</sup>; <sup>1</sup>*Rockefeller University, New York, NY*
- WOC am 10:35 **Kinase-Specific Phosphoproteomics: Direct Purification and Identification of Kinase-Specific Subsets of the Phosphoproteome;** Justin D Blethrow<sup>1</sup>; David O Morgan<sup>1</sup>; Kevan M Shokat<sup>1</sup>; <sup>1</sup>*University of California San Francisco, San Francisco, CA*
- WOC am 10:55 **Peptidomics of Salmonella under Phagosome-Mimicking Culture Conditions;** Nathan P Manes<sup>1</sup>; Jean K Gustin<sup>2</sup>; Joanne Rue<sup>2</sup>; Heather M Mottaz<sup>1</sup>; Samuel O Purvine<sup>1</sup>; Angela D Norbeck<sup>1</sup>; Joshua N Adkins<sup>1</sup>; Fred Heffron<sup>2</sup>; Richard D Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Oregon Health and Science University, Portland, OR*
- WOC am 11:15 **Profiles of Cardioprotection: Integrated Proteomic and Metabonomic Study of the Effects of Nitrite Treatment on the Heart;** David H. Perlman<sup>1</sup>; Selena Bauer<sup>1</sup>; Hua Huang<sup>1</sup>; Maria Francisca Garcia-Saura<sup>1</sup>; Nathan S. Bryan<sup>1</sup>; Bernadette O. Fernandez<sup>1</sup>; Mark E. McComb<sup>1</sup>; Martin Feelisch<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*
- WOC am 11:35 **Study Metabolic Pathway Alteration Resulted from the Development of Hepatocellular Carcinoma;** Rong Wang<sup>1</sup>; Heyi Yang<sup>1</sup>; Yezhou Sun<sup>1</sup>; Gregg Czerwieniec<sup>1</sup>; Weijia Zhang<sup>1</sup>; Josep M. Llovet<sup>1</sup>; <sup>1</sup>*Mount Sinai School of Medicine, New York, NY*
- WOC am 11:55 **A novel role of Autophagy in Axonal Degeneration;** Qingjun Wang<sup>1</sup>; Yaomei Ding<sup>2</sup>; Yun Zhong<sup>1</sup>; Stave Kohtz<sup>2</sup>; Noboru Mizushima<sup>3</sup>; Ileana M. Cristea<sup>1</sup>; Michael P. Rout<sup>1</sup>; Nathaniel Heintz<sup>1</sup>; Zhenyu Yue<sup>2</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*Mount Sinai School of Medicine, New York, NY*; <sup>3</sup>*Tokyo Metropolitan Institute of Medical Science, Tokyo, Japan*

## Session Room D: 10:15 am – 12:15 pm BIOINFORMATICS

Michael J. MacCoss, presiding

- WOD am 10:15 **A New Approach to Protein Identification;** Pavel Pevzner<sup>1</sup>; <sup>1</sup>*University of California San Diego, La Jolla, CA*
- WOD am 10:35 **Reference Library Searching Strategies in Proteomics;** Jeffrey R. Johnson<sup>1</sup>; Greg T. Cantin<sup>1</sup>; John D. Venable<sup>1</sup>; Daniel Cociorva<sup>1</sup>; John R. Yates<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*
- WOD am 10:55 **Improved Peptide Identification and Spectrum Prediction Using a Probabilistic Model of Peptide Fragmentation;** Aaron A. Klammer<sup>1</sup>; Barbara E. Frewen<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; William S. Noble<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- WOD am 11:15 **GEQUEST: Using Proteomics to Annotate Genomic Sequences;** Joel R Sevinsky<sup>1</sup>; Benjamin J Cargile<sup>1</sup>; Maureen K Bunker<sup>1</sup>; Jonathan L Bundy<sup>1</sup>; James L Stephenson Jr.<sup>1</sup>; <sup>1</sup>*Research Triangle Institute, Research Triangle Park, NC*
- WOD am 11:35 **ChromAlign - A Two-Step, Three Dimensional Chromatographic Time Alignment Algorithm;** Rovshan Sadygov<sup>1</sup>; Andreas Huhmer<sup>1</sup>; <sup>1</sup>*Thermo Electron Corp, San Jose, CA*
- WOD am 11:55 **End-to-End Data Analysis of Label Free Biomarker Discovery Experiments: Both Cross Sectional and Longitudinal Designs;** Nathan A Yates<sup>1</sup>; Andrey Bondarenko<sup>2</sup>; Lee Weng<sup>2</sup>; Joyce Y Peng<sup>2</sup>; Andrew Keller<sup>2</sup>; Matthew Mazur<sup>1</sup>; Robert E Settlege<sup>1</sup>; Yelena Shevelenko<sup>2</sup>; Ronald C Hendrickson<sup>1</sup>; <sup>1</sup>*Merck & Co. Inc., Rahway, NJ*; <sup>2</sup>*Rosetta Biosoftware, Seattle, WA*

# WEDNESDAY ORAL SESSIONS

| <b>Session Room E: 10:15 am – 12:15 pm</b><br><b>FLUORINATED ORGANICS IN THE ENVIRONMENT</b><br>William L. Budde, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | <b>Session Room F: 10:15 am – 12:15 pm</b><br><b>FROM NUCLEIC ACIDS TO DNA/RNA COMPLEXES</b><br>Kristina Håkansson, presiding                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
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| WOE am 10:15 <b>Tracking the Dirty Byproducts of a World Trying to Stay Clean ~ Environmental Fate of Fluorinated Chemicals;</b> <u>Scott A. Mabury</u> <sup>1</sup> ; <sup>1</sup> University of Toronto, Toronto, Canada                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | WOF am 10:15 <b>Analysis of Nucleic Acid Based Noncovalent Complexes as a Tool in the Drug Discovery Arena;</b> Steven A Hofstadler <sup>1</sup> ; <u>Kristin A. Sannes-Lowery</u> <sup>1</sup> ; Jared J. Drader <sup>1</sup> ; <sup>1</sup> Ibis Division of Isis Pharmaceuticals, Carlsbad, CA                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| WOE am 10:55 <b>Measuring Perfluorinated Chemicals in Biological Matrices by SPE-HPLC-MS/MS. Applications to Epidemiologic Studies for Exposure Assessment in Human Populations;</b> <u>Antonia M. Calafat</u> <sup>1</sup> ; Zsuzsanna Kuklenyik <sup>1</sup> ; Xavier A. Bryant <sup>1</sup> ; Larry L. Needham <sup>1</sup> ; <sup>1</sup> Centers for Disease Control and Prevention, Atlanta, GA                                                                                                                                                                                                                                                                                                                              | WOF am 10:35 <b>Using Transition Metal Complexes to Generate Radical Ions of Nucleic Acids;</b> <u>Christopher K. Barlow</u> <sup>1</sup> ; Adrian Lam <sup>1</sup> ; Brittany D.M. Hodges <sup>2</sup> ; Richard A.J. O'Hair <sup>1</sup> ; W. David McFadyen <sup>1</sup> ; Scott A. McLuckey <sup>2</sup> ; <sup>1</sup> University of Melbourne, Melbourne, Australia; <sup>2</sup> Purdue University, West Lafayette, IN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| WOE am 11:15 <b>Determination of Perfluorinated Carboxylic Acids, Fluorotelomer Acids, and Fluorotelomer Alcohols in Biological Matrices by LC/MS/MS;</b> <u>Bogdan Szostek</u> <sup>1</sup> ; Charles R. Powley <sup>1</sup> ; Timothy Snow <sup>1</sup> ; Keith B. Prickett <sup>1</sup> ; Steve George <sup>1</sup> ; Robert C. Buck <sup>2</sup> ; <sup>1</sup> DuPont Haskell Laboratory, Newark, DE; <sup>2</sup> DuPont Chemical Solutions Enterprise, Wilmington, DE                                                                                                                                                                                                                                                       | WOF am 10:55 <b>ESI-FTMS Investigation of the Structural Determinants of Deoxyribozyme Activity;</b> Kevin B. Turner <sup>1</sup> ; Nathan A. Hagan <sup>1</sup> ; <u>Daniele Fabris</u> <sup>1</sup> ; <sup>1</sup> University of Maryland, Baltimore County, Baltimore, MD                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| WOE am 11:35 <b>Isomer-Specific Determination of Perfluorinated Chemicals in Environmental Matrices;</b> <u>Mehran Alaei</u> <sup>1</sup> ; Christine Spencer <sup>1</sup> ; Takeo Sakuma <sup>2</sup> ; Gordana Ivosev <sup>2</sup> ; Robert Ellis <sup>2</sup> ; Andre Schreiber <sup>2</sup> ; Yves Leblanc <sup>2</sup> ; Chris Marvin <sup>1</sup> ; Patrick Crozier <sup>3</sup> ; Eric Reiner <sup>3</sup> ; Corina Lucaciu <sup>3</sup> ; Vasile Furdui <sup>3</sup> ; Magali Houde <sup>1</sup> ; Derek Muir <sup>1</sup> ; <sup>1</sup> National Water Research Institute, Burlington, Canada; <sup>2</sup> Applied Biosystems-MDS-SCIEX, Concord, Canada; <sup>3</sup> Ontario Ministry of Environment, Toronto, Canada | WOF am 11:15 <b>Footprinting of DNA/Drug Complexes by ESI-Mass Spectrometry;</b> <u>Jennier Brodbelt</u> <sup>1</sup> ; Carolyn Mazzitelli <sup>1</sup> ; <sup>1</sup> University of Texas, Austin, TX                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| WOE am 11:55 <b>Benchmark GC-ECNI-IDMS Analysis of PBDEs in Fish from Remote Mountain Lakes: Effects of Ion Source Parameters and Bromine Substitution Patterns;</b> <u>Luke K. Ackerman</u> <sup>1</sup> ; Dan C. Koch <sup>1</sup> ; Staci L. Simonich <sup>1</sup> ; <sup>1</sup> Oregon State University, Corvallis, OR                                                                                                                                                                                                                                                                                                                                                                                                        | WOF am 11:35 <b>G-Quadruplex Targeting Drugs: From the Gas Phase Structure of Non Covalent Complexes to <i>in vitro</i> Activity;</b> Gabriel Mazzucchelli <sup>1</sup> ; Nicolas Smargiasso <sup>1</sup> ; Frédéric Rosu <sup>1</sup> ; Valérie Gabelica <sup>1</sup> ; Pierre Colson <sup>1</sup> ; Marie-Paule Teulade-Fichou <sup>2</sup> ; Marie-Claire Gillet <sup>1</sup> ; <u>Edwin De Pauw</u> <sup>1</sup> ; <sup>1</sup> University of Liège, Liège, Belgium; <sup>2</sup> Collège de France, Paris, France<br><br>WOF am 11:55 <b>MALDI-ToF Analysis of Cross-Linked Peptide–Oligoribonucleotides Derived from Various UV-Irradiated Ribonucleoprotein Particles;</b> <u>Eva Kühn-Hölsken</u> <sup>1</sup> ; Florian Richter <sup>1</sup> ; Björn Sander <sup>1</sup> ; Olexandr Dybkov <sup>1</sup> ; Cindy L. Will <sup>1</sup> ; Reinhard Lührmann <sup>1</sup> ; Henning Urlaub <sup>1</sup> ; <sup>1</sup> Max-Planck-Institute for Biophysical Chemistry, Goettingen, Germany |

## WEDNESDAY ORAL SESSIONS

### Session Room G: 10:15 am – 12:15 pm

#### ION SOLVATION

Paul Wenthold, presiding

- WOG am 10:15 **Hydration of DNA Nucleotides;** Thomas Wytttenbach<sup>1</sup>; Dengfeng Liu<sup>1</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>*University of California Santa Barbara, Santa Barbara, CA*
- WOG am 10:35 **Superoxide Hydration Studied by Velocity-Mapped Photoelectron Imaging;** Fatma A Akin<sup>1</sup>; <sup>1</sup>*University of Arizona, Tucson, AZ*
- WOG am 10:55 **Modulation of Peptide Charge State and Dissociation Behavior Through Binding with Cucurbit[6]uril or  $\alpha$ -Cyclodextrin: an FTICR/MS Study;** Haizhen Zhang<sup>1</sup>; David V. Dearden<sup>1</sup>; R. Jon Willes<sup>1</sup>; <sup>1</sup>*Brigham Young University, Provo, UT*
- WOG am 11:15 **Helix Macro-Dipolar Effects on the Gas-Phase Acidity of Cysteine-Polyalanine Peptides: An Investigation of Internal Solvation;** Jianhua Ren<sup>1</sup>; John Tan<sup>1</sup>; C. Michael McCallum<sup>1</sup>; <sup>1</sup>*University of the Pacific, Stockton, CA*
- WOG am 11:35 **Time-Resolved Recombination Dynamics of  $\text{IBr}^{\text{&minus}}$ ;  $(\text{CO}_2)_n$  Clusters;** Jack Barbera<sup>1</sup>; Vladimir Dribinski<sup>1</sup>; Joshua P. Martin<sup>1</sup>; Annette Svendsen<sup>2</sup>; Matt A. Thompson<sup>1</sup>; Robert Parson<sup>1</sup>; W. Carl Lineberger<sup>1</sup>; <sup>1</sup>*JILA/University of Colorado, Boulder, CO*; <sup>2</sup>*University of Aarhus, Aarhus, Denmark*
- WOG am 11:55 **Reaction of Protonated Water Clusters with Methylamine: Observation of Ion Solvation as Cluster Growth Inhibitor;** Chi-Tung Chiang<sup>1</sup>; Robert L. DeLeon<sup>1</sup>; James F. Garvey<sup>1</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*

## WEDNESDAY AFTERNOON, MAY 31

### 12:30 – 1:30 pm: INTEREST GROUP MEETING

#### Clinical Chemistry Interest Group Meeting

Donald Chace, presiding  
Room 620

### 1:30 – 3:00 pm: POSTER SESSION AND EXHIBITS

Wednesday posters.

Authors of even-numbered posters present.  
See list beginning on page 108.

### 3:00 – 5:00 pm: PARALLEL SESSIONS

#### Session Room A: 3:00 – 5:00 pm

#### QUANTITATIVE PROTEIN PROFILING

Arthur Moseley, presiding

- WOA pm 03:00 **Comparison of Quantitative Approaches for High Throughput Proteomics;** Jon Jacobs<sup>123</sup>; Weijin Qian<sup>123</sup>; Tao Liu<sup>123</sup>; Stephen Callister<sup>123</sup>; Vlad Petyuk<sup>123</sup>; Joshua Adkins<sup>123</sup>; Matthew Monroe<sup>123</sup>; Deep Jaitly<sup>123</sup>; Mary Lipton<sup>123</sup>; David Camp<sup>123</sup>; Richard D. Smith<sup>123</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>3</sup>*Pacific Northwest National Laboratory, Richland, WA*
- WOA pm 03:40 **Optimization of Antibody-Based Enrichment of Peptides on Magnetic Beads for Mass Spectrometry-Based Quantification of Serum Biomarkers;** Amanda G. Paulovich<sup>1</sup>; Lei Zhao<sup>1</sup>; Heidi Y. Zhang<sup>1</sup>; Li-chia Feng<sup>1</sup>; Brian D. Piening<sup>1</sup>; Jeffrey R. Whiteaker<sup>1</sup>; Leigh Anderson<sup>2</sup>; <sup>1</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>2</sup>*Plasma Proteome Institute, Washington, DC*
- WOA pm 04:00 **Quantitative Analysis of Cell Signaling;** Ming Zhou<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; David A. Lucas<sup>1</sup>; King C. Chan<sup>1</sup>; Haleem J. Issaq<sup>1</sup>; Daniel Ritt<sup>2</sup>; Deborah K. Morrison<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>*SAIC-Frederick, Inc., Frederick, MD*; <sup>2</sup>*National Cancer Institute at Frederick, Frederick, MD*
- WOA pm 04:20 **PEPPeR: A Platform for Experimental Proteomics Pattern Recognition;** Jacob D. Jaffe<sup>1</sup>; D.R. Mani<sup>1</sup>; Kyriacos C. Leptos<sup>2</sup>; Betty Chang<sup>1</sup>; Vamsi K. Mootha<sup>3</sup>; John Aach<sup>2</sup>; George M. Church<sup>2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*The Broad Institute of Harvard and MIT, Cambridge, MA*; <sup>2</sup>*Harvard Medical School Dept. of Genetics, Boston, MA*; <sup>3</sup>*Massachusetts General Hospital, Boston, MA*
- WOA pm 04:40 **Diagnostic Protein Signatures of Mammary Carcinoma Characterized by Mass Spectrometric Proteome Analysis – On the Way towards Clinical Marker Sets;** Katharina M. Dreschler<sup>1</sup>; Cornelia Koy<sup>1</sup>; Annika Kasten<sup>1</sup>; Johannes Vissers<sup>2</sup>; Marc Kipping<sup>2</sup>; Jim L. Langridge<sup>2</sup>; Toralf Reimer<sup>3</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, University of Rostock, Rostock, Germany*; <sup>2</sup>*Waters Corporation, Manchester, United Kingdom*; <sup>3</sup>*Gynecology, University of Rostock, Rostock, Germany*

## WEDNESDAY ORAL SESSIONS

### Session Room B: 3:00 – 5:00 pm PHOSPHORYLATION OF PROTEINS

Forest White, presiding

- WOB pm 03:00 **Temporal Dynamics of Tyrosine Phosphorylation in the Insulin Signaling Pathway;** Katrin Schmelzle<sup>1</sup>; Susan Kane<sup>2</sup>; Scott Gridley<sup>2</sup>; Gustav E. Lienhard<sup>2</sup>; Forest M. White<sup>1</sup>; <sup>1</sup>*Massachusetts Institute of Technology, Cambridge, MA*; <sup>2</sup>*Dartmouth Medical School, Hanover, NH*
- WOB pm 03:20 **Highly Selective Enrichment of Phosphopeptides Involved in the Very Early Cytokine Signaling Event Using an Optimized TiO<sub>2</sub> Purification Protocol;** Lene Jacobsen<sup>1</sup>; Peter Heding<sup>2</sup>; Flemming Pociot<sup>2</sup>; Peter Roepstorff<sup>1</sup>; Martin R. Larsen<sup>1</sup>; <sup>1</sup>*Biochemistry and Molecular Biology, Odense, Denmark*; <sup>2</sup>*Steno Diabetes Center, Copenhagen, Denmark*
- WOB pm 03:40 **Activitomics: Multiplexed Quantification of Protein Kinase Activities by Mass Spectrometry;** Pedro Cutillas<sup>1</sup>; Bart Vanhaesebroeck<sup>1</sup>; <sup>1</sup>*Ludwig Institute for Cancer Research, London, United Kingdom*
- WOB pm 04:00 **Large-Scale Data Evaluation of Mass Spectra for Shotgun Phosphoproteomics;** Yoshiya Oda<sup>1</sup>; Yasushi Ishihama<sup>1</sup>; Tsuyoshi Tabata<sup>1</sup>; Ken Aoshima<sup>1</sup>; Toshitaka Sato<sup>1</sup>; Junro Kuromitsu<sup>1</sup>; <sup>1</sup>*Eisai Co Ltd, Tsukuba, Japan*
- WOB pm 04:20 **A Novel Method of Enrichment and Identification for Phosphoprotein by Two-dimensional LC-MS-MS Based on pH Gradient and Reverse Phase Chromatography;** Rong Zeng<sup>1</sup>; Wen-Hai Jin<sup>1</sup>; Jie Dai<sup>1</sup>; Chia-Hui Shieh<sup>1</sup>; <sup>1</sup>*Shanghai Institutes for Biological Sciences, Shanghai, China*
- WOB pm 04:40 **Motif-Driven Multisite Phosphorylation Analysis from Thousands of Unambiguous Sites;** Judit Villén<sup>1</sup>; Sean A. Beausoleil<sup>1</sup>; Daniel Schwartz<sup>1</sup>; Scott A. Gerber<sup>2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Dartmouth Medical School, Hanover, NH*

### Session Room C: 3:00 – 5:00 pm METHODS TO INCREASE THROUGHPUT FOR PK ANALYSIS

Wilmin P. Bartolini, presiding

- WOC pm 03:00 **Rapid *in vivo* PK Analysis Using LC-MS/MS in Drug Discovery;** Xiaoying Xu<sup>1</sup>; <sup>1</sup>*Schering-Plough Research Institute, Kenilworth, NJ*
- WOC pm 03:20 **It's What's Before the Mass Spectrometer that Improves Productivity;** Lucinda H Cohen<sup>1</sup>; Dave Weller<sup>1</sup>; Joe Palandra<sup>1</sup>; Jeff Li<sup>2</sup>; Lisa Buchholz<sup>1</sup>; Min Zhong<sup>1</sup>; Steve Michael<sup>1</sup>; <sup>1</sup>*Pfizer Global Research and Development, Ann Arbor, MI*; <sup>2</sup>*Michigan State University, East Lansing, MI*
- WOC pm 03:40 **An Optimized Solution for High-Throughput Qualitative and Quantitative Analysis of Pharmaceuticals;** Kenneth C. Lewis<sup>1</sup>; Joseph D. Simpkins<sup>1</sup>; <sup>1</sup>*OpAns, Durham, NC*
- WOC pm 04:00 **A Novel Approach for Bisphosphonate Bioanalysis Using LC-MS/MS;** Venjamin Lapko<sup>1</sup>; Lee Zhu<sup>1</sup>; Yousef Basir<sup>1</sup>; Rick Olsen<sup>1</sup>; Chris Kafonek<sup>1</sup>; Chad Briscoe<sup>1</sup>; Jean Lee<sup>2</sup>; <sup>1</sup>*MDS Pharma Services, Lincoln, NE*; <sup>2</sup>*Amgen, Carmarillo, CA*
- WOC pm 04:20 **Rapid Quantification in a Discovery Pharmaceutical Setting Using Nanoelectrospray and FAIMS;** Panos Hatsis<sup>1</sup>; Jing-Tao Wu<sup>1</sup>; Adam Brockman<sup>1</sup>; <sup>1</sup>*Millennium Pharmaceuticals, Inc., Cambridge, MA*
- WOC pm 04:40 **Pooling Strategy to Increase Throughput and Reduce Interference for Microsomal Stability Assay by High-Resolution Chromatography/ Tandem Mass Spectrometry;** Rongda Xu<sup>1</sup>; Kheng Lim<sup>1</sup>; Melinda Manuel<sup>1</sup>; Shaokun Pang<sup>1</sup>; Joshua Cramlett<sup>1</sup>; Dan Hascall<sup>1</sup>; Daniel B. Kassel<sup>1</sup>; <sup>1</sup>*Takeda San Diego, Inc., San Diego, CA*

# WEDNESDAY ORAL SESSIONS

## Session Room D: 3:00 – 5:00 pm IMPURITY/DEGRADATION IN DRUG PRODUCTS AND PACKAGING

Fenghe Qiu, presiding

- WOD pm 03:00 **The Impact of Modern Mass Spectrometry on the Regulation and Control of Impurities in Pharmaceutical Products;** Daniel L. Norwood<sup>1</sup>; <sup>1</sup>*Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*
- WOD pm 03:20 **Identification of Packaging Related Drug Product Impurities;** Alan D. Hendricker, Ph.D.<sup>1</sup>; John D. Lennon, Ph.D.<sup>1</sup>; Thomas N. Feinberg, Ph.D.<sup>1</sup>; <sup>1</sup>*Cardinal Health, Morrisville, NC*
- WOD pm 03:40 **Determination of Trace Leacheable Impurities in Prefillable Plastic Medical Device Containers;** Peter Lu<sup>1</sup>; Stilianos Roussis<sup>1</sup>; Roger Groskopf<sup>1</sup>; <sup>1</sup>*BD, Franklin Lakes, NJ*
- WOD pm 04:00 **HPLC combined with Travelling Wave Ion-Mobility Separator and an oa-ToF for Identification of Trace Impurities in Zidovudine Formulated Drug Products;** Christine Eckers<sup>1</sup>; Alice Laures<sup>1</sup>; Kevin Giles<sup>2</sup>; Hilary Major<sup>2</sup>; Jose Castro-Perez<sup>2</sup>; Robert Bateman<sup>2</sup>; Steven Pringle<sup>2</sup>; <sup>1</sup>*GlaxoSmithKline Research and Development, Stevenage, UK*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- WOD pm 04:20 **Rapid Identification of Metabolites and Drug Product and Substance Impurities by Hybrid Techniques: Three Case Studies;** Paul M Bigwarfe Jr<sup>1</sup>; Christopher M McGinley<sup>1</sup>; Oystein Loe<sup>1</sup>; Samantha A Leidner<sup>1</sup>; David M Loffredo<sup>1</sup>; David P White<sup>1</sup>; <sup>1</sup>*Hospira, Inc.; One 2 One(R) Product Development, Lake Forest, IL*
- WOD pm 04:40 **Identification of Impurities in Drug Products Using LC/DAD/MS and Headspace SPME/GC/MS;** Peter Zhou<sup>1</sup>; Wencan Chen<sup>1</sup>; Kirby Wong-Moom<sup>1</sup>; Nina Cauchon<sup>1</sup>; <sup>1</sup>*Amgen Inc., Thousand Oaks, CA*

## Session Room E: 3:00 – 5:00 pm INSTRUMENTATION AND METHODOLOGY FOR IMAGING MS

Ron M. A. Heeren, presiding

- WOE pm 03:00 **Imaging Mass Spectrometry: Exploiting Modern Developments to Generate High Mass, High Spatial Resolution Images;** Liam A McDonnell<sup>1</sup>; Ian W Fletcher<sup>2</sup>; AF Maarten Altelaar<sup>1</sup>; Sander R Piersma<sup>1</sup>; Ron MA Heeren<sup>1</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, The Netherlands*; <sup>2</sup>*ICI PLC, Redcar, Great Britain*
- WOE pm 03:20 **Imaging Mass Spectrometry: Benchmarking to Autoradiography;** Josephine Bunch<sup>1</sup>; Hazel Dickson<sup>1</sup>; Sarah Stokes<sup>1</sup>; Cameron W. McLeod<sup>1</sup>; <sup>1</sup>*The University of Sheffield, Sheffield, UK*
- WOE pm 03:40 **Profiling and Imaging Neuropeptides in the Brain;** Jonathan V. Sweedler<sup>1</sup>; Eric B. Monroe<sup>1</sup>; Nathan Hatcher<sup>1</sup>; Stanislav S. Rubakhin<sup>1</sup>; <sup>1</sup>*University of Illinois, Urbana, IL*
- WOE pm 04:00 **Histology Directed MALDI-MS Tissue Profiling for Improved Throughput and Cellular Specificity: Focus on Breast Cancer;** Dale S. Cornett<sup>1</sup>; Eduardo C. Dias<sup>1</sup>; James A. Mobley<sup>1</sup>; Melinda E. Sanders<sup>1</sup>; Carlos L. Arteaga<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- WOE pm 04:20 **Imaging Mass Spectrometry with a New Intermediate-Pressure MALDI Linear Ion Trap Mass Spectrometer;** Richard A. Yost<sup>1</sup>; Timothy A. Garrett<sup>1</sup>; Viatcheslav V. Kovtoun<sup>2</sup>; Huy Bui<sup>2</sup>; Nick Izgarian<sup>2</sup>; Maria C. Prieto Conaway<sup>2</sup>; George C. Stafford<sup>2</sup>; <sup>1</sup>*University of Florida, Department of Chemistry, Gainesville, FL*; <sup>2</sup>*ThermoFinnigan, San Jose, CA*
- WOE pm 04:40 **Chemical Mapping and Differentiation of Tissue Sections Using Imaging Time-of-Flight Secondary Ion Mass Spectrometry;** Ligang Wu<sup>3</sup>; Kris Kulp<sup>1</sup>; Mark Knize<sup>1</sup>; Erik Nelson<sup>1</sup>; James Felton<sup>1</sup>; Xiaochen Lu<sup>1</sup>; Elena Berman<sup>1</sup>; David Seligson<sup>2</sup>; David Chia<sup>2</sup>; Sheila Tze<sup>2</sup>; Lee Goodglick<sup>2</sup>; Kuang Jen Wu<sup>1</sup>; <sup>1</sup>*Lawrence Livermore National Lab, Livermore, CA*; <sup>2</sup>*University of California - Los Angeles, Los Angeles, CA*; <sup>3</sup>*University of California - Davis, Davis, CA*

# WEDNESDAY ORAL SESSIONS

## Session Room F: 3:00 – 5:00 pm ON-LINE ANALYSIS OF ORGANIC AEROSOLS

Giuseppe Petrucci, presiding

- WOF pm 03:00 **Chemical Characterization of Nanoparticles in the Early Stage of Biogenic Secondary Organic Aerosol Formation**; Katherine Heaton<sup>1</sup>; Matthew Dreyfus<sup>1</sup>; Shenyi Wang<sup>1</sup>; Michael Tolocka<sup>1</sup>; Murray Johnston<sup>1</sup>; <sup>1</sup>University of Delaware, Newark, DE
- WOF pm 03:20 **New Methods for On-Line Analysis of Organic Aerosol Constituents Based on Vaporisation followed by Soft Post-Ionisation and TOFMS**; Matthias Bente<sup>1</sup>; Jochen Weh<sup>1</sup>; Martin Sklorz<sup>1</sup>; Thorsten Streibel<sup>1</sup>; Ralf Zimmermann<sup>1</sup>; <sup>1</sup>GSF-Research Centre and University of Augsburg, Oberschleissheim, Germany
- WOF pm 03:40 **A Minimal Fragmentation Approach to Real Time Aerosol Mass Spectrometry: A New Tool for Laboratory Studies of Organic Aerosol Aging**; Pedro Campuzano-Jost<sup>1</sup>; Sarah Hanna<sup>1</sup>; Emily Simpson<sup>1</sup>; Damon Robb<sup>1</sup>; Mike W. Blades<sup>1</sup>; John W. Hepburn<sup>1</sup>; Allan K. Bertram<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC, Canada
- WOF pm 04:00 **Recent Developments and Improved Understanding of Photoelectron Resonance Capture Ionization Aerosol Mass Spectrometry for the Analysis of Organic Particles**; Brian W. LaFranchi<sup>1</sup>; James Zahardis<sup>1</sup>; Giuseppe A. Petrucci<sup>1</sup>; <sup>1</sup>University of Vermont, Burlington, VT
- WOF pm 04:20 **Studies of Oxidative Processing of Organic Aerosols Using Aerosol CIMS**; Geoffrey D. Smith<sup>1</sup>; John D. Hearn<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- WOF pm 04:40 **Applications of Thermal Desorption Particle Beam Mass Spectrometry to Studies of Atmospheric Organic Aerosol Chemistry**; Paul J Ziemann<sup>1</sup>; <sup>1</sup>University of California-Riverside, Riverside, CA

## Session Room G: 3:00 – 5:00 pm FUNDAMENTALS OF ION MOLECULE REACTIONS

Steven R. Kass, presiding

- WOG pm 03:00 **New Adventures in Gas Phase Organocuprate Chemistry: What Makes a Good Dummy Ligand?**; Richard A.J. O'Hair<sup>1</sup>; Nicole Rijs<sup>1</sup>; George N. Khairallah<sup>1</sup>; Tom Waters<sup>1</sup>; <sup>1</sup>University of Melbourne, Melbourne, Australia
- WOG pm 03:20 **Investigation of Gas-phase Reactions of Charged Phenyl Radicals with Peptides in a Fourier-Transform Ion Cyclotron Resonance Mass Spectrometer**; Sen Li<sup>1</sup>; Hilkka I. Kenttämä<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WOG pm 03:40 **Controversies in the Reactions of Peroxides in Solution and in vivo: A Gas Phase Ion Chemistry Approach and Biological Implications**; Shuji Kato<sup>1</sup>; Veronica M. Bierbaum<sup>1</sup>; G. Barney Ellison<sup>1</sup>; Stephen J. Blanksby<sup>2</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>University of Wollongong, Wollongong, Australia
- WOG pm 04:00 **Exploring the Roles of the Exchange Mechanism and Reaction Environment in the Hydrogen-Deuterium Exchange Reactions of Oligonucleotides**; Joseph E. Chipuk<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas, Austin, TX
- WOG pm 04:20 **Hydrogen Bonding and Steric Restriction in Gas Phase Chiral Recognition**; Nannan Fang<sup>1</sup>; David V. Dearden<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- WOG pm 04:40 **Negative Ion Chemistry of Simple Organogermanes and Gas-Phase Synthesis of Novel Oxy-Germanium Anions**; Jose M. Riveros<sup>1</sup>; Luciano A. Xavier<sup>1</sup>; Nelson H. Morgon<sup>2</sup>; <sup>1</sup>University of Sao Paulo, Sao Paulo, Brazil; <sup>2</sup>University of Campinas, Campinas, Brazil

5:15 – 6:00 pm: ASMS MEETING

Session Room C

Free beverages.

## THURSDAY ORAL SESSIONS

### THURSDAY MORNING, JUNE 1

**No Plenary Session this morning**

#### **8:45 – 10:15am: POSTER SESSION AND EXHIBITS**

Thursday posters.

Authors of odd-numbered posters present.

See list beginning on page 135.

#### **10:15 am – 12:15 pm: PARALLEL SESSIONS**

##### Session Room A: 10:15 am – 12:15 pm **BIOMARKERS FOR DRUG SAFETY AND EFFICACY**

Nathan Yates, presiding

- ThOA am 10:15 **The Plasma Proteome: Challenges for Biomarker Discovery and Validation;** N. Leigh Anderson<sup>1</sup>; <sup>1</sup>*Plasma Proteome Institute, Washington, DC*
- ThOA am 10:55 **Relative Quantification of Proteins in Plasma from Pancreatic Cancer Patients Using <sup>18</sup>O/<sup>16</sup>O Labeling and 2-Dimensional Liquid Chromatography Tandem Mass Spectrometry;** Kenneth L. Johnson<sup>1</sup>; Christopher J. Mason<sup>1</sup>; Jeanette E. Eckel-Passow<sup>1</sup>; Douglas W. Mahoney<sup>1</sup>; Ann L. Oberg<sup>1</sup>; Terry M. Therneau<sup>1</sup>; Janet E. Olson<sup>1</sup>; David C. Muddiman<sup>2</sup>; H. Robert Bergen, III<sup>1</sup>; <sup>1</sup>*Mayo Clinic College of Medicine, Rochester, MN*; <sup>2</sup>*North Carolina State University, Raleigh, NC*
- ThOA am 11:15 **ITRAQ Analysis Facilitates Discovery of Biomarkers from Clinical Samples;** Leroi V. DeSouza<sup>1</sup>; Shaun Ghanny<sup>1</sup>; Valerie Dube<sup>2</sup>; Alexander D. Romaschin<sup>3</sup>; Terence J. Colgan<sup>2</sup>; K. W. Michael Siu<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*; <sup>2</sup>*Mt. Sinai Hospital, Toronto, Canada*; <sup>3</sup>*Hospital for Sick Children, Toronto, Canada*
- ThOA am 11:35 **Validated CNS Lymphoma Biomarkers Discovered in Cerebrospinal Fluid by DeepLook™ Mass Spectrometry;** Sushmita Mimi Roy<sup>1</sup>; Christopher H. Becker<sup>1</sup>; Howard Schulman<sup>1</sup>; James Rubenstein<sup>2</sup>; <sup>1</sup>*Biomarker Discovery Sciences, PPD, Menlo Park, CA*; <sup>2</sup>*University of California, San Francisco, San Francisco, CA*
- ThOA am 11:55 **High Resolution Differential Mass Spectrometry (dMS) Reveals Markers of Alzheimer's Disease in Humans;** Ronald C Hendrickson<sup>1</sup>; Cloud P Paweletz<sup>1</sup>; Matthew C Wiener<sup>1</sup>; Anita Lee<sup>1</sup>; Li Jenny<sup>1</sup>; Robert E Settlege<sup>1</sup>; Jeffrey R Sachs<sup>1</sup>; Xuemei Zhao<sup>1</sup>; Fanyu Meng<sup>1</sup>; Ekaterina G Deyanova<sup>1</sup>; Jayshree Mistry<sup>1</sup>; Gary J Romano<sup>1</sup>; Seeburger Jeff<sup>1</sup>; Mark S Shearman<sup>1</sup>; Adam J Simon<sup>1</sup>; Omar Laterza<sup>1</sup>; Jeff Zhang<sup>1</sup>; Matthew T Mazur<sup>1</sup>; Vijay Modur<sup>1</sup>; Elizabeth

King<sup>2</sup>; Catharine Joachim<sup>2</sup>; David A Smith<sup>2</sup>; Alan B Sachs<sup>1</sup>; Nathan A Yates<sup>1</sup>; <sup>1</sup>*Merck Research Laboratories, Rahway, NJ*; <sup>2</sup>*OPTIMA, University of Oxford, Oxford, UK*

##### Session Room B: 10:15 am – 12:15 pm **PROTEIN NETWORKS AND THEIR REGULATION** Natalie Ahn, presiding

- ThOB am 10:15 **Investigation of Protein Interaction Network of Macromolecular Protein Complex Using a Newly Developed Proteomic Approach-QTAX;** Lan Huang<sup>1</sup>; Cortnie Guerrero<sup>1</sup>; Xiaorong Wang<sup>1</sup>; Christian Tagwerker<sup>1</sup>; Peter Kaiser<sup>1</sup>; <sup>1</sup>*University of California, Irvine, Irvine, CA*
- ThOB am 10:35 **An Interaction Map of the Lid of the 19S Proteasome from MS of Intact Complexes;** Michal Sharon<sup>1</sup>; Xavier I. Ambroggio<sup>2</sup>; Raymond J. Deshaies<sup>2</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>*University of Cambridge, Cambridge, United Kingdom*; <sup>2</sup>*California Institute of Technology, Pasadena, CA*
- ThOB am 10:55 **Regulation of PPAR/RXR/Co-Activator Complex by Partial Agonists;** Patrick R. Griffin<sup>1</sup>; Swati Prasad<sup>1</sup>; Scott A Busby<sup>1</sup>; Michael J. Chalmers<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, Jupiter, FL*
- ThOB am 11:15 **Discovering Protein-Protein Interactions Using MuDPIT;** James Wohlschlegel<sup>1</sup>; Lani C. Keller<sup>2</sup>; Edwin P. Romijn<sup>1</sup>; Ivan Zamora<sup>2</sup>; Wallace F. Marshall<sup>2</sup>; John R. Yates<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, LaJolla, CA*; <sup>2</sup>*University of California San Francisco, San Francisco, CA*
- ThOB am 11:35 **Probing Non-Covalent Interactions and Post-Translational Modifications in the Heterogeneous Yeast Exosome Protein Complex;** Silvia A. Synowsky<sup>1</sup>; Robert H. H. van den Heuvel<sup>1</sup>; Shabaz Mohammed<sup>1</sup>; Pim W. W. M. Pijnappel<sup>1</sup>; Albert J. R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, The Netherlands*
- ThOB am 11:55 **Assembling Protein Interactions Networks from Shotgun Proteomics Datasets;** Mihaela E. Sardi<sup>1</sup>; Laurence Florens<sup>1</sup>; Ronald C. Conaway<sup>1</sup>; Joan Weliky Conaway<sup>1</sup>; Michael P. Washburn<sup>1</sup>; <sup>1</sup>*Stowers Institute for Medical Research, Kansas City, MO*

## THURSDAY ORAL SESSIONS

### Session Room C: 10:15 am – 12:15 pm MS IMAGING OF SMALL MOLECULES

Michelle Reyzer, presiding

- ThOC am 10:15 **Direct Visualization of First-Pass Drug Metabolism by Imaging Mass Spectrometry**; Jiwen Chen<sup>1</sup>; Walter Korfmacher<sup>1</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, NJ
- ThOC am 10:35 **Utility of Multistage Mass Spectrometric Imaging by MALDI Ion-Trap MS in the Analysis of Drugs and Metabolites in Biological Tissues**; Dieter Drexler<sup>1</sup>; Timothy J. Garrett<sup>2</sup>; Joseph Cantone<sup>1</sup>; Richard Ditters<sup>3</sup>; James Mitroka<sup>4</sup>; Maria Prieto Conaway<sup>5</sup>; Stephen Adams<sup>1</sup>; Richard A. Yost<sup>2</sup>; Mark Sanders<sup>4</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Wallingford, CT; <sup>2</sup>University of Florida, Gainesville, FL; <sup>3</sup>Bristol-Myers Squibb Company, Syracuse, NY; <sup>4</sup>Bristol-Myers Squibb Company, Princeton, NJ; <sup>5</sup>ThermoElectron Finnigan, San Jose, CA
- ThOC am 10:55 **Tissue Imaging of Small Molecules by High Mass Accuracy MALDI**; Catherine Stacey<sup>1</sup>; Taeman Kim<sup>1</sup>; Melvin Park<sup>1</sup>; <sup>1</sup>Bruker Daltonics Inc, Billerica, MA
- ThOC am 11:15 **Imaging Phospholipids in Brain Tissue by Intermediate-Pressure MALDI/MS<sup>n</sup> on a Linear Ion Trap**; Timothy J. Garrett<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- ThOC am 11:35 **Sampling and Imaging of Tissue Sections Using a Surface Sampling Probe Electrospray Ionization Mass Spectrometry System**; Gary J. Van Berkel<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- ThOC am 11:55 **Biological Cluster-TOF-SIMS Imaging**; David Touboul<sup>1</sup>; Alain Brunelle<sup>1</sup>; Olivier Laprévote<sup>1</sup>; <sup>1</sup>ICSN-CNRS, Gif-sur-Yvette, France

### Session Room D: 10:15 am – 12:15 pm LIPIDOMICS

Richard B. Cole, presiding

- ThOD am 10:15 **In Situ Structural Characterization of Lipids in Brain Tissue Using MALDI-MS/MS**; Amina S. Woods<sup>1</sup>; Hay-Yan J. Wang<sup>1</sup>; Mark Little<sup>1</sup>; Shelley N. Jackson<sup>1</sup>; <sup>1</sup>NIDA IRP, NIH, Baltimore, MD
- ThOD am 10:35 **Nano-LC-MS/MS/MS for the Characterisation of Cholestetriols and Cholestenolones in Rat Brain**; William Griffiths<sup>1</sup>; Kersti Karu<sup>1</sup>; John Turton<sup>1</sup>; Yuqin Wang<sup>1</sup>; <sup>1</sup>University of London, London, UK
- ThOD am 10:55 **Taking Advantage of the High Resolving Power of MALDI FTMS for Analyzing Phospholipid Profiles from Mouse Tissues**; Sabine Borgmann<sup>1</sup>; Jeffrey J. Jones<sup>1</sup>; Charles L. Wilkins<sup>1</sup>; Richard M. O'Brien<sup>2</sup>; <sup>1</sup>University of Arkansas, Fayetteville, AR; <sup>2</sup>Vanderbilt University, Nashville, TN
- ThOD am 11:15 **Profiling and Identification of Lipids Associated with M. Tuberculosis Hypervirulence Using FT-MS and FAAT: A New Lipid Analysis Algorithm**; Michael D. Leavell<sup>1</sup>; Sally Cantrell<sup>2</sup>; Lee W. Riley<sup>2</sup>; Julie A. Leary<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>University of California, Berkeley, CA
- ThOD am 11:35 **Towards the Accurate Lipidome: Profiling by High Mass Accuracy Measurements**; Dominik Schwudke<sup>1</sup>; J. Thomas Hannich<sup>1</sup>; Teymuraz Kurzchalia<sup>1</sup>; Thomas Moehring<sup>3</sup>; Jeffrey Oegema<sup>2</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>Max Planck Institute of Molecular Cell Biology, Dresden, Germany; <sup>2</sup>Scionics Computer Innovation GmbH, Dresden, Germany; <sup>3</sup>Thermo Electron GmbH, Bremen, Germany
- ThOD am 11:55 **Hyphenated Lipidomics: Characterization of Sphingomyelins in Lipid Extracts**; Jan Willmann<sup>1</sup>; Kerstin Mahlstedt<sup>1</sup>; Manfred Spraul<sup>3</sup>; Herbert Thiele<sup>2</sup>; Dieter Leibfritz<sup>1</sup>; <sup>1</sup>University of Bremen, Bremen, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Bruker BioSpin GmbH, Karlsruhe, Germany



## THURSDAY ORAL SESSIONS

### Session Room E: 10:15 am – 12:15 pm NANOSPRAY LC/MS OF SMALL MOLECULES

Paul Vourros, presiding

- ThOE am 10:15 **Correlation between Spraying Modes and Ion Chemistry in Electrosprays;** Peter Nemes<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, DC
- ThOE am 10:35 **Extending the Benefits of Nanoelectrospray to High-Flow Chromatography Using Multiple Nozzle Arrays to Improve Spray Stability and Mass Sensitivity;** Gary A. Schultz<sup>1</sup>; Ellen Pace<sup>1</sup>; Christopher Alpha<sup>1</sup>; Jack Henion<sup>1</sup>; <sup>1</sup>Advion BioSystems, 22 Thornwood Drive, Ithaca, NY
- ThOE am 10:55 **An Integrated Method for Quantification and Identification of Radiolabeled Metabolites: Application of Chip-based Nanoelectrospray and Mass Defect Filter Techniques;** Weiping Zhao<sup>1</sup>; Haiying Zhang<sup>1</sup>; Mingshe Zhu<sup>1</sup>; Bethanne Warrack<sup>1</sup>; Li Ma<sup>1</sup>; W. Griffith Humphreys<sup>1</sup>; Mark Sanders<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ
- ThOE am 11:15 **Carbon Nanotube Liquid Chromatography-FT-ICR: Novel Chromatography in a Microfluidic Chip Coupled to FT-ICR, Fundamental Studies and Applications;** Nicolas L. Young<sup>3</sup>; Micheal Stadermann<sup>1</sup>; Bryan Dick<sup>1</sup>; Carlito B. Lebrilla<sup>2</sup>; Alexandr Noy<sup>1</sup>; Olga Bakajin<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory, Livermore, CA; <sup>2</sup>University of California, Davis, CA; <sup>3</sup>Both LLNL & UC Davis, Livermore/Davis, CA
- ThOE am 11:35 **Nanospray Ionization Combined with Nanobore Column Switching Chromatography for the Quantitative Analysis of Paclitaxel in Plasma;** Dan J. Magiera<sup>1</sup>; Adam A. Peral<sup>2</sup>; Gary A. Valaskovic<sup>2</sup>; Mike S. Lee<sup>3</sup>; <sup>1</sup>Spherics, Inc., Lincoln, RI; <sup>2</sup>New Objective Inc., Woburn, MA; <sup>3</sup>Milestone Development Services Inc., New Town, PA
- ThOE am 11:55 **Assessment of Human Exposure to Chemical Agents by High Throughput Chip-Based Nanoelectrospray Mass Spectrometry;** Douglas B. Mawhinney<sup>1</sup>; Elizabeth I. Hamelin<sup>2</sup>; Robert J. Kobelski<sup>1</sup>; <sup>1</sup>U.S. Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>Battelle/U.S. Centers for Disease Control, Atlanta, GA

### Session Room F: 10:15 am – 12:15 pm SPECTROSCOPY OF IONS

Robert C. Dunbar, presiding

- ThOF am 10:15 **Collision-Induced Dissociation and H/D Exchange Elucidated by Infrared Photodissociation Spectroscopy;** Jos Oomens<sup>1</sup>; Nick C. Polfer<sup>1</sup>; Bela Paizs<sup>2</sup>; Robert C. Dunbar<sup>3</sup>; <sup>1</sup>FOM Institute for Plasma Physics, Nieuwegein, Netherlands; <sup>2</sup>German Cancer Research Center, Heidelberg, Germany; <sup>3</sup>Case Western Reserve University, Cleveland, OH
- ThOF am 10:35 **Probing the Structures of Simple Ion Complexes Using Infrared Spectroscopy;** Evan J. Bieske<sup>1</sup>; <sup>1</sup>University of Melbourne, Melbourne, Australia
- ThOF am 10:55 **IRMPD Studies of Actinide Ligand Complexes;** Michael J. Van Stipdonk<sup>1</sup>; Winnie Chien<sup>1</sup>; Gary S. Groenewold<sup>2</sup>; Anita K. Gianotto<sup>2</sup>; Jos Oomens<sup>3</sup>; Nick Polfer<sup>3</sup>; David T. Moore<sup>3</sup>; Wibe A. de Jong<sup>4</sup>; Lucas Visscher<sup>5</sup>; <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>3</sup>FOM Institute for Plasma Physics, Nieuwegein, The Netherlands; <sup>4</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>5</sup>Free University of Amsterdam, Amsterdam, The Netherlands
- ThOF am 11:15 **Infrared Multiphoton Dissociation Spectroscopy: Probing the Tautomeric States of Protonated and Alkali Metalated Heterocycles (2-Hydroxypyridine/2-Pyridone, Cytosine, and 1-Methylcytosine);** Mary T. Rodgers<sup>1</sup>; Nick C. Polfer<sup>2</sup>; Jos Oomens<sup>2</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>FOM Institute for Plasma Physics "Rijnhuizen", Nieuwegein, Netherlands
- ThOF am 11:35 **Spectroscopy of PAH Ions: From Laboratory Studies to Astronomical Observations;** Farid Salama<sup>1</sup>; <sup>1</sup>NASA Ames Research Center, Space Science Division, Moffett Field, CA
- ThOF am 11:55 **IR Photodissociation Spectroscopy. Unique Characterization of Hydrogen Bonding in Gaseous Protein Ions;** Giuseppe Infusini<sup>1</sup>; Cheng Lin<sup>3</sup>; Xuemei Han<sup>1</sup>; Mi Jin<sup>1</sup>; Harold Y. Hwang<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Barry K. Carpenter<sup>1</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, Austria; <sup>3</sup>Boston University Medical College, Boston, MA

## THURSDAY ORAL SESSIONS

### Session Room G: 10:15 am – 12:15 pm ATMOSPHERIC CHEMISTRY

Shuji Kato, presiding

ThOG am 10:15 **Measurements of Volatile Organic Compounds in the Atmosphere using PTR-MS (Proton-Transfer-Reaction Mass Spectrometry) and PIT-MS (Proton-Transfer Ion Trap Mass Spectrometry);** Carsten Warneke<sup>1</sup>; Joost A de Gouw<sup>2</sup>; <sup>1</sup>NOAA Earth System Research Laboratory, Boulder, CO; <sup>2</sup>CIRES, University of Colorado, Boulder, CO

ThOG am 10:35 **Development of an Automated Sampling MS System for the Measurement of Atmospheric Volatile Organic Compounds;** Gavin D. Edwards<sup>1</sup>; Paul B. Shepson<sup>1</sup>; Garth E. Patterson<sup>2</sup>; J. Mitchell Wells<sup>2</sup>; John W. Grossenbacher<sup>2</sup>; Dennis J. Barket, Jr.<sup>2</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Griffin Analytical Technologies, Inc., West Lafayette, IN

ThOG am 10:55 **CIMS as a Tool to Study Atmospheric Aerosol Nucleation Mechanisms;** Rhonda Hirschl<sup>1</sup>; Shan-Hu Lee<sup>1</sup>; Dave Tanner<sup>2</sup>; Greg Huey<sup>2</sup>; <sup>1</sup>Kent State University, Department of Chemistry, Kent, OH; <sup>2</sup>Georgia Tech, School of Earth, Atmospheric Science, Atlanta, GA

ThOG am 11:15 **Chemical and Physical Characterization of Aerosols with the Aerodyne Aerosol Mass Spectrometer: Laboratory and Field Applications;** Douglas R. Worsnop<sup>1</sup>; John T. Jayne<sup>1</sup>; Manjula R. Canagaratna<sup>1</sup>; Timothy Onasch<sup>1</sup>; Leah Williams<sup>1</sup>; Megan Northway<sup>1</sup>; Achim Trimborn<sup>1</sup>; Jay Slowik<sup>2</sup>; Paul Davidovits<sup>2</sup>; Peter DeCarlo<sup>3</sup>; Jose L. Jimenez<sup>3</sup>; Qi Zhang<sup>4</sup>; <sup>1</sup>Aerodyne Research Inc., Billerica, MA; <sup>2</sup>Boston College, Chestnut Hill, MA; <sup>3</sup>University of Colorado, Boulder, CO; <sup>4</sup>State University of New York, Albany, NY

ThOG am 11:35 **Aerosol Mass Spectrometric Analysis of Atmospheric Particles: New Techniques and Field Results;** Jose-Luis Jimenez<sup>1</sup>; Qi Zhang<sup>2</sup>; Peter DeCarlo<sup>1</sup>; Joel Kimmel<sup>1</sup>; Allison Aiken<sup>1</sup>; D.R. Worsnop<sup>3</sup>; Eiko Nemitz<sup>5</sup>; Marc Gonin<sup>4</sup>; Kathrin Fuhrer<sup>4</sup>; Kenneth Docherty<sup>1</sup>; J. Alex Huffman<sup>1</sup>; Ingrid Ulbrich<sup>1</sup>; Edward Dunlea<sup>1</sup>; Achim Trimborn<sup>3</sup>; <sup>1</sup>Dept. of Chemistry & CIRES; Univ. of Colorado, Boulder, CO; <sup>2</sup>Atmos. Sci. Res. Ctr.; Univ. at Albany, Albany, NY; <sup>3</sup>Aerodyne Research, Billerica, MA; <sup>4</sup>Tofwerk, Thun, Switzerland; <sup>5</sup>CEH, Edinburgh, UK

ThOG am 11:55 **Electrospray Ionization with Ultrahigh Resolution Fourier Transform Mass Spectrometry as a New Characterization Technique for Rainwater Dissolved Organic Matter;** Patrick G. Hatcher<sup>1</sup>;

Amanda Grannas<sup>2</sup>; Eunjee Lee<sup>3</sup>; <sup>1</sup>Old Dominion University, Norfolk, VA; <sup>2</sup>Villanova University, Philadelphia, PA; <sup>3</sup>Massachusetts Institute of Technology, Boston, MA

### THURSDAY AFTERNOON, JUNE 1

#### 1:00 – 2:30 pm: POSTER SESSION AND EXHIBITS

Thursday posters.

Authors of even-numbered posters present.

See list beginning on page 135.

#### 2:30 – 4:30 pm: PARALLEL SESSIONS

### Session Room A: 2:30 – 4:30 pm REACTIVE METABOLITES AND TOXICOLOGICAL LINKS

Ajai K. Chaudhary, presiding

ThOA pm 02:30 **Mass Spectrometry in the Study of Chemically-Reactive Metabolites. Applications in Drug Discovery and Early Development;** Thomas A Baillie<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA

ThOA pm 03:10 **The Formation of Endogenous Glutathione-Adducts By Lipid Hydroperoxide-Derived Reactive Intermediates;** Ian A. Blair<sup>1</sup>; Tomoyuki Oe<sup>1</sup>; Clementina Mesaros<sup>1</sup>; Wenying Jian<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA

ThOA pm 03:30 **Negative Ion Tandem Mass Spectrometry for the Detection of Glutathione Conjugates;** Christine Dieckhaus<sup>1</sup>; <sup>1</sup>Merck, West Point, PA

ThOA pm 03:50 **Detection of Reactive Intermediates as Thioethers Generated by Neutrophils and Microsomes Using a Specific CNL-Scan Combined with Product-Ion-Scans;** Karoline Scholz<sup>1</sup>; Eva K. Kopp<sup>1</sup>; Axel Paehler<sup>2</sup>; Wolfgang Voelkel<sup>1</sup>; <sup>1</sup>University of Wuerzburg, Wuerzburg, Germany; <sup>2</sup>F. Hofmann-La Roche Ltd, Pharmaceuticals, Basel, Switzerland

ThOA pm 04:10 **Application of Mass Spectrometry and Stable Isotope Labeled Compounds in Mechanistic and Predictive Toxicology Studies;** Abdul E. Mutlib<sup>1</sup>; <sup>1</sup>Pfizer Global Research and Development, Ann Arbor, MI

## THURSDAY ORAL SESSIONS

### Session Room B: 2:30 – 4:30 pm NOVEL MS INSTRUMENTATION

Susanne Moyer, presiding

- ThOB pm 02:30 **Infrared Laser Desorption Ionization Ion Mobility Mass Spectrometry and Its Applications;** Michael Ugarov<sup>1</sup>; Thomas Egan<sup>1</sup>; J. Albert Schultz<sup>1</sup>; Shelley Jackson<sup>2</sup>; Hay-Yan J. Wang<sup>2</sup>; Amina S. Woods<sup>2</sup>; <sup>1</sup>*Ionwerks, Inc., Houston, TX*; <sup>2</sup>*NIDA IRP, Baltimore, MD*
- ThOB pm 02:50 **New Ionization Sources and Detection Strategies in Mass Spectrometry;** Francisco J. Andrade<sup>1</sup>; Gary M. Hieftje<sup>1</sup>; Steven Ray<sup>1</sup>; Gregory D. Schilling<sup>1</sup>; William C. Wetzel<sup>1</sup>; Michael R. Webb<sup>1</sup>; Gerardo G. Gamez<sup>1</sup>; David W. Koppelaar<sup>2</sup>; Charles J. Barinaga<sup>2</sup>; Roger P. Sperline<sup>3</sup>; M. Bonner Denton<sup>3</sup>; James H. Barnes IV<sup>4</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>3</sup>*University of Arizona, Tucson, AZ*; <sup>4</sup>*Los Alamos National Laboratory, Los Alamos, NM*
- ThOB pm 03:10 **Charge Detection Mass Spectrometry of Microparticles;** Wen-Ping Peng<sup>1</sup>; Ming-Lee Chu<sup>2</sup>; Huan-Chang Lin<sup>1</sup>; Huan-Cheng Chang<sup>3</sup>; Chung-Hsuan Winston Chen<sup>1</sup>; <sup>1</sup>*Genomics Research Center, Academia Sinica, Taipei, Taiwan, R.O.C.*; <sup>2</sup>*Institute of Physics, Academia Sinica, Taipei, Taiwan, R.O.C.*; <sup>3</sup>*IAMS, Academia Sinica, Taipei, Taiwan, R.O.C.*
- ThOB pm 03:30 **Towards a Levitated Droplet Ion Source for Electrospray Ionization Mass Spectrometry;** Ryan T. Hilger<sup>1</sup>; Brian L. Frey<sup>1</sup>; Michael S. Westphall<sup>1</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*
- ThOB pm 03:50 **MEMS Assembled Mass Spectrometry: A Novel Approach to Miniaturization and Construction of Electron and Ion Optics;** Guido F. Verbeck<sup>1</sup>; Rahul Saini<sup>1</sup>; James Wylde<sup>1</sup>; Ken Tsui<sup>1</sup>; Mathew Ellis<sup>1</sup>; <sup>1</sup>*Zyvex, Richardson, TX*
- ThOB pm 04:10 **Fragmentation of Peptide Ions via Interaction with Metastable Atoms;** Vadym D. Berkout<sup>1</sup>; <sup>1</sup>*MassTech, Inc., Columbia, MD*

### Session Room C: 2:30 – 4:30 pm METHODS FOR PROBING PROTEIN CONFORMATIONS

Lars Konermann, presiding

- ThOC pm 02:30 **Mass spectrometry of higher order protein structures;** Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>*University of Massachusetts at Amherst, Amherst, MA*
- ThOC pm 03:10 **Protein Interaction Studies by Chemical Cross-Linking Using Isotope-Labeled and Trifunctional Cross-Linkers Combined with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Andrea Sinz<sup>1</sup>; Daniela M. Schulz<sup>1</sup>; Stefan Kalkhof<sup>1</sup>; Andreas Schmidt<sup>1</sup>; Christian Ihling<sup>1</sup>; <sup>1</sup>*University of Leipzig, Leipzig, Germany*
- ThOC pm 03:30 **Monitoring Protein Motions by Hydrogen Exchange Mass Spectrometry;** Thomas Lee<sup>1</sup>; Andrew N. Hoofnagle<sup>1</sup>; Katheryn A. Resing<sup>1</sup>; Natalie G. Ahn<sup>1</sup>; <sup>1</sup>*University of Colorado at Boulder, Boulder, CO*
- ThOC pm 03:50 **A Combined Use of Spectroscopy, Tandem MS and Molecular Dynamics Simulations in Probing Protein Structures in Solution and Vacuum;** Christopher M Adams<sup>1</sup>; Frank Kjeldsen<sup>1</sup>; Alexandra Patriksson<sup>1</sup>; David van der Spoel<sup>1</sup>; Roman A. Zubarev<sup>1</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*
- ThOC pm 04:10 **Casting an Eye on Cataractogenesis by Radical Probe Mass Spectrometry;** Sam Issa<sup>1</sup>; Wai-Kei Shum<sup>1</sup>; Simin Maleknia<sup>2</sup>; Kevin Downard<sup>1</sup>; <sup>1</sup>*The University of Sydney, Sydney, Australia*; <sup>2</sup>*Griffith University, Brisbane, Australia*

## THURSDAY ORAL SESSIONS

### Session Room D: 2:30 – 4:30 pm ATMOSPHERIC PRESSURE IONIZATION TECHNIQUES

Charles N. McEwen, presiding

- ThOD pm 2:30 **Atmospheric Pressure IR Laser Ablation of Water-Rich Targets for Mass Spectrometry;** Zhaoyang Chen<sup>1</sup>; Annemie Bogaerts<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>The George Washington University, Washington, DC; <sup>2</sup>University of Antwerp, Antwerp, Belgium
- ThOD pm 2:50 **Atmospheric Pressure Laser Ionization (APLI): Current Status, New Applications, and Major Improvements;** Thorsten Benter<sup>1</sup>; Matthias Lorenz<sup>1</sup>; Klaus J. Brockmann<sup>1</sup>; Marc Schellenträger<sup>2</sup>; Ralf Schiewek<sup>2</sup>; Stefan Droste<sup>2</sup>; Marc Constapel<sup>2</sup>; Oliver J. Schmitz<sup>2</sup>; Siegmär Gäß<sup>2</sup>; <sup>1</sup>University of Wuppertal, Physical Chemistry, Wuppertal, Germany; <sup>2</sup>University of Wuppertal, Analytical Chemistry, Wuppertal, Germany
- ThOD pm 3:10 **Use of a novel APCI-MS Interface for the Normal Phase LC-MS of Ceramides;** Mark Busman<sup>1</sup>; <sup>1</sup>USDA - ARS - NCAUR, Peoria, IL
- ThOD pm 3:30 **Atmospheric Pressure Photoionization for Enhanced Compatibility in Capillary Electrophoresis – Mass Spectrometry;** Roelof Mol<sup>1</sup>; Govert W. Somsen<sup>1</sup>; Gerhardus J. de Jong<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, the Netherlands
- ThOD pm 3:50 **Effects of Mobile Phase Solvents and Vacuum UV lamps on APPI-MS—Implications of Photoabsorption Cross Sections and Photon Energies;** Luke C Short<sup>1</sup>; Sheng-Suan Cai<sup>1</sup>; Jack A. Syage<sup>1</sup>; <sup>1</sup>Syagen Technology, Inc., Tustin, CA
- ThOD pm 4:10 **The Role of Atmospheric Oxygen in Negative Ion Formation in APPI and APCI: A Comparison;** Eleanor Riches<sup>1</sup>; Adam W. McMahon<sup>2</sup>; Richard J. Dennis<sup>3</sup>; <sup>1</sup>Manchester Metropolitan University, Manchester, United Kingdom; <sup>2</sup>University of Manchester, Manchester, United Kingdom; <sup>3</sup>GlaxoSmithKline, Stevenage, United Kingdom

### Session Room E: 2:30 – 4:30 pm MECHANISMS OF PEPTIDE FRAGMENTATION

Vicki H. Wysocki, presiding

- ThOE pm 2:30 **Gas-phase peptide chemistry;** Bela Paizs<sup>1</sup>; <sup>1</sup>German Cancer Research Center, Heidelberg, Germany
- ThOE pm 2:50 **Enhanced Protein Identification Using Electron Transfer Dissociation and Collision Induced Dissociation: A Study of the Trypanosoma brucei Flagellar Proteome;** Sarah R Hart<sup>1</sup>; Zhiqi Hao<sup>2</sup>; Andreas FR Huhmer<sup>2</sup>; Richard Broadhead<sup>3</sup>; Paul McKean<sup>3</sup>; Keith Gull<sup>4</sup>; Simon J Gaskell<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom; <sup>2</sup>Thermo Electron, San Jose, CA; <sup>3</sup>University of Lancaster, Lancaster, United Kingdom; <sup>4</sup>University of Oxford, Oxford, United Kingdom
- ThOE pm 3:10 **Lysine, Histidine, and Arginine Residues as H-Atom Donors in ECD and ETD;** Frantisek Turecek<sup>1</sup>; Xiaohong Chen<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThOE pm 3:30 **Mechanisms for the Selective Gas-phase Fragmentation Reactions of Side Chain Fixed Charge Sulfonium Ion Containing Peptides;** Mahasilu Amunugama<sup>1</sup>; Kade D. Roberts<sup>1</sup>; James J. Sierakowski<sup>1</sup>; Gavin E. Reid<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- ThOE pm 3:50 **Dissociation Pathways of Singly Charged Dilithiated Peptides;** Chrys Wesdemiotis<sup>1</sup>; Ping Wang<sup>1</sup>; Alyson Leigh<sup>1</sup>; Michael J. Polce<sup>1</sup>; Christian Bleiholder<sup>2</sup>; Bela Paizs<sup>2</sup>; <sup>1</sup>The University of Akron, Akron, OH; <sup>2</sup>German Cancer Research Center, Heidelberg, Germany
- ThOE pm 4:10 **Fragmentation Energetics of Peptide Radical Cations from Time-and Energy-Resolved Surface-Induced Dissociation Studies;** Julia Laskin<sup>1</sup>; Ivan. K. Chu<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>The University of Hong-Kong, Hong-Kong, China

## THURSDAY ORAL SESSIONS

### Session Room F: 2:30 – 4:30 pm FLAVORS AND FRAGRANCES Raymond E. March, presiding

- ThOF pm 2:30 **Identification of Compounds in Giraffe (*Giraffa camelopardalis*) Pelage for Candidate Mosquitoes Repellents;** Ulrich R. Bernier<sup>1</sup>; Brian P. Quinn<sup>1</sup>; Matthew M. Booth<sup>2</sup>; Paul J. Weldon<sup>3</sup>; <sup>1</sup>USDA-ARS-CMAVE, Gainesville, FL; <sup>2</sup>University of Florida, Dept of Anesthesiology, Gainesville, FL; <sup>3</sup>Smithsonian Institution, Front Royal, VA
- ThOF pm 2:50 **Automated Sample Preparation Techniques coupled to GC-MS for the Determination of Allergens in Cosmetics Containing Plant Extracts and/or Essential Oils;** Nieves Sarrión<sup>1</sup>; José Antonio Muñoz<sup>1</sup>; Ariadna Galve<sup>2</sup>; Jordi Reverter<sup>1</sup>; <sup>1</sup>KONIK-TECH, S.A., Sant Cugat del Vallés, Spain; <sup>2</sup>IKAI, Sant Cugat del Vallés, Spain
- ThOF pm 3:10 **A Shake and Shoot Approach for Screening Antibiotic Residues in Honey Using Turbulent Flow Liquid Chromatography with Tandem Mass Spectrometry;** Yves-Alexis Hammel<sup>1</sup>; Amy Davies<sup>2</sup>; Byron Kieser<sup>3</sup>; Gary Impey<sup>3</sup>; Philippe A. Guy<sup>1</sup>; <sup>1</sup>Nestle Research Center, Lausanne, Switzerland; <sup>2</sup>Cohesive Technologies, Milton Keynes, UK; <sup>3</sup>Applied Biosystems/MDS SCIEX, Concord, Canada
- ThOF pm 3:30 **Wine Astringency Approached by MS/MS Analysis of Peptide-Tannins Supramolecular Complexes;** Benoit Plet<sup>1</sup>; Jean-Marie Schmitter<sup>1</sup>; <sup>1</sup>Institut Européen de Chimie et Biologie, UMR 5144, Pessac, France
- ThOF pm 3:50 **Identification and Quantification of a ‘Pepper’ Marker Compound in Shiraz Grape Berries by Combination of Chemometrics and GC-MS;** Alan P Pollnitz<sup>1</sup>; Mango Parker<sup>1</sup>; Tracey E Siebert<sup>1</sup>; Daniel Cozzolino<sup>1</sup>; I Leigh Francis<sup>1</sup>; Markus J Herderich<sup>1</sup>; <sup>1</sup>The Australian Wine Research Institute, Glen Osmond (Adelaide), Australia
- ThOF pm 4:10 **Multi-residue Pesticide Analysis- Comparison of LC/MS with Time-of-Flight and LC/MS/MS with a Triple Quadrupole;** Paul Zavitsanos<sup>1</sup>; Michael Thurman<sup>2</sup>; Imma Ferrer<sup>2</sup>; Jerry Zweigenbaum<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc, Wilmington, DE; <sup>2</sup>University of Almeria, Almeria, Spain

### Session Room G: 2:30 – 4:30 pm MASS SPECTROMETRY (AND THEORETICAL) METHODS FOR PROBING THE CONFORMATIONS OF IONS IN THE GAS PHASE Mary T. Rodgers, presiding

- ThOG pm 2:30 **Interaction of Divalent Metal Ions with the Hormone Oxytocin: Hormone Receptor Binding;** Michael T. Bowers<sup>1</sup>; Dengfeng Liu<sup>1</sup>; Thomas Wytenbach<sup>1</sup>; <sup>1</sup>University of California at Santa Barbara, Santa Barbara, CA
- ThOG pm 2:50 **Hydration Energies of Metallated Amino Acids;** Sha Ye<sup>1</sup>; Peter B. Armentrout<sup>1</sup>; <sup>1</sup>Chemistry Dept, U of Utah, Salt Lake City, UT
- ThOG pm 3:10 **Conformations of Metal Cation/Tryptophan Complexes From IRMPD Spectroscopy with the Free Electron Laser;** Nick C. Polfer<sup>1</sup>; Jos Oomens<sup>1</sup>; Robert C. Dunbar<sup>2</sup>; <sup>1</sup>FOM-Institute for Plasmaphysics, Nieuwegein, Netherlands; <sup>2</sup>Case Western Reserve University, Cleveland, OH
- ThOG pm 3:30 **Fluorescence Measurements and Molecular Dynamics Simulations of Protein Conformational Fluctuations;** Anthony T. Iavarone<sup>1</sup>; Alexandra Patriksson<sup>2</sup>; David van der Spoel<sup>2</sup>; Joel H. Parks<sup>1</sup>; <sup>1</sup>Rowland Institute at Harvard, Cambridge, MA; <sup>2</sup>Uppsala University, Uppsala, Sweden
- ThOG pm 3:50 **Charge-State Resolved Mid-Infrared Spectroscopy of a Gas-Phase Protein;** Gert von Helden<sup>1</sup>; Jos Oomens<sup>2</sup>; Nick Polfer<sup>2</sup>; David T. Moore<sup>2</sup>; Lex van der Meer<sup>2</sup>; Alan G. Marshall<sup>3</sup>; John R. Eyler<sup>4</sup>; Gerard Meijer<sup>1</sup>; <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; <sup>2</sup>FOM Institute for Plasma Physics Rijnhuizen, Nieuwegein, Netherlands; <sup>3</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>4</sup>University of Florida, Gainesville, FL
- ThOG pm 4:10 **Probing Peptide Conformational Dynamics in the Gas-Phase;** Janel R. McLean<sup>1</sup>; John A. McLean<sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A & M University, College Station, TX

## THURSDAY ORAL SESSIONS

### 4:45 – 5:30 pm: PLENARY LECTURE

**Diane Evans, NASA**

*Exploring Earth*

Session Room C

### 6:00 pm: Closing Event

**Museum of Flight**

Buses depart from lobby level bus entrance of the convention center beginning at 5:45 pm

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# MONDAY POSTERS

## POSTER SPACE

## POSTER SPACE

### THESE POSTERS DISPLAYED MONDAY - THURSDAY

- 1 **ABRF-sPRG2006 Study: A Proteomics Standard;** Jeffrey A Kowalak<sup>1</sup>; Philip C. Andrews<sup>2</sup>; David Arnott<sup>3</sup>; Mary Ann Gawinowicz<sup>4</sup>; William S. Lane<sup>5</sup>; Kathryn S. Lilley<sup>6</sup>; Larry Martin<sup>7</sup>; Steven E. Stein<sup>8</sup>; <sup>1</sup>National Institute of Mental Health, Bethesda, MD; <sup>2</sup>University of Michigan School of Medicine, Ann Arbor, MI; <sup>3</sup>Genentech, Inc, So. San Francisco, CA; <sup>4</sup>Columbia University, New York, NY; <sup>5</sup>Harvard University, Cambridge, MA; <sup>6</sup>Cambridge University, Cambridge, UK; <sup>7</sup>East-West University, Chicago, IL; <sup>8</sup>National Institute of Standards and Technology, Gaithersburg, MD
- 2 **Teach Protein Identification, Polymer Analysis and the Analysis of Cocaine in Hair Using an Internet Based Mass Spectrometry Lab;** Mark E. Bier<sup>1</sup>; Joseph Grabowski<sup>2</sup>; <sup>1</sup>Carnegie Mellon University, Pittsburgh, PA; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA
- 3 **The Bendix Time-of-Flight Mass Spectrometer;** Michael A. Grayson<sup>1</sup>; <sup>1</sup>Washington University, St Louis, MO
- 4 **ABRF-PRG2006: Quantitative Proteomics Study;** A.M. Falick<sup>1</sup>; J.A. Kowalak<sup>2</sup>; W.S. Lane<sup>3</sup>; K.S. Lilley<sup>4</sup>; B.S. Phinney<sup>5</sup>; C.W. Turck<sup>6</sup>; S.T. Weintraub<sup>7</sup>; H.E. Witkowska<sup>8</sup>; <sup>1</sup>HHMI Mass Spec Lab., Univ. of California, Berkeley, CA; <sup>2</sup>National Institutes of Health (NIMH), Bethesda, MD; <sup>3</sup>Harvard University, Cambridge, MA; <sup>4</sup>Cambridge University, Cambridge, UK; <sup>5</sup>University of California, Davis, CA; <sup>6</sup>Max Planck Institute of Psychiatry, Munich, Germany; <sup>7</sup>Univ. of Texas Health Science Center, San Antonio, TX; <sup>8</sup>BRC, University of California, San Francisco, CA
- 5 **Proposal for a Common Nomenclature of Fragment Ions in the Mass Spectra of Synthetic Polymers;** Anthony T. Jackson<sup>1</sup>; Robert P. Lattimer<sup>2</sup>; Philip C. Price<sup>3</sup>; William E. Wallace<sup>4</sup>; Chrys Wesdemiotis<sup>5</sup>; <sup>1</sup>ICI Measurement Science Grp., Wilton, UK; <sup>2</sup>Noveon, Inc., Cleveland, OH; <sup>3</sup>Dow Chemical Co., South Charleston, WV; <sup>4</sup>National Institute of Standards & Technology, Gaithersburg, MD; <sup>5</sup>University of Akron, Akron, OH
- 6 **Francis William Aston - International Man of Mystery;** Kevin M Downard<sup>1</sup>; <sup>1</sup>The University of Sydney, Sydney, Australia
- 7 **International Mass Spectrometry Conference**

### MONDAY POSTERS

These posters should be set up at 7:30 am on Monday and removed at 7:30 pm. Be sure to use the poster space number next to the title.

### QUANTITATIVE ANALYSIS OF DRUGS AND METABOLITES I

- MP 9 **The Quantitation of Fentanyl in Equine Serum using Linear Ion Trap Mass Spectrometry;** Brooks H Nelson<sup>1</sup>; Keith D Zientek<sup>1</sup>; David Pirman<sup>1</sup>; L. Chris Sanchez<sup>1</sup>; Cynthia Cole<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- MP 10 **Withdrawn**
- MP 11 **Stabilization of the Clopidogrel Active Metabolite in Whole Blood and its Assay in Human Plasma by LC-MS/MS;** Makoto Takahashi<sup>1</sup>; Henrianna Pang<sup>2</sup>; Akiko Kikuchi<sup>3</sup>; Kiyoshi Kawabata<sup>1</sup>; Atsushi Kurihara<sup>1</sup>; Nagy A. Farid<sup>4</sup>; Toshihiko Ikeda<sup>1</sup>; <sup>1</sup>Sankyo Co., Ltd., Tokyo, Japan; <sup>2</sup>LLBR, Eli Lilly Canada, Toronto, Canada; <sup>3</sup>Hitachi Science Systems, Ltd., Ibaraki, Japan; <sup>4</sup>Lilly Research Laboratories, Indianapolis, IN

- MP 12 **A Novel Validated Liquid Chromatographic-Tandem Mass Spectroscopy Method for the Quantification of Abiraterone Acetate and Abiraterone in Human Plasma;** Florence Raynaud<sup>1</sup>; Vanessa Martins<sup>1</sup>; Nicola Wilsher<sup>1</sup>; Yasmin Asad<sup>1</sup>; <sup>1</sup>The Institute of Cancer Research, Sutton, Surrey, England
- MP 13 **A New LC/MS/MS Method for Quantitation of Moxifloxacin in Human Plasma;** Yong-Xi Li<sup>1</sup>; Dawei Zhou<sup>1</sup>; <sup>1</sup>XenoBiotic Laboratories, Inc., Plainsboro, NJ
- MP 14 **Monitoring Antineoplastic Benzyl Styryl Sulfone Analog ON 01910.Na in Phase I Clinical Trial;** Sool Yeon Cho<sup>1</sup>; John Roboz<sup>1</sup>; Stanely C. Bell<sup>2</sup>; Premkumar Reddy<sup>3</sup>; Takao Ohnuma<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY; <sup>2</sup>Onconova Therapeutics Inc., Lawrenceville, NJ; <sup>3</sup>Temple University, Philadelphia, PA
- MP 15 **Analysis of Nanomolar Drug Compound A in a Complex Ophthalmic Formulation Using Quantitative Tandem Mass Spectrometry;** Leah A. Buhler<sup>1</sup>; John M. Ballard<sup>2</sup>; Brian T. Hill<sup>1</sup>; Qingxi Wang<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA; <sup>2</sup>M-Scan, Inc., West Chester, PA
- MP 16 **Quantitation of Loratadine and Descarboethoxy Loratadine in Human Plasma by HPLC-Tandem Mass Spectrometry using an API 5000;** Melissa J. Meyer<sup>1</sup>; Matthew J. Amundson<sup>1</sup>; Laura V. Baum<sup>1</sup>; Darren J. Hoffman<sup>1</sup>; Andrew M. Osenga<sup>1</sup>; Ardeshir Khadang<sup>1</sup>; <sup>1</sup>PRACS Institute, Ltd., Fargo, ND
- MP 17 **Quantitative Analysis of Total Phenylephrine in Human Plasma by Turbo Ion Spray LC-MS-MS;** William K Haisch<sup>1</sup>; Dan J Aufman<sup>1</sup>; Ardeshir Khadang<sup>1</sup>; Jessie S Lindemann<sup>2</sup>; <sup>1</sup>PRACS Institute, Ltd., Fargo, ND; <sup>2</sup>EraGen Biosciences, Madison, WI
- MP 18 **Simultaneous LC-MS/MS Quantitation of Sulfuraphane and its Metabolites: Investigation of Sulfuraphane Metabolism in Rat Tissues;** Karolina M. Krasinska<sup>1</sup>; Suvama Bhamre<sup>2</sup>; James D. Brooks<sup>2</sup>; Allis S. Chien<sup>1</sup>; <sup>1</sup>Vincent Coates Foundation Mass Spectrometry Lab, Stanford, CA; <sup>2</sup>Department of Urology, Stanford School of Medicine, Stanford, CA
- MP 19 **Quantitative Analysis of the Chemoprevention Agent Isoliquiritigenin in Rat Plasma Using Liquid Chromatography-Tandem Mass Spectrometry;** Jian Guo<sup>1</sup>; John M. Pezzuto<sup>2</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>Purdue University School of Pharmacy, West Lafayette, IN
- MP 20 **Automated Solid Phase Extraction of Fexofenadine, Pseudoephedrine, and Cetirizine from Human Plasma and Subsequent Quantitation by LC/MS/MS;** Robert J. Brooks<sup>1</sup>; Daniel Pederson<sup>1</sup>; Darren Hoffman<sup>1</sup>; Melisa Meyer<sup>1</sup>; Laura Baum<sup>1</sup>; Scott Kragerud<sup>2</sup>; Autumn Dinnel<sup>1</sup>; Ardeshir Khadang<sup>1</sup>; <sup>1</sup>PRACS Institute, Ltd., Fargo, ND; <sup>2</sup>Array-Biopharma, Boulder, CO
- MP 21 **Analysis of Naloxone and Nornaloxone by High Performance Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry;** Wenfeng B. Fang<sup>1</sup>; David E. Moody<sup>1</sup>; Elinore F. McCance-Katz<sup>2</sup>; <sup>1</sup>Center for Human Toxicology, University of Utah, Salt Lake City, UT; <sup>2</sup>Virginia Commonwealth University, Richmond, VA
- MP 22 **LC-MS Method-Selectivity Enhancement by Combining FAIMS with Highly-Selective Reaction Monitoring (H-SRM) for Drug Urinalysis;** Randy W. Purves<sup>1</sup>; David A. Barnett<sup>1</sup>; James T. Kapron<sup>1</sup>; <sup>1</sup>Thermo Electron, Ottawa, Canada

# MONDAY POSTERS

## POSTER SPACE

- MP 23 **LC-ES/MS/MS Analysis of Synephrine and Octopamine in Rat Serum;** Nathan C Twaddle<sup>1</sup>; Deborah K Hansen<sup>1</sup>; Daniel R Doerge<sup>1</sup>; <sup>1</sup>National Center for Toxicological Research, Jefferson, AR
- MP 24 **Improved Signal-to-Noise Ratio in the Analysis of Clenbuterol in Urine using LC-FAIMS-H-SRM;** Rohan Thakur<sup>1</sup>; James Kapron<sup>2</sup>; <sup>1</sup>Thermo Electron Corp, San Jose, CA; <sup>2</sup>Thermo Electron, Ottawa, Canada
- MP 25 **Automated 96-Well SPE and LC-MS/MS Determination of Artemether and its Active Metabolite Dihydroartemisinin in Human Plasma;** Ojitkumar Lukram<sup>1</sup>; Ashok K<sup>1</sup>; Nagnath B<sup>1</sup>; Padgaonkar K<sup>1</sup>; M.C Agarwal<sup>2</sup>; D Kumar<sup>2</sup>; Asha Oroskar<sup>3</sup>; Anil Oroskar<sup>3</sup>; Saurabh Parikh<sup>3</sup>; Nirav Thakkar<sup>3</sup>; <sup>1</sup>Drug Monitoring Research Institute, Mumbai, India; <sup>2</sup>Department of Chemistry Government Model Science, Gwalior, India; <sup>3</sup>Orochem Technologies Inc, Lombard, IL
- MP 26 **A Rapid and Selective Method for the Analysis of GGTI-2418 in Mouse Plasma by HPLC/MS/MS;** Lori Coward<sup>1</sup>; Corenna Kerstner-Wood<sup>1</sup>; Lea Cork<sup>1</sup>; Greg Gorman<sup>1</sup>; Pat Noker<sup>1</sup>; Andrew Hamilton<sup>3</sup>; Said Sebt<sup>2</sup>; Lee Jia<sup>4</sup>; <sup>1</sup>Southern Research Institute, Birmingham, AL; <sup>2</sup>Moffitt Research Institute, University of South FL, Tampa, FL; <sup>3</sup>Yale University, New Haven, CT; <sup>4</sup>National Cancer Institute, Bethesda, MD
- MP 27 **LC-MS/MS Method for the Simultaneous Quantitation of Butorphanol, Morphine, Morphine-3-Glucuronide, Morphine-6-Glucuronide in Human Plasma and Urine;** Minghong Jia<sup>1</sup>; Roger B. Fillingim<sup>1</sup>; George N. Henderson<sup>1</sup>; <sup>1</sup>Univ. of Florida, Gainesville, FL
- MP 28 **Ultrasensitive (<1 pg/ml) Determination of a Drug in Human Plasma Utilizing HPLC Combined with Q TRAP Mass Spectrometry using SRM;** Manfred Zell<sup>1</sup>; Christophe Husser<sup>1</sup>; Bernd Steinhuber<sup>1</sup>; <sup>1</sup>F. Hoffmann-La Roche Ltd, Basel, Switzerland
- MP 29 **High Throughput Analysis of Rabeprazole in Human Plasma by LC-MS/MS;** Dan J. Aufman<sup>1</sup>; Gabriel Hardmeyer<sup>2</sup>; Cindy A. Ackerland<sup>1</sup>; Matthew J. Amundson<sup>1</sup>; Ardesir Khadang<sup>1</sup>; <sup>1</sup>PRACS Institute, Fargo, ND; <sup>2</sup>A.T. Still University, Mesa, AZ
- MP 30 **Development of a LC/MS Method for the Quantitation of Compound A, Ketoconazole, and Pentobarbital Using the Spiderling Column Selection System;** Chengwei Fang<sup>1</sup>; James Bostick<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, Merck &Co., Inc, West Point, PA

## QUANTITATIVE ANALYSIS OF DRUGS: METHOD DEVELOPMENT I

- MP 31 **A Fully Automated Assay to Evaluate Drug Candidate Stability in Biological Matrices;** Jinnan Cai<sup>1</sup>; Huidong Gu<sup>1</sup>; Yuzhong Deng<sup>1</sup>; Steve Unger<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ
- MP 32 **The Impact of Liposomes in Matrix on the Application of Hydrophilic Interaction Liquid Chromatography / Tandem Mass Spectrometric Analysis;** Jiongwei Pan<sup>1</sup>; Mark Leahy<sup>1</sup>; Jacob Maguigad<sup>1</sup>; Xiangyu Jiang<sup>1</sup>; <sup>1</sup>Covance The Development Services Company, Madison, WI
- MP 33 **Identification and Solution of Metabolite Overestimation During Support of Clinical Sample Analysis by LC/MS/MS;** Michael J Avery<sup>1</sup>; Debra Carson<sup>1</sup>; <sup>1</sup>Pfizer PGRD, Groton, CT
- MP 34 **Assessment of The Effect of Matrix Components on Accuracy of Quantitation;** Kimberly L. Norwood<sup>1</sup>; Edward G. Green<sup>1</sup>; David M. Wilson<sup>1</sup>; Richard S. Hucker<sup>2</sup>; John R Perkins<sup>1</sup>; <sup>1</sup>Advion BioSciences, Ithaca,

## POSTER SPACE

- NY; <sup>2</sup>Pfizer Global Research & Development, Sandwich, England
- MP 35 **Quantitative Analysis of 4-Trifluoromethylumbelliferyl Glucuronide Using HPLC-MS/MS: In vitro Evaluation of Inhibition of Glucuronidation by P450 Chemical Inhibitors;** Anthony Barros<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Lawrenceville, NJ
- MP 36 **Probing Electrospray Lipid Matrix Ionization Effects in the Analysis of Drugs in Plasma Samples;** James L. Little<sup>1</sup>; Michael F. Wempe<sup>1</sup>; Charles Buchanan<sup>1</sup>; <sup>1</sup>Eastman Chemical Company, Kingsport, TN
- MP 37 **Principal Component Analysis Tools to Visualize Matrix Effects in Quantitative LC-MS Bioanalysis;** Emmanuel Bourgogne<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>LSMS, EPGL-University of Geneva, Geneva, Switzerland
- MP 38 **Minimizing Matrix Effects on Bioanalysis of Drug Entities to Support Drug Discovery;** Hong Gao<sup>1</sup>; Licong Jiang<sup>2</sup>; Jianbo Zhang<sup>1</sup>; Christopher Brummel<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals Inc., Cambridge, MA; <sup>2</sup>Vertex Pharmaceuticals Inc, San Diego, CA
- MP 39 **Ion Suppression Mapping: A Tool for Assessing the Transferability of Quantitative ESI-LC/MS Methods;** David N. Heller<sup>1</sup>; <sup>1</sup>FDA Center for Veterinary Medicine, Laurel, MD
- MP 40 **Multiple Plasma Analyses using Rat Plasma Calibration Standards: Killing Three Birds with One Stone;** Christine M. Gambino<sup>1</sup>; <sup>1</sup>Memory Pharmaceuticals, Montvale, NJ
- MP 41 **Monitoring LC-MS Matrix-Effect Causing Phospholipids of Different Classes via Neutral Loss and Precursor Ion Scans in Positive and Negative Electrospray;** Mohammed Jemal<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Yuan-Qing Xia<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ
- MP 42 **Highly Selective LC/MS/MS Method with Resolution of 1'-Hydroxy and 4-Hydroxymidazolam for CYP3A Activity Assessment In vitro;** Girish Gudi<sup>1</sup>; Kenneth Matuszak<sup>1</sup>; Patricia Stuart<sup>1</sup>; Zhiwen Guan<sup>1</sup>; Maria Beconi<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
- MP 43 **Using Supercritical Fluid Chromatography MS to Alleviate the Imprecision in Bioanalysis Resulting from the Matrix Effect of Phospholipids;** Rui Chen<sup>1</sup>; Jennifer VanAnda<sup>1</sup>; Patrick Bennett<sup>23</sup>; Edward Brewer<sup>23</sup>; <sup>1</sup>Mettler Toledo Autochem, Inc., Newark, DE; <sup>2</sup>Tandem Labs, A Division of NWT Inc., Salt Lake City, UT; <sup>3</sup>Tandem Labs, A Division of NWT Inc., West Trenton, NJ
- MP 44 **Application of Weak Reversed-Phase Retention on Silica Column to Remove Matrix Suppression in LC-MS/MS;** Earl Moore<sup>1</sup>; Khanh Nguyen<sup>1</sup>; Patrick Lin<sup>1</sup>; <sup>1</sup>Alta Analytical Laboratories, El Dorado Hills, CA
- MP 45 **Obstacles to Lowering the Preclinical LLOQ from 500 TO 50 PG/ML for a Clinical Study;** David P Wolford<sup>1</sup>; Michael J Avery<sup>1</sup>; <sup>1</sup>Pfizer PGRD, Groton, CT
- MP 46 **Ionization Effects of Mobile Phase Additives on Stable Isotopically Labeled Internal Standards in Quantitative LC/MS/MS Analysis;** Danny W. Choo<sup>1</sup>; Chinedu D. Nriagu<sup>1</sup>; Irina R. Miksa<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA
- MP 47 **Matrix Effect Caused by Freeze-Thaw? A Case Study for Plasma Sample Analysis Using Direct-Injection LC/MS/MS;** Guowen Liu<sup>1</sup>; Anthony Barros<sup>1</sup>; Mike-Qingtao Huang<sup>1</sup>; Naidong Weng<sup>1</sup>; Mark E. Arnold<sup>1</sup>; Steve Unger<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Co., New Brunswick, NJ
- MP 48 **Optimization for the Quantitative Analysis of Zwitter Ion Compounds in DMPK on the Drug Discovery;**



# MONDAY POSTERS

## POSTER SPACE

- Hiroya Miura<sup>1</sup>; Toshiko Yahata<sup>1</sup>; Kazuyo Nakagawa<sup>2</sup>; Masayuki Kubota<sup>2</sup>; <sup>1</sup>Astellas Pharm Inc, Tsukuba, Japan; <sup>2</sup>Thermo Electron Corp., Yokohama, Japan
- MP 49 **Alternatives to Standard Bioanalysis;** Michael L. Bass<sup>1</sup>; Lara D. Penn<sup>1</sup>; David Weller<sup>1</sup>; Changyu Quang<sup>1</sup>; Roger Winters<sup>1</sup>; Lucinda H. Cohen<sup>1</sup>; <sup>1</sup>Pfizer Global Research and Development, Ann Arbor, MI
- MP 50 **High Throughput Cytochrome P450 Inhibition Study Analysis with Capillary LC-MSMS;** Themis Flarakos<sup>1</sup>; Ari Gritsas<sup>1</sup>; Tanya N Gamble<sup>2</sup>; Peter Kovarik<sup>2</sup>; J.C. Yves Le Blanc<sup>2</sup>; <sup>1</sup>MDS Pharma Services, Montreal, Canada; <sup>2</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- MP 51 **Factors Affecting Quantification in Atmospheric Pressure Chemical Ionization Mass Spectrometry;** Lisandra Cubero Herrera<sup>1</sup>; J. Stuart Grossert<sup>1</sup>; Louis Ramaley<sup>1</sup>; <sup>1</sup>Dalhousie University, Halifax, NS, Canada
- MP 52 **Quantification of a Cytochrome P450 3A4 Substrate, Buspirone, in Human Plasma by LC-MS/MS;** Wade M. Chew<sup>1</sup>; Min-Jian Xu<sup>1</sup>; H-H. Sherry Chow<sup>1</sup>; <sup>1</sup>Arizona Cancer Center, The University of Arizona, Tucson, AZ
- MP 53 **Comparative Evaluation of Four SPE Micro-Extraction Procedures for Biological Sample Extraction with LC/MS/MS Analysis;** Ming Wang<sup>1</sup>; Kasia Hopek<sup>1</sup>; Chinedu D. Nriagu<sup>1</sup>; Irina R. Miksa<sup>1</sup>; Harold D. Lanzoni<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA
- MP 54 **Rapid Detection and Quantitation of Glucuronides Utilizing ESI In-Source Fragmentation;** Eugene J. Eisenberg<sup>1</sup>; Lani M. Wieman<sup>1</sup>; Melody S. Lee<sup>1</sup>; Bernard P. Murray<sup>1</sup>; Gerry Rhodes<sup>1</sup>; <sup>1</sup>Gilead Sciences, Inc., Foster City, CA
- MP 55 **Evaluation of Dried Blood Spots for Quantitation in Drug Discovery by LC-MS/MS;** Elizabeth A. Mahan<sup>1</sup>; Joan Ellis<sup>1</sup>; Laquisha Hamilton<sup>1</sup>; Carmen Fernandez-Metzler<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA

## QUANTITATION OF ENDOGENOUS COMPOUNDS AND NATURAL PRODUCTS

- MP 56 **Development of a High-Throughput SPE-LC-MS/MS Method to Quantify Trace Levels of Endogenous Thiocyanate in Complex Biological Fluids;** Frank A. Kero<sup>1</sup>; Matthew M. Booth<sup>1</sup>; Donn M. Dennis<sup>1</sup>; Bruce A. Goldberger<sup>1</sup>; Gregory E. Conner<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, Florida; <sup>2</sup>University of Miami, Miami, FL
- MP 57 **Method Development for Quantification of Asparagine Synthetase in Leukemia Cell Lines;** Susan E. Abbatiello<sup>1</sup>; Thomas P Conrads<sup>2</sup>; Timothy D Veenstra<sup>2</sup>; John R Eyler<sup>1</sup>; Nigel G J Richards<sup>1</sup>; <sup>1</sup>University of Florida, Department of Chemistry, Gainesville, FL; <sup>2</sup>SAIC-Frederick, Inc., Frederick, MD
- MP 58 **Quantitation of Cellular Redox Intermediates and Nucleotide Phosphates in Cultured Cells;** Anthony J. Romanelli Jr.<sup>1</sup>; Richard G. Kibbey<sup>2</sup>; Gary W. Cline<sup>2</sup>; James A. Ferguson<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>Yale University, New Haven, CT
- MP 59 **Enantiomeric Determination of Salsolinols in Plasma by High-Performance Liquid Chromatography-Electrospray-Tandem Mass Spectrometry (HPLC-ESI-MS/MS);** Jeongrim Lee<sup>1</sup>; Bill Huang<sup>1</sup>; Zhixin Yuan<sup>1</sup>; Hee-Yong Kim<sup>1</sup>; <sup>1</sup>NIH/NIAAA, Rockville, MD
- MP 60 **Direct-Injection LC/MS/MS Determination of M+4 Stable Isotope Labeled Cortisone and Cortisol in Human Microdialysate;** Amy Y. Yang<sup>1</sup>; Li Sun<sup>1</sup>; Jin Zhang<sup>1</sup>; Donald G. Musson<sup>1</sup>; Jamie J. Zhao<sup>1</sup>; Eric J. Woolf<sup>1</sup>; <sup>1</sup>Merck & Co., Inc, West Point, PA

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- MP 61 **Rapid LC-MS/MS Method for the Detection of GL-3 Biomarker in Fabry Disease – Advantages of using Urine Filter Paper Samples;** Christiane Auray-Blais<sup>1</sup>; Denis Cyr<sup>1</sup>; Robert Giguère<sup>1</sup>; Bernard Lemieux<sup>1</sup>; Régen Drouin<sup>1</sup>; <sup>1</sup>Université de Sherbrooke, Sherbrooke, Quebec, Canada
- MP 62 **Quantifying the Concentration of Glucose in Tears by ESI-MS;** Christopher R. Taormina<sup>1</sup>; Justin T. Baca<sup>1</sup>; David N. Finegold<sup>1</sup>; Sanford A. Asher<sup>1</sup>; Joseph J. Grabowski<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA
- MP 63 **The Application of GC/MS to Quantify 17β-estradiol within the Thyroid-Gonad Signaling Pathway of the American Alligator (*Alligator mississippiensis*);** John A. Bowden<sup>1</sup>; Dieldrich S. Bermudez<sup>1</sup>; Louis J. Guille Jr.<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- MP 64 **Ultra-Performance Liquid Chromatography/Tandem Mass Spectrometric Determination of Testosterone and its Metabolites in in vitro Samples;** Ganfeng Wang<sup>1</sup>; Yunsheng Hsieh<sup>1</sup>; Xiaoming Cui<sup>1</sup>; Kuo-Chi Cheng<sup>1</sup>; Walter A. Korfmacher<sup>1</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, NJ
- MP 65 **Increased Organic Content Mobile Phases for Optimum Ionization Efficiency Allowing for Rapid Analysis of Pyridoxine in Human Plasma;** John Chapdelaine<sup>1</sup>; Evgueni Fedorov<sup>1</sup>; Jean-François Larocque<sup>1</sup>; Michael Mancini<sup>1</sup>; <sup>1</sup>Warnex, Laval, Quebec, Canada
- MP 66 **Development of Liquid Chromatography/Tandem Mass Spectrometry Methods for Quantitation of Cyclic Nucleotides (cGMP and cAMP) as Biomarkers;** Yanhua Zhang<sup>1</sup>; Brian Sanchez<sup>2</sup>; Charles Stankovic<sup>1</sup>; Wenlin Li<sup>1</sup>; Gabriella Szekely-Klepser<sup>1</sup>; Scott Fountain<sup>1</sup>; Nalini Sadagopan<sup>1</sup>; <sup>1</sup>Pfizer Inc. Biomarker Implementation Group, Ann Arbor, MI; <sup>2</sup>Pfizer Inc. Inflammation Biology, Ann Arbor, MI
- MP 67 **Biomarkers of Ethanol in Equine Urine by Liquid Chromatography-Tandem Mass Spectrometry;** Youwen You<sup>1</sup>; Cornelius Ubob<sup>1</sup>; Lawrence Soma<sup>1</sup>; Fuyu Guan<sup>1</sup>; Jeffrey Rudy<sup>2</sup>; <sup>1</sup>School of Veterinary Medicine, University of Penn., Kennett Square, PA; <sup>2</sup>PA Equine Toxicology and Research Center, West Chester, PA
- MP 68 **Bioanalytical Analysis of Non-Polar Lipids in Tears using LC/MS;** Feng Zhong<sup>1</sup>; Yu Gu<sup>2</sup>; Janusz Pawlisyzyn<sup>2</sup>; Terry McMahon<sup>2</sup>; Lyndon W. Jones<sup>2</sup>; <sup>1</sup>MDS Sciex, Concord, ON, Canada; <sup>2</sup>University of Waterloo, Waterloo, ON, Canada
- MP 69 **Surface Activated Chemical Ionization in the Analysis of Markers of Cardiac Diseases;** Lorenzo Zingaro<sup>1</sup>; Viviana Cavalca<sup>1</sup>; Luigi Rossi Bernardi<sup>2</sup>; Cristina Canton<sup>3</sup>; Marco Cantu<sup>4</sup>; Simone Cristoni<sup>5</sup>; <sup>1</sup>Monzino Cardiology Center, Milan, Italy; <sup>2</sup>University of Milan, Milan, Italy; <sup>3</sup>CNR of Milan, Milan, Italy; <sup>4</sup>Biotrack, Lodi Milan, Italy; <sup>5</sup>ISB, Milan, Italy
- MP 70 **A Sensitive 96-well MicroElute SPE-LC-MS/MS Method for the Quantitation of Cortisone and Cortisol in Rat Plasma;** Xiao Ding<sup>1</sup>; Mark Rose<sup>1</sup>; Maurice Emery<sup>1</sup>; Robert Kimura<sup>2</sup>; Christopher James<sup>1</sup>; <sup>1</sup>Amgen, Inc., Thousand Oaks, CA; <sup>2</sup>Rush Medical College, Chicago, IL
- MP 71 **Validation of Calcitriol (Vitamin-D3) in Human Serum by HPLC-MS-MS and UPLC-MS-MS and Subsequent Analysis of Samples From a Clinical Study;** David J Browne<sup>1</sup>; Mohammed Abrar<sup>1</sup>; Sunetha Diaram<sup>1</sup>; David

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- Bakes<sup>1</sup>; Morten Carlsen<sup>2</sup>; <sup>1</sup>Covance Laboratories, Harrogate, UK; <sup>2</sup>Leo Pharma A/S, Ballerup, Denmark
- MP 72 **Quantification Of Corticosteroids From Ex Vivo Activity Assay**; Lan Gao<sup>1</sup>; William Chiou<sup>1</sup>; Xueheng Cheng<sup>1</sup>; Heidi Camp<sup>1</sup>; David Burns<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
- MP 73 **Quantitative Analysis using LC-MS-MS of PGE2 and PGD2 in Cellular Supernatant Samples**; Hongmei Cao<sup>1</sup>; Gye Young Park<sup>2</sup>; Anser Azim<sup>2</sup>; Bijl Mathew<sup>2</sup>; Xuerong Wang<sup>2</sup>; John W. Christman<sup>2</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>University of Illinois College of Medicine, Chicago, IL
- MP 74 **Quantification of Fatty Acid Ethyl Esters as Biomarkers by HPLC/ Electrospray Mass Spectroscopy**; Whitney V Milec<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH
- MP 76 **Quantitative Analysis of Malachite Green and its Metabolite in Aquaculture Samples from Asia**; Matthew E Grigg<sup>1</sup>; YanLing Yu<sup>2</sup>; Charles C Liu<sup>2</sup>; <sup>1</sup>Applied Biosystems, Singapore, Singapore; <sup>2</sup>Applied Biosystems, Shanghai, China
- MP 77 **Quantification of Heart Fatty Acid Binding Protein as a Biomarker for Drug-Induced Cardiac and Musculoskeletal Necroses**; Yuejun Zhen<sup>1</sup>; Michael J Berna<sup>1</sup>; Zhaoyan Jin<sup>1</sup>; David E Watson<sup>1</sup>; Bradley L Ackermann<sup>1</sup>; John E Hale<sup>1</sup>; <sup>1</sup>Eli Lilly and Company, Indianapolis, IN
- MP 78 **High Throughput LC-MS/MS Quantitative Analysis of Amino Acids in Arabidopsis Seeds and Leaves**; Lijun Chen<sup>1</sup>; Liping Gu<sup>1</sup>; Yan Lu<sup>1</sup>; Robert L. Last<sup>1</sup>; A. Daniel Jones<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- MP 79 **Quantitative Determination of 7 $\alpha$ -OH Dehydroepiandrosterone and 7 $\beta$ -OH Dehydroepiandrosterone in Rat Brain Microsome Mixtures Using LC/MS/MS**; Aiqun Li<sup>1</sup>; James C Bigelow<sup>1</sup>; <sup>1</sup>Idaho State University, College of Pharmacy, Pocatello, ID
- MP 80 **Withdrawn**
- MP 81 **Quantification of Prebiotic Oligosaccharides by Negative Ion Mode LC-MS Multiple Reaction Monitoring (MRM)**; Bernd Stahl<sup>1</sup>; Marko Mank<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; <sup>1</sup>Numico Research Germany, Friedrichsdorf, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- MP 82 **Identification and Quantification of Soy Isoflavonoids in Human Urine Using Triple Quadrupole-Linear Ion-Trap Mass Spectrometer**; Sudha S Marimanikkuppam<sup>1</sup>; Michael L Wachter<sup>1</sup>; Mindy S Kurzer<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN

## CLINICAL CHEMISTRY I

- MP 83 **Avoiding Artifacts in Acylcarnitine Profiling**; Martin Sadilek<sup>1</sup>; Katerina Sadilkova<sup>2</sup>; Rhona M. Jack<sup>2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Children's Hospital and Regional Medical Center, Seattle, WA
- MP 84 **Improvement in the Analysis of 4-Aminobiphenyl in Hemoglobin Adducts and Urine in Nonsmokers by On-Column GC Tandem Mass Spectrometry**; Tiffany H. Seyler<sup>1</sup>; J. Thomas Bernert<sup>1</sup>; <sup>1</sup>CDC/NCEH/DLS, Atlanta, GA
- MP 85 **Separation and Quantitation of Complex Amino Acid Derivatives in Plasma**; Ray Chen<sup>1</sup>; Jennifer Huang<sup>1</sup>; Charlie Van Wandelen<sup>1</sup>; Chris Loran<sup>1</sup>; <sup>1</sup>Thermo Electron Corp, San Jose, CA
- MP 86 **Determination of New Anabolic Agents in Urine – SARMS and Synthetic Insulins**; Mario Thevis<sup>1</sup>; Matthias Kamber<sup>2</sup>; Andreas Thomas<sup>1</sup>; Philippe Delahaut<sup>3</sup>; Alain

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- Bosseloir<sup>4</sup>; Wilhelm Schänzer<sup>1</sup>; <sup>1</sup>Institute of Biochemistry/ German Sport University, Cologne, Germany; <sup>2</sup>Federal Office of Sports, Magglingen, Switzerland; <sup>3</sup>Centre d'Economie Rurale, Marloie, Belgium; <sup>4</sup>ZenTech, Angleur, Belgium
- MP 87 **Prenatal Variability and the Stability of Human Plasma Proteins: Mass Spectrometry Changes of Peptides Post Blood Collection**; Jizu Yi<sup>1</sup>; Changki Kim<sup>1</sup>; Craig A Gelfand<sup>1</sup>; <sup>1</sup>BD Diagnostics, Preanalytic System, Franklin Lakes, NJ
- MP 88 **Withdrawn**
- MP 89 **Diagnosis of Chronic Hepatorenal Tyrosinemia Type 1 in Urine by Flow Injection Tandem Mass Spectrometry**; David W Johnson<sup>1</sup>; <sup>1</sup>Women's and Children's Hospital, North Adelaide, Australia
- MP 90 **Evaluation of a Multiplexed Enhanced Pressure Pumping System in Clinical Diagnostics**; Russell P Grant<sup>1</sup>; Mary K Morr<sup>1</sup>; Andrew D Wagner<sup>1</sup>; <sup>1</sup>Esoterix inc., Calabasas Hills, CA
- MP 91 **Measuring Endogenous Free and Total Estrogens and Estrogen Metabolites in Human Serum by High-Performance Liquid Chromatography-Tandem Mass Spectrometry**; Xia Xu<sup>1</sup>; John M. Roman<sup>1</sup>; Haleem J. Issaq<sup>1</sup>; Roni Falk<sup>2</sup>; Larry K. Keefer<sup>3</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; <sup>3</sup>National Cancer Institute at Frederick, Frederick, MD
- MP 92 **Characterization of Hemoglobin Variants Using Hyphenated LC-MS/MS Technologies**; Sonja Hess<sup>1</sup>; Ruth Huettnerich<sup>2</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>University of Bonn, Bonn, Germany
- MP 93 **A Quantitative Method For Simultaneous Determination of Seven Vitamins Including D2, D3, Mono-Hydroxy Metabolites and Dihydroxy Metabolites in Human Serum**; Yan Ling Zhang<sup>1</sup>; Valerie Burns<sup>1</sup>; Leah Swanson<sup>1</sup>; Michol Rothman<sup>1</sup>; Margaret Wierman<sup>1</sup>; Chester Ridgeway<sup>1</sup>; Uwe Christians<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, CO
- MP 94 **Rapid Determination of Steroids for Newborn Screening for Congenital Adrenal Hyperplasia (CAH) by Turbulent Flow Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; Jean M. Lacey<sup>1</sup>; Mark J. Magera<sup>1</sup>; Joseph M. Di Bussolo<sup>2</sup>; Silvia Tortorelli<sup>1</sup>; SiHoun Hahn<sup>1</sup>; Piero Rinaldo<sup>1</sup>; Dietrich Matern<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Cohesive Technologies, Franklin, MA
- MP 95 **Measurement of Serum Dehydroepiandrosterone (DHEA) by LC-MS/MS**; Ravinder J. Singh<sup>1</sup>; Robert E. Nelson<sup>1</sup>; Stefan K. Grebe<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN
- MP 96 **Fragmentation Specific Stable Isotope Dilution Measurement of Asymmetric and Symmetric Dimethylarginines Using Electrospray Mass Spectrometry-Mass Spectrometry**; R Neil Dalton<sup>1</sup>; Charles Turner<sup>2</sup>; <sup>1</sup>King's College London, London, UK; <sup>2</sup>Guy's & St Thomas' NHS Foundation Trust, London, UK

## SAMPLE PREPARATION FOR LC/MS I

- MP 97 **Vial to File - A New Paradigm for Sample Analysis in a GLP Laboratory**; Roger N. Hayes<sup>1</sup>; James E. Schiller<sup>1</sup>; Hui Lin<sup>1</sup>; Dirk Hiemstra<sup>2</sup>; Steven Eendhuizen<sup>2</sup>; Rob Castien<sup>2</sup>; <sup>1</sup>Schering-Plough Research Institute, Lafayette, NJ; <sup>2</sup>Spark Holland, Emmen, The Netherlands
- MP 98 **Direct Injection of the Organic Phase From Liquid-Liquid Extraction of Biological Samples onto a Reversed Phase Column in Drug Discovery**; Henrik

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- Zackari<sup>1</sup>; Gunilla Jerndal<sup>1</sup>; <sup>1</sup>AstraZeneca R&D, Molndal, Sweden
- MP 99 **Optimization of Sample Preparation for LC-MS/MS Analysis of Basic Pharmaceuticals from Serum using Solid Phase Extraction;** Jason Blodgett<sup>1</sup>; Vivek Joshi<sup>1</sup>; Nanyang Bian<sup>2</sup>; <sup>1</sup>Millipore Corporation, Danvers, MA; <sup>2</sup>Millipore Corp., Bedford, MA
- MP 100 **Determination of Antibiotic Compounds in Water by On-Line SPE(Solid-Phase Extraction)-Liquid Chromatography Mass Spectrometry;** Keun-Joo Choi<sup>1</sup>; Sang-Goo Kim<sup>1</sup>; Hee-Jong Son<sup>1</sup>; Pyung-Jong You<sup>1</sup>; Chang-Won Kim<sup>2</sup>; Seung-Hyun Kim<sup>3</sup>; Sook-Hwa Kweon<sup>4</sup>; <sup>1</sup>Water Quality Research Institute, Busan, Korea; <sup>2</sup>Department of Environmental Engineering, Busan, Korea; <sup>3</sup>Department of civil Engineering, Kyungnam, Korea; <sup>4</sup>Application Support Team, Seoul, Korea
- MP 101 **A Novel Method for Quantifying Reduced and Oxidized Glutathione in Plasma by LC-MS-MS;** Roy C Bogseth<sup>1</sup>; Kelly L Balla<sup>1</sup>; Todd S Wielgos<sup>1</sup>; <sup>1</sup>Baxter Healthcare, Round Lake, IL
- MP 102 **Evaluation of Chemical Stability and Assay Quality Using Focused Acoustic Energy Tissue Homogenization and LC-MS/MS Analysis;** Hang Zeng<sup>1</sup>; Kristen MacFarland<sup>1</sup>; Joe Gallagher<sup>1</sup>; Ping Wang<sup>1</sup>; Daksha Desai-Krieger<sup>1</sup>; <sup>1</sup>Johnson & Johnson Pharmaceutical R&D, PCD, Spring House, PA
- MP 103 **Quantitative Determination of Gaboxadol in Biological Samples by LC-MS/MS;** Morten A. Kall<sup>1</sup>; Patrick Vallano<sup>2</sup>; Irong Fu<sup>2</sup>; Tina Dige<sup>1</sup>; Eric Woolf<sup>2</sup>; Martin Jørgensen<sup>1</sup>; <sup>1</sup>Drug ADME Research, H. Lundbeck, Copenhagen, Denmark; <sup>2</sup>Dept. of Drug Metabolism, Merck Research Laboratory, West Point, PA
- MP 104 **Matrix Removal and Matrix Effect Elimination by HTLC/MS/MS;** John Brann<sup>1</sup>; Chris Esposito<sup>1</sup>; Francois A. Espourteille<sup>1</sup>; <sup>1</sup>Cohesive Technologies, Inc., Franklin, MA
- MP 105 **Strategies for Method Developments in High Speed and Robust On-Line Solid Phase Extraction - LC-MS/MS;** Huqun Liu<sup>1</sup>; Dave Jones<sup>1</sup>; Raegan Goodell<sup>1</sup>; Chris Lee<sup>1</sup>; <sup>1</sup>Varian, Inc., Lake Forest, CA
- MP 106 **A Simple Strategy to Quantify a Solubility-Limited Pharmaceutical in Human Urine;** Eliza N. Fung<sup>1</sup>; Yongjun Xue<sup>1</sup>; Nick Duczak<sup>2</sup>; Steve Unger<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, New Brunswick, NJ; <sup>2</sup>Thermo Electron Corporation, Somerset, NJ
- MP 107 **Development and Validation of Quantitative Methods for Digoxin in Human Serum and Urine by LC/MS/MS: Challenges and Considerations;** Steve Lowes<sup>1</sup>; Brian T. Hoffman<sup>1</sup>; Sara L. Jones<sup>1</sup>; George P. Hade<sup>1</sup>; Daniel E. Mulvana<sup>1</sup>; <sup>1</sup>Advion BioServices, Ithaca, NY
- MP 108 **Reduction of Matrix Effects due to Phospholipids: A Comparison of Sample Preparation Techniques;** Lee Williams<sup>1</sup>; Scott Merriman<sup>1</sup>; Helen Lodder<sup>1</sup>; Anne Howells<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Matthew Clevee<sup>1</sup>; Richard Calverley<sup>1</sup>; <sup>1</sup>Argonaut Technologies, now a Biotage company, Hengoed, UK
- MP 109 **Enhancing Extraction Efficiencies of HTLC-MS Assays using Turbulent-Flow Mixing;** Kimberly M. Navaline<sup>1</sup>; Kathryn Black<sup>2</sup>; Jessica Barwell<sup>2</sup>; Matthew Ercolino<sup>2</sup>; Joseph M. Di Bussolo<sup>1</sup>; <sup>1</sup>Cohesive Technologies, Franklin, MA; <sup>2</sup>West Chester University of Pennsylvania, West Chester, PA
- MP 110 **Fluorous Derivatization for Improved Detection and Isolation of Small Molecules by Functional Class;**

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- Daniel E. Mason<sup>1</sup>; <sup>1</sup>Genomics Institute of Novartis, San Diego, CA
- MP 111 **Determination and Impact Evaluation of Interfering Contaminants Leached from Plastic Materials used during LC-MS/MS Sample Preparation;** Fabio Garofolo<sup>1</sup>; Véronique Gauvreau<sup>1</sup>; Marie-Pierre Taillon<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval Montreal, Canada
- MP 112 **Overcoming Challenges During Development of Plasma and Urine Assays for a Drug Candidate Indicated for Migraine Using Turbulent Flow LC-MS/MS;** Yang Xu<sup>1</sup>; Donald G. Musson<sup>1</sup>; Cynthia M. Miller-Stein<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- MP 113 **Automated 96- Well Plate Solid-Phase Extraction of Aflatoxin B1-Lysine Adduct for Liquid Chromatography Tandem Mass Spectrometric Analysis;** Leslie F. McCoy<sup>1</sup>; Carissa D. Powers<sup>1</sup>; Rosemary L. Schleicher<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA
- MP 114 **Development and Validation of a Sensitive Automated On-line SPE-LC/MS/MS Method to Support Early Candidate Selection in Drug Discovery;** Carrie Xu<sup>1</sup>; Baomin Xin<sup>1</sup>; Timothy Olah<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Lawrenceville, NJ
- MP 115 **Total Drug Analysis of Pharmaceutical Compounds from Whole Blood using Solid Phase Extraction (SPE) Coupled with LC-MS/MS;** Vivek Joshi<sup>1</sup>; Jason Blodgett<sup>1</sup>; Nanyang Bian<sup>2</sup>; <sup>1</sup>Millipore Corporation, Danvers, MA; <sup>2</sup>Millipore Corp., Bedford, MA
- MP 116 **Common Methods of Peptide Extraction from Clinical Samples can Cause Notable Omissions and Artifactual Additions in the Peptidome;** Jeffrey P Henderson<sup>1</sup>; Richard Brasington<sup>1</sup>; John Turk<sup>1</sup>; Jan R Crowley<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO
- MP 117 **Withdrawn**
- MP 118 **Can ion Suppression be Quantitated? Part II – Vials;** Claude R. Mallet<sup>1</sup>; Diane M. Diehl<sup>1</sup>; Jeff R. Mazzeo<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- MP 119 **Comparison of Methods to Examine the Endogenous Peptides of Fetal Serum;** Declan Williams<sup>1</sup>; Peihong Zhu<sup>1</sup>; Peter Bowden<sup>1</sup>; June McCallum<sup>1</sup>; Catherine Stacey<sup>23</sup>; Michael E McDonell<sup>23</sup>; Paul Kowalski<sup>23</sup>; JaneMarie Kowalski<sup>23</sup>; Ken Evans<sup>4</sup>; Eleftherios Diamandis<sup>5</sup>; Michael Siu<sup>6</sup>; John Marshall<sup>1</sup>; <sup>1</sup>Ryerson University, Toronto, Canada; <sup>2</sup>Bruker Daltonics, Milton, Ontario, Ca; <sup>3</sup>Bruker Daltonics, Billerica, Ma; <sup>4</sup>Ontario Cancer Biomarker Network, Toronto, Canada; <sup>5</sup>Mt Sinai Hospital, Toronto, Canada; <sup>6</sup>York University, Toronto, Canada
- MP 120 **Extraction and HPLC-MS/MS Detection of Antibiotics from Bovine Fodder: Methods Comparison;** Valeria Catanzaro<sup>1</sup>; Marco Pazzi<sup>1</sup>; Marco Vincenti<sup>1</sup>; <sup>1</sup>Università degli Studi di Torino, Torino, Italy

### HOMELAND SECURITY AND FORENSICS

- MP 121 **Comparison of High Resolution MS and MS/MS for Chemical Weapons (CW) Air Monitoring Applications;** William R. Creasy<sup>1</sup>; Scott Cantwell<sup>2</sup>; Ralph Spafford<sup>2</sup>; Richard O'Connor<sup>3</sup>; <sup>1</sup>EAI Corp. Division of SAIC, Abingdon, MD; <sup>2</sup>FOCIS Division of SAIC, Newton, MA; <sup>3</sup>R&T Directorate, ECBC, Aberdeen Proving Ground, MD
- MP 122 **Degradation of Tabun in Aqueous Matrices Studied by LC/ESI/ITMS and LC/ESI/MS<sup>n</sup>;** Anne Bossée<sup>1</sup>;

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- Dominique Somnard<sup>1</sup>; Arlette Bégos<sup>1</sup>; Bruno Bellier<sup>1</sup>;  
<sup>1</sup>Centre d'Etudes du Bouchet, Vert Le Petit, France
- MP 123 **Whole-Cell Protein Profiling of Forensically Relevant Microorganisms Using LC-ESI MS**; Douglas B. Henderson<sup>1</sup>; Danielle N. Dickinson<sup>1</sup>; Peter Leopold<sup>2</sup>; Brian A. Eckenrode<sup>3</sup>; <sup>1</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>2</sup>BioAnalyte, Inc., Portland, ME; <sup>3</sup>Federal Bureau of Investigation, Quantico, VA
- MP 124 **MALDI/TOF Analysis followed by Correlation Analysis for the Characterization of Foodborne Pathogens**; Shane A. Wyatt<sup>1</sup>; Elise Smith<sup>1</sup>; Denise M. Toney<sup>1</sup>; Timothy R. Croley<sup>1</sup>; Dan Buzatu<sup>2</sup>; Jon Wilkes<sup>2</sup>; <sup>1</sup>Commonwealth of Virginia, Richmond, VA; <sup>2</sup>Food and Drug Administration, Jefferson, AR
- MP 125 **Novel Methods for the Rapid Characterization of Viruses**; Stephen J. Swatkoski<sup>1</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD
- MP 126 **Bacterial Spore Culture Condition Differentiation by MALDI-TOFMS**; Catherine E Petersen<sup>1</sup>; Kristin H Jarman<sup>1</sup>; Nancy B Valentine<sup>1</sup>; David S Wunschel<sup>1</sup>; Karen L Wahl<sup>1</sup>; James M Robertson<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>CFSRU/FBI Academy, Quantico, VA
- MP 127 **Detection of Trace Agar on Bacillus Spores by Agarase Digestion ESI-MS**; Heather C. Edberg<sup>1</sup>; Catherine E. Petersen<sup>1</sup>; Nancy B. Valentine<sup>1</sup>; David S. Wunschel<sup>1</sup>; Karen L. Wahl<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 128 **A New Diagnostic Francisella Peptide Chip Assay Allowing Sensitive, Quantitative, and Specific Detection of Francisella in Clinical and Environmental Samples**; Jian Jiang<sup>1</sup>; Carol E. Parker<sup>1</sup>; James R. Fuller<sup>1</sup>; Tomas H. Kawula<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- MP 129 **Optimization of Enzymatic Sample Processing for the Detection of Bioagents Using AP-MALDI-MS/MS**; Constance M. Murphy<sup>1</sup>; Nelli I. Taranenko<sup>1</sup>; Appavu K. Sundaram<sup>1</sup>; Berk Oktem<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; <sup>1</sup>MassTech Inc., Columbia, MD
- MP 130 **Towards the Optimization of an LC-MS/MS Strategy for the Classification of BACT Group Serotypes Based on Proteogenomic Similarities**; Danielle N. Dickinson<sup>1</sup>; Jacek P. Dworzanski<sup>2</sup>; Heather L. Hartman<sup>1</sup>; Ducote Matt<sup>1</sup>; Samir V. Deshpande<sup>3</sup>; Brian A. Eckenrode<sup>4</sup>; <sup>1</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>2</sup>SAIC, Aberdeen Proving Ground, MD; <sup>3</sup>Science and Technology Corporation, Edgewood, MD; <sup>4</sup>FBI Counterterrorism and Forensic Science Research, Quantico, VA
- MP 131 **Detection and Identification of Chemical Warfare Agent Degradation Products by Capillary Electrophoresis Coupled To Mass Spectrometry**; Mélanie Lagarrigue<sup>1</sup>; Anne Bossée<sup>1</sup>; Arlette Bégos<sup>1</sup>; Anne Varenne<sup>2</sup>; Jean-Claude Tabet<sup>3</sup>; Pierre Gareil<sup>2</sup>; Bruno Bellier<sup>1</sup>; <sup>1</sup>Centre d'Etudes du Bouchet, Vert le Petit, France; <sup>2</sup>Ecole Nationale Supérieure de Chimie de Paris, Paris, France; <sup>3</sup>Université Pierre et Marie Curie, Paris, France
- MP 132 **Effective and Sensitive Detection of Enterobacteriophage MS2 by Atmospheric Pressure MALDI Ion Trap Mass Spectrometry**; Nelli I. Taranenko<sup>1</sup>; Olga V. Protchenko<sup>2</sup>; Appavu K. Sundaram<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; <sup>1</sup>MassTech, Inc., Columbia, MD; <sup>2</sup>NIH/NIDDK, Bethesda, MD

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- MP 133 **High Performance Electrospray Ionization Mass Spectrometry Analysis of Multiplexed PCR for the Forensic Discrimination of Human Mitochondrial DNA**; Thomas A. Hall<sup>1</sup>; Kristin Sannes-Lowery<sup>1</sup>; Brian A. Eckenrode<sup>2</sup>; Kerri A. Dugan<sup>2</sup>; Douglas Henderson<sup>3</sup>; Amy Schink<sup>1</sup>; Steven A. Hofstadler<sup>1</sup>; <sup>1</sup>Ibis Division of Isis Pharmaceuticals, Inc., Carlsbad, CA; <sup>2</sup>Federal Bureau of Investigation, Quantico, VA; <sup>3</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN
- MP 134 **MALDI Analysis of Impacted Bioaerosols for Bacteria Identification**; Alton J. Dugas<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- MP 135 **Detection of Ricin in Clinical and Food Samples**; Suzanne R. Kalb<sup>1</sup>; Adrian R. Woolfitt<sup>1</sup>; John R. Barr<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA

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- MP 136 **Detection of Improvised Explosives and Pyrotechnic Compositions on Passengers**; Karl Hanold<sup>1</sup>; <sup>1</sup>Syagen Technology Inc, Tustin, CA
- MP 137 **High-Throughput Analysis of Methamphetamine by Liquid Chromatography-Time of Flight Mass Spectrometry**; Miho Ebata<sup>1</sup>; Osamu Shirota<sup>1</sup>; Kazuko Tanaka<sup>2</sup>; Akihiko Kusai<sup>2</sup>; Rae-Ann Baldwin<sup>3</sup>; <sup>1</sup>Shiseido HPLC Application Lab, Yokohama, Japan; <sup>2</sup>Application and Research Group, JEOL, Akishima, Tokyo, Japan; <sup>3</sup>JEOL USA, Peabody, MA
- MP 138 **High Throughput Drugs-of-Abuse Screening: The Combination of Scheduled MRM Transitions and Fast Chromatography**; Byron Kieser<sup>1</sup>; Sandra Chu<sup>2</sup>; Gary Impey<sup>1</sup>; Yves LeBlanc<sup>2</sup>; Nic Bloomfield<sup>2</sup>; <sup>1</sup>Applied Biosystems / MDS Sciex, Toronto, Canada; <sup>2</sup>MDS Sciex, Toronto, Canada
- MP 139 **Characterization of the Degradation Process and Products in Urine of the Metabolite from the Nerve Agent GA by LC/MS/MS**; Elizabeth I. Hamelin<sup>1</sup>; Douglas B. Mawhinney<sup>2</sup>; Robert J. Kobelski<sup>2</sup>; <sup>1</sup>Battelle Memorial Institute/CDC, Atlanta, GA; <sup>2</sup>CDC, Atlanta, GA
- MP 140 **Laser-Ionization Mass Spectrometry of Explosives and Chemical Warfare Simulants**; Harald Oser<sup>1</sup>; Christopher Mullen<sup>1</sup>; Michael J. Coggiola<sup>1</sup>; <sup>1</sup>SRI International, Menlo Park, CA
- MP 141 **Screening for 4-Hydroxycoumarin-based Commercial Rodenticides in Food or Drug Products Using High Performance Liquid Chromatography / Negative Ion Mass Spectrometry**; Mantai Mesmer<sup>1</sup>; R. Duane Satzger<sup>1</sup>; <sup>1</sup>Forensic Chemistry Center USFDA, Cincinnati, OH
- MP 142 **Quick Screening and Quantification of Explosive Samples Using Rapid Resolution LC/MS and Simultaneous ESI/APCI Detection**; Andre Szczesniowski<sup>1</sup>; Sheher Mohsin<sup>1</sup>; Michael Woodman<sup>1</sup>; <sup>1</sup>Agilent Technologies, Schaumburg, IL
- MP 143 **Screening and Quantitation of Multiple Drugs of Abuse and Their Metabolites in Urine by LC/MS/MS**; June Feng<sup>1</sup>; Lanqing Wang<sup>1</sup>; Yingkun Dai<sup>1</sup>; John T Bernert<sup>1</sup>; <sup>1</sup>DLS, NCEH/ATSDR, Centers for Disease Control, Atlanta, GA
- MP 144 **Multi Target Screening for the Detection of 400 Drugs in Serum/Urine Extracts and Identification with a New MS/MS Library**; Sebastian Dresen<sup>1</sup>; André Schreiber<sup>2</sup>; Wolfgang Weinmann<sup>1</sup>; <sup>1</sup>Institute of Forensic Medicine, Freiburg, Germany; <sup>2</sup>MDS SCIEX, Toronto, Canada
- MP 145 **Waterborne Biomarkers as Triggers for Online MS-Monitoring of Drinking Water**; Ronny Robbins<sup>1</sup>; William Lagna<sup>1</sup>; <sup>1</sup>U.S. Army, Gunpowder, MD

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- MP 146 **A Novel Method to Extend the Detection Window of Drug Administration with LC-MS Technology, Combining Triple Quad and Trap Technology;** Sophie Turfus<sup>1</sup>; Simon Elliott<sup>1</sup>; Frans Schoutsen<sup>2</sup>; Stephen Lock<sup>2</sup>; <sup>1</sup>Regional Laboratory for Toxicology, Birmingham, UK; <sup>2</sup>Applied Biosystems, Warrington, UK
- MP 147 **Simultaneously Analyzing of Various Kinds of Abused Drugs in Urine by Liquid Chromatography-Mass Spectrometry;** Chung-Yu Chen<sup>1</sup>; Maw-Rong Lee<sup>1</sup>; Chien-Chun Shen<sup>1</sup>; <sup>1</sup>National Chung-Hsing University, Taichung, Taiwan, ROC
- MP 148 **Quantitative Determination of Amphetamine, Methylene-Dioxy-Methamphetamine (MDMA), Morphine, Cocaine and Tetrahydrocannabinol (THC) from Saliva Using LC-MS;** Harald C. Köfeler<sup>2</sup>; Gerald N. Rechberger<sup>4</sup>; Günter Fauler<sup>3</sup>; Manfred Kollroser<sup>1</sup>; <sup>1</sup>Medical University, Legal Medicine, Graz, Austria; <sup>2</sup>Medical University, ZMF, Graz, Austria; <sup>3</sup>Medical University, Clinical Chemistry, Graz, Austria; <sup>4</sup>Karl Franzens University, Biochemistry, Graz, Austria
- MP 149 **Analysis of a Challenging Subset of World Anti-Doping Agency-Banned Steroids and Anti-Estrogens by LC/MS/MS;** Chad R. Borges<sup>1</sup>; Nicole Miller<sup>1</sup>; Megan Hansen<sup>1</sup>; Claudia White<sup>1</sup>; Melinda Shelby<sup>1</sup>; Matthew H. Slawson<sup>1</sup>; Dennis J. Crouch<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT
- MP 150 **Determination of Four Metabolites of Dipyrone in a Suspected Pediatric Poisoning Case by LC-MS/MS on a Q-ToF;** Loan T. Nguyen<sup>1</sup>; Laura Labay<sup>1</sup>; Kevin D. Ballard<sup>1</sup>; <sup>1</sup>National Medical Services, Willow Grove, PA
- MP 151 **Ultrafast Laser Photoionization Time of Flight Mass Spectrometry of Triacetone Triperoxide (TATP) and Nitro-Containing Explosives;** Christopher Mullen<sup>1</sup>; Michael J. Coggiola<sup>1</sup>; Harald Oser<sup>1</sup>; <sup>1</sup>SRI International, Menlo Park, CA
- MP 152 **A Rapid Method of Detecting Drinking Water Adulteration by LC/MS/MS;** Michael Baynham<sup>2</sup>; Stephen Lock<sup>2</sup>; David Evans<sup>1</sup>; Clive Thompson<sup>1</sup>; Pat Cummings<sup>1</sup>; <sup>1</sup>ALcontrol Laboratories, Rotherham, UK; <sup>2</sup>Applied Biosystems, Warrington, UK
- MP 153 **Application of Isotope Ratio Mass Spectrometry (&delta; <sup>13</sup>C & &delta;D) to Discrimination Between PVC Electrical Tape Backings;** Alexandra H Thompson<sup>1</sup>; Mark L. Miller<sup>2</sup>; <sup>1</sup>Oak Ridge Institute for Science & Education, Oak Ridge, TN; <sup>2</sup>FBI Laboratory, CFSRU, Quantico, VA

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- MP 154 **Use of Ion Mobility Spectrometry to Characterize Odor Plumes from Field Release of Compounds that Modify Mosquito Host-Seeking Behavior;** Samaret M. Otero-Santos<sup>1</sup>; Richard A. Yost<sup>1</sup>; Ulrich R. Bernier<sup>2</sup>; Sandra A. Allan<sup>2</sup>; Daniel L. Kline<sup>2</sup>; Gary G. Clark<sup>2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>USDA-ARS-CMAVE, Gainesville, FL
- MP 155 **Development of a Hybrid Quadrupole-Linear Ion Trap-Ion Mobility-TOFMS for Structural Mass Spectrometry;** Jody C. May<sup>1</sup>; John A. McLean<sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- MP 156 **A Method to Separate Protein Ions with Similar Ion Mobilities via Mass-Selective Ejection from an Ion Trap;** Qin Zhao<sup>1</sup>; Matthew Soyk<sup>1</sup>; Gregg Schieffer<sup>1</sup>; Ethan Badman<sup>1</sup>; <sup>1</sup>Iowa State University, Ames, IA
- MP 157 **Structure Activity Relationships of Tryptic Peptide Behavior in High Field Asymmetric Waveform Ion Mobility Mass Spectrometry (FAIMS);** Jennifer A.

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- Garrett<sup>1</sup>; Christopher K. Hilton<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- MP 158 **Separation and Fragmentation of Isomeric Peptides with a Two Gate Ion Mobility Quadrupole Ion Trap Mass Spectrometer;** Matthew J. Pollard<sup>1</sup>; Brian H. Clowers<sup>2</sup>; Bharath Kumar<sup>1</sup>; Herbert H. Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>University of California, Davis, CA
- MP 159 **Ion-Mobility Measurements of Functionalized Pentacene Cations with a Modified Electrospray/Triple Quadrupole Mass Spectrometer;** Svitlana Shcherbyna<sup>1</sup>; Diethard Bohme<sup>1</sup>; Vladimir Baranov<sup>2</sup>; <sup>1</sup>York University, Toronto, ON; <sup>2</sup>IBBME, University of Toronto, Toronto, ON
- MP 160 **Analytical Detection by Liquid Phase Ion Mobility Spectrometry;** Maggie Tam<sup>1</sup>; Herbert H. Hill, Jr. <sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- MP 161 **Effect of Carrier Gas Composition in FAIMS/MS on Separation of Charge States and Conformers of Intact Proteins;** Rachelle R. Landgraf<sup>1</sup>; Christopher K. Hilton<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, Florida
- MP 162 **Isoprene Analysis by Secondary Electrospray Ionization-Ion Mobility-Mass Spectrometry;** Maggie Tam<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Jack Chen<sup>1</sup>; Hal Westberg<sup>1</sup>; Herbert H. Hill, Jr. <sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- MP 163 **Multi-Dimensional Ion Mobility Spectrometry Coupled to Time-of-Flight Mass Spectrometry;** Stormy L. Koeniger<sup>1</sup>; Samuel I. Merenbloom<sup>1</sup>; Stephen J. Valentine<sup>2</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Predictive Physiology and Medicine (PPM), Bloomington, IN
- MP 164 **Instrument Control and Data Acquisition System for ESI/FAIMS/IMS/Q-TOF MS;** David C. Prior<sup>1</sup>; Michael A. Buschbach<sup>1</sup>; Fumin Li<sup>1</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Battelle, Richland, WA
- MP 165 **-Electrospray Ionization Coupled to Ion Mobility Mass Spectrometry for Chiral Preference Determination of Amino Acid Clusters;** Sunnie Myung<sup>1</sup>; Marco Fioroni<sup>1</sup>; Ryan R. Julian<sup>2</sup>; Stormy L. Koeniger<sup>1</sup>; Mu-Hyun Baik<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Department of Chemistry, Indiana University, Bloomington, IN; <sup>2</sup>Department of Chemistry, UCR, Riverside, CA
- MP 166 **A Hybrid Atmospheric IMS-FTICR-MS Instrument for Biological Samples;** Xiaoting Tang<sup>1</sup>; James E. Bruce<sup>1</sup>; Herbert H. Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- MP 167 **Characterization of Explosive Compounds Using High-Field Asymmetric Waveform Ion Mobility Spectrometry;** Jared J. Boock<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- MP 168 **Fast Qualitative Determination of Over-the-Counter Drugs and Cosmetics;** Roberto Fernandez-Maestre<sup>1</sup>; Herbert H. Hill<sup>1</sup>; Prabha Dwivedi <sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- MP 169 **Using IMS-CID-IMS-MS to Dissociate Noncovalent Complexes for Enhanced Resolution of Tryptic Peptides;** Brian C. Bohrer<sup>1</sup>; Samuel I. Merenbloom<sup>1</sup>; Stormy L. Koeniger<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- MP 170 **Evaluation of Resolving Powers for Atmospheric Pressure Ion Mobility Spectrometry (APIMS);** Abu B. Kanu<sup>1</sup>; Herbert H. Hill<sup>1</sup>; Molly Grib<sup>2</sup>; Robert Walters<sup>2</sup>; Jerome Imonigie<sup>2</sup>; Kevin Ryan<sup>2</sup>; <sup>1</sup>Washington State

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University, Pullman, WA; <sup>2</sup>Boise State University, Boise, ID

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- MP 171 **Improvement of Energy Linearity in Kinetic Energy Measurement with Superconducting Detectors for TOF MS;** Yiner Chen<sup>1</sup>; Masataka Ohkubo<sup>1</sup>; Masahiro Ukibe<sup>1</sup>; Akihiro Kushino<sup>1</sup>; <sup>1</sup>National Institute of AIST, Tsukuba, Ibaraki Japan
- MP 172 **Improved Ion Transmission with a RF Frequency Switchable Hexapole Ion Guide;** Shida Shen<sup>1</sup>; Robert Valley<sup>1</sup>; Craig Whitehouse<sup>1</sup>; <sup>1</sup>Analytica of Branford, Inc., Branford, CT
- MP 173 **Fragmentation Analysis using Superconducting Detectors in MALDI-TOF MS for a Range of 1 k to 1 MDa;** Masataka Ohkubo<sup>1</sup>; Hiroaki Sato<sup>1</sup>; Yasushi Shigeri<sup>1</sup>; Tomoya Kinumi<sup>1</sup>; Yiner Chen<sup>1</sup>; Masahiro Ukibe<sup>1</sup>; Shingo Ichimura<sup>1</sup>; <sup>1</sup>AIST, Tsukuba, Japan
- MP 174 **Statistical Limits of Isotopic/Isobaric Quantification in Counting Detectors;** Brian Carrillo<sup>1</sup>; Corey Yanofsky<sup>1</sup>; Daniel Boismenu<sup>1</sup>; Martin Latterich<sup>1</sup>; Robert E. Kearney<sup>1</sup>; <sup>1</sup>McGill University, Montreal, Quebec
- MP 175 **Improving Mass Resolution in ortho-TOF Mass Spectrometer;** Vadym D. Berkout<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; <sup>1</sup>MassTech, Inc., Columbia, MD
- MP 176 **Application of Multivariate Regression for Improved Mass Calibration in Electrospray Time-of-Flight Mass Spectrometry;** Matthew Giardina<sup>1</sup>; Viatcheslav Artaev<sup>1</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI
- MP 177 **Selective Ion Filtering by Digital Thresholding: New Method to Unwind Complex ESI-Mass Spectra and Eliminate Signals from Low MW Contaminants;** Jared J. Drader<sup>1</sup>; Amy Schink<sup>1</sup>; Steven A. Hofstadler<sup>1</sup>; <sup>1</sup>Ibis Division of Isis Pharmaceuticals, Carlsbad, CA
- MP 178 **Improved Performance of an Aerosol MALDI Mass Spectrometer;** Ineke Kleefman<sup>1</sup>; Michael A. Stowers<sup>1</sup>; Arjan L. van Wuijckhuijs<sup>2</sup>; Charles E. Kientz<sup>2</sup>; Jan C.M. Marijnissen<sup>1</sup>; <sup>1</sup>Delft University of Technology, Delft, The Netherlands; <sup>2</sup>TNO Prins Maurits Laboratory, Rijswijk, The Netherlands
- MP 179 **Quantitative Time-of-flight Mass Spectrometry of Aerosols Using a Digitally Thresholded Analog-to-Digital Converter;** Joel Kimmel<sup>1</sup>; Peter DeCarlo<sup>1</sup>; Achim Trimborn<sup>2</sup>; Megan Northway<sup>2</sup>; Douglas Worsnop<sup>2</sup>; Jose-Luis Jimenez<sup>1</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>Aerodyne Research, Billerica, MA
- MP 180 **A Multiple-Reflection Time-of-Flight Mass Spectrometer for Separation and Precision Measurement of Exotic Nuclei;** Wolfgang R. Plass<sup>1</sup>; Timo Dickel<sup>1</sup>; Christian Jesch<sup>1</sup>; Hans Geissel<sup>2</sup>; Martin Petrick<sup>1</sup>; Christoph Scheidenberger<sup>2</sup>; <sup>1</sup>Justus-Liebig-Universität Giessen, Giessen, Germany; <sup>2</sup>GSI, Darmstadt, Germany
- MP 181 **Analysis of Intact Proteins and Protein Multimers Using a Conventional UV MALDI Instrument in Reflector Mode;** Matthias Glueckmann<sup>1</sup>; Dietmar Waidelich<sup>1</sup>; Dietrich Merkel<sup>1</sup>; Christof Lenz<sup>1</sup>; <sup>1</sup>Applied Biosystems, Darmstadt, Germany
- MP 182 **The Combination of Ion-Mobility with Orthogonal TOF Mass Spectrometry to improve the Limits of Detection for MALDI-MS and MS/MS Analysis;** Daniel J. Kenny<sup>1</sup>; Jeffery M. Brown<sup>1</sup>; Kevin Giles<sup>1</sup>; Steven D. Pringle<sup>1</sup>; Jason L. Wildgoose<sup>1</sup>; Robert H. Bateman<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK
- MP 183 **A Novel Ion Gate Comprising a Small Orthogonal TOF With Ion Mirror;** Jeffery M. Brown<sup>1</sup>; Daniel J.

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- MP 184 **Development of a Compact Time-of-Flight Mass Spectrometer with Ion Attachment Ionization Technique;** Naoaki Saito<sup>1</sup>; Jyun-ichi Nanjyo<sup>2</sup>; Yasuyuki Taneda<sup>3</sup>; Yoshiro Shiokawa<sup>3</sup>; <sup>1</sup>RIIF/AIST, Tsukuba, Japan; <sup>2</sup>Fac. Sci. Tech./ Tokyo Univ. Sci., Noda, Chiba, Japan; <sup>3</sup>Canon Anelva Technix Corp., Fuchu, Tokyo, Japan
- MP 185 **Hot Laminar Flow Sampling of a QqTOF Electrospray Ion Source;** John Merritt<sup>1</sup>; Matt Smyth<sup>1</sup>; Lisa Cousins<sup>2</sup>; Ilia Tomski<sup>2</sup>; <sup>1</sup>mSPEC Group, Concord, Canada; <sup>2</sup>IONICS Mass Spectrometry Group, Concord, Canada
- MP 186 **Impurity Profiling of Pharmaceuticals with a Quadrupole Time-of-Flight Mass Spectrometer;** Jian Bai<sup>1</sup>; Jean-Claude Wolff<sup>2</sup>; John Fjeldsted<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>GlaxoSmithKline, Medicines Research Centre, Hertfordshire, England
- MP 187 **Comparison of Sensitivity and Saturation of MALDI-TOF Detectors for High Mass Ions;** Ryan J. Wenzel<sup>1</sup>; Alexis Nazabal<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>Swiss Institute of Technology, Zürich, Switzerland
- MP 188 **A Multi-anode Detection Scheme for Increased Resolution and Sensitivity in TOFMS;** Stacy D. Sherrod<sup>1</sup>; Greg Matthijetz<sup>1</sup>; John A. McLean<sup>1</sup>; Tom Egan<sup>2</sup>; Agnes Tempez<sup>2</sup>; Valerie Vaughn<sup>2</sup>; J. Albert Schultz<sup>2</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Ionwerks, Houston, TX
- MP 189 **High Speed Faraday Cup Detector for Time of Flight Mass Spectrometry;** Michael S. Westphall<sup>1</sup>; Mark Scalf<sup>1</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- MP 190 **Focusing Analysis of Tandem Time-Of-Flight Instruments by Taking Advantage of the Correlation between Velocity and Position in the Second TOF;** Cristian P. Santacruz<sup>1</sup>; Edy Ayala<sup>1</sup>; Cesar Costa<sup>1</sup>; <sup>1</sup>Escuela Politecnica Nacional, Quito, Ecuador
- MP 191 **Evaluation of the Agilent LC/MSD/TOF as an Alternative to LC/MS/MS for Quantitation in Various Matrices;** Dan A. Markham<sup>1</sup>; Fagen Zhang<sup>1</sup>; <sup>1</sup>The Dow Chemical Company, Midland, Michigan
- MP 192 **Development of a High Performance TOF-SIMS System using Multi-turn Mass Analyzer;** Kousuke Kumondai<sup>1</sup>; Mariko Higashigaki<sup>1</sup>; Kiichiro Uchino<sup>2</sup>; Hisayoshi Yurimoto<sup>3</sup>; Morio Ishihara<sup>1</sup>; <sup>1</sup>Osaka University, Toyonaka, Osaka, Japan; <sup>2</sup>Kyushu University, Kasuga, Fukuoka, Japan; <sup>3</sup>Hokkaido University, Sapporo, Hokkaido, Japan
- MP 193 **The Development of a Method for Designing TOF-Detectors;** Masahiro Hayashi<sup>1</sup>; Akio Suzuki<sup>1</sup>; Masahiko Iguchi<sup>2</sup>; <sup>1</sup>Hamamatsu Photonics K.K., Iwata, Japan; <sup>2</sup>Hamamatsu Corporation, Bridgewater, NJ
- MP 194 **On-Line Aerosol MALDI TOF-MS Analysis of Protein and Other Biological Samples;** Theresa G. Evans-Nguyen<sup>1</sup>; Robert J. Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD
- MP 195 **Design and Development of High-Throughput LC-TOF MS for Fully-Automated Accurate Mass Measurement;** Tetsuichiro Morita<sup>1</sup>; Kenji Nagatomo<sup>1</sup>; Keiko Kaneda<sup>1</sup>; Robert DiPasquale<sup>2</sup>; Toshinobu Honda<sup>1</sup>; Jun Tamura<sup>1</sup>; <sup>1</sup>JEOL Ltd., Tokyo, Japan; <sup>2</sup>JEOL USA Inc., Peabody, MA
- MP 196 **A Direct Comparison of a Resitive Glass and Stacked-Ring Reflectron;** Stephen M. Ritzau<sup>1</sup>; Bruce N. Laprade<sup>1</sup>;

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- MP 197 **Simple Template-Based Method to Fabricate Bradbury-Nielson Gates and Applications in Mass Spectrometry [1];** Oh Kyu Yoon<sup>1</sup>; Ignacio A. Zuleta<sup>1</sup>; Matthew D. Robbins<sup>1</sup>; Griffin K. Barbula<sup>1</sup>; Richard N. Zare<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA

### INSTRUMENTATION: FTMS

- MP 198 **Electronics for the Cryogenic Fourier Transform Mass Spectrometer;** Raman Mathur<sup>2</sup>; Peter B. O'Connor<sup>1</sup>; Ronald W. Knepper<sup>2</sup>; <sup>1</sup>Boston University, School of Medicine, Boston, MA; <sup>2</sup>Boston University, College of Engineering, Boston, MA
- MP 199 **Modification of ICR Trapping Potential to Generate a Local Electrostatic Field Minimum to Improve Signal Resolving Power;** Sunghwan Kim<sup>1</sup>; Myoung Choul Choi<sup>1</sup>; Seung Yong Kim<sup>1</sup>; Jong Shin Yoo<sup>1</sup>; Hyun Sik Kim<sup>1</sup>; Greg T. Blankney<sup>2</sup>; Christopher L. Hendrickson<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>Korea Basic Science Institute, Daejeon, Korea; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL
- MP 200 **Combined IRMPD and ECD Using Co-Linear and Overlapping Beams in FTICR Mass Spectrometry;** Yuri van der Burgt<sup>1</sup>; Liam A. McDonnell<sup>1</sup>; Romulus Mihalca<sup>1</sup>; Marc Duursma<sup>1</sup>; Illyia Cerjak<sup>1</sup>; Albert J.R. Heck<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, the Netherlands; <sup>2</sup>Dept Biomolecular Mass Spectrometry, Utrecht, the Netherlands
- MP 201 **Implementation of the SWIFT on LTQ/FT;** Shenheng Guan<sup>1</sup>; Alma L. Burlingame<sup>1</sup>; <sup>1</sup>University of California, San Francisco, CA
- MP 202 **Atmospheric Pressure Ionization Permanent Magnet FTICR Mass Spectrometer: A Way to High Performance Mass Spectrometry in a Bench-Top Size;** Andrey N. Vilkov<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; Irina A. Tarasova<sup>2</sup>; Dmitry A. Tolmachev<sup>2</sup>; Mikhail V. Gorshkov<sup>2</sup>; <sup>1</sup>MassTech, Inc., Columbia, MD; <sup>2</sup>Institute of Energy Problems of Chemical Physics, Moscow, Russia
- MP 203 **Photodissociation study of Peptides and Oligosaccharides by Infrared Spectroscopy using FTMS-FEL-SUT;** Kazuhiko Fukui<sup>1</sup>; Katsutoshi Takahashi<sup>1</sup>; <sup>1</sup>AIST, Tokyo, Japan
- MP 204 **Mass Accuracy Improvement via Pseudo-Internal Calibration in FTICR;** Richard L. Wong<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- MP 205 **MALDI-FTMS with In-Cell Accumulation Techniques: Optimized Conditions for Calibration and Ion Trapping;** Elizabeth A. Stemmler<sup>1</sup>; <sup>1</sup>Bowdoin College, Brunswick, ME
- MP 206 **Rapid de-novo Terminal Domain Assignment of CAD Fragments from Intact Proteins;** Michael L. Easterling<sup>1</sup>; Christian Berg<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Inc., Billerica, MA
- MP 207 **A Unique FTMS Cylindrical Trap Compensation Design That Minimized Compensation Voltages and Trapping Fields at End Cap Apertures;** Don L. Rempel<sup>1</sup>; Adam M. Brustkern<sup>1</sup>; Michael L. Gross<sup>1</sup>; Robert T. McIver<sup>2</sup>; <sup>1</sup>Washington University, Saint Louis, MO; <sup>2</sup>IonSpec Corp., Lake Forest, CA
- MP 208 **A Fourier Transform Ion Cyclotron Resonance Mass Spectrometer Designed to Operate at Cryogenic Temperatures;** Peter B. O'Connor<sup>1</sup>; Cheng Lin<sup>1</sup>; Raman Mathur<sup>1</sup>; Konstantine Aizikov<sup>1</sup>; Jason J. Cournoyer<sup>1</sup>; Parminder Kaur<sup>1</sup>; Vera B. Ivleva<sup>1</sup>; Cheng Zhao<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA

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- MP 209 **A Multi-Region Recalibration Approach for Obtaining Ppm-Range Mass Measurement Accuracy For LC-MS Analyses of Complex Proteomics Mixtures;** Aleksey V. Tolmachev<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 210 **Coaxial Multi-Electrode FTICR Cell for High-Sensitivity Detection at a Multiple Frequency: Main Design and Modeling Results;** Alexander Misharin<sup>1</sup>; Roman Zubarev<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden
- MP 211 **Characterization and Optimization of Broadband Phase Correction of FT-ICR MS Spectra via Simultaneous Excitation and Detection;** Greg T. Blakney<sup>1</sup>; Steven C. Beu<sup>2</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>ICR Group at NHMFL, Tallahassee, FL; <sup>2</sup>S.C. Beu Consulting, Austin, TX
- MP 212 **SIMION Modeling of Image Charge Detection in FT-ICR MS;** Steven C. Beu<sup>1</sup>; Christopher L. Hendrickson<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>S C Beu Consulting, Austin, TX; <sup>2</sup>ICR Group at NHMFL, Tallahassee, FL
- MP 213 **A New Open Cylindrical ICR Cell with Electrodes of Different Diameters;** Karl P. Wanczek<sup>1</sup>; Basem Kanawati<sup>1</sup>; <sup>1</sup>Inorganic & Physical Chemistry, University, D-28334 Bremen, Germany
- MP 214 **A Source of Sub Part Per Million Error in Accurate Mass Measurements in Externally Injected MALDI FTMS Experiments;** Adam M. Brustkern<sup>1</sup>; Don L. Rempel<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO
- MP 215 **Electron Capture Dissociation Implementation Evolution in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Oleg Yu. Tsybin<sup>2</sup>; Yury O. Tsybin<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; John P. Quinn<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>State Polytechnical University, Saint-Petersburg, Russia
- MP 216 **Stability of ion motion in FTICR-MS;** Nathan K. Kaiser<sup>1</sup>; Si Wu<sup>1</sup>; Kai Zhang<sup>1</sup>; James E. Bruce<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- MP 217 **Progress Toward Real Time Bioerosol Analysis Using the Novel Fourier Transform Ion Cyclotron Resonance Bioerosol Mass Spectrometer;** Richard Seipert<sup>1</sup>; Xin Cong<sup>1</sup>; Gregg Czerweineic<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- MP 218 **The Grid Cell: a New Cell Design for Reduced Z-Axis Ejection in Fourier Transform Ion Cyclotron Mass Spectrometry;** Andreas Wiegand<sup>1</sup>; Ulf Fröhlich<sup>1</sup>; Robert Malek<sup>1</sup>; Stevan R. Horning<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, Bremen, Germany
- MP 219 **The New Approach to Analytical Treatment of Peak Coalescence and Phase Locking Phenomena in FT ICR Mass Spectrometry;** Alexander A. Vedenov<sup>2</sup>; Eugene N. Nikolaev<sup>1</sup>; <sup>1</sup>The Institute for Energy Probl. Chem.Phys., Moscow, Russia; <sup>2</sup>Kurchatov Institute for Atomic Energy, Moscow, Russia
- MP 220 **Simulation Study to Improve Ion Transmission Efficiency through the Gate Valve for an External Ion Injection FTICR-MS;** Myoung Choul Choi<sup>1</sup>; Hyun Sik Kim<sup>1</sup>; Sunghwan Kim<sup>1</sup>; Jong Shin Yoo<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Daejeon, Republic of Korea

### SYNTHETIC POLYMERS

- MP 221 **MALDI-TOF Analysis of Aromatic Polyesters by Using Fluorinated Azobenzene and Stilbene Matrices;** Arpad Somogyi<sup>1</sup>; El-Hadj Elandaloussi<sup>1</sup>; Anne Padias<sup>1</sup>; Doug Hall<sup>1</sup>; Henry Hall, Jr. <sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ



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- MP 222 **Selective Monitoring of Proteins, Peptides, Polymers and Their Interactions;** Sara E. Tomechko<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH*
- MP 223 **Mild Pyrolysis/ Mass Spectrometry Investigation of Poly(Ethylene Glycol), Polydimethylsiloxane, and Their Copolymer Assemblies;** Panthida Thomya<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; Gabor Erdodi<sup>1</sup>; Joseph P. Kennedy<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH*
- MP 224 **Characterization of Synthetic Aliphatic Co-polyamides by MALDI-ToF Mass Spectrometry;** Vladimir G. Zaikin<sup>1</sup>; Roman S. Borisov<sup>1</sup>; Nikolai Yu. Polovkov<sup>1</sup>; Vladislav V. Lobodin<sup>2</sup>; <sup>1</sup>*Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia*; <sup>2</sup>*Moscow State University, Moscow, Russia*
- MP 225 **Measurement of Environmentally Relevant Partition and Diffusion Coefficients Using Membrane Introduction Mass Spectrometry;** Erik T. Krogh<sup>1</sup>; Derek M. van Pel<sup>1</sup>; Michael S. Lynch<sup>1</sup>; Chris G. Gill<sup>1</sup>; Chris J. Durning<sup>2</sup>; Dustin Janes<sup>2</sup>; <sup>1</sup>*Applied Environmental Research Labs, Malaspina, Nanaimo, B.C., Canada*; <sup>2</sup>*Columbia University, New York, NY*
- MP 226 **Isomeric Recognition of Polyacrylates and Polymethacrylates by MALDI Post Source Decay Measurements;** Ryuichi Arakawa<sup>1</sup>; Yohei Okuyama<sup>1</sup>; Koichi Ute<sup>2</sup>; Masato Kiuchi<sup>3</sup>; Shoji Okuno<sup>3</sup>; <sup>1</sup>*Kansai Univ. Applied chemistry, Suita, Osaka Japan*; <sup>2</sup>*Osaka Univ. Materials Eng. Science, Toyonaka, Osaka Japan*; <sup>3</sup>*AIST, Ikeda, Osaka Japan*
- MP 227 **Analysis of Polyisobutylenes by Laser-induced Acoustic Desorption Coupled with Chemical Ionization in a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer;** Putuma P. Gqamana<sup>1</sup>; Hilkka I. Kenttamaa<sup>1</sup>; David J. Aaserud<sup>2</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*The Lubrizol Corporation, Wickliffe, OH*
- MP 228 **Monitoring Aniline Polymerization with MALDI-TOF Mass Spectrometry;** Leonard J Soltzberg<sup>1</sup>; Richard W Gurney<sup>1</sup>; Katia L Doerr<sup>1</sup>; Marcy B Keddy<sup>1</sup>; <sup>1</sup>*Simmons College, Boston, MA*
- MP 229 **Characterization of Polymer for Organic Light Emitting Device Using MALDI MS and 1,1,4,4-Tetraphenyl-1,3-butadiene Matrix;** JungBae Song<sup>1</sup>; <sup>1</sup>*Samsung Advanced Institute of Technology, Yongin-City, Korea*
- MP 230 **Resolution and Mass Accuracy of High Mass Ions in TOF Mass Spectrometry: Applications to PAMAM Dendrimers;** Robin J. Hood<sup>1</sup>; J. Throck Watson<sup>2</sup>; A. Daniel Jones<sup>2</sup>; <sup>1</sup>*Central Michigan University, Mount Pleasant, MI*; <sup>2</sup>*Michigan State University, East Lansing, MI*
- MP 231 **Tandem Mass Spectrometry of Poly(methyl methacrylates);** Kittisak Chaicharoen<sup>1</sup>; Michael J. Polce<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, OH*
- MP 232 **Analytical Study of Photoinitiating Systems Using a MALDI-TOFMS Technique;** Akihiro Unno<sup>1</sup>; Osamu Hirai<sup>1</sup>; Makoto Kaji<sup>1</sup>; Yukiko Muramatsu<sup>1</sup>; Shinichi Kinugasa<sup>2</sup>; Kayori Shimada<sup>2</sup>; <sup>1</sup>*Hitachi Chemical Co., Ltd., Hitachi, Japan*; <sup>2</sup>*AIST, Tsukuba, Japan*
- MP 233 **Collision Induced Dissociation for Structural Information from Synthetic Oligomer using Matrix-assisted Laser Desorption/Ionization Quadrupole Ion Trap Time-Of-Flight Mass Spectrometry;** Hiroki Nakajima<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Masaki Yamada<sup>1</sup>; Yuzo Yamazaki<sup>1</sup>; Shinichiro Kawabata<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*

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### MICROBIAL ANALYSIS: METHODS AND CHARACTERIZATION

- MP 234 **Investigation of Non-Volatile Pyrolysis Products of Proteins Using Electrospray Ionization-Multistep Tandem Mass Spectrometry;** Shaofeng Zhang<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>*University of Wyoming, Laramie, WY*
- MP 235 **Exploring C1-Metabolism - Shotgun Proteomics of the Methylophilic Prokaryote Methylobacterium Extorquens;** Gundula Bosch<sup>1</sup>; Tiansong Wang<sup>1</sup>; Jonathan Miller<sup>1</sup>; Greg Crowther<sup>1</sup>; Elizabeth Skovran<sup>1</sup>; Kelly Fitzgerald<sup>1</sup>; Mary Lidstrom<sup>1</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 236 **Characterization of Cyanobacterial Species Using Whole Cell MALDI Mass Spectrometry;** Brady D. Lee<sup>1</sup>; David W. Reed<sup>1</sup>; Vicki S. Thompson<sup>1</sup>; Michelle R. Walton<sup>1</sup>; William A. Apel<sup>1</sup>; <sup>1</sup>*Idaho National Laboratory, Idaho Falls, ID*
- MP 237 **Differential Proteomics of the Plant Pathogen Agrobacterium tumefaciens;** Murray Hackett<sup>1</sup>; Gundula Bosch<sup>1</sup>; Tiansong Wang<sup>1</sup>; Pu Liu<sup>1</sup>; Gene Nester<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 238 **Utilization of Combined Proteomic and Glycomic Analyses to Identify Subclasses of Bacteria;** Deborah M Post<sup>1</sup>; Robert S Munson, Jr.<sup>2</sup>; Bradford W Gibson<sup>1</sup>; <sup>1</sup>*Buck Institute for Age Research, Novato, CA*; <sup>2</sup>*The Ohio State University, Columbus, OH*
- MP 239 **Detection of Cellular Pathways Utilizing Quantitative Protein Profiling in Yersinia pestis, Shewanella oneidensis, and Rhodobacter sphaeroides;** Mary S. Lipton<sup>1</sup>; Margie F. Romine<sup>1</sup>; Stephen J. Callister<sup>1</sup>; Kim K. Hixson<sup>1</sup>; Samuel O. Purvine<sup>1</sup>; Angela D. Norbeck<sup>1</sup>; Joshua N. Adkins<sup>1</sup>; Matthew E. Monroe<sup>1</sup>; Carrie D. Nicora<sup>1</sup>; Timothy Donohue<sup>2</sup>; Miguel Dominguez<sup>2</sup>; Christine Tavano<sup>2</sup>; Samuel Kaplan<sup>3</sup>; Xiaohua Zeng<sup>3</sup>; Jung Hyeob Roh<sup>3</sup>; Richard Ding<sup>4</sup>; Derek Lovley<sup>4</sup>; Jim K. Fredrickson<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*University of Wisconsin, Madison, WI*; <sup>3</sup>*UT-Medical School, Houston, TX*; <sup>4</sup>*University of Massachusetts, Amherst, MA*
- MP 240 **A Statistical Framework for Integrating Diverse Mass Spectral Data;** Kristin H. Jarman<sup>1</sup>; Karen L. Wahl<sup>1</sup>; Nancy B. Valentine<sup>1</sup>; John B. Clifton<sup>1</sup>; Helen Kreuzer<sup>1</sup>; Catherine E. Petersen<sup>1</sup>; Heather C. Edberg<sup>1</sup>; David S. Wunschel<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Lab, Richland, WA*
- MP 241 **Fluoroquinolone Resistance in Salmonella Enterica: A Top-Down Proteomic Investigation;** Tracie L. Williams<sup>1</sup>; Rebecca L. Bell<sup>1</sup>; Denis Andrezjewski<sup>1</sup>; Steven M. Musser<sup>1</sup>; <sup>1</sup>*Center for Food Safety and Applied Nutrition, FDA, College Park, MD*
- MP 242 **Identification and Quantification of Quorum-sensing Peptides in Microbial Biofilms;** Praneeth D. Edirisinghe<sup>1</sup>; Luke Hanley<sup>1</sup>; Jerry F. Moore<sup>2</sup>; Kelly A. Skinner-Nemec<sup>3</sup>; Carl B. Lindberg<sup>3</sup>; Carol S. Giometti<sup>3</sup>; Jerry E. Hunt<sup>3</sup>; Wallis F. Calaway<sup>3</sup>; Michael J. Pellin<sup>3</sup>; <sup>1</sup>*University of Illinois at Chicago, Chicago, IL*; <sup>2</sup>*MassThink, Naperville, IL*; <sup>3</sup>*Argonne National Laboratory, Argonne, IL*
- MP 243 **Quantitative Proteomics of a Hyperthermophilic Archeon Enabled By A New Two-Step Digestion Procedure;** Alice Lee<sup>2</sup>; Jonathan L Bundy<sup>1</sup>; Joel R Sevinsky<sup>1</sup>; Benjamin J Cargile<sup>1</sup>; Kristy J Brown<sup>3</sup>; Amy Grunden<sup>2</sup>; James L Stephenson Jr.<sup>2</sup>; <sup>1</sup>*Research Triangle Institute, RTP, NC*; <sup>2</sup>*North Carolina State University,*



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- Raleigh, NC; <sup>3</sup>Cognition Therapeutics LLC, Rockville, MD
- MP 244 **Immobilization of Microorganisms with Magnetic Metal Hydroxides for Detection by MALDI-MS;** Cheng-Tung Chen<sup>1</sup>; Alan A.L. Lo<sup>1</sup>; Chia-Liang Cheng<sup>1</sup>; Yen-Peng Ho<sup>1</sup>; <sup>1</sup>National Dong Hwa University, Hualien, Taiwan, ROC
- MP 245 **Identification and Classification of Clostridia Strains Based on MALDI-TOF MS Fingerprint Spectra and a Dedicated Pattern Matching Software;** Thomas Maier<sup>1</sup>; Anke Große-Herrenthey<sup>2</sup>; Monika Krueger<sup>2</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Leipzig, Germany; <sup>2</sup>Institute of Bacteriology and Mycology, University Leipzig, Germany
- MP 246 **ESI-LCMS for Genetically Modified Bacteria: Determination of 3-Deoxy-D-Arabino-Heptulosonate-7-Phosphate (DAHP) and 3-Dehydroquinone (DHQ) in Escherichia coli Cultures;** Georgina Hernández-Chávez<sup>1</sup>; Jose Luis Báez-Viveros<sup>1</sup>; Eugenio Meza Mora<sup>1</sup>; Francisco Bolívar-Zapata<sup>1</sup>; Guillermo Gosset Lagarda<sup>1</sup>; <sup>1</sup>Instituto de Biotecnología, UNAM, Cuernavaca, Morelos, Mexico
- MP 247 **Application of High Resolution Proteomics to Characterize Microbial Systems under Differing Metabolic Paradigms;** Samuel O. Purvine<sup>1</sup>; Mary S. Lipton<sup>1</sup>; Margie F. Romine<sup>1</sup>; Stephen J. Callister<sup>1</sup>; Kim K. Hixson<sup>1</sup>; Angela D. Norbeck<sup>1</sup>; Joshua N. Adkins<sup>1</sup>; Matthew E. Monroe<sup>1</sup>; Yuri A. Gorby<sup>1</sup>; Carrie D. Nicora<sup>1</sup>; Jim K. Fredrickson<sup>1</sup>; Richard D. Smith<sup>1</sup>; Derek Lovely<sup>2</sup>; Richard Ding<sup>2</sup>; Timothy Donohue<sup>3</sup>; Miguel Dominguez<sup>3</sup>; Christine Tavano<sup>3</sup>; Samuel Kaplan<sup>4</sup>; Xiaihua Zeng<sup>4</sup>; Jung Hyeob Roh<sup>4</sup>; Frank Larimer<sup>5</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Massachusetts, Amherst, MA; <sup>3</sup>University of Wisconsin-Madison, Madison, WI; <sup>4</sup>University of Texas-Houston Medical School, Houston, TX; <sup>5</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- MP 248 **The Discriminatrix: A System for Discovering Microbial Biomarkers;** Zachary O. Waldon<sup>1</sup>; Felix Bonowski<sup>2</sup>; Marc Kirchner<sup>2</sup>; Fred A. Hamprecht<sup>2</sup>; Hanno Steen<sup>1</sup>; Judith Steen<sup>1</sup>; <sup>1</sup>Children's Hospital Boston/Harvard Medical School, Boston, MA; <sup>2</sup>University of Heidelberg, Heidelberg, Germany
- MP 249 **Rapid Detection of Bacterial Pathogens in Drinking Water and Wastewater by a Simultaneous Multiple Enzyme Activity Measurement;** Hao Zhang<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY
- MP 250 **Electrochemically Induced Digestion of Proteins for the Rapid Identification of Bacteria;** Nicolas J. Hauser<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY
- MP 251 **Extraction Methods for Intact Protein LC/MS of Bacterial Cells;** Denis Andrejewski<sup>1</sup>; Tracie L. Williams<sup>1</sup>; Steven M. Musser<sup>1</sup>; <sup>1</sup>Center for Food Safety and Applied Nutrition, FDA, College Park, MD
- MP 252 **Clinical Evaluation of Direct LDMS for Malaria Diagnosis in Humans;** Andrew Feldman<sup>1</sup>; Jeff Lin<sup>1</sup>; John Pisciotta<sup>2</sup>; Peter Scholl<sup>2</sup>; David Sullivan<sup>2</sup>; Nirbhay Kumar<sup>2</sup>; Plamen Demirev<sup>1</sup>; <sup>1</sup>Applied Physics Lab, Johns Hopkins University, Laurel, MD; <sup>2</sup>Bloomberg School of Public Health, Johns Hopkins U, Baltimore, MD
- MP 253 **Proteomic Examination of Complex Microbial Communities – an In-Silico and Applied Approach;** Carrie D Nicora<sup>1</sup>; Angela D Norbeck<sup>1</sup>; Philip E Long<sup>2</sup>; Mary S Lipton<sup>1</sup>; Heather M Mottaz<sup>1</sup>; Richard D Smith<sup>1</sup>; <sup>1</sup>Pacific NW National Lab, Biological Sciences, Richland,

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- WA; <sup>2</sup>Pacific NW National Lab, Environmental Technology, Richland, WA
- MP 254 **Food Poisoning and Typhoid Fever – Proteomic Exploration of Virulence in Salmonella typhimurium and typhi;** Angela D. Norbeck<sup>1</sup>; Heather M. Mottaz<sup>1</sup>; Kenneth J. Auberry<sup>1</sup>; Samuel O. Purvine<sup>1</sup>; Jean Gustin<sup>2</sup>; Joanne Rue<sup>2</sup>; Joshua N. Adkins<sup>1</sup>; Fred Heffron<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Oregon Health Sciences University, Portland, OR

### UNDERGRADUATE POSTERS

- MP 269 **Methyl Esterification and Acetylation Reactions to Improve Detection and SORI-CID Efficiency for the Analysis of Orcokinin Family Neuropeptides using MALDI-FTMS;** Emily A. Bruns<sup>1</sup>; Christopher R. Cashman<sup>1</sup>; Lucas M. Amundson<sup>1</sup>; Noah P. Gardner<sup>1</sup>; Patsy S. Dickinson<sup>1</sup>; Elizabeth A. Stemmler<sup>1</sup>; <sup>1</sup>Bowdoin College, Brunswick, ME
- MP 270 **LC/QIT/TOF Determination of the Efficacy of Drug Test Kits for the Rapid Screening of Food;** Jessica B. Zuckschwerdt<sup>2</sup>; Christopher E. Nixon<sup>1</sup>; Frederic L. Ciner<sup>1</sup>; Timothy R. Croley<sup>1</sup>; <sup>1</sup>Commonwealth of Virginia, Richmond, VA; <sup>2</sup>Eastern Kentucky University, Richmond, KY
- MP 271 **Determination of the Gas-Phase Acidities of the Cysteine-Polyalanine Peptides;** John Tan<sup>1</sup>; Jianhua Ren<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA
- MP 280 **Targeting Phytoplankton with Shotgun Proteomics and LTQ FT MS;** Jocelyn R. Aker<sup>1</sup>; Brook Nunn<sup>2</sup>; Scott Shaffer<sup>1</sup>; Mitch Brittnacher<sup>1</sup>; Dave Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Otago, Dunedin, New Zealand
- MP 281 **A Novel Chromophoric Affinity-Tagged Isotopically-Coded Crosslinker DGDNBS;** Evgeniy V. Petrotchenko<sup>1</sup>; Truc Doant<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- MP 282 **Membrane Introduction Mass Spectrometry (MIMS) Analysis of Low-Volatility and Hydrophilic Esters Using an Enzyme Derivatized PDMS Interface;** A. Skye Creba<sup>1</sup>; Alexandra Weissfloch<sup>1</sup>; Erik T. Krogh<sup>1</sup>; Chris G. Gill<sup>1</sup>; <sup>1</sup>Applied Environmental Research Labs, Malaspina, Nanaimo, BC, Canada
- MP 283 **The Determination of the Chirality of Amino Acids in Neuropeptides;** Jane Wang<sup>1</sup>; Michael A. Ewing<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana-Champaign, IL
- MP 284 **Temperature and pH Dependence of the Cyclization of Creatine: A Study Via Mass Spectrometry;** William J. Meadows<sup>1</sup>; Brian J. Diamond<sup>1</sup>; David Rupp<sup>1</sup>; William D. Price<sup>1</sup>; <sup>1</sup>Marshall University, Huntington, WV
- MP 285 **Characterization of Hindered amine Light Stabilisers in polymer Coatings By DESI, ESI and Tandem Mass Spectrometry;** Troy A. Lowe<sup>1</sup>; Philip J. Barker<sup>2</sup>; Stephen J. Blanksby<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Wollongong, Wollongong, Australia; <sup>2</sup>BlueScope Steel, Port Kembla, Australia
- MP 286 **A Coaxially Heated Hollow Fibre Membrane Interface for Real-Time, Ultra-Trace Membrane Introduction Mass Spectrometry of Less Volatile Analyte Molecules;** Alexander J. Thompson<sup>1</sup>; A. Skye Creba<sup>1</sup>; Robyn M. Ferguson<sup>1</sup>; Erik T. Krogh<sup>1</sup>; Chris G. Gill<sup>1</sup>; <sup>1</sup>Applied Environmental Research Labs, Malaspina, Nanaimo, BC, Canada
- MP 287 **Comparison of Human Serum Proteome Identification Fractionated by Immunodepletion Followed by Three**

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- MP 288 **Dimensional and Linear Ion Trap Mass Spectrometry;** Quanhu Sheng<sup>1</sup>; Jie Dai<sup>1</sup>; Yixue Li<sup>1</sup>; Haixu Tang<sup>2</sup>; Rong Zeng<sup>1</sup>; <sup>1</sup>Shanghai Institutes for Biological Sciences, CAS, Shanghai, China; <sup>2</sup>Indiana University, Bloomington, IN
- MP 289 **Direct Reaction Monitoring of Dis-Infection By-Product Formation using Membrane Introduction Mass Spectrometry;** Owen D. M. Stechishin<sup>1</sup>; Lydia Rockwell<sup>1</sup>; Robyn M. Ferguson<sup>1</sup>; Chris G. Gill<sup>1</sup>; Erik T. Krogh<sup>1</sup>; <sup>1</sup>Applied Environmental Research Labs, Malaspina, Nanaimo, B.C.
- MP 290 **Examining Protein Conformations in Mixtures by Hydroxyl Radical Surface Mapping with High Resolution Mass Spectrometry;** Christine Shook<sup>1</sup>; Carlee McClintock<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>Chemical Sciences Division, Oak Ridge National Lab, Oak Ridge, TN
- MP 291 **Protein Digestion by Microwave-Assisted Acid Hydrolysis;** Megan Roberts<sup>1</sup>; Kate Smetana<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY

## HIGH THROUGHPUT ANALYSIS

- MP 292 **A SUPREX-Based HTS Assay for the Discovery of Novel Molecular Imaging Probes;** Michael C. Fitzgerald<sup>1</sup>; Erin D. Hopper<sup>1</sup>; Petra L. Roulhac<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- MP 293 **Open Access LC/MS/MS Quantification Using an Ultra-High Pressure Chromatography System to boost Laboratory Throughput and Maintain Data Quality;** Ed Sprake<sup>1</sup>; Steve Preece<sup>1</sup>; <sup>1</sup>Waters Corp., Manchester, UK
- MP 294 **High Throughput, Robust HPLC Electrospray Ionization Time-of-Flight Mass Spectrometry for the Sensitive Analysis of Antibodies and other Proteins;** Andy Gieschen<sup>1</sup>; Greg W Kilby<sup>1</sup>; Jim Lau<sup>1</sup>; Lorenzo Chen<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Merck & Co, West Point, PA
- MP 295 **A New Nano LC MALDI Approach to Investigate the Mammalian Peptidome;** Stephan Poetsch<sup>1,2</sup>; Johan Axelman<sup>1,2</sup>; <sup>1</sup>GE Healthcare Europe GmbH, Munich, Germany; <sup>2</sup>GE Healthcare Europe GmbH, Uppsala, Sweden
- MP 296 **Evaluation of Three Detectors in High Throughput Quantitative Measurements: Comparison of ELSD, CAD, and CLND;** Baiwei Lin<sup>1</sup>; Hong Phan<sup>1</sup>; Min Wan<sup>1</sup>; <sup>1</sup>Berlex Biosciences, Richmond, CA
- MP 297 **Fast LC with Ultra-Short Cycle Times;** Masayuki Nishimura<sup>1</sup>; William A Hedgepeth<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- MP 298 **An LC/MS/MS Method for Quantitative Analysis of Capecitabine and Its Three Major Metabolites in Human Plasma;** Ling Zhang<sup>1</sup>; Tom Smith<sup>2</sup>; Wei Wu<sup>1</sup>; Jiang Luo<sup>1</sup>; Jinsong Xing<sup>1</sup>; Francis Tse<sup>2</sup>; Ning Zhao<sup>1</sup>; <sup>1</sup>WuXi PharmaTech Co., Ltd., Shanghai, China; <sup>2</sup>Novartis Pharmaceuticals, East Hanover, NJ
- MP 299 **Automated Peak Identification in a TOF-SIMS Spectrum;** Haijian Chen<sup>1</sup>; Eugene Tracy<sup>1</sup>; William Cooke<sup>1</sup>; Dariya Malyarenko<sup>1</sup>; Maciek Sasinowski<sup>2</sup>; Dennis Manos<sup>1</sup>; Michael Trosset<sup>1</sup>; John Semmes<sup>3</sup>; <sup>1</sup>College of William and Mary, Williamsburg, VA; <sup>2</sup>INCOGEN, Inc., Williamsburg, VA; <sup>3</sup>Eastern Virginia Medical School, Norfolk, VA
- MP 300 **Hardware and Software Improvements on the Waters ZQ Walk-up LC/MS Purification System that Enhance Efficiency and Throughput;** Lu Zeng<sup>1</sup>; Yinong Zhang<sup>1</sup>; Rongda Xu<sup>1</sup>; Warren Potts<sup>2</sup>; Daniel B. Kassel<sup>1</sup>; <sup>1</sup>Takeda SD, Inc., San Diego, CA; <sup>2</sup>Waters Corporation, Milford, MA

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- MP 301 **A Rapid and Improved LC-MS/MS Platform for the Therapeutic Drug Monitoring of Five Major Immunosuppressants;** Wolfgang M. Stoegg<sup>1</sup>; Christoph Seger<sup>2</sup>; Klaus Weinberger<sup>1</sup>; Andrea Griesmacher<sup>2</sup>; Armin Graber<sup>1</sup>; Steven L. Ramsay<sup>1</sup>; <sup>1</sup>Biocrates Life Sciences GmbH, Innsbruck, Austria; <sup>2</sup>Zentralinstitut fuer med. u. chem. Labordiagnostik, Innsbruck, Austria
- MP 302 **Ultra high throughput autosampler utilizing multiple independent parallel injection channels;** Peter Kovarik<sup>1</sup>; Yves LeBlanc<sup>1</sup>; Mauro Aiello<sup>1</sup>; Thomas Covey<sup>1</sup>; Thomas Londo<sup>2</sup>; <sup>1</sup>MDS SCIEX, Concord, ON, Canada; <sup>2</sup>Parker Life Sciences, Hollis, NH
- MP 303 **High Throughput Concurrent Determination of Compound Solubility and Purity Employing a Low Volume Parallel Liquid Chromatography System with MS Capability;** Sergio A. Guazzoti<sup>1</sup>; Sheila Bilbao<sup>1</sup>; <sup>1</sup>Nanostream, Inc., Pasadena, CA
- MP 304 **Fast Analytical Quality Preparative UV, ELSD, and/or MS Directed Purification for 100 mg Injections;** Mark J. Hayward<sup>1</sup>; David P. Budac<sup>1</sup>; <sup>1</sup>Lundbeck Research USA, Paramus, NJ
- MP 305 **Sample Throughput Improvements for Determination of &ALPHA;&NU&BETA3 Bone Integrin Antagonist in Human Plasma using Protein Precipitation Coupled with LC-MS/MS;** Jin Zhang<sup>1</sup>; Yang Xu<sup>1</sup>; Cynthia M. Miller-Stein<sup>1</sup>; Donald G. Musson<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- MP 306 **Use of a Multimode Ionization Source for Open Access LC-MS in a Pharmaceutical Chemistry Environment;** Patrick D. Wheeler<sup>1</sup>; Muhammad Alimuddin<sup>1</sup>; <sup>1</sup>Pfizer, San Diego, CA
- MP 307 **Non-Multiplexed DAD-ToF Analysis of >1000 Samples/Day - Accurate Mass with Simultaneous APCI and ESI Detection;** Michael G. Frank<sup>1</sup>; Edgar Naegel<sup>1</sup>; Doug McIntyre<sup>2</sup>; <sup>1</sup>Agilent Technologies, Waldbronn, Germany; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- MP 308 **Ion Funnel Interface for a Linear Ion Trap Enabling Faster, High Resolution LC-MS Analyses;** Jason S. Page<sup>1</sup>; Yufeng Shen<sup>1</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 309 **Development of High-Throughput Single Time-Point Phase II Metabolic Stability Assay;** Susan Q. Li<sup>1</sup>; Li Di<sup>1</sup>; Edward Kerns<sup>1</sup>; <sup>1</sup>Wyeth research, Princeton, NJ
- MP 310 **Designing a Flexible High-Throughput Open Access LCMS Platform for Drug Discovery;** Mark Zambrowski<sup>1</sup>; <sup>1</sup>AstraZeneca R&D Boston, Waltham, MA
- MP 311 **Automated Sample Preparation and Purification of Homogenized Brain Tissues;** Suoyu Xu<sup>1</sup>; S. Zheng<sup>1</sup>; X. Shen<sup>1</sup>; Z. Yao<sup>1</sup>; X. Tong<sup>1</sup>; <sup>1</sup>Merck & Co. Inc., Rahway, NJ
- MP 312 **Lead Discovery Screening Using Column Chromatography - Mass Spectrometry Measurement in Functional Biomolecular Assays;** Mark J. Hayward<sup>1</sup>; Stuart P. Coleman<sup>2</sup>; <sup>1</sup>Biomolecular Discovery Technologies, Boston, MA; <sup>2</sup>Matrix BioAnalytical, New Haven, CT
- MP 313 **A Novel High Throughput MD-MALDI-ToF Platform for Serum Biomarker Discovery;** Fumiko Taguchi<sup>1</sup>; James A. Mobley<sup>1</sup>; Pierre P. Masson<sup>1</sup>; David P. Carbone<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- MP 314 **Fully Automated Walk Away SPE for Psuedoephedrine in Porcine Plasma Using The OMIX Tomtec Tip and Tomtec Quadra 96;** William Hudson<sup>1</sup>; <sup>1</sup>Varian Inc, Lake Forest, CA

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- MP 314 **Investigation of and Solution to the Sample Dilution Problem of Automated Multi-Channel Liquid Handler used for LC-MS/MS Bioanalysis;** Zheng Ouyang<sup>1</sup>; Huijin Dong<sup>2</sup>; Mohammed Jemal<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb Company, New Brunswick, NJ
- MP 315 **Let the Robot Do the Work: Automated Biological Sample Preparation;** David Weller<sup>1</sup>; Joe Palandra<sup>1</sup>; Jeff Li<sup>2</sup>; Lisa Buchholz<sup>1</sup>; Min Zhong<sup>1</sup>; Lucinda Cohen<sup>1</sup>; Steven Michael<sup>1</sup>; <sup>1</sup>Pfizer Global Research & Development, Ann Arbor, MI; <sup>2</sup>Michigan State University, East Lansing, MI
- MP 316 **Micro Parallel Chromatography and Fraction Collection Coupled Off-Line with Mass Spectrometry for Rapid Sample Clean Up of Complex Mixtures;** John T. Mehl<sup>1</sup>; Rick C. King<sup>1</sup>; Nicole Trainor<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- MP 317 **Overcoming Sample Preparation Bottleneck: Elimination of Organic Solvent Evaporation and Reconstitution for SPE and LLE Automation Using HILIC-MS/MS;** Qi Song<sup>1</sup>; Yong Tang<sup>1</sup>; Naidong Weng<sup>2</sup>; <sup>1</sup>Covance Bioanalytical Services, LLC, Indianapolis, IN; <sup>2</sup>Bristol-Myers Squibb Company, New Brunswick, NJ
- MP 318 **Ultra Fast Gradient LC/MS Separations using your Existing LC/MS;** Mark J. Hayward<sup>1</sup>; <sup>1</sup>Lundbeck Research USA, Paramus, NJ
- MP 319 **The Effect of Sampling Rotor Moving Speed on the Acquisition of Total Ion Current in a LCT/MUX System;** Min Wan<sup>1</sup>; Baiwei Lin<sup>1</sup>; Gary Phillips<sup>1</sup>; <sup>1</sup>Berlex Biosciences, Richmond, CA
- MP 320 **System Management Tools for a High Throughput Open Access UPLC/MS System Used During the Analysis of Thousands of Samples;** Ronan Cleary<sup>1</sup>; Darcy Shave<sup>1</sup>; Warren Potts<sup>1</sup>; Michael D. Jones<sup>1</sup>; Paul Lefebvre<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- MP 321 **A Dual Staggered LC/MS with Online Extraction for High Throughput Bioanalysis;** Jun Zhang<sup>1</sup>; Mitch Friedman<sup>1</sup>; <sup>1</sup>deCODE genetics, Inc., Woodridge, IL

## BIOINFORMATICS I

- MP 322 **Assessment of Tandem Mass Spectra Quality Using Intelligent Algorithms;** Cheolhwan Oh<sup>1</sup>; Hamid Mirzaei<sup>1</sup>; Fred E Regnier<sup>1</sup>; Xiang Zhang<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- MP 323 **A Proteomic Reporting System with Heuristic and BLAST-based Protein Clustering;** Roger E Moore<sup>1</sup>; Mary K Young<sup>1</sup>; Terry D Lee<sup>1</sup>; <sup>1</sup>Beckman Research Institute, City of Hope, Duarte, CA
- MP 324 **Probability-Based Protein Identification for Post-Translation Modifications and Amino Acid Variants Using Peptide Mass Fingerprint Data;** Weiwei Tong<sup>2</sup>; Mark E. McComb<sup>1</sup>; David Perlman<sup>1</sup>; Hua Huang<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Zhiping Weng<sup>2</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston University, Boston, MA
- MP 325 **The SeqR – a Software Tool for the Analysis of High Accuracy Mass Spectral Data;** Flavio Monigatti<sup>1</sup>; Bogdan Budnik<sup>1</sup>; Richard Lee<sup>1</sup>; Thomas Patterson<sup>1</sup>; Judith Steen<sup>1</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Children's Hospital Boston, Boston, MA
- MP 326 **De novo Peptide Sequencing Using Exhaustive Enumeration of Peptide Composition and MALDI-TOF/TOF;** Matthew T Olson<sup>1</sup>; Jonathan A Epstein<sup>1</sup>; Alfred L Yergey<sup>1</sup>; <sup>1</sup>NICHD, NIH, Bethesda, MD
- MP 327 **Intact Peptide Charge Determination from Ion Trap MS/MS;** Weiwei Chen<sup>1</sup>; Iain Rogers<sup>2</sup>; Bin Ma<sup>1</sup>;

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- <sup>1</sup>University of Western Ontario, London, ON; <sup>2</sup>Bioinformatics Solutions Inc., Waterloo, Canada
- MP 328 **Drastically Increased Coverage by Using Four Programs in an Amalgamative Approach to Protein Identification;** Iain Rogers<sup>1</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, Canada
- MP 329 **Removing Deficient MS/MS Spectra Before Database Search;** Weiwei Chen<sup>2</sup>; Iain Rogers<sup>1</sup>; John Morey<sup>1</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, Canada; <sup>2</sup>University of Western Ontario, London, ON
- MP 330 **High-Throughput De novo Sequencing Using Bioinformatics and Database Searching;** John M Asara<sup>1</sup>; Matthew Phillips<sup>1</sup>; Mary H Schweitzer<sup>2</sup>; Lewis C Cantley<sup>1</sup>; <sup>1</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>2</sup>North Carolina State University, Raleigh, NC
- MP 331 **A Computational Approach to Glycoprotein Identification Using Mass Spectrometry;** Yin Wu<sup>1</sup>; Yehia Mechref<sup>1</sup>; Iveta Klouckova<sup>1</sup>; Milos V. Novotny<sup>1</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN
- MP 332 **Identification of Proteins Without Specific Enzymatic Digestion;** Vinh An Thieu<sup>1</sup>; Dieter Kirsch<sup>1</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>University of Giessen, Giessen, Germany
- MP 333 **An Overlaying Method to Improve Protein Identification from Mass Spectra Peaks by using the Theoretical Protein/Peptide Structural Information;** Seiji Okuizumi<sup>1</sup>; Akihisa Kenmochi<sup>1</sup>; Masao Satoh<sup>1</sup>; Kenji Miyazaki<sup>1</sup>; Kenichi Kamijo<sup>1</sup>; <sup>1</sup>NEC, Tsukuba, Japan
- MP 334 **Improving the Reliability of Protein Identification using Peptide Mass Fingerprinting by Probability Based Scoring of Amino Acid Modifications;** Christian Bleiholder<sup>1</sup>; Sabine Fiedler<sup>1</sup>; Bela Paizs<sup>1</sup>; Martina Schnolzer<sup>1</sup>; <sup>1</sup>German Cancer Research Center, Heidelberg, Germany
- MP 335 **Evaluation of Different Interpretation Strategies to Discover PTM in MS/MS Peptide Fragmentation Data;** Daniel C. Chamrad<sup>1</sup>; Gerhard Körtling<sup>1</sup>; Ken Fantom<sup>2</sup>; Andy West<sup>2</sup>; Klaus Schneider<sup>2</sup>; Ulrike Schweiger-Hufnagel<sup>3</sup>; Herbert Thiele<sup>3</sup>; Martin Blüggel<sup>1</sup>; <sup>1</sup>Protagen AG, Dortmund, Germany; <sup>2</sup>GlaxoSmithKline, Harlow, Great Britain; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany
- MP 336 **Improved Automated Validation of MS/MS Search Results Employing High Precursor Ion Mass Accuracy;** Andrew Keller<sup>1</sup>; Jennifer Sutton<sup>2</sup>; Manor Askenazi<sup>2</sup>; Andrey Bondarenko<sup>1</sup>; Lee Weng<sup>1</sup>; <sup>1</sup>Rosetta Biosoftware, Seattle, WA; <sup>2</sup>Thermo Electron Corporation, Cambridge, MA
- MP 337 **PepTiger: Search Engine for Error-Tolerant Protein Identification from de novo Sequences;** Irina Fedulova<sup>1</sup>; Hamid Mirzaei<sup>2</sup>; Sergey Pevtsov<sup>1</sup>; Zheng Ouyang<sup>2</sup>; Xiang Zhang<sup>2</sup>; <sup>1</sup>Moscow State University, Moscow, Russia; <sup>2</sup>Purdue University, West Lafayette, IN
- MP 338 **Novel Strategy to Simplify the Spectrum for Denovo Peptide Sequence using MS<sup>n</sup> Measurement;** Shigeki Kajihara<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Mike May<sup>2</sup>; <sup>1</sup>Shimadzu corporation, Kyoto, JAPAN; <sup>2</sup>Shimadzu Research Laboratory (Europe) Ltd, Manchester, UK
- MP 339 **Protein Scoring and Clustering for OMSSA;** ming xu<sup>1</sup>; Lewis Y. Geer<sup>1</sup>; Stephen H. Bryant<sup>1</sup>; Jeffrey A. Kowalak<sup>2</sup>; Sanford P. Markey<sup>2</sup>; <sup>1</sup>NCNI/NLM/NIH, Bethesda, MD; <sup>2</sup>National Institute of Mental Health, NIH, Bethesda, MD
- MP 340 **Improving Mass Accuracy for LC-MS Based Protein Identification;** Harald Pettersen<sup>1</sup>; Lennart Björkstén<sup>1</sup>;

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- Malin Söderström<sup>1</sup>; Anders Kaplan<sup>1</sup>; <sup>1</sup>GE Healthcare, Uppsala, Sweden
- MP 341 **Composite Target/Decoy Database Searching Explained**; Joshua E. Elias<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Taplin Biological Mass Spectrometry Facility, Boston, MA
- MP 342 **RAID\_GIDB: A PTM-Capable Library Search Tool For Peptide Identifications with de novo Based Statistics**; Gelio Alves<sup>1</sup>; Yi-Kuo Yu<sup>1</sup>; <sup>1</sup>NCBI/NLM/NIH, Bethesda, MD
- MP 343 **Instrument Specific Calibration of PeptideProphet**; Bryan J. Prazan<sup>1</sup>; Erik J. Nilsson<sup>1</sup>; Brian S. Pratt<sup>1</sup>; Daniel Martin<sup>2</sup>; John Klimek<sup>2</sup>; Andrew Gemmill<sup>2</sup>; Laura Hohmann<sup>2</sup>; Jennifer Jackson<sup>2</sup>; Martin Sadilek<sup>3</sup>; <sup>1</sup>Insilicos, Seattle, WA; <sup>2</sup>Institute for Systems Biology, Seattle, WA; <sup>3</sup>University of Washington, Chemistry, Seattle, WA
- MP 344 **Withdrawn**
- MP 345 **MS/MS Database Search Strategies for High-accuracy Mass Spectrometry**; Sajani Swamy<sup>1</sup>; Lu Yu<sup>1</sup>; Vivek Iyer<sup>1</sup>; Mercedes Pardo<sup>1</sup>; Jyoti Choudhary<sup>1</sup>; <sup>1</sup>Wellcome Trust Sanger Institute, Hinxton, UK
- MP 346 **An On-Line Algorithm for Peptide Identification by Fourier Transform Mass Spectrometry**; Ari Frank<sup>1</sup>; Michael L. Nielsen<sup>2</sup>; Mikhail Savitski<sup>2</sup>; Pavel Pevzner<sup>1</sup>; Roman Zubarev<sup>2</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>Uppsala University, Uppsala, Sweden
- MP 347 **byOnic: Fast and Sensitive Identification of Peptide Spectra Using Lookup Peaks**; Marshall Bern<sup>1</sup>; David Goldberg<sup>1</sup>; Hua Lin<sup>2</sup>; Thomas Shaler<sup>2</sup>; Ted Jones<sup>2</sup>; Christopher Becker<sup>2</sup>; <sup>1</sup>Palo Alto Research Center, Palo Alto, CA; <sup>2</sup>PPD, Inc., Menlo Park, CA
- MP 348 **Improved Positional Confidence Score in De novo Sequencing by Tandem Mass Spectrometry**; Bin Ma<sup>1</sup>; Gilles Lajoie<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, ON
- MP 349 **MassMatrix – Rapid Characterization of Post-Translationally Modified Proteins from Tandem Mass Spectra**; Hua Xu<sup>1</sup>; Michael A. Freitas<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- MP 350 **Shotgun Protein Sequencing by de-novo Assembly of MS/MS Spectra from Modified and Unmodified Overlapping Peptides**; Nuno Bandeira<sup>1</sup>; Pavel Pevzner<sup>1</sup>; Karl Clauser<sup>2</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>Broad Institute, Cambridge, MA
- MP 351 **Protein Prospector and Ways of Calculating Expectation Values**; Aenoch J. Lynn<sup>1</sup>; Robert J. Chalkley<sup>1</sup>; Peter R. Baker<sup>1</sup>; Mark R. Segal<sup>1</sup>; Alma L. Burlingame<sup>1</sup>; <sup>1</sup>University of California, San Francisco, San Francisco, CA

## NON-COVALENT INTERACTIONS I

- MP 352 **Screening for Protein/Ligand Binding by Automated Nanospray Mass Spectrometry**; Farzin Gharahdaghi<sup>1</sup>; Russell Spreen<sup>1</sup>; <sup>1</sup>AstraZeneca Pharmaceuticals, Wilmington, DE
- MP 353 **Gas Phase Dissociation Pathways and Relative Stabilities of Alkaline Earth Metal Complexes with the Polyether Ionophores Lasalocid and Monensin**; Matthew W. Forbes<sup>1</sup>; Dietrich A. Volmer<sup>2</sup>; J. Stuart Grossert<sup>3</sup>; Diethard K. Bohme<sup>4</sup>; <sup>1</sup>Dept. of Chemistry, University of Toronto, Toronto, ON, Canada; <sup>2</sup>Institute for Marine Biosciences, Halifax, NS, Canada; <sup>3</sup>Dept. of Chemistry, Dalhousie University, Halifax, NS, Canada; <sup>4</sup>Dept. of Chemistry, York University, Toronto, ON, Canada

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- MP 354 **Metal Binding Properties of Human Centrin-2 Determined by Micro-Electrospray Ionization Mass Spectrometry and UV Spectroscopy**; Linda M Benson<sup>1</sup>; Theodore A Craig<sup>1</sup>; Sergei Yu Venyaminov<sup>1</sup>; Zachary C Ryan<sup>1</sup>; Justin Sperry<sup>2</sup>; James R Thompson<sup>1</sup>; Jeffrey L Salisbury<sup>1</sup>; H. Robert Bergen III<sup>1</sup>; Michael L Gross<sup>2</sup>; Rajiv Kumar<sup>1</sup>; <sup>1</sup>Mayo Clinic College of Medicine, Rochester, MN; <sup>2</sup>Washington University in St. Louis, St Louis, MO
- MP 355 **Super-Shifting: A New Method to Characterize Protein Complexes using High-Mass MALDI ToF Mass Spectrometry and Immunochemistry**; Alexis Nazabal<sup>1</sup>; Markus Schlumberger<sup>1</sup>; Wolf Hardt<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>Swiss Federal Institute of Technology-ETHZ, Zürich, Switzerland
- MP 356 **Characterization of Small Heat Shock Protein Oligomers by Mass Spectrometry**; Richard L. Beardsley<sup>1</sup>; Christopher M. Jones<sup>1</sup>; Guilong Cheng<sup>1</sup>; Eman Basha<sup>1</sup>; Elizabeth Vierling<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- MP 357 **Probing Individual Hydrogen Bonds between Cex and Three Inhibitors in Gas Phase Noncovalent Complexes**; Milica Tesic<sup>1</sup>; Jacqueline Wicki<sup>1</sup>; Stephen G. Withers<sup>1</sup>; Donald J. Douglas<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada
- MP 358 **Development of a Mass Spectrometry-Based Assay for the Analysis and Screening of Endocrine Disruptors**; Cédric Bovet<sup>1</sup>; Arno Wortmann<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zürich, Zürich, Switzerland
- MP 359 **Study of the Non-Covalent Interactions between Polyalanine and Arginine by ESI-FTMS**; Edgardo Rivera-Tirado<sup>1</sup>; David J. Aaserud<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH; <sup>2</sup>The Lubrizol Corporation, Wickliffe, OH
- MP 360 **NMR Spectroscopic and Mass Spectrometric Characterization of the Epitope&Minus;Paratope Interaction Structure of a Plaque&Minus;Specific &Beta;&Minus;Amyloid Antibody**; Irina Perdivara<sup>1</sup>; Marilena Manea<sup>1</sup>; Heiko Möller<sup>1</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>University of Konstanz, Konstanz, Germany
- MP 361 **Interactions of Deprotonated Amino Acids with Cyclodextrins: The Acidity of Aspartic and Glutamic Acid**; Carlos Afonso<sup>1</sup>; Sandra Alves<sup>1</sup>; Françoise Fournier<sup>1</sup>; Denis Lesage<sup>1</sup>; Adelaide Fagin<sup>2</sup>; Scott Gronert<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>Université Pierre et Marie Curie, Paris, France; <sup>2</sup>San Francisco State University, San Francisco, CA
- MP 362 **Identification of Subunits in Non-Covalent Complexes by Solution and Gas Phase Dissociation**; Rachael C. Leverence<sup>1</sup>; Anne B. Mason<sup>2</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>University of Vermont Medical School, Burlington, VT
- MP 363 **Multiplexed MS Approach to Probe Ligand and Redox Controlled Induction of Active CprK1 Conformations**; Robert H. H. van den Heuvel<sup>1</sup>; Hortense Mazon<sup>1</sup>; Krisztina Gabor<sup>2</sup>; John van der Oost<sup>2</sup>; Albert J. R. Heck<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>Wageningen University, Wageningen, Netherlands
- MP 364 **Mass Spectrometry of Sticky Protein-Ligand Complexes: Nucleotide Binding**; Sheng Yin<sup>1</sup>; Yongming Xie<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California-Los Angeles, Los Angeles, CA
- MP 365 **SUPREX Analysis of Bcl-x<sub>L</sub> Interactions with Bak-Derived Peptides**; Erin D. Hopper<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC

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- MP 366 **Learning an Old Q-ToF New Tricks;** Hortense Mazon<sup>1</sup>; Robert H. H. van den Heuvel<sup>1</sup>; Esther van Duijn<sup>1</sup>; Cees Versluis<sup>1</sup>; John Hoyes<sup>2</sup>; Albert J. R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, Netherlands*; <sup>2</sup>*MS Horizons, Stockport, UK*
- MP 367 **The Formation and Gas Phase Stability of Trypsin-Benzamidine Complexes;** Jiangxiao Sun<sup>1</sup>; Elena N Kitova<sup>1</sup>; John S Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*
- MP 368 **A Stability-Toxicity Study of the Shiga Toxins 1 and 2;** Elena N Kitova<sup>1</sup>; Igor Sinelnikov<sup>1</sup>; John S Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*
- MP 369 **Comparison of Dissociation Constants of Noncovalent Complexes Determined using ESI-MS, NanoESI-MS, MALDI-SUPREX, SPR and CD Spectrometry;** Sonal Mathur<sup>1</sup>; Michael Scott<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*Swiss Federal Institute of Technology (ETH), Zurich, Switzerland*; <sup>2</sup>*Functional Genomics Center, Zurich, Switzerland*
- MP 370 **Electrospray Ionization and Ion Mobility Analysis of Vaults, MDa Ribonucleoprotein Complexes;** Catherine S. Kaddis<sup>1</sup>; Shirley Lomeli<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>*University of California Los Angeles, Los Angeles, CA*
- MP 371 **NanoESI Gas-phase Electrophoretic Mobility Analysis (GEMMA) of an Intact Specific Human Rhinovirus (HRV)-Monoclonal Antibody (mAB) Complex;** Christian Laschober<sup>1</sup>; Dieter Blaas<sup>3</sup>; Wladyslaw W. Szymanski<sup>2</sup>; Günter Allmaier<sup>1</sup>; <sup>1</sup>*Chemical Technology and Analytics, TU, Vienna, Austria*; <sup>2</sup>*Experimental Physics, University, Vienna, Austria*; <sup>3</sup>*Medical University, Vienna, Austria*
- MP 372 **Native Electrospray Ionization Mass Spectrometry for the Analysis of Metals and Inhibitors Binding to Metallo-β-Lactamases;** Nathalie Selevsek<sup>1</sup>; Benoît Liénard<sup>2</sup>; Andreas Tholey<sup>1</sup>; Elmar Heinzel<sup>1</sup>; Hans-Werner Adolph<sup>3</sup>; Neil J. Oldham<sup>2</sup>; Christopher J. Schofield<sup>2</sup>; <sup>1</sup>*Technische Biochemie, Universität des Saarlandes, Saarbrücken, Germany*; <sup>2</sup>*Chemistry Research Laboratory, Oxford, UK*; <sup>3</sup>*Organische Makromolekulare Chemie, Saarbrücken, Germany*
- MP 373 **Probing the Interaction between TRAIL and its Receptor DR5 by MS;** Zhili Li<sup>1</sup>; Dexian Zheng<sup>1</sup>; Yanxin Liu<sup>1</sup>; <sup>1</sup>*Chinese Academy of Medical Sciences, Beijing, China*
- MP 374 **Using Solution and Gas Phase Hydrogen/Deuterium Exchange with NanoESI to Study Hydrogen Bonds;** Honghai Jiang<sup>1</sup>; Anthony R. Dolan<sup>2</sup>; Minfeng Li<sup>1</sup>; Marie A. Moy<sup>2</sup>; Bing Gong<sup>1</sup>; Troy D. Wood<sup>1</sup>; <sup>1</sup>*State University of New York at Buffalo, Buffalo, NY*; <sup>2</sup>*Nanogenesys Inc., Amherst, NY*

## PEPTIDES: FRAGMENTATION AND SEQUENCING I

- MP 375 **Fragmentation of N-terminal Labeled Tryptic Peptides with Various Isocyanates;** Ting Liu<sup>1</sup>; Bert C. Lynn<sup>1</sup>; <sup>1</sup>*University of Kentucky, Lexington, KY*
- MP 376 **Charge State Effects on Peptide Conformational Dynamics: Fluorescence Measurements and Molecular Dynamics Simulations;** Anthony T. Iavarone<sup>1</sup>; Joel H. Parks<sup>1</sup>; <sup>1</sup>*Rowland Institute at Harvard, Cambridge, MA*
- MP 377 **Identification of Cross-Linked Peptides by Systematic Screening of Fragmentation Spectra;** Alessio Maiolica<sup>1</sup>; Dario Borsotti<sup>2</sup>; Claudio Ciferri<sup>2</sup>; Andrea Musacchio<sup>2</sup>; Juri Rappsilber<sup>1</sup>; <sup>1</sup>*Wellcome Trust Centre for Cell Biology, Edinburgh, UK*; <sup>2</sup>*F.I.R.C. Institute of Molecular Oncology Foundatio, Milan, IT*
- MP 378 **Peptide Dimethylation Yields Enhanced y-Ion Series and Greater Sequence Coverage in Proteomics;** Jeremy

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- E. Melanson<sup>1</sup>; J. Stuart Grossert<sup>1</sup>; Kenneth A. Chisholm<sup>1</sup>; Devanand M. Pinto<sup>1</sup>; <sup>1</sup>*NRC Institute for Marine Biosciences, Halifax, NS, Canada*
- MP 379 **Can Metal Ions be used as Gas Phase Disulfide Bond Cleavage Reagents?;** Hadi Lioe<sup>1</sup>; Mubing Duan<sup>1</sup>; Richard, A. J. O'Hair<sup>1</sup>; <sup>1</sup>*The University of Melbourne, Parkville, VIC, Australia*
- MP 380 **Secondary Structure of Gas-Phase Peptide and Protein Cations Probed by Electron Capture Dissociation Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Yury O. Tsybin<sup>1</sup>; Mark R. Emmett<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Oleg Yu. Tsybin<sup>2</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*State Polytechnical University, Saint-Petersburg, Russia*
- MP 381 **Behavior of Peptide/Copper Complexes in the Gas Phase: Evidencing of Zwitterionic Forms from Doubly Charged Species;** Michel Boutin<sup>1</sup>; Claudia Bich<sup>1</sup>; Julien Franck<sup>1</sup>; Carlos Afonso<sup>1</sup>; Françoise Fournier<sup>1</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>*University Paris 6, UMR 7613, Paris, France*
- MP 382 **Facilitated de novo Sequencing of Peptides by Charge Derivatization and C-Terminal Digestion;** John C. Gebler<sup>1</sup>; Peter J. Lee<sup>1</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*
- MP 383 **Recognition of Individual Amino Acid Isomeric Form in Peptides by FT ICR Mass Spectrometry. Application to Alzheimer's Disease Peptides;** Igor A. Popov<sup>1</sup>; Sergey Kozin<sup>2</sup>; Oleg N. Kharybin<sup>2</sup>; Aleksey S. Kononikhin<sup>1</sup>; Eugene N. Nikolaev<sup>1</sup>; <sup>1</sup>*The Institute for Energy Problems of Chem. Physics, Moscow, Russia*; <sup>2</sup>*The Institute for Biomedical Chemistry, Moscow, Russia*
- MP 384 **Sequencing Unknown Marine Peptide Based on Accurate Mass and Natural Tag of Halogen Atoms;** Xidong Feng<sup>1</sup>; Damian Laid<sup>2</sup>; Tim Bugni<sup>2</sup>; Guy Carter<sup>1</sup>; Mary Kay Harper<sup>2</sup>; Chris Ireland<sup>2</sup>; <sup>1</sup>*Discovery Analytical Chemistry, Wyeth Research, Pearl River, NY*; <sup>2</sup>*Department of Medicinal Chemistry, U. of Utah, Salt Lake City, UT*
- MP 385 **Sequencing of New Antibacterial Peptides by Mass Spectrometry;** Christin Stegemann<sup>1</sup>; Alexander Kolobov<sup>2</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*
- MP 386 **Odd-Electron Radical Fragments and charge Site Locations Investigated in 157 nm Photodissociation of Peptide Ions;** Liangyi Zhang<sup>1</sup>; Matthew S. Thompson<sup>1</sup>; James P. Reilly<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*
- MP 387 **Gastro-Analogous in vitro Digestion Of Bovine & Beta;-Casein as Studied by Nano-ES-MS/MS and MALDI-PSD;** Christian E. H. Schmelzer<sup>1</sup>; Regina Schöps<sup>1</sup>; Lucy Reynell<sup>1</sup>; Reinhard H. H. Neubert<sup>1</sup>; Klaus Raith<sup>1</sup>; <sup>1</sup>*Martin Luther University Halle-Wittenberg, Halle (Saale), Germany*
- MP 388 **Misassignment of Oxidized Residues by MS/MS can be Eliminated using N-terminal Derivatization to Simplify Peptide Dissociation Patterns;** Juma D. Bridgewater<sup>1</sup>; R. Srikanth<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*
- MP 389 **Immonium Ion Intensity is a Strong Predictor of Associated Amino Acid Presence using a QSTAR Hybrid TOF Mass Spectrometer;** Laura J. Hohmann<sup>1</sup>; Jimmy K. Eng<sup>2</sup>; Andrew B. Gemmill<sup>1</sup>; Jennifer Jackson<sup>1</sup>; John E. Klimek<sup>1</sup>; Olga Vitek<sup>1</sup>; Daniel B. Martin<sup>1</sup>;

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- <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 390 **Novel Tags for Analysis of Peptides by ESI Mass Spectrometry Enhance MS Signals and Promote Gas-Phase Edman Cleavage;** Dongxia Wang<sup>1</sup>; Sunan Fang<sup>1</sup>; Robert M. Wohlhueter<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention (CDC), Atlanta, GA
- MP 391 **Improved MS/MS Spectra for De novo Interpretation Through Photodissociation of N-Sulfonated Peptides in a Quadrupole Ion Trap;** Jeffrey J Wilson<sup>1</sup>; Jennifer S Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, Tx
- MP 392 **Withdrawn**
- MP 393 **Facile Generation and Characterization of Cationic Radical Peptides: Ligand Effect and Peptide Structures;** Corey. N.W. Lam<sup>1</sup>; Galina Orlova<sup>2</sup>; Julia Laskin<sup>3</sup>; Ivan K. Chu<sup>1</sup>; <sup>1</sup>Dep. of Chemistry/The University of Hong Kong, Hong Kong, China; <sup>2</sup>Dep. of Chemistry/St. Francis Xavier University, Antigonish, Canada; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 394 **Peptide de-novo Sequencing using a Lys specific Protease and N-Terminal Tagging;** Pau-Miau Yuan<sup>1</sup>; Philip Ross<sup>1</sup>; Xunming Chen<sup>1</sup>; Darryl Pappin<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA
- MP 395 **Using Molecular Dynamics to Probe Fragmentation Mechanisms of Peptide Ozonolysis Products;** Jeffrey M. Spraggins II<sup>1</sup>; Julia Laskin<sup>2</sup>; Murray V. Johnston<sup>1</sup>; Douglas P. Ridge<sup>1</sup>; <sup>1</sup>The University of Delaware, Newark, DE; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 396 **Observation of Changes in Deuteration during Oligomerization of VP40 by Hydrogen-Deuterium Exchange Mass Spectrometry;** Leslie P. Silva<sup>1</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, Canada
- MP 397 **Identification and Structural Elucidation of CD22-Binding Proteins from Human, Bovine, and Camel Milk by Composition Based Sequencing;** Andreas Roempp<sup>1</sup>; Marko Mank<sup>2</sup>; Nadine Bock<sup>3</sup>; Bernd Stahl<sup>2</sup>; Soerge Kelm<sup>3</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>Justus Liebig University, Giessen, Germany; <sup>2</sup>Numico Research, Friedrichsdorf, Germany; <sup>3</sup>University of Bremen, Bremen, Germany

## MODIFIED PROTEINS I

- MP 398 **Identification and Characterization of Bacteriophage Proteins by Mass Spectrometry;** Susan T. Weintraub<sup>1</sup>; Christopher A. Carroll<sup>1</sup>; Elena T. Wright<sup>1</sup>; Julie A. Thomas<sup>1</sup>; Mandy Rolando<sup>1</sup>; Stephen C. Hardies<sup>1</sup>; Philip Serwer<sup>1</sup>; <sup>1</sup>University of Texas Health Science Center, San Antonio, TX
- MP 399 **Site Specific Determination of Tyrosine-O-sulfation Resulting from Tyrosylprotein Sulfotransferases;** Yonghao Yu<sup>1</sup>; Julie A. Leary<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA
- MP 400 **Photo-Crosslinkable Proteins to Reveal Protein-Nucleic Acids Interactions: The Case of HIV-1 Nucleocapsid Protein and Genomic RNA;** Prajakta C. Chaudhari<sup>1</sup>; Zhishi Guo<sup>1</sup>; Eizadora T. Yu<sup>1</sup>; Daniele Fabris<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore County, Baltimore, MD
- MP 401 **Identification of Non-Enzymatically Glycosylated Protein Residues using Characteristic MS/MS Fragmentation Patterns;** Andrej Frolov<sup>1</sup>; Peter Hoffmann<sup>2</sup>; Ralf Hoffmann<sup>1</sup>; <sup>1</sup>University of Leipzig, Leipzig, Germany; <sup>2</sup>The University of Adelaide, Adelaide, Australia
- MP 402 **Identification of New Glycated Proteins in Human Diabetic Plasma;** Thomas A. Shaler<sup>1</sup>; Weixun Wang<sup>1</sup>;

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- Perry J. Blackshear<sup>2</sup>; Christopher H. Becker<sup>1</sup>; <sup>1</sup>PPD, Inc., Menlo Park, CA; <sup>2</sup>NIEHS, RTP, NC
- MP 403 **Assessing Selenomethionine Labeling using LC-ESI-MS;** Medha J. Tomlinson<sup>1</sup>; Mark E. Michalak<sup>1</sup>; Margaret Pietras<sup>1</sup>; Richard A. Petrillo<sup>1</sup>; David L. Banach<sup>1</sup>; David W. Borhani<sup>1</sup>; John A. Mankovich<sup>1</sup>; <sup>1</sup>Abbott Bioresearch Center, Worcester, MA
- MP 404 **Redox Signalling in Dormant and Germinating Wheat Seeds Studied by a Disulfide Proteomic Approach;** Natalia V Bykova<sup>1</sup>; Brenda Hoehn<sup>1</sup>; Jo-Ann Stebbing<sup>1</sup>; Christof Rampitsch<sup>1</sup>; Ron Knox<sup>2</sup>; Mark Jordan<sup>1</sup>; Werner Ens<sup>3</sup>; <sup>1</sup>Agriculture and Agri-Food Canada, CRC, Winnipeg, Canada; <sup>2</sup>Agriculture and Agri-Food Canada, SPARC, Swift Current, Canada; <sup>3</sup>University of Manitoba, Winnipeg, Canada
- MP 405 **A Differential Tandem Mass Spectrometry Technique for Studying Protein Interaction with Arsenic;** Zhongwen Wang<sup>1</sup>; Hongquan Zhang<sup>1</sup>; Xingfang Li<sup>1</sup>; X. Chris Le<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB, Canada
- MP 406 **Post-Translational Modifications (PTMs) of MeCP2 Protein in vivo;** Yuan Gao<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA
- MP 407 **A Universal Method for the Determination of Posttranslational Modification by the Small Ubiquitin-Related Modifier SUMO;** Wendell P. Griffith<sup>1</sup>; Robert J. Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- MP 408 **Characterization by Mass Spectrometry of Tetanus Toxoid, the Immunogenic Component of Tetanus Vaccine;** Morten Thaysen-Andersen<sup>1</sup>; Sys Borchert Jørgensen<sup>2</sup>; Jesper Westphal Petersen<sup>2</sup>; Peter Højrup<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Statens Seruminstitut, Copenhagen, Denmark
- MP 409 **Electron Capture Dissociation (ECD) and the Challenge of Posttranslational Proteome Complexity;** Xin Zhang<sup>1</sup>; Shenheng Guan<sup>1</sup>; Robert J Chalkley<sup>1</sup>; Keith Vosseller<sup>2</sup>; Jonathan C Trinidad<sup>1</sup>; Alma L Burlingame<sup>1</sup>; <sup>1</sup>University of California, San Francisco, San Francisco, CA; <sup>2</sup>Drexel University College of Medicine, Philadelphia, PA
- MP 410 **Characterization of a Rare Modification on a Variant Human TNF Protein;** Melissa D Zolodz<sup>1</sup>; Helen Chung<sup>1</sup>; Michael L Klein<sup>1</sup>; <sup>1</sup>Xencor, Monrovia, CA
- MP 411 **Characterization of a Novel S hydroxylsyl-Methionine Crosslink in Collagen IV using an LTQ-FT;** Amy-Joan L. Ham<sup>1</sup>; Roberto Vanacore<sup>1</sup>; Thomas P. Conrads<sup>2</sup>; Timothy D. Veenstra<sup>2</sup>; Billy Hudson<sup>1</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>2</sup>SAIC Frederick, Inc, Frederick, MD
- MP 412 **Identification of S-Nitrosylated Cysteines in Human Endothelial Nitric Oxide Synthase (eNOS);** Manorama Tummala<sup>1</sup>; Victor Ryzhov<sup>1</sup>; Kandasamy Ravi<sup>2</sup>; Stephen Black<sup>3</sup>; <sup>1</sup>Northern Illinois University, DeKalb, IL; <sup>2</sup>Cold Spring Harbor Laboratories, Cold Spring Harbor, NY; <sup>3</sup>University of Montana, Missoula, MT
- MP 413 **Identification of Post-Translational Modifications of High Mobility Group A1 Proteins from Human Breast Cancer Tissues by Tandem Mass Spectrometry;** Yan Zou<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA
- MP 414 **Locating the Ritonavir Modification Site on Cytochrome P450 3A4 by LC-MS/MS;** Stone D.-H. Shi<sup>1</sup>; Wei O. Chen<sup>1</sup>; Michael J. Greig<sup>1</sup>; Darin Vanderpool<sup>1</sup>; Jacques Ermolieff<sup>1</sup>; <sup>1</sup>Pfizer Global R&D, La Jolla Labs, San Diego, CA

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- MP 415 **Characterization of CMD-193, a Calicheamicin-Anti-Lewis Y Monoclonal Antibody Conjugate Using MS Based Methods;** Jason X. Tang<sup>1</sup>; Eugene Vidunas<sup>1</sup>; Parimal Desai<sup>1</sup>; Mark Ruppen<sup>1</sup>; <sup>1</sup>Wyeth Research, Pearl River, NY
- MP 416 **The Study of Post-Translational Modifications of Human 20S Proteasome by Mass Spectrometry;** Qingchun Zhang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA

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- MP 417 **Protein Identification via Ion Trap Collision-induced Dissociation and Examination of Low Mass Product Ion Spectra;** Jeremiah J. Bowers<sup>1</sup>; Jian Liu<sup>1</sup>; Harsha P. Gunawardena<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- MP 418 **Top Down Identification and Characterization of Intact Human Saliva Proteins;** Jennifer Zhang<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Thomas C. McClure<sup>1</sup>; Joseph A. Loo<sup>2</sup>; Kym F. Faull<sup>2</sup>; David T. Wong<sup>2</sup>; Julian P. Whitelegge<sup>2</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA; <sup>2</sup>University of California, Los Angeles, CA
- MP 419 **Disulphide Bridge Determination and Characterisation of Low Mass Heterogeneity in Intact Mouse Urinary Proteins by FTICR-MS;** Duncan H. Robertson<sup>1</sup>; Steve C. Wong<sup>2</sup>; Jane L. Hurst<sup>1</sup>; Robert J. Beynon<sup>1</sup>; Simon J. Gaskell<sup>2</sup>; <sup>1</sup>University of Liverpool, Liverpool, UK; <sup>2</sup>University of Manchester, Manchester, UK
- MP 420 **Extending Top Down Mass Spectrometry to Larger (229 kDa) Proteins;** Xuemei Han<sup>1</sup>; Mi Jin<sup>1</sup>; Giuseppe Infusini<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, Austria
- MP 421 **Optimum Dissociation of Noncovalent and Backbone Bonds in Gaseous 144 kDa Protein Ions;** Mi Jin<sup>1</sup>; Xuemei Han<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Valerie C. Clark<sup>1</sup>; Fred W. McLafferty<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Innsbruck University, Innsbruck, Austria
- MP 422 **Towards Fast Mapping of Protein Disulfide Bonds using Negative Ion Fragmentation with a Broad-Band precursor Selection;** Mingxuan Zhang<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA
- MP 423 **Studying the Effects of Small Ligands on the Chaperone Activity of HIV-1 Nucleocapsid Protein p7 by ESI-FTMS;** Kevin B. Turner<sup>1</sup>; Nathan A. Hagan<sup>1</sup>; Katherine A. Kellersberger<sup>1</sup>; Daniele Fabris<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore County, Baltimore, MD
- MP 424 **Disulfide Bond Mapping of Recombinant Monoclonal Antibodies and Recombinant Proteins using Multiple Enzymatic Digestion, LC/MS and Principal Component Analysis (PCA);** Li Zang<sup>1</sup>; Damian Houde<sup>1</sup>; Tyler Carlage<sup>1</sup>; Yelena Lyubarskaya<sup>1</sup>; <sup>1</sup>Analytical Development Depart., BiogenIdec, Inc., Cambridge, MA
- MP 425 **Top-Down Analysis of Transthyretin using a Quadrupole/Orthogonal Acceleration TOF Mass Spectrometer;** Roger Theberge<sup>1</sup>; Jon Kingsbury<sup>1</sup>; Elena Klimtchuk<sup>1</sup>; Lawreen H Connors<sup>1</sup>; Martha Skinner<sup>1</sup>; Peter O'Connor<sup>1</sup>; Bogdan Budnik<sup>2</sup>; Catherine E Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- MP 426 **Study of Free and Albumin-Complexed Antineoplastic Benzyl Styryl Sulfone in Patient Sera from Phase I Clinical Trial;** John Roboz<sup>1</sup>; Sool Yeon Cho<sup>1</sup>; Stanely C Bell<sup>2</sup>; Premkumar Reddy<sup>3</sup>; Takao Ohnuma<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY; <sup>2</sup>Onconova

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- Therapeutics, Inc., Lawrenceville, NJ; <sup>3</sup>Temple University, Philadelphia, PA*
- MP 427 **Liquid Chromatography/Mass Spectrometry Methods for the Detailed Characterization of Intact Proteins in the Development of Recombinant Glycoprotein Therapeutics;** Joseph E. McClellan<sup>1</sup>; Colleen Steimmeyer<sup>1</sup>; Judith Gallant<sup>1</sup>; Heather Eichert<sup>1</sup>; Himakshi K. Patel<sup>1</sup>; Michael A. Jankowski<sup>1</sup>; Thomas J. Porter<sup>1</sup>; Jason C. Rouse<sup>1</sup>; <sup>1</sup>Wyeth Biotech, Andover, MA
- MP 428 **The Application of Intact Mass Analysis to Characterize Product-Related Impurities in Cell Culture Harvest;** Yonghui Wang<sup>1</sup>; Darryl Davis<sup>2</sup>; Minhong Zhuang<sup>1</sup>; David Jan<sup>1</sup>; Michael Lewis<sup>2</sup>; Michael D. Bond<sup>2</sup>; Sham-Yuen Chan<sup>1</sup>; <sup>1</sup>Cell Biology, Centocor R&D Inc., Radnor, PA; <sup>2</sup>Analytical Development, Centocor R&D Inc., Radnor, PA
- MP 429 **Identification of Secretome During Skeletal Muscle Development;** Chi Yuet Chan<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; John C. McDermott<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- MP 430 **Intact Mass Analysis of Whole Antibodies by SEC-MS Analysis;** Lowell J. Brady<sup>1</sup>; Alain Balland<sup>1</sup>; Theresa Martinez<sup>1</sup>; <sup>1</sup>Amgen, Inc., Seattle, WA

## PROTEINS: MEMBRANE

- MP 431 **Characterizing the Mitochondrial Inner-Membrane Kinase, PARL by Mass Spectrometry;** Eric A. Berg<sup>1</sup>; Jordan B. Fishman<sup>1</sup>; Luca Pellegrini<sup>2</sup>; <sup>1</sup>21st Century Biochemicals, Marlboro, MA; <sup>2</sup>Université Laval, Quebec, QC, CAN
- MP 432 **Investigation of Drug Metabolizing Enzymes using Chemical Crosslinking, Isotope Labeling and Mass Spectrometry;** Qiuxia Gao<sup>1</sup>; Catalin Doneanu<sup>1</sup>; Scott Shaffer<sup>1</sup>; Elinor Adman<sup>1</sup>; David Goodlett<sup>1</sup>; Sidney Nelson<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- MP 433 **Molecular Architecture of Pancreatic Zymogen Granule Membranes;** Xuequn Chen<sup>1</sup>; Eric S. Simon<sup>1</sup>; Donna M. Veine<sup>1</sup>; John A. Williams<sup>1</sup>; P. C. Andrews<sup>1</sup>; <sup>1</sup>The University of Michigan, Ann Arbor, MI
- MP 434 **Enhancing Sequence Coverage of Integral Membrane Proteins Using Proteomic Approaches: Application to the G-protein Coupled Receptor for Neurotensin;** Jenny TC Ho<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>NIDDK/NIH, Bethesda, MD
- MP 435 **Identification of the the Ciliary Membrane Proteome in Rat Olfactory Sensory Neurons;** Uwe Warnken<sup>1</sup>; Ulrich Mayer<sup>2</sup>; Nicole Ungerer<sup>2</sup>; Daniel Klimmeck<sup>2</sup>; Frank Mohrlen<sup>2</sup>; Stephan Frings<sup>2</sup>; Martina Schnolzer<sup>1</sup>; <sup>1</sup>German Cancer Research Center, Prot.Anal.Facility, Heidelberg, Germany; <sup>2</sup>University of Heidelberg, Inst. of Zoology, Heidelberg, Germany
- MP 436 **Characterization of the Outer Membrane Protein Profile of Clinical *Helicobacter pylori* Isolates by Subcellular Fractionation and Nano-LC FT-ICR MS Analysis;** Elisabet Carlsson<sup>1</sup>; Johanna Nystrom<sup>1</sup>; Hasse Karlsson<sup>1</sup>; Carol L Nilsson<sup>2</sup>; Ann-Mari Svennerholm<sup>1</sup>; <sup>1</sup>Inst. Biomedicine, Goteborg University, Goteborg, Sweden; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL
- MP 437 **Identification of Protein Transmembrane Domain Segments Using Shotgun Proteomics;** Adele R Blackler<sup>1</sup>; Christine C Wu<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Aurora, CO
- MP 438 **Identification and Validation of the Antiproliferative Factor Bladder Epithelial Cell Receptor in Interstitial Cystitis;** Thomas P. Conrads<sup>1</sup>; Brian L. Hood<sup>1</sup>; Gillian Tocci<sup>2</sup>; Li Guo<sup>3</sup>; Chen-Ou Zhang<sup>3</sup>; Christopher J. Michejda<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; Susan K. Keay<sup>3</sup>;



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- <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>NCI-Frederick, Frederick, MD; <sup>3</sup>University of Maryland School of Medicine, Baltimore, MD
- MP 439 **Proteomic Analysis of Early and Late Endocytic Vesicles Purified from Rat Liver by a Novel Fluorescence Cell Sorter Technique;** Jin J. Wang<sup>1</sup>; Lianji Jin<sup>1</sup>; Edward Nieves<sup>1</sup>; Linda Siconolfi-Baez<sup>1</sup>; Yansen Xiao<sup>1</sup>; Kristie Gordon<sup>2</sup>; Ruth H. Angeletti<sup>1</sup>; Allan W. Wolkoff<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY; <sup>2</sup>Columbia University, New York, NY
- MP 440 **Association of CatSper with Cav3.3 leads to Suppression of T-Type Calcium Channel Activity;** Anita Saraf<sup>1</sup>; Di Zhang<sup>1</sup>; Jun Chen<sup>1</sup>; Steve Cassar<sup>1</sup>; Ping Han<sup>1</sup>; Jorge D Brioni<sup>1</sup>; James P Sullivan<sup>1</sup>; Murali Gopalakrishnan<sup>1</sup>; John C Rogers<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
- MP 441 **New 1D and 2D Gels for the Characterization of Hydrophobic Proteins;** Caroline Tokarski<sup>1</sup>; Anne-Gaëlle Fournial<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- MP 442 **A New Strategy for Intact Mass Measurement of Hydrophobic Proteins by MALDI-MS;** Yibai Chen<sup>1</sup>; Tony Yeung<sup>1</sup>; <sup>1</sup>Fox Chase Cancer Center, Philadelphia, PA
- MP 443 **Proteomic Analysis of Torpedo Californica Electroplaque as a Model for the Neuromuscular Junction;** Javad Nazarian<sup>1</sup>; Yetrib Hathout<sup>1</sup>; Eric P Hoffman<sup>1</sup>; Bindesh Shrestha<sup>2</sup>; Akos Vertes<sup>2</sup>; <sup>1</sup>Children's National Medical Center, Washington, DC; <sup>2</sup>George Washington University, Washington, DC
- MP 444 **Proteomic Studies of Cell Surface Proteins of Prostate Cancer Cells;** Zhenyu Huang<sup>1</sup>; Xiaoning Lu<sup>1</sup>; Jianjun Zhai<sup>1</sup>; Natasha Kyprianou<sup>1</sup>; Haining Zhu<sup>1</sup>; <sup>1</sup>University of Kentucky, Lexington, KY
- MP 445 **Toxoplasma Gondii Membrane Subproteome Analysis Improved by Membrane Isolation and Pre-Fractionation Prior to Mass Spectrometry;** L. J. Jin<sup>1</sup>; T. Huang<sup>1</sup>; B. Burd<sup>1</sup>; H. Zhang<sup>1</sup>; L. M. Weiss<sup>1</sup>; R. H. Angeletti<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY
- MP 446 **A Ligand Based Structural Biology Approach for the Characterization of the Cannabinoid Receptor Binding Domains;** John Williams<sup>1</sup>; Suma Yaddanapudi<sup>1</sup>; Wei Xu<sup>1</sup>; Ganesh Thakur<sup>1</sup>; Nikolai Zvonok<sup>1</sup>; Paul Vouros<sup>2</sup>; Alexandros Makriyannis<sup>1</sup>; <sup>1</sup>Center for Drug Discovery, Northeastern University, Boston, MA; <sup>2</sup>Barnett Institute, Northeastern University, Boston, MA
- MP 447 **A Mass Spectrometry Study on the Topology of Cytochrome P450 17 $\alpha$ -Cytochrome b5 Complex by Using Crosslinker;** Hajime Mizuno<sup>1</sup>; Shunsuke Izumi<sup>1</sup>; Takeshi Yamazaki<sup>1</sup>; Toshifumi Hirata<sup>1</sup>; Shiro Kominami<sup>1</sup>; <sup>1</sup>Hiroshima Univ., Higashihiroshima, Japan
- MP 448 **Investigating the Function of Lipids in the Membrane Protein Cytochrome c Oxidase via Mass Spectrometry and Lipid Profile Modification;** Xi Zhang<sup>1</sup>; Carrie Hiser<sup>1</sup>; Banita Tamot<sup>1</sup>; Christoph Benning<sup>1</sup>; Shelagh M. Ferguson-Miller<sup>1</sup>; Gavin E. Reid<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- MP 449 **Proteomic Analysis of Plasma Membrane and Secretory Vesicles from Human Neutrophils;** Deepa Jethwaney<sup>1</sup>; Md. Rafiqul Islam<sup>2</sup>; Kevin G. Leidal<sup>2</sup>; Daniel B-V de Bernade<sup>3</sup>; Kevin P. Campbell<sup>3</sup>; William M Nauseef<sup>2</sup>; Bradford W Gibson<sup>1</sup>; <sup>1</sup>Buck Institute of Age Research, Novato, CA; <sup>2</sup>University of Iowa, Department of

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- Medicine, Iowa City, IA; <sup>3</sup>University of Iowa, Howard Hughes Med. Institute, Iowa City, IA
- MP 450 **The Proteins of the Phagosome as Detected by LC-MS/MS and Confirmed by Confocal Microscopy;** Andy Jankowski<sup>1</sup>; John G Marshall<sup>1</sup>; <sup>1</sup>Ryerson University, Toronto, Canada
- MP 451 **Mass Spectrometry and Stem Cells: Identification of Differentially Expressed Membrane and Membrane-associated Proteins Using 2-DGE and LC/MS-MS;** Lori D Shoemaker<sup>2</sup>; Harley I Kornblum<sup>1</sup>; Daniel H Geschwind<sup>1</sup>; Julian P Whitelegge<sup>2</sup>; Kym F Faull<sup>2</sup>; <sup>1</sup>School of Medicine, UCLA, Los Angeles, CA; <sup>2</sup>Pasarrow Mass Spectrometry Laboratory, UCLA, Los Angeles, CA
- MP 452 **Large scale Analysis of Olfactory Receptors in Human Sperm Membranes;** Andreas Kyas<sup>1</sup>; Jon Barbour<sup>2</sup>; Hanns Hatt<sup>2</sup>; Eva Neuhaus<sup>2</sup>; Dirk Wolters<sup>1</sup>; <sup>1</sup>Analytical Chemistry, University of Bochum, Bochum, Germany; <sup>2</sup>Cellphysiology, University of Bochum, Bochum, Germany
- MP 453 **Application of Quantitative Mass Spectrometry to Cancer Metastasis;** Hui Liu<sup>1</sup>; Forest M. White<sup>2</sup>; Richard O. Hynes<sup>1</sup>; <sup>1</sup>Center for Cancer Research, MIT, Cambridge, MA; <sup>2</sup>Biological Engineering, MIT, Cambridge, MA
- MP 454 **Optimized Protocols for Identification and Relative Quantification of Plasma Membrane Proteins from Minute Amounts of Frozen Tissues;** Jacek R. Wisniewski<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Martinsried, Germany
- CARBOHYDRATES/OLIGOSACCHARIDES I**
- MP 455 **New Ionic Liquid Matrix for Direct UV-MALDI-TOF-MS Analysis of Dermatan Sulfate Oligosaccharides;** Tatiana N. Laremore<sup>1</sup>; Fuming Zhang<sup>1</sup>; Robert J. Linhardt<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute, Troy, NY
- MP 456 **Miniaturized Graphitized Carbon LC-MS of Chondroitin Sulfate Oligosaccharides from Enzymatically Treated Aggrecan;** Ruby P. Estrella<sup>1</sup>; John M. Whitelock<sup>1</sup>; Nicolle H. Packer<sup>2</sup>; Niclas G. Karlsson<sup>2</sup>; <sup>1</sup>GSBME, University of New South Wales, Sydney, Australia; <sup>2</sup>Proteome Systems Ltd., Sydney, Australia
- MP 457 **Analysis of Gangliosides by Capillary Electrophoresis / Electrospray Ionization Mass Spectrometry with Volatile Buffers;** Mei-Chun Tseng<sup>1</sup>; Gour-Rong Her<sup>2</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan
- MP 458 **Predicting Infrared Spectra of Alkali-Attached Methylated Pyranoside Ions: Conformational Analysis with Computational Methods;** Cesar S. Contreras<sup>1</sup>; Jose J. Valle<sup>1</sup>; John R. Eyler<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- MP 459 **A Glycomics Application to Glycosaminoglycan Expression in *Caenorhabditis elegans*;** Gregory O Staples<sup>1</sup>; John F. Cipollo<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- MP 460 **The Development of ESI-FTICR-MS Methods for Structural Characterization of the Oligosaccharide Antibiotic Everninomicin;** Li-Kang Zhang<sup>1</sup>; Larry Heimark<sup>1</sup>; Birendra N Pramanik<sup>1</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, NJ
- MP 461 **Mass Spectrometric Characterization of Lipophosphoglycan from *Trichomonas vaginalis*;** Ulf Sommer<sup>1</sup>; Bibhuti N. Singh<sup>2</sup>; Gary R. Hayes<sup>2</sup>; John F. Cipollo<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University



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- School of Medicine, Boston, MA; <sup>2</sup>SUNY Upstate Medical University, Syracuse, NY
- MP 462 **Optimized Extraction of Glycosaminoglycans from Cartilage for Disease State Glycomics**; Alicia M. Hitchcock<sup>1</sup>; Sonya Shortkroff<sup>2</sup>; Karen E. Yates<sup>2</sup>; Catherine E. Costello<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Brigham and Women's Harvard Medical School, Boston, MA
- MP 463 **Characterization of Minor Glycan Structures on Monoclonal Antibodies by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry**; Danielle L. Pace<sup>1</sup>; Paul Kodama<sup>1</sup>; Theresa Martinez<sup>1</sup>; Alain Balland<sup>1</sup>; Wesley Wang<sup>1</sup>; <sup>1</sup>Amgen Washington, Seattle, WA
- MP 464 **ESI QTOF MS/MS of Protonated Calicheamicin Derivatives**; Qiang Fu<sup>1</sup>; Changsheng Zhang<sup>1</sup>; Jon S. Thorson<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin at Madison, Madison, Wisconsin
- MP 465 **Quantitative Determination of Endogenous Glucose in Human Nerve Tissues and Erythrocytes by Turboionspray LC/MS/MS**; Laixin Wang<sup>1</sup>; Min Meng<sup>1</sup>; K C Van Horne<sup>1</sup>; Patrick Bennett<sup>1</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT; <sup>2</sup>Dainippon Pharmaceuticals Company Limited, Osaka, Japan
- MP 466 **Investigation by Mass Spectrometry of New Molecular Hosts: Cyclic Oligomer of Sugar Amino Acid and Sugar-Aza-Crown Ethers**; Françoise Fournier<sup>1</sup>; Carlos Afonso<sup>1</sup>; Mickaël Ménand<sup>1</sup>; Louis Hamon<sup>2</sup>; Juan Xie<sup>3</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris 6, UMR 7613, Paris, France; <sup>2</sup>University Paris 6, UMR 7611, Paris, France; <sup>3</sup>Ecole normale supérieure, Cachan, France
- MP 467 **Development of a System for Accurate and Highly Sensitive Measurements of Non-Human Glycoprotein Modifications on Cultured Human Embryonic Stem Cells**; W. Travis Berggren<sup>1</sup>; Kevin R. Conard<sup>1</sup>; Tenneille E. Ludwig<sup>2</sup>; Jennifer L. Frane<sup>2</sup>; Lloyd M. Smith<sup>3</sup>; James A. Thomson<sup>2</sup>; <sup>1</sup>WiCell Research Institute, Madison, WI; <sup>2</sup>Nat. Primate Res. Cntr/Univ. of Wisconsin, Madison, WI; <sup>3</sup>Dept. of Chemistry-Univ. of Wisconsin, Madison, WI
- MP 468 **Analysis of Protonated and Cationized Glycoconjugate (Macrolide) Antibiotics by ESI-LE-CID (IT), Vacuum MALDI-HE-CID (TOF/RTOF) and Mass Frontier Fragmentation Library**; Ernst Pittenauer<sup>1</sup>; Omar Belgacem<sup>2</sup>; Robert Mistrik<sup>3</sup>; Guenter Allmaier<sup>1</sup>; <sup>1</sup>Vienna University of Technology, Vienna, Austria; <sup>2</sup>Shimadzu Biotech Kratos Analytical, Manchester, UK; <sup>3</sup>HighChem, Bratislava, Slovakia

## PROTEOMICS: NEW METHODS I

- MP 469 **Incorporating Theoretical Peptide pI Information in PeptideProphet to Improve Validation of MS/MS Samples Separated by Isoelectric Focusing**; David Shteynberg<sup>1</sup>; Alexey Nesvizhskii<sup>3</sup>; Johan Malmstroem<sup>2</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Swiss Federal Institute for Technology Zürich ETHZ, Zürich, Switzerland; <sup>3</sup>University of Michigan, Ann Arbor, MI
- MP 470 **Two-Dimensional Mapping (pI and m/Z) of Human Serum by Combining Microchip and MALDI-TOF-MS**; Machiko Fujita<sup>1</sup>; Wataru Hattori<sup>1</sup>; Hiroko Someya<sup>1</sup>; Tohru Sano<sup>1</sup>; Yo Tabuse<sup>1</sup>; Kenji Miyazaki<sup>1</sup>; Hirotaka Minagawa<sup>1</sup>; Masahiko Kuroda<sup>2</sup>; Hisao Kawaura<sup>1</sup>; Ken'ichi Kamijo<sup>1</sup>; <sup>1</sup>Fundamental and Environmental Res.Labs., NEC Corp., Tsukuba, Ibaraki, Japan; <sup>2</sup>Tokyo Medical University, Shinjuku-ku, Tokyo, Japan
- MP 471 **Combining Microfluidic HPLC Chip Technology with a Hybrid Triple Quadrupole Fourier Transform Ion**

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- Cyclotron Resonance Mass Spectrometer**; J. Larry Campbell<sup>1</sup>; Paula P. Pittock<sup>1</sup>; Hongfeng Yin<sup>2</sup>; Kevin Killeen<sup>2</sup>; Reid Brennen<sup>2</sup>; Gilles A. Lajoie<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Ontario; <sup>2</sup>Agilent Technologies, Palo Alto, CA
- MP 472 **Low Mass Error Tolerance and the Mass Sieve Approach to Peptide Mass Fingerprinting with MALDI-FTICR-MS**; Eric D. Dodds<sup>1</sup>; Hyun Joo An<sup>1</sup>; Paul J. Hagerman<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California Davis, Davis, CA
- MP 473 **De novo Sequencing of Tryptic Digests: A Method for Amino Acid Sequencing by Coupling The CAF Method with Affinity-isolation**; Daisuke Nakayama<sup>1</sup>; Minoru Yamaguchi<sup>1</sup>; Hiroki Kuyama<sup>1</sup>; Eiji Ando<sup>1</sup>; Taka-aki Okamura<sup>2</sup>; Norikazu Ueyama<sup>2</sup>; Takashi Nakazawa<sup>3</sup>; Osamu Nishimura<sup>1</sup>; Susumu Tsunasawa<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Osaka University, Toyonaka, Japan; <sup>3</sup>Nara Women's University, Nara, Japan
- MP 474 **Extended-pH-range Chromatofocusing Combined with MS for the Analysis of Complex Protein Mixtures**; Ying Zhang<sup>1</sup>; Zhihui Wen<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Alberta
- MP 475 **Application of (CE-MS)<sup>n</sup> to the High Throughput Analysis of Complex Protein Digests Utilizing Narrow Mass Range Scans**; Selynda Soto<sup>1</sup>; Mehdi Moini<sup>1</sup>; <sup>1</sup>University of Texas, Austin, TX
- MP 476 **A "Middle-Down" Platform for Interrogation of the Human Nucleus Using 2-Dimensional LC-FTICR-MS/MS**; Paul M Thomas<sup>1</sup>; Craig D Wenger<sup>1</sup>; Bryan A Parks<sup>1</sup>; Dana E Robinson<sup>1</sup>; Ryan T Fellers<sup>1</sup>; Yong-bin Kim<sup>1</sup>; Leonid Zamdborg<sup>1</sup>; Richard D LeDuc<sup>1</sup>; Andrew J Forbes<sup>2</sup>; Neil L Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana-Champaign, Urbana, IL; <sup>2</sup>Center for Top Down Proteomics, Urbana, IL
- MP 477 **A New Device for LC-MALDI by Heated Droplet Concentration and Impulse-Driven Deposition**; J. Bryce Young<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada
- MP 478 **An Investigation of Travelling Wave and Drift Tube IMS Separations of Protein Ion Charge States and their Fragments**; Steven D Pringle<sup>1</sup>; Kevin Giles<sup>1</sup>; Stormy L Koeniger<sup>2</sup>; Stephen J Valentine<sup>3</sup>; Robert H Bateman<sup>1</sup>; David E Clemmer<sup>2</sup>; <sup>1</sup>Waters MS Technologies Centre, Manchester, UK; <sup>2</sup>Department of Chemistry, Indiana University, Bloomington, IN; <sup>3</sup>Predictive Physiology and Medicine, Bloomington, IN
- MP 479 **Comprehensive Analysis of Glycosylated and Phosphorylated Proteins Using Extended Range Proteomic Analysis with Combined Collisional-Induced Dissociation and Electron Transfer Dissociation**; Shiaw-Lin Wu<sup>1</sup>; Barry Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- MP 480 **Efficient Prefractionation of Proteomes According to pI and MW without 2D-Gels: Application to E. coli and Arabidopsis**; Laurence V Bindschedler<sup>1</sup>; Magnus Palmblad<sup>1</sup>; Rainer K Cramer<sup>1</sup>; <sup>1</sup>The University of Reading, Reading, UK
- MP 481 **Improved Protein Separation and Identification by use of 2D Liquid Protein Fractionation and Ion Mobility Mass Spectrometry Approaches**; Susan E. Slade<sup>1</sup>; Konstantinos Thalassinos<sup>1</sup>; Jonathan P. Williams<sup>1</sup>; Robert H. Bateman<sup>2</sup>; Kevin Giles<sup>2</sup>; James H. Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Waters MS Technologies, Manchester, UK

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- MP 482 **Determining Single Amino Acid Polymorphisms (SAAPs) with Ion Mobility Spectrometry/Mass Spectrometry Techniques;** Stephen J. Valentine<sup>1</sup>; Sevugarajan Sundarapandian<sup>2</sup>; Ruwan T. Kurulugama<sup>2</sup>; David E. Clemmer<sup>2</sup>; <sup>1</sup>Predictive Physiology and Medicine, Inc., Bloomington, IN; <sup>2</sup>Indiana University, Bloomington, IN
- MP 483 **Comparison of Various Amine Reactive Modifications for Increased Verification of N-terminal Sequence Identification by Mass Spectrometry;** Peter S. Liu<sup>1</sup>; Wendy Sandoval<sup>1</sup>; Anita Izrael-Tomasevic<sup>1</sup>; Jennie R. Lill<sup>1</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA
- MP 484 **Determination of Sites of Modification of Human Keap1 by Electrophiles Using FT ICR Mass Spectrometry;** Yan Luo<sup>1</sup>; Aimee L. Egger<sup>1</sup>; Andrew D. Mesecar<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL
- MP 485 **Sub-organellar Protein Localization in Arabidopsis Thaliana Chloroplasts using an Accurate Mass and Time Tag Approach;** Christophe D. Masselon<sup>1</sup>; Myriam Ferro<sup>1</sup>; Sabine Brugiere<sup>1</sup>; Christophe Bruley<sup>1</sup>; Magali Court<sup>1</sup>; Veronique Dupieris<sup>1</sup>; Sylvie Kieffer-Jaquinet<sup>1</sup>; Norbert Rolland<sup>2</sup>; Daniel Salvi<sup>2</sup>; Daphne Seigneurin-Berny<sup>2</sup>; Jacques Joyard<sup>2</sup>; Jerome Garin<sup>1</sup>; <sup>1</sup>Lab. Chimie des Proteines, ERM-0201 INSERM/UJF/CEA, Grenoble, France; <sup>2</sup>Lab Physiologie vegetale UMR5168 CNRS/INRA/UJF/CEA, Grenoble, France
- MP 486 **Intact Protein Profiling with an Online CIEF-RPLC-MS System;** Feng Zhou<sup>1</sup>; Murray Johnston<sup>1</sup>; <sup>1</sup>University of Delaware, Newark, DE
- MP 487 **Targeting Proteome Dynamic Range Via Isotachopheresis-Based Analyte Enrichment;** Xueping Fang<sup>1</sup>; Paul A. Rudnick<sup>2</sup>; Brian M. Balgley<sup>2</sup>; Cheng S. Lee<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>Calibrant Biosystems, Gaithersburg, MD
- MP 488 **Improved Laser Desorption/Ionization Conditions for High Throughput Analyses of Large Peptides and Intact Proteins by MALDI-TOF-MS;** Eckhard Nordhoff<sup>1</sup>; Johan Gobom<sup>1</sup>; Hans Lehrach<sup>1</sup>; Armin Holle<sup>2</sup>; Jens Hoehndorf<sup>2</sup>; <sup>1</sup>Max Planck Institute for Molecular Genetics, Berlin, Germany; <sup>2</sup>Bruker Daltonics, Bremen, Germany
- MP 489 **Combined Top-Down/Bottom-Up Proteome Analysis using Electrokinetic-Based Multidimensional Separations;** Tong Guo<sup>1</sup>; Xueping Fang<sup>1</sup>; Yueju Wang<sup>1</sup>; Paul A. Rudnick<sup>2</sup>; Brian M. Balgley<sup>2</sup>; Cheng S. Lee<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>Calibrant Biosystems, Gaithersburg, MD
- MP 490 **Analysis of Intact Mouse Urinary Proteins: A Combined Electron Transfer/ Collision-Induced Dissociation Strategy with Linear Ion Trap Mass Spectrometry;** Zhiqi Hao<sup>1</sup>; Sarah R. Hart<sup>2</sup>; Duncan HL Robertson<sup>3</sup>; Andreas FR Hühner<sup>1</sup>; Robert J Beynon<sup>3</sup>; Simon J Gaskell<sup>2</sup>; <sup>1</sup>Thermo Electron Corp, San Jose, CA; <sup>2</sup>University of Manchester, Manchester, UK; <sup>3</sup>University of Liverpool, Liverpool, UK
- MP 491 **High-Resolution Protein Separation Coupled to On-Line, Top-Down Protein Analysis;** Karl E V Burgess<sup>1</sup>; Logan Mackay<sup>2</sup>; Stefan Weidt<sup>2</sup>; Ken Cook<sup>3</sup>; Remco Swart<sup>4</sup>; Patrick RR Langridge-Smith<sup>2</sup>; Andrew R Pitt<sup>1</sup>; <sup>1</sup>University of Glasgow, Glasgow, UK; <sup>2</sup>University of Edinburgh, Edinburgh, UK; <sup>3</sup>Dionex UK, Camberley, UK; <sup>4</sup>Dionex, Amsterdam, Netherlands
- MP 492 **Top-Down Proteomics Experiments Using LC-ESI-ETD/CID MS/MS;** Julie A. Horner<sup>1</sup>; Roger Biringer<sup>1</sup>;

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- Zhiqi Hao<sup>1</sup>; Jae C. Schwartz<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA
- MP 493 **Improving Protein Identification Using a Combination of Collision Induced Dissociation and Electron Transfer Dissociation MS/MS;** Ning Tang<sup>1</sup>; Paul C. Goodley<sup>1</sup>; David Horn<sup>1</sup>; Christine Miller<sup>1</sup>; Patric Hoerth<sup>1</sup>; Sheher Mohsin<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- MP 494 **A Proteomics Platform Based on Spectrum Alignment for de novo Sequencing by LTQ FT MS;** Bogdan A. Budnik<sup>1</sup>; Flavio Monigatti<sup>1</sup>; Richard Lee<sup>1</sup>; Thomas Patterson<sup>1</sup>; Judith Steen<sup>1</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Childrens Hospital Boston, Boston, MA
- MP 495 **Proteome Analysis of the Salmonella typhimurium by Ion Mobility Spectrometry - Time of Flight Mass Spectrometry;** Olesya Y. Chornoguz<sup>1</sup>; Heather M. Mottaz<sup>1</sup>; Samuel O. Purvine<sup>1</sup>; Michael A. Buschbach<sup>1</sup>; Angela D. Norbeck<sup>1</sup>; Navdeep Jaitly<sup>1</sup>; Fred Heffron<sup>2</sup>; Joshua N. Adkins<sup>1</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Oregon Health Sciences University, Portland, OR
- MP 496 **Time Series Filtering of Linear MALDI-TOF Records for Full Mass Range Enhancement of Protein Survey;** Dariya I Malyarenko<sup>1</sup>; William E. Cooke<sup>1</sup>; Eugene R. Tracy<sup>1</sup>; Richard R. Drake<sup>2</sup>; Susanna Shin<sup>2</sup>; O. John Semmes<sup>2</sup>; Maciek Sasinowski<sup>3</sup>; Dennis M. Manos<sup>1</sup>; <sup>1</sup>College of William and Mary, Williamsburg, VA; <sup>2</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>3</sup>INCOGEN, Inc., Williamsburg, VA
- MP 497 **Identification of Cognate Tumor-Associated Antigens using ProteomeLab™ PF-2D in Tandem with Mass Spectrometry;** Francina C Chahal<sup>1</sup>; Diana Lipniczky<sup>1</sup>; Jeannick Cizeau<sup>1</sup>; Nick Glover<sup>2</sup>; Glen C MacDonald<sup>1</sup>; <sup>1</sup>Viventia Biotech Inc., Winnipeg, Canada; <sup>2</sup>Viventia Biotech Inc., Toronto, Canada

## PROTEOMICS: LOWER ORGANISMS

- MP 498 **Comparative Subcellular Proteomic Analysis of Virulent Mycobacterium Tuberculosis and Corresponded Vaccine Strain Mycobacterium Bovis BCG Reveals New MTB Pathogenicity;** Sheng Gu<sup>1</sup>; Christian Forst<sup>1</sup>; Karen M. Dobos-Elder<sup>2</sup>; John T. Belisle<sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Colorado State University, Fort Collins, CO
- MP 499 **A Proteomic View of L-lysine Production with Corynebacterium Glutamicum;** Ansgar Poetsch<sup>1</sup>; Dirk Wolters<sup>2</sup>; Daniela Schluesener<sup>1</sup>; Frank Fischer<sup>1</sup>; Matthias Roegner<sup>1</sup>; <sup>1</sup>Ruhr University Bochum, Plant Biochemistry, Bochum, Germany; <sup>2</sup>Ruhr University Bochum, Analytical Chemistry, Bochum, Germany
- MP 500 **Proteomic Analysis of Aeromonas salmonicida type III Secretion Protein Complex in a Secretion Competent vs Secretion Non-Competent State;** Roger O Ebanks<sup>1</sup>; Devanand M. Pinto<sup>1</sup>; <sup>1</sup>National Research Council Canada, Halifax, Canada
- MP 501 **Proteome Characterization of Cyanobacteria Bicarbonate Transporters Under Varying Carbon Dioxide Conditions;** David W. Reed<sup>1</sup>; Vicki S. Thompson<sup>1</sup>; Michelle R. Walton<sup>1</sup>; Kastli D. Schaller<sup>1</sup>; Cody J. Permann<sup>1</sup>; Brady D. Lee<sup>1</sup>; William A. Apel<sup>1</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID
- MP 502 **Can a Protein Chemist get by with an LCQ-DUO for Shotgun Proteomics or is an LTQFT Really Needed?;** Brook Nunn<sup>2</sup>; Byron Gallis<sup>1</sup>; Manhong Wu<sup>1</sup>; Alexander Scherl<sup>1</sup>; Jinzhi Chen<sup>3</sup>; Samuel Miller<sup>1</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA;

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- <sup>2</sup>University of Otago, Dunedin, New Zealand; <sup>3</sup>Fred Hutchinson Cancer research Institute, Seattle, WA
- MP 503 **Proteomic Analysis of the Periplasm of the Yersinia Pestis Strain KIM6+;** Rembert Pieper<sup>1</sup>; Tina L. Gatlin<sup>1</sup>; David J. Clark<sup>1</sup>; Prashanth P. Parmar<sup>1</sup>; Hamid Alami<sup>1</sup>; Elizabeth M. Gebregorgis<sup>1</sup>; Shih-Ting Huang<sup>1</sup>; Srilatha Kuntumalla<sup>1</sup>; Robert D. Perry<sup>2</sup>; Scott N. Peterson<sup>1</sup>; <sup>1</sup>The Institute for Genomic Research, Rockville, MD; <sup>2</sup>University of Kentucky, Lexington, KY
- MP 504 **Catabolic Pathways of an Environmental Bacterium: Protein Identification and Quantitative Analyses in a Complex Proteomics Project;** Peter Hufnagel<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Oksana Gvozdyak<sup>2</sup>; Ralf Rabus<sup>3</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Max-Planck-Institute for Marine Microbiology, Bremen, Germany
- MP 505 **Experimental Annotation of a Herpesvirus Genome;** Dusan Kunec<sup>1</sup>; Bindu Nanduri<sup>1</sup>; Larry A. Hanson<sup>1</sup>; Shane C. Burgess<sup>1</sup>; <sup>1</sup>Mississippi State University, Mississippi State, MS
- MP 506 **Differentiation of Specific and Non-Specific Protein Interactions in Bacteria by Isotopic Labeling and Mass Spectrometry;** W. Judson Hervey, IV<sup>1</sup>; Chongle Pan<sup>1</sup>; Patricia K. Lankford<sup>2</sup>; Dale A. Pelletier<sup>2</sup>; Gregory B. 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 507 **Pox Proteomics: Mass Spectrometric Analysis and Identification of Vaccinia Virion Proteins;** Jennifer Yoder<sup>1</sup>; Tsefang Chen<sup>1</sup>; Cliff Gagnier<sup>1</sup>; Srilakshmi Vemulapalli<sup>1</sup>; Claudia Maier<sup>1</sup>; Dennis Hruby<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- MP 508 **Proteomic Analysis of Stress Response of Bacillus stearothermophilus TLS33;** Supachai Topanurak<sup>1</sup>; Suree Phutrakul<sup>1</sup>; Pinmanee Boonthueung<sup>2</sup>; Joseph A. Loo<sup>2</sup>; <sup>1</sup>Chiang Mai University, Chiang Mai, Thailand; <sup>2</sup>University of California-Los Angeles, Los Angeles, CA
- MP 509 **Identifications of Low Level Virulence Factors in Protein Fractions of Burkholderia cepacia using Mass Spectrometric Techniques;** Samanthi I Wickramasekara<sup>1</sup>; Amy Hilderbrand<sup>1</sup>; Julie Neilson<sup>1</sup>; Raina M Maier<sup>1</sup>; Vicki H Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- MP 510 **Proteomic Profiling of Methicillin Sensitive (MSSA) and Methicillin Resistant (MRSA) Staphylococcus Aureus Strains By LC-MS and LC-MS/MS;** Therese McKenna<sup>1</sup>; Christopher Hughes<sup>1</sup>; Vesela Encheva<sup>2</sup>; Haroun N Shah<sup>2</sup>; James Langridge<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Molecular Identification Services Unit, HPA, London, UK
- MP 511 **Proteomic Analysis of a Novel Anaerobic Bacterium, Syntrophus aciditrophicus;** Yanan Yang<sup>1</sup>; Yongming Xie<sup>1</sup>; Michael J. McNerney<sup>2</sup>; Robert Gunsalus<sup>3</sup>; Joseph A. Loo<sup>1</sup>; Rachel R. Ogorzalek Loo<sup>4</sup>; <sup>1</sup>UCLA, Department of Chemistry and Biochemistry, Los Angeles, CA; <sup>2</sup>University of Oklahoma, Botany and Microbiology, Norman, OK; <sup>3</sup>UCLA, Dept. of Microbiology and Molecular Genetics, Los Angeles, CA; <sup>4</sup>UCLA, Dept. of Biological Chemistry, Los Angeles, CA
- MP 512 **Dynamic Analysis for the Expression of the Heat Shock Proteins in Thermoanaerobacter Tengcongensis Corresponding with Temperature Elevated;** Bo Meng<sup>1</sup>; Jingqiang Wang<sup>1</sup>; Na Li<sup>1</sup>; Ningzhi Xu<sup>1</sup>; Yanhe Ma<sup>3</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>Beijing Genomics Institute, CAS, Beijing, China;

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- <sup>2</sup>Beijing Proteomics Institute, Beijing, China; <sup>3</sup>Institute of Microbiology, CAS, Beijing, China
- MP 513 **Sub-speciating Campylobacter Jejuni by Proteomic Analysis of Its Protein Biomarkers and Their Post-Translational Modifications;** Clifton K. Fagerquist<sup>1</sup>; Anna H. Bates<sup>1</sup>; Sekou Heath<sup>1</sup>; Bryan C. King<sup>1</sup>; Brandon Garbus<sup>1</sup>; Leslie A. Harden<sup>1</sup>; <sup>1</sup>Western Regional Research Center, ARS, USDA, Albany, CA
- MP 514 **Proteomic and Genomic Investigation of the Hydrogen Producing Thermophile Carboxydothermus hydrogenoformans;** Kevin L. Epting<sup>1</sup>; David W Reed<sup>1</sup>; Joni M Barnes<sup>1</sup>; Kastli D Schaller<sup>1</sup>; Jeff A Lacey<sup>1</sup>; Heather G Silverman<sup>1</sup>; Cody J Perman<sup>1</sup>; A S Colman<sup>2</sup>; Dennis L Maeder<sup>2</sup>; Frank T Robb<sup>2</sup>; Deborah T Newby<sup>1</sup>; Vicki S Thompson<sup>1</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>2</sup>Center of Marine Biotechnology, Univ. of Maryland, Baltimore, MD
- MP 515 **Post-Translational Modification of the Streptococcus pneumoniae Enolase;** Karen Homer<sup>1</sup>; Susmitha Rao<sup>1</sup>; Renata Soares<sup>1</sup>; <sup>1</sup>King's College London, London, UK
- MP 516 **The Cytoskeletal Scaffold of Toxoplasma gondii;** Tianmin Huang<sup>1</sup>; Berta Burd<sup>1</sup>; Jun Zhai<sup>1</sup>; Lianji Jin<sup>1</sup>; Hongshan Zhang<sup>1</sup>; Pascal Verdier-Pinard<sup>1</sup>; Hui Xiao<sup>1</sup>; Edward Nieves<sup>1</sup>; Kami Kim<sup>1</sup>; Andras Fiser<sup>1</sup>; Louis M. Weiss<sup>1</sup>; Ruth Hogue Angeletti<sup>1</sup>; <sup>1</sup>Einstein Biodefense Proteomic Research Center, Bronx, NY
- MP 517 **Proteome Analysis of Zebrafish (Danio rerio) Liver;** Andrea G. De Souza<sup>1</sup>; Nan Wang<sup>1</sup>; Lauren J. MacKenzie<sup>1</sup>; Greg G. Goss<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada
- MP 518 **Comprehensive proteome analysis of Brevibacillus brevis 47;** Hanako Ataku<sup>1</sup>; Miyako Mise<sup>1</sup>; Keiko Nishijima<sup>1</sup>; Rie Otsuka<sup>1</sup>; Jun Yamazaki<sup>1</sup>; Syuji Yamazaki<sup>1</sup>; Kazumi Sasaki<sup>1</sup>; Shinichi Tago<sup>1</sup>; Nobuyuki Fujita<sup>1</sup>; <sup>1</sup>National Institute of Technology and Evaluation, Tokyo, Japan
- MP 519 **Cellular Localization of MS/MS Identified Cilia Proteins in Tetrahymena Thermophila;** Hongyan Li<sup>1</sup>; Jeffrey C. Smith<sup>1</sup>; Wei Li<sup>1</sup>; Ronald E. Pearlman<sup>1</sup>; K.W.Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- MP 520 **The Dynamic Range Challenges for Proteomics in Microbial Communities: From Extreme Environments to Common Pond Water;** Nathan C. VerBerkmoes<sup>1</sup>; Rachna J. Ram<sup>2</sup>; Melissa Thompson<sup>1</sup>; Christine Shook<sup>1</sup>; Vincent Deneff<sup>2</sup>; Michael P. Thelen<sup>3</sup>; A. Borole<sup>1</sup>; Babu Raman<sup>1</sup>; Manesh Shah<sup>1</sup>; Brian Davison<sup>1</sup>; Jillian F. Banfield<sup>2</sup>; Robert L. Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>Lawrence Livermore National Laboratory, Livermore, CA
- MP 521 **Combination of Mass Spectrometric Approaches to Study Protein Complexes in Yeast Hybrids;** Elzbieta Piatkowska<sup>1</sup>; Francesco L Brancia<sup>2</sup>; Daniela Delneri<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>Shimadzu Research Laboratory (Europe) LTD, Manchester, UK
- MP 522 **A Quantitative Proteomic Study of Escherichia coli Expressing an Exogenous Pathway for Amorphadiene Production;** Christopher J. Petzold<sup>1</sup>; Lance Kizer<sup>1</sup>; Wenqing Shui<sup>1</sup>; Wes Marner<sup>1</sup>; Rob Dahl<sup>1</sup>; David Garcia<sup>1</sup>; Jay D. Keasling<sup>1</sup>; <sup>1</sup>University of California, Berkeley, CA
- MP 523 **Application of Proteomics Mass Spectrometry in Transcription Factor Discovery in Pyrococcus furiosus;** Meiyao Wang<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; Robert A. Scott<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA

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- MP 524 **Orthopox Proteomics and Host-Pathogen Interactions Investigated by Reversed-Phase LC-LTQ-OrbiTrap Mass Spectrometry;** Ryan D Estep<sup>2</sup>; Nathan P Manes<sup>1</sup>; Harold R Udseth<sup>1</sup>; Heather M Mottaz<sup>1</sup>; Joshua N Adkins<sup>1</sup>; Scott W Wong<sup>2</sup>; Richard D Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Oregon Health and Science University, Portland, OR*
- MP 525 **High-Throughput Proteome Analysis of *Pseudomonas putida* KT 2440 by Multidimensional Separation Coupled with ESI-MS/MS;** Jin Young Kim<sup>1</sup>; Gun Wook Park<sup>1</sup>; Sung-Ho Yun<sup>1</sup>; Seung-Il Kim<sup>1</sup>; <sup>1</sup>*Korea Basic Science Institute, Daejeon, Korea*
- MP 526 **Probing the AI-2 Regulatory Network in *Porphyromonas gingivalis* by a Proteomics Approach;** Weibin Chen<sup>1</sup>; Yoonsuk Park<sup>2</sup>; Richard J. Lamont<sup>2</sup>; John C. Gebler<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*University of Florida, Gainesville, FL*
- MP 527 **Use of 2DGE and MALDI TOF-TOF MS To Create a Comprehensive Map of The Grape Berry Proteome;** Matthew D Wheatley<sup>1</sup>; Delphine Vincent<sup>1</sup>; David R. Quilici<sup>1</sup>; David A Schooley<sup>1</sup>; Grant R Cramer<sup>1</sup>; <sup>1</sup>*University of Nevada, Reno, Reno, NV*
- MP 528 **Tracking Infection Dynamics: New Approaches for Studying Viral-Host Interactions;** Ileana M. Cristea<sup>1</sup>; John-William N. Carroll<sup>1</sup>; Michael P. Rout<sup>1</sup>; Charles M. Rice<sup>1</sup>; Margaret R. MacDonald<sup>1</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*

## PROTEOMICS: SAMPLE PREPARATION AND METHODOLOGIES I

- MP 529 **Evaluating the Variability in Commercial Trypsin Preparations;** David M. Bunk<sup>1</sup>; Paul C. Kline<sup>2</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*; <sup>2</sup>*Middle Tennessee State University, Murfreesboro, TN*
- MP 530 **Comparison of LC-MALDI vs. Sample Fractionation by Step Elution using ZipTips(TM) for the Analysis of Peptide Mixtures;** Matthew E. Openshaw<sup>1</sup>; Joanne B Connolly<sup>1</sup>; Helen Montgomery<sup>2</sup>; <sup>1</sup>*Shimadzu Biotech, Manchester, UK*; <sup>2</sup>*Koichi Tanaka Mass Spec Research Lab, Manchester, UK*
- MP 531 **Out-of-Gel Experience: Optimization Studies to Achieve Improved Peptide Recovery from Digests of Gel-Separated Proteins;** Alexander V. Lazarev<sup>1</sup>; Tomas Rejtar<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>*Barnett Institute, Northeastern University, Boston, MA*
- MP 532 **Improving Protein Identification for *Methanococcus maripaludis* Using Trypsin to Mimic Arg-C Digestion and by Isolation of the N-terminal Peptides;** Dhanashri Bagal<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*
- MP 533 **Monolithic LC-ES-MS/MS in Proteomic Analysis of Nodulation Factor-Treated Soybean Roots;** James Ault<sup>1</sup>; David Sumpton<sup>1</sup>; Joao Rodrigues<sup>1</sup>; Jerry Thomas<sup>1</sup>; Clara Diaz<sup>2</sup>; Herman Spaik<sup>2</sup>; Jane Thomas-Oates<sup>1</sup>; <sup>1</sup>*University of York, York, UK*; <sup>2</sup>*Universiteit Leiden, Leiden, The Netherlands*
- MP 534 **High Throughput Protein Identification using 2-Dimensional Difference Gel Electrophoresis and Robotic Spot Picking for Aluminum Tolerance-Related Maize Root Tip Proteins;** Yong Yang<sup>1</sup>; Robert Sherwood<sup>2</sup>; Sheng Zhang<sup>2</sup>; Issa Isaac<sup>3</sup>; Theodore Thannhauser<sup>1</sup>; <sup>1</sup>*US Plant Soil and Nutrition Laboratory, Ithaca, NY*; <sup>2</sup>*Proteomics Core Facility, Cornell University, Ithaca, NY*; <sup>3</sup>*Genomic Solutions, Inc., Ann Arbor, MI*
- MP 535 **Single Analysis Protein Profiling with Low Sample Amounts: GeLC/MS/MS or MudPIT?;** Richard C.

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- Jones<sup>1</sup>; Jason T. Taylor<sup>1</sup>; Sheeno Thyparambil<sup>1</sup>; Ricky D. Edmondson<sup>1</sup>; <sup>1</sup>*FDA/NCTR, Jefferson, AR*
- MP 536 **Positional Proteomics: Addressing the Problem of Proteome Complexity by Selective Recovery and Analysis of N-Terminal Peptides;** Lucy McDonald<sup>1</sup>; Amy Claydon<sup>1</sup>; Rachel Gore<sup>1</sup>; Robert J Beynon<sup>1</sup>; Simon J Gaskell<sup>2</sup>; <sup>1</sup>*The University of Liverpool, Liverpool, UK*; <sup>2</sup>*The University of Manchester, Manchester, UK*
- MP 537 **Detergent Extraction and 1D SDS-PAGE for the Enrichment of Plant Membrane Proteins and their Subsequent Detection by Tandem Mass Spectrometry;** Joohyun Lee<sup>1</sup>; Wesley Garrett<sup>1</sup>; Jian Feng<sup>2</sup>; Daniel Naiman<sup>2</sup>; Bret Cooper<sup>1</sup>; <sup>1</sup>*USDA-ARS, Beltsville, MD*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*
- MP 538 **"MS-tern-Blotting" for Efficient Sample Transfer and Rapid Protein Identification by Peptide Mass Fingerprinting and Peptide Sequencing;** Thomas Deierling<sup>1</sup>; Helen V. Montgomery<sup>2</sup>; Cornelia Koy<sup>1</sup>; Peter Lorenz<sup>4</sup>; Koichi Tanaka<sup>3</sup>; Hans-Juergen Thiesen<sup>4</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, University of Rostock, Rostock, Germany*; <sup>2</sup>*Shimadzu Biotech, Manchester, UK*; <sup>3</sup>*Shimadzu Corp., Kyoto, Japan*; <sup>4</sup>*Institute for Immunology, University of Rostock, Rostock, Germany*
- MP 539 **25-Sample On-Target Parallel Homogenization/Transfer Method for Solvent-free MALDI-MS Analysis of Proteins and Peptides;** Sarah Trimpin<sup>1</sup>; Charles N. McEwen<sup>2</sup>; Michael Hare<sup>3</sup>; Peter S. Spencer<sup>1</sup>; Max L. Deinzer<sup>3</sup>; <sup>1</sup>*Oregon Health & Science University, CROET, Portland, OR*; <sup>2</sup>*DuPont Corporate Center for Analytical Sciences, Wilmington, DE*; <sup>3</sup>*Oregon State University, Corvallis, OR*
- MP 540 **MALDIplex™: Automated Parallel Sample Preparation of Biofluids for MALDI Mass Spectrometry;** Dean G. Hafeman<sup>1</sup>; James B. Harkins<sup>1</sup>; Donald Loveday<sup>1</sup>; Jeremy L. Norris<sup>1</sup>; Sheila N. Baker<sup>1</sup>; <sup>1</sup>*Protein Discovery, Inc., Knoxville, TN*
- MP 541 **Multiple Applications for the Use of Magnetic Streptavidin Microparticles in Combination with MALDI-TOF and -TOF/TOF MS;** Katrin Sparbier<sup>1</sup>; Ronald Aardema<sup>2</sup>; Irina Kessler<sup>1</sup>; Thomas Wenzel<sup>1</sup>; Thomas Maier<sup>1</sup>; Chris G. de Koster<sup>2</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Leipzig, Germany*; <sup>2</sup>*Swammerdam Institute for Life Sciences, Amsterdam, The Netherlands*
- MP 542 **Highly Sensitive and Selective Analysis of Peptides by MALDI-TOF Using Polymeric Micelles for Extraction and Concentration;** Marianny Y. Combariza<sup>1</sup>; Elamprakash Savariar<sup>1</sup>; Sankaran Thayumanavan<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*
- MP 543 **Pattern-Based Identification of Protein Structural Variations by Mass Spectrometry;** Hua Huang<sup>1</sup>; Mark E. McComb<sup>1</sup>; David H. Perlman<sup>1</sup>; Hongyuan Luo<sup>1</sup>; Timothy P. Skelton<sup>1</sup>; Martin H. Steinberg<sup>1</sup>; David H. K. Chui<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*
- MP 544 **Standardization and Evaluation of Magnetic Bead-Based Urine Proteome Profiling with MALDI-TOF MS for the Detection of New Biomarkers;** Sven Baumann<sup>1</sup>; Uta Ceglarek<sup>1</sup>; Georg Martin Fiedler<sup>1</sup>; Alexander Leichte<sup>1</sup>; Christof Mayer<sup>2</sup>; Michael Stumvoll<sup>2</sup>; Joachim Thiery<sup>1</sup>; <sup>1</sup>*University Hospital Leipzig, Leipzig, Germany*; <sup>2</sup>*University of Leipzig, Leipzig, Germany*

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- MP 545 **MS Analysis of the TNF- $\alpha$  Signaling Complex Following a Novel Isolation Approach Combining Biotin and Cross-Linking Methodologies;** Julie K Freed<sup>1</sup>; Andrew S Greene<sup>2</sup>; <sup>1</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>2</sup>Biotechnology & Bioengineering Center, Milwaukee, WI
- MP 546 **Cross-linking Site Mapping of Sindbis Virus Structural Proteins;** Young Jin Lee<sup>1</sup>; Christopher B. Whitehurst<sup>2</sup>; Erik J. Soderblom<sup>2</sup>; Michael B. Goshe<sup>2</sup>; Dennis T. Brown<sup>2</sup>; Brett S. Phinney<sup>1</sup>; <sup>1</sup>University of California, Davis, CA; <sup>2</sup>North Carolina State University, Raleigh, NC
- MP 547 **Is Subtractive Affinity Depletion of Abundant Serum Proteins Useful and Reproducible?** Asish B. Chakraborty<sup>1</sup>; Scott J. Berger<sup>1</sup>; Craig Dorschel<sup>1</sup>; Scott Geromanos<sup>1</sup>; Guo-Zhong Li<sup>1</sup>; John C. Gebler<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- MP 548 **Characterization of Immobilized Carboxypeptidase Reactors for Protein Sequencing;** Marites J. Ayson<sup>1</sup>; Richard B. Jacobsen<sup>1</sup>; Joseph S. Schoeniger<sup>1</sup>; Renee Shediach<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Livermore, CA
- MP 549 **In-Solution Isoelectric Focusing of Peptides as a First Separation Dimension in Shotgun Proteomics;** Mikkel Nissum<sup>1</sup>; Robert Wildgruber<sup>1</sup>; Gerhard Weber<sup>1</sup>; Christoph Eckerskorn<sup>1</sup>; <sup>1</sup>BD Diagnostics, Martinsried, Germany
- MP 550 **Differential Protein Expression Between Male and Female Human Lumbar Cerebrospinal Fluid after Abundant Protein Depletion;** Yuko Ogata<sup>1</sup>; David C. Muddiman<sup>2</sup>; LeeAnn Higgins<sup>3</sup>; Lee Lomas<sup>4</sup>; B. Mark Keegan<sup>5</sup>; Steven A. Vernino<sup>6</sup>; H. Robert Bergen<sup>5</sup>; <sup>1</sup>Seattle Biomedical Research Institute, Seattle, WA; <sup>2</sup>North Carolina State University, Raleigh, NC; <sup>3</sup>University of Minnesota, St. Paul, MN; <sup>4</sup>Ciphergen Biosystems, Fremont, CA; <sup>5</sup>Mayo Clinic, Rochester, MN; <sup>6</sup>UT Southwestern Medical Center, Dallas, TX
- MP 551 **Free Flow Electrophoresis (FFE) for MS-based Top-Down Proteomics;** Matthew P. Torres<sup>1</sup>; Jun Han<sup>1</sup>; Hung-Hiang Quek<sup>2</sup>; Craig A. Gelfand<sup>2</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>BD Diagnostics, Preanalytical Systems, Franklin Lakes, NJ

## PROTEOMICS: QUANTITATIVE TECHNIQUES I

- MP 552 **Quantitative Proteomics Identifies Actively Translating (Polysome-Associated) and Polysome-Free mRNA-Binding Proteins (mRBPs) Upon Stimulation of the Ras/Akt-Signaling-Pathways in Glial Progenitor Cells;** Ivo Fierro-Monti<sup>1</sup>; Fabienne Brenet<sup>2</sup>; Eric C. Holland<sup>2</sup>; Peter Roepstorff<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Memorial Sloan-Kettering Cancer Center, New York, NY
- MP 553 **Quantitative Carbamylation for Comparative Proteomics;** Peggy M. Angel<sup>1</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center/UGA, Athens, GA
- MP 554 **A New Method for Quantitative Proteomics by Using Metal Element Chelated Tags Coupled with Mass Spectrometry;** Huiling Liu<sup>3</sup>; Yangjun Zhang<sup>1</sup>; Jinglan Wang<sup>1</sup>; Chunxi Zhou<sup>2</sup>; Yun Cai<sup>1</sup>; Xiaohong Qian<sup>1</sup>; <sup>1</sup>Beijing Institute of Radiation Medicine, Beijing, China; <sup>2</sup>Beijing Proteome Research Center, Beijing, China; <sup>3</sup>Beijing Institute of Transfusion Medicine, Beijing, China
- MP 555 **Combined Proteomic Strategies for Studying Embryo Implantation in Mice;** Kristin E. Burnum<sup>1</sup>; Susanne Tranguch<sup>1</sup>; Takiko Daikoku<sup>1</sup>; Dale S. Cornett<sup>1</sup>; S. K. Dey<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN

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- MP 556 **Quantitation of Cysteine Oxidation within Redox Sensitive Zinc Finger Domain of Estrogen Receptor by Stable Isotope and Immuno-Affinity Techniques;** Christian Atsriku<sup>1</sup>; David Britton<sup>1</sup>; Gary Scott<sup>1</sup>; Brad Gibson<sup>1</sup>; Christopher Benz<sup>1</sup>; Mike Baldwin<sup>2</sup>; <sup>1</sup>Buck Institute for Age Research, Novato, CA; <sup>2</sup>UCSF Mass Spec. facility, San Francisco, CA
- MP 557 **Identification and Quantitative Analysis of Acrylamide Isotope Labeled Serum Proteins Covering Five Logs of Protein Abundance;** Vitor M. Faca<sup>1</sup>; Marc Coram<sup>1</sup>; Doug Phanstiel<sup>1</sup>; Veronika Glukhova<sup>1</sup>; Qing Zhang<sup>1</sup>; Matthew Fitzgibbon<sup>1</sup>; Martin McIntosh<sup>1</sup>; Samir Hanash<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 558 **Reproducibility of Relative Quantification of Membrane Proteomes by Isotope-labeling and LC-MALDI MS;** Nan Zhang<sup>1</sup>; Chengjie Ji<sup>2</sup>; Sambasivarao Damaraju<sup>1</sup>; Vijaya L. Damaraju<sup>2</sup>; Pat Carpenter<sup>2</sup>; Carol E. Cass<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta & Cross Cancer Institute, Edmonton, Canada; <sup>2</sup>University of Alberta, Edmonton, Canada
- MP 559 **A Novel Strategy for the Quantitative Analyses of the Oxidized Proteins;** Akio Hayashi<sup>1</sup>; Takaaki Kawai<sup>3</sup>; Hiroyuki Matsumoto<sup>2</sup>; Kazuo Tsujimoto<sup>1</sup>; <sup>1</sup>JAIST, Nomi, Japan; <sup>2</sup>University of Oklahoma, Oklahoma City, OK; <sup>3</sup>AIST, Tokyo, Japan
- MP 560 **MeCAT - A Novel Technique for Quantification on Protein Level;** Robert Ahrends<sup>1</sup>; Stefan Pieper<sup>1</sup>; Andreas Kuehn<sup>1</sup>; Christian Scheler<sup>2</sup>; Meike Hamester<sup>3</sup>; Torsten Lindemann<sup>3</sup>; Michael W. Linscheid<sup>1</sup>; <sup>1</sup>Humboldt-Universitaet, Berlin, Germany; <sup>2</sup>Proteome Factory AG, Berlin, Germany; <sup>3</sup>Thermo, Bremen, Germany
- MP 561 **Mass Spectrometry-Based Strategies for Semiquantitative, Statistical and Clustering Characterization of Complex Proteomes;** Michael W. Schmidt<sup>1</sup>; E. Andres Houseman<sup>1</sup>; Keita Kono<sup>1</sup>; Katie Doud<sup>1</sup>; Dieter A. Wolf<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Harvard School of Public Health, Boston, MA
- MP 562 **Analysis Platform for Differential Quantitative Proteomics Analysis;** Ruihua Fang<sup>1</sup>; Petra Mannová<sup>1</sup>; Hong Wang<sup>1</sup>; Matthew P. Fitzgibbon<sup>1</sup>; Samir M. Hanash<sup>1</sup>; Laura Beretta<sup>1</sup>; Martin W. McIntosh<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 563 **Protein Identification and Quantification Based on C-Terminal Isotope-Coded Tagging;** Alexandre Panchaud<sup>1</sup>; Michael Affolter<sup>2</sup>; Philippe Moreillon<sup>1</sup>; Martin Kussmann<sup>2</sup>; <sup>1</sup>University of Lausanne, Lausanne, Switzerland; <sup>2</sup>Nestlé Research Centre, Lausanne, Switzerland
- MP 564 **Top Down Identification of Methanosarcina Acetivorans Proteins Using Carbon Monoxide vs. Carbon-13 Labeled Methanol as Growth Substrates;** Jonathan T. Ferguson<sup>1</sup>; Bryan A. Parks<sup>1</sup>; Jun-Kai Zhang<sup>1</sup>; William W. Metcalf<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL
- MP 565 **A New Proteomic Method for Quantitative Analysis of Peptides and Proteins Using D-labeled and unlabeled N-Naphthylidoacetamides and MALDI MS;** Sadamu Kurono<sup>1</sup>; Hanjoung Cho<sup>2</sup>; Hiroyuki Matsumoto<sup>3</sup>; Satomi Niwayama<sup>2</sup>; <sup>1</sup>IBERICA Co., Ltd., Kurume-Shi, Fukuoka, Japan; <sup>2</sup>Texas Tech University, Lubbock, TX; <sup>3</sup>University of Oklahoma HSC, Oklahoma City, OK
- MP 566 **Quantitation and Dynamic Visualization of Proteomics Data;** Brian Halligan<sup>1</sup>; Yetrib Hathout<sup>2</sup>; Kristy Brown<sup>2</sup>; Eric Hoffman<sup>2</sup>; Andrew Greene<sup>1</sup>; <sup>1</sup>Medical College of

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- Wisconsin, Milwaukee, WI; <sup>2</sup>Children's National Medical Center, Washington, DC
- MP 567 **Isotope-Differentiated Binding Energy Shift Tags (IDBEST) in Biomarker Validation and Isoform Discovery;** Michael P. Hall<sup>1</sup>; John P. Wilson<sup>1</sup>; Luke V. Schneider<sup>1</sup>; <sup>1</sup>Target Discovery, Inc., Palo Alto, CA
- MP 568 **Beyond Stable Isotope Labeling: A Mathematical Algorithm Capable of Extracting Biological Signal From Noise Inherent in Genetically Diverse Populations;** Eric J Foss<sup>1</sup>; Dragan Radulovic<sup>3</sup>; Scott Shaffer<sup>2</sup>; Antonio Bedalov<sup>5</sup>; Leonid Kruglyak<sup>4</sup>; David R. Goodlett<sup>2</sup>; <sup>1</sup>University of Washington/Fred Hutchinson Center, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Florida Atlantic University, Boca Raton, FL; <sup>4</sup>Princeton University, Princeton, NJ; <sup>5</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 569 **A Computational Tool for Quantitative Proteomics Using Stable-Isotope Labeling and LC-MSn;** Guanghui Wang<sup>1</sup>; Wells W. Wu<sup>1</sup>; Trairak Pisitkun<sup>1</sup>; Mark A. Knepper<sup>1</sup>; Rong-Fong Shen<sup>1</sup>; <sup>1</sup>National Heart, Lung, and Blood Institute, Bethesda, MD
- MP 570 **Label-free Quantitation of Proteins in the Striatum of Rats Administrated with Drugs of Abuse;** John Flensburg<sup>1</sup>; Jenny Samskog<sup>1</sup>; Petra Villani<sup>2</sup>; Fred Nyberg<sup>2</sup>; Pierre LeGrevés<sup>2</sup>; <sup>1</sup>GE Healthcare Bio-sciences AB, Uppsala, Sweden; <sup>2</sup>Pharmaceutical Biosciences, BMC, Uppsala, Sweden
- MP 571 **Evaluation of Different Stable Isotopic Labeling Approaches to Protein Quantification in LC-MS/MS Workflows;** Wolfgang Jabs<sup>1</sup>; Stephanie Hahner<sup>1</sup>; Sven Brand<sup>1</sup>; Lars Vorwerg<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany
- MP 572 **Mining the Quantitative Information Inherent in LC-MS/MS Data using Informatics for Peak Area with Internal Standard (PAIS);** Pedro Cutillas<sup>1</sup>; Bart Vanhaesebroeck<sup>1</sup>; <sup>1</sup>Ludwig Institute for Cancer Research, London, UK
- MP 573 **Global Isotopic Labeling of Protein Digests: Application in Quantitative Proteomics and Phosphoproteomics;** Michael Fedjaev<sup>1</sup>; Eugene Kanshin<sup>1</sup>; Alexander Mazur<sup>1</sup>; Ilya Nifant'ev<sup>2</sup>; Alexey Pshezhetsky<sup>1</sup>; <sup>1</sup>St-Justine Hospital, Montreal, Canada; <sup>2</sup>Moscow State University, Moscow, Russia
- MP 574 **Automatic and Manual Curation to Improve the Significance and Reliability of Relative Protein Abundance Measurements;** Alexander Loboda<sup>1</sup>; Wilfred Tang<sup>1</sup>; Alpesh Patel<sup>1</sup>; Sean Seymour<sup>1</sup>; Ignat Shilov<sup>1</sup>; Daniel Schaeffer<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA
- MP 575 **Absolute Quantification of ADH Isoenzymes in Human Liver using Multiple Reaction Monitoring (MRM) Method;** Dariusz J Janecki<sup>1</sup>; Tony Tegeler<sup>1</sup>; Thomas D. Hurley<sup>2</sup>; William F. Bosron<sup>2</sup>; Mu Wang<sup>1</sup>; <sup>1</sup>Indiana Centers for Applied Protein Sciences, Indianapolis, IN; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- MP 576 **Using Repeated Sequencing to Assess the Accuracy of emPAI Abundance Estimates from Single Samples;** Deborah H. Lundgren<sup>1</sup>; Linfeng Wu<sup>1</sup>; Viveka Maya<sup>1</sup>; Karim Rezaul<sup>1</sup>; Sunil Hwang<sup>1</sup>; David K. Han<sup>1</sup>; <sup>1</sup>UCHC, Farmington, CT
- MP 577 **Reproducible FTMS-Based Plasma Profiling of Proteins Responsive to 17 $\beta$ -estradiol (E2) or an ER  $\alpha$ -Selective Agonist in Female Rats;** Ekaterina G. Deyanova<sup>1</sup>; Xuemei Zhao<sup>1</sup>; Laura S Lubbers<sup>1</sup>; Pete T.

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- Zafian<sup>1</sup>; Gerry G Hickey<sup>1</sup>; Nathan A Yates<sup>1</sup>; Ronald C Hendrickson<sup>1</sup>; <sup>1</sup>Merck & Co. Inc, Rahway, NJ
- MP 578 **A Probabilistic Framework for Protein and Peptide Quantitation;** Keith Richardson<sup>1</sup>; Richard Denny<sup>1</sup>; John Skilling<sup>2</sup>; Iain Campuzano<sup>1</sup>; Thérèse McKenna<sup>1</sup>; Phillip Young<sup>1</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Maximum Entropy Data Consultants Ltd, Kenmare, Ireland
- MP 579 **Mass Profiling Approach to the Study of Differential Expression in Biologically Relevant Systems – A Study of Blood Platelet Aging;** Greg W Kilby<sup>1</sup>; David A Weil<sup>1</sup>; David A Engler<sup>2</sup>; Rise K Matsunami<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Texas Heart Institute, Houston, TX
- MP 580 **Label-Free Mass Spectrometry-Based Differential Proteome Analysis of Secreted Proteins Following Interferon Alpha Treatment of HepaRG Liver Cells;** Hong Wang<sup>1</sup>; Romain Parent<sup>1</sup>; Samir Hanash<sup>1</sup>; Laura Beretta<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- MP 581 **Duty Cycle Optimization for the Quantitation of Protein Abundance by LC-MS/MS and Spectral Counting;** Simon Letarte<sup>1</sup>; Mathieu Drapeau<sup>2</sup>; Peter S. McPherson<sup>2</sup>; Francois R. Blondeau<sup>2</sup>; <sup>1</sup>Universite de Montreal, Montreal, CA; <sup>2</sup>McGill University, Montreal, CA
- MP 582 **Improved NBS (2-nitrobenzenesulfonyl) Method and a New MALDI Matrix for Selective Ionization/Detection of NBS-labeled Peptides;** Ei-ichi Matsuo<sup>1</sup>; Chikako Toda<sup>1</sup>; Makoto Watanabe<sup>1</sup>; Noriyuki Ojima<sup>1</sup>; Shunsuke Izumi<sup>2</sup>; Tetsuo Iida<sup>1</sup>; Taro Masuda<sup>1</sup>; Toshikazu Minohata<sup>1</sup>; Eiji Ando<sup>1</sup>; Koichi Tanaka<sup>1</sup>; Susumu Tsunasawa<sup>1</sup>; Osamu Nishimura<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Hiroshima University, Higashi-hiroshima, Japan; <sup>3</sup>Osaka University, Osaka, Japan
- MP 583 **A New Protein Quantification Software Analysis Tool for Label-Free MS/MS-Directed Protein Quantification for Nanospray Tandem Mass Spectroscopy;** Benbo Gao<sup>1</sup>; Edward P Feener<sup>1</sup>; <sup>1</sup>Joslin Diabetes Center, Harvard Medical School, Boston, MA
- MP 584 **Proteome Analyses of LC/MS/MS Data by Multiple Search Engine Comparison and Label-Free Peptide Relative Quantification;** Melinda A. McFarland<sup>1</sup>; Xiaoyu Yang<sup>2</sup>; Jeffrey A. Kowalak<sup>2</sup>; Anthony J. Makusky<sup>2</sup>; Robert L. Nussbaum<sup>1</sup>; Lewis Y. Geer<sup>3</sup>; Sanford P. Markey<sup>2</sup>; <sup>1</sup>National Human Genome Research Institute, Bethesda, MD; <sup>2</sup>National Institute of Mental Health, Bethesda, MD; <sup>3</sup>National Center for Biotechnology Information, Bethesda, MD

## PROTEOMICS: MAMMALIAN

- MP 585 **Proteomic Analysis of Estrogen-Dependent MNAR Complexes;** Yongjing Guo<sup>1</sup>; James Greger<sup>1</sup>; Christophor McNally<sup>1</sup>; Ioannis Moutsatsos<sup>1</sup>; Patrick Cody<sup>1</sup>; Yongchang Qiu<sup>1</sup>; John F. Ross<sup>1</sup>; <sup>1</sup>Wyeth Research, Cambridge, MA
- MP 586 **Proteomic Identification of Redox-Sensitive Proteins in Experimental Animal Model of Parkinsonism;** JoungLL Choi<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA
- MP 587 **The Development of Peptide Aptamers for the Affinity Purification of Anterior Gradient-2 Protein from Barrett's Epithelium;** Euan Murray<sup>1</sup>; Lindsay R. Burch<sup>1</sup>; Ted R. Hupp<sup>1</sup>; Borek Vojtesek<sup>2</sup>; <sup>1</sup>University of Edinburgh, Cancer Research Centre, Edinburgh, UK; <sup>2</sup>Masaryk Memorial Cancer Institute, Brno, Czech Republic

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- MP 588 **Metal Status of Superoxide Dismutase From Rat Spinal Cord Determined by a ZipTip Trap and ESI-MS;** Keith E. Nylin<sup>1</sup>; Jeffrey Morré<sup>1</sup>; Joseph S. Beckman<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*
- MP 589 **Intensive Proteomic Approach to Identify Secreted Peptide/Protein from 3T3-L1 Adipocyte and Primary Adipocyte and the Influence of Thiazolidinediones on Secretome;** Hyun-Ho Hwang<sup>1</sup>; Pyong-Gon Moon<sup>1</sup>; Hye-Jeong Kim<sup>1</sup>; Sun-Jin Kim<sup>2</sup>; Seung-Jin Lee<sup>3</sup>; Jung-Guk Kim<sup>1</sup>; Wan Lee<sup>4</sup>; Je-Yoel Cho<sup>3</sup>; Sung-Ho Ryu<sup>2</sup>; Moon-Chang Baek<sup>1</sup>; <sup>1</sup>*School of Medicine, Kyungpook National University, Daegu, South Korea*; <sup>2</sup>*Pohang University of Science and Technology, Pohang, South Korea*; <sup>3</sup>*School of Dentistry, Kyungpook National University, Daegu, South Korea*; <sup>4</sup>*College of Medicine, Dongguk University, Gyeongju, South Korea*
- MP 590 **Effect of Protein Oxidation on Catalase Activity: Survey of Oxidative Modifications of Catalase with HOCl Treatment;** Suma Kaveti<sup>1</sup>; Sudakshina Ghosh<sup>1</sup>; Serpil, C. Erzurum<sup>1</sup>; Michael, T. Kinter<sup>1</sup>; <sup>1</sup>*Cleveland Clinic Foundation, Cleveland, OH*
- MP 591 **Proteomic Analysis of HDAC2 Interaction Partners;** Robert Sprung<sup>1</sup>; Junmei Zhang<sup>1</sup>; Yingda Xu<sup>1</sup>; Sungchan Kim<sup>1</sup>; Yingming Zhao<sup>1</sup>; <sup>1</sup>*UT Southwestern Medical Center, Dallas, TX*
- MP 592 **Proteomic Analysis Of MMP-9 Mediated Shedding In Macrophages;** Tomas Vaisar<sup>1</sup>; Sean Kassim<sup>1</sup>; Ivan Gomez<sup>1</sup>; Carole Wilson<sup>1</sup>; Peter Gough<sup>1</sup>; Elaine Raines<sup>1</sup>; Jay Heinecke<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 593 **Monitoring Enzymatic Turnover of Large Protein Substrate by Mass Spectrometry;** Rong-Fang Gu<sup>1</sup>; Gejing Deng<sup>1</sup>; <sup>1</sup>*Infection Discovery, AstraZeneca R&D Boston, Waltham, MA*
- MP 594 **Relative Stoichiometric Determination of the Transcriptional Cofactor Complex Mediator by Mass Spectral Analysis;** Andrew C. Paoletti<sup>1</sup>; Shigeo Sato<sup>1</sup>; Chieri Tomomori-Sato<sup>1</sup>; Tari J. Parmely<sup>1</sup>; Laurence Florens<sup>1</sup>; Ronald C. Conaway<sup>1</sup>; Joan W. Conaway<sup>1</sup>; Michael P. Washburn<sup>1</sup>; <sup>1</sup>*Stowers Institute for Medical Research, Kansas City, MO*
- MP 595 **ESI qToF and MALDI ToF/ToF MS/MS Analysis of the Rat Cardiac Mitochondrial Proteome;** Kevin Marley<sup>1</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*
- MP 596 **BlueNative-Gel and LC-MS/MS to Analyze Plasma Membrane Protein Complexes in Plants;** Sylwia Bem<sup>1</sup>; Waltraud Schulze<sup>1</sup>; <sup>1</sup>*Max-Planck Institut mol. Plant Physiology, Golm, Germany*; <sup>2</sup>*Carnegie Institute of Washington, Stanford, CA*
- MP 597 **Comparative Proteomic Analysis of an in vitro Mouse Model of Glial Tumorigenesis;** Joshua K. McBee<sup>1</sup>; Li-Rong Yu<sup>2</sup>; Takuma Uo<sup>1</sup>; Zhen Xiao<sup>2</sup>; Timothy D. Veenstra<sup>2</sup>; Yoshito Kinoshita<sup>1</sup>; Thomas P. Conrads<sup>2</sup>; Richard S. Morrison<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*SAIC-Frederick, Inc., Frederick, MD*
- MP 598 **Quantitative Proteomic Analysis of the Effect of Oxysterols on Neurons;** Yugin Wang<sup>1</sup>; Jasmina Jovanovic<sup>1</sup>; Sabina Muneton<sup>1</sup>; William Griffiths<sup>1</sup>; <sup>1</sup>*University of London, London, UK*
- MP 599 **Study of ephrinB1 Reverse Pathway using Stable Isotope Labeling and Mass Spectrometry;** Guoan Zhang<sup>1</sup>; Thomas A. Neubert<sup>1</sup>; <sup>1</sup>*New York University School of Medicine, New York, NY*
- MP 600 **The Proteomics of Proliferation and Malignancy: Analysis of Tumor-Specific and Proliferation-Specific**

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- Transcription Complexes in Normal and Malignant B Cells;** Paul B. Romesser<sup>1</sup>; David Perlman<sup>1</sup>; Anupama Sinha<sup>1</sup>; Mark E. McComb<sup>1</sup>; Douglas V. Faller<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Gerald V. Dennis<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*
- MP 601 **Comparative Proteome Profiling of Mouse Epididymal Tissues;** Shakey Quazi<sup>1</sup>; Ashok Bapat<sup>2</sup>; Panayiotis Stevis<sup>2</sup>; Gregory Kopf<sup>2</sup>; Yongchang Qiu<sup>1</sup>; Lin Liu<sup>1</sup>; <sup>1</sup>*Biological Technologies, Wyeth Research, Cambridge, MA*; <sup>2</sup>*Women's Health and Musculoskeletal Biology, Wyeth, Collegeville, PA*
- MP 602 **Using 2-D LC/MS/MS to Elucidate Tumor Necrosis-alpha and Interleukin-1 Signaling Pathways;** Lee W. Ott<sup>1</sup>; Alicia Sizemore<sup>1</sup>; Mark Goebel<sup>1</sup>; Nathan Pedrick<sup>1</sup>; Frank Witzmann<sup>1</sup>; Maureen Harrington<sup>1</sup>; <sup>1</sup>*Indiana University School of Medicine, Indianapolis, IN*
- MP 603 **Withdrawn**
- MP 604 **Proteomic Analysis of Lipid Droplet (LD) Biogenesis;** Mark S Lowenthal<sup>1</sup>; Christine Wu<sup>1</sup>; Kathryn Howell<sup>1</sup>; <sup>1</sup>*University of Colorado, Health Sciences Center, Denver, CO*
- MP 605 **HPLC-MS Detection of Light-Stimulated Cone Opsin Phosphorylation in Mouse Retinas;** Junhua Wei<sup>1</sup>; James B Hurley<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- MP 606 **Abundance Changes of Proteins in Rat Aorta in Association with Aging;** Zongming Fu<sup>1</sup>; Mingyi Wang<sup>2</sup>; Jing Zhang<sup>2</sup>; Edward Lakatta<sup>2</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*; <sup>2</sup>*National Institute on Aging, Baltimore, MD*
- MP 607 **Proteomics Analysis of Prostate Derived Ets Transcription Factor-Interacting Protein Complex;** Minjung Lee<sup>1</sup>; Seung-Jin Lee<sup>1</sup>; Byung-Gyu Kim<sup>1</sup>; Sun Hee Her<sup>1</sup>; Youn-Jeong Kim<sup>1</sup>; Hye-Jeong Park<sup>1</sup>; Hyun-Mo Ryoo<sup>2</sup>; Je-Yoel Cho<sup>1</sup>; <sup>1</sup>*Kyungpook National University, Daegu, South Korea*; <sup>2</sup>*Seoul National University, Seoul, South Korea*
- MP 608 **The Determination of the Membrane Proteome of Natural Killer Cells;** Lorraine B Anderson<sup>1</sup>; Troy C Lund<sup>1</sup>; Valarie Johnson<sup>1</sup>; Gong H Yun<sup>1</sup>; Michael R Verneris<sup>1</sup>; Bartek Grzywacz<sup>1</sup>; LeeAnn Higgins<sup>1</sup>; Jeffrey S Miller<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*

## PROTEOMICS: CANCER BIOMARKERS

- MP 609 **Characterizing Oral Cancer Progression by Free Flow Electrophoresis-Based Quantitative Saliva Proteomics;** Hongwei Xie<sup>1</sup>; Nelson L. Rhodus<sup>1</sup>; Robert J. Griffin<sup>1</sup>; John V. Carlis<sup>1</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*
- MP 610 **Differential Protein Mapping Method in Ovarian Serous Carcinoma Tissue: Identification of Potential Markers for Distinct Groups;** Yanfei Wang<sup>1</sup>; Kathleen Cho<sup>1</sup>; David Lubman<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*
- MP 611 **A Proteomic Study of Global Protein Expression Profiles in Metastatic WM 266-4 and Primary WM 115 Melanoma Cell Lines;** Victor Asirvatham<sup>1</sup>; Mohammad Al-Ghoul<sup>1</sup>; Thomas Brueckl<sup>1</sup>; Janelle Lauer-Fields<sup>1</sup>; Gregg Fields<sup>1</sup>; <sup>1</sup>*Florida Atlantic University, Boca Raton, FL*
- MP 612 **Protein Expression Profiles of Primary and Metastatic Colon Cancer Cell Lines;** Priska D. von Haller<sup>1</sup>; David Meyer<sup>1</sup>; Nadine Tuaillon<sup>2</sup>; David H. Inzunza<sup>2</sup>; Lisa A. Schubert<sup>1</sup>; Larry W. Tjoelker<sup>1</sup>; <sup>1</sup>*MacroGenics, Seattle, WA*; <sup>2</sup>*MacroGenics, Rockville, MD*
- MP 613 **A novel MS- and Affinity-based Peptide (MAP)-Chip for Clinical Cancer Diagnostic;** Jian Jiang<sup>1</sup>; Carol E.



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- MP 614 **Serum Protein Biomarkers for the Diagnosis of Pancreatic Cancer;** Unnikrishnan Gopinathan<sup>1</sup>; Suresh Chari<sup>1</sup>; Larry Ward<sup>2</sup>; Mai Persson<sup>2</sup>; Sreekumar Raghavakaimal<sup>2</sup>; <sup>1</sup>Division of Gastroenterology, Mayo Clinic, Rochester, MN; <sup>2</sup>Division of Endocrinology, Mayo Clinic, Rochester, MN
- MP 615 **Characterizing Breast Tumor Metastasis to Bone by Direct Analysis of Decalcified Tissues Using MALDI Mass Spectrometry;** Sarah A. Schwartz<sup>1</sup>; Leasa A. Greene<sup>1</sup>; Patricia A. Veno<sup>2</sup>; Jill R. Guthrie<sup>1</sup>; Lynda F. Bonewald<sup>2</sup>; Sarah L. Dallas<sup>2</sup>; <sup>1</sup>Midwest Research Institute, Kansas City, MO; <sup>2</sup>University of Missouri, Kansas City, Kansas City, MO
- MP 616 **Differential Phosphoproteomic Analysis Of Rat Traumatic Brain Injury Utilizing Fluorescent Phosphoprotein Stain and Mass Spectrometry;** Firas H. Kobeissy<sup>1</sup>; Andrew K. Ottens<sup>2</sup>; Issa Isaac<sup>5</sup>; Stanley M. Stevens Jr.<sup>6</sup>; Marjorie Chow<sup>6</sup>; Gitte Kitlen<sup>6</sup>; Neil Sharma<sup>5</sup>; Kevin K. K. W. Wang<sup>7</sup>; <sup>1</sup>Department of Psychiatry, Gainesville, FL; <sup>2</sup>Center of Neuroproteomics & Biomarkers Research, Gainesville, FL; <sup>3</sup>University of Florida, Gainesville, FL; <sup>4</sup>Department of Neuroscience, Gainesville, FL; <sup>5</sup>Genomic Solutions, Ann Arbor, MI; <sup>6</sup>Proteomics Core Facility, Gainesville, FL; <sup>7</sup>Department of Neuroscience & Psychiatry, Gainesville, FL
- MP 617 **Glycomic Profiling of Invasive and Noninvasive Breast Cancer Cells;** John A. Goetz<sup>1</sup>; Yehia Mechref<sup>1</sup>; Zuzana Kyselova<sup>1</sup>; Meei-huey Jeng<sup>2</sup>; Milos Novotny<sup>1</sup>; <sup>1</sup>Indiana University Dept. of Chemistry, Bloomington, IN; <sup>2</sup>National Center for Glycomics and Glycoproteomics, Bloomington, IN; <sup>3</sup>Indiana University Dept. of Medicine, Indianapolis, IN
- MP 618 **Oral Cancer Proteomics;** Shen Hu<sup>1</sup>; Roger Li<sup>2</sup>; Yongming Xie<sup>2</sup>; Joseph A Loo<sup>2</sup>; David T Wong<sup>1</sup>; <sup>1</sup>UCLA School of Dentistry, Los Angeles, CA; <sup>2</sup>UCLA Department of Chemistry and Biochemistry, Los Angeles, CA
- MP 619 **Identification Of Candidate Human Metastatic Melanoma Biomarkers From A Xenograft Mouse Model Using A Multi-dimensional Protein Profiling Strategy;** Hsin-Yao Tang<sup>1</sup>; Lynn Echan<sup>1</sup>; Glenn Tan<sup>1</sup>; David W. Speicher<sup>1</sup>; <sup>1</sup>The Wistar Institute, Philadelphia, PA
- MP 620 **Large Scale Proteomic Profiling of Endothelial Cells in Lung Cancer for Discovery of Cancer-Specific Protein Biomarkers;** Hye-jeong Park<sup>1</sup>; Byung-gyu Kim<sup>1</sup>; Seung-jin Lee<sup>1</sup>; Sun-hee Her<sup>1</sup>; Eung-bae Lee<sup>2</sup>; Jae-yong Park<sup>2</sup>; Hyun-mo Ryoo<sup>3</sup>; Je-yoel Cho<sup>1</sup>; <sup>1</sup>School of Dentistry Kyungpook National University, Daegu, South Korea; <sup>2</sup>Kyungpook National University Hospital, Daegu, South Korea; <sup>3</sup>School of Dentistry Seoul National University, Seoul, South Korea
- MP 621 **Toward Markers Discovery for Childhood Brain Tumors: a Proteomic Study of Cerebrospinal Fluids;** Xiaoning Lu<sup>1</sup>; Brian Rood<sup>1</sup>; Tobey MacDonald<sup>1</sup>; Yetrib Hathout<sup>1</sup>; <sup>1</sup>Children's National Medical Center, Washington, DC
- MP 622 **Assessing Protein Signatures of Metastatic Melanoma by MALDI MS;** William M. Hardesty<sup>1</sup>; Mark C. Kelley<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- MP 623 **Identification of Race-Specific Alterations in Human Prostate Cancer Proteome by 2D-PAGE and LC-MS/MS;** Amira Wohabrebbi<sup>1</sup>; Sarka Beranova-

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- Giorgianni<sup>1</sup>; <sup>1</sup>The University of Tennessee Health Science Center, Memphis, TN
- MP 624 **The Proteomic Profiling of Human Colorectal Cancer Tissue using NBS Method;** Makoto Watanabe<sup>1</sup>; Ichiro Takemasa<sup>2</sup>; Toshiya Matsubara<sup>1</sup>; Noriko Nishimura<sup>1</sup>; Shinichi Yoshioka<sup>2</sup>; Masakazu Miyake<sup>2</sup>; Taro Masuda<sup>1</sup>; Ei-ichi Matsuo<sup>1</sup>; Katsuya Nagai<sup>3</sup>; Morito Monden<sup>2</sup>; Susumu Tsunasawa<sup>1</sup>; Osamu Nishimura<sup>3</sup>; <sup>1</sup>Life Science Lab / Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Dept. of Surg. and Clin. Oncol. / Osaka University, Osaka, Japan; <sup>3</sup>Institute for Protein Research / Osaka University, Osaka, Japan
- MP 625 **Proteomic Analysis of Metastatic Breast Cancer Variants using a Novel LC-MALDI-MS/MS System;** Jane Y. Zhao<sup>1</sup>; George Scott<sup>1</sup>; Kenneth A. Chisholm<sup>2</sup>; Moulay Aloui-Jamali<sup>3</sup>; Peter Kovarik<sup>4</sup>; Tom Covey<sup>4</sup>; Devanand M. Pinto<sup>2</sup>; <sup>1</sup>Applied Biosystems/MDS Sciex, Concord, ON, Canada; <sup>2</sup>IMB, National Research Council, Halifax, NS, Canada; <sup>3</sup>McGill University, Montreal, QC, Canada; <sup>4</sup>MDS Sciex, Concord, ON, Canada
- MP 626 **Detection Of Expression Changes In Human Salivary Proteome Using Quantitative 2D-Chromatography;** Puneet Souda<sup>1</sup>; Kym Faull<sup>1</sup>; Joseph Loo<sup>1</sup>; David Wong<sup>1</sup>; Julian P Whitelegge<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- MP 627 **Ionizing Radiation-Induced Protein Profiling Using Two-Dimensional Liquid Chromatography Separation;** Xiaoping Ao<sup>1</sup>; Mary A Davis<sup>1</sup>; Theodore S Lawrence<sup>1</sup>; David M Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- MP 628 **Identification of Changes in Glycosylation Associated with Prostate Cancer Biomarkers;** Julio C Ruiz<sup>1</sup>; Tina R Hubler<sup>1</sup>; Amra Zuzo<sup>1</sup>; Lalita Samant<sup>1</sup>; Lewis K Pannell<sup>1</sup>; <sup>1</sup>Cancer Research Institute, Mobile, AL
- MP 629 **Identification of Biomarker Candidate, Catechol Estrogen-DNA Adduct, in Human Breast Tissue;** Qiang Zhang<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- MP 630 **The Comparison of Expression Changes in Endometrioid Ovarian Cancer Across Different Stages;** Hyeveung Kim<sup>1</sup>; Rong Wu<sup>2</sup>; Kathleen R. Cho<sup>2</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Department of Chemistry, Ann Arbor, MI; <sup>2</sup>University of Michigan, Department of Pathology, Ann Arbor, MI
- MP 631 **Ovarian Cancer Biomarker Discovery using Abundant Plasma Protein Depletion, 2D-PAGE and Post-Translational Modification Specific Stains;** David C Muddiman<sup>1</sup>; Yuko Ogata<sup>2</sup>; M. Cristine Charlesworth<sup>3</sup>; William A Cilby<sup>3</sup>; Benjamin J Madden<sup>3</sup>; Carrie J Heppelmann<sup>3</sup>; H Robert Bergen III<sup>3</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Seattle Biomedical Research Institute, Seattle, WA; <sup>3</sup>Mayo Clinic College of Medicine, Rochester, MN
- MP 632 **A Mass Spectrometry Based Platform for Biomarker Discovery in Archived Prostate Tissues;** Armann A. Andaya<sup>1</sup>; Harry D. Martinez<sup>1</sup>; Rohini J. Jasavala<sup>1</sup>; David K. Han<sup>2</sup>; Michael E. Wright<sup>1</sup>; <sup>1</sup>University of California Davis Genome Center, Davis, CA; <sup>2</sup>University of Connecticut Health Center, Farmington, CT
- MP 633 **Search for Inflammation Biomarkers in Lymphoma-Bearing SJL Mice Plasma using iTRAQ;** Monica H Kristiansson<sup>1</sup>; Vadiraja B Bhat<sup>2</sup>; Ramesh B Indrakanti<sup>3</sup>; John S Wishnok<sup>3</sup>; Steven R Tannenbaum<sup>3</sup>; <sup>1</sup>Lund University, Lund, Sweden; <sup>2</sup>Scott & White Memorial



# MONDAY POSTERS

## POSTER SPACE

- Hospital, Temple, TX; <sup>3</sup>Massachusetts Institute of Technology, Cambridge, MA
- MP 634 **Proteomic Analysis of Three Breast Cancer Cell Lines for Biomarker Discovery;** Kyu H. Park<sup>1</sup>; Fred R. Miller<sup>2</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Barbara Ann Karmanos Cancer Institute, Detroit, MI
- MP 635 **Identification of Protein Profiles for Breast Cancer Therapy-Response from Microdissected Tumor Cells using Nano LC-FTICR;** Arzu Umar<sup>1</sup>; Hyuk Kang<sup>2</sup>; Theo M. Luider<sup>1</sup>; John A. Foekens<sup>1</sup>; Ljiljana Pasa-Tolic<sup>2</sup>; <sup>1</sup>Erasmus University Medical Center, Rotterdam, Netherlands; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 636 **Elucidating Humoral Response in Prostate Cancer using Protein Microarrays and Liquid Phase Fractionation of Tissue Lysates;** Manoj Pal<sup>1</sup>; Arun Sreekumar<sup>1</sup>; Arul M. Chinnaiyan<sup>1</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- MP 637 **Quantitative Proteomic Approaches for the Determination of Carcinogenesis Biomarkers in Prostate Tissue;** Spiros D. Garbis<sup>1</sup>; Panagiotis Zerefos<sup>1</sup>; Aggeliki Papadopoulou<sup>1</sup>; Antonia Vlahou<sup>1</sup>; Constantin Tamvakopoulos<sup>1</sup>; Sophia Kossida<sup>1</sup>; Jose Diaz<sup>3</sup>; Kitty Pavlaki<sup>4</sup>; Stavros Tyritzis<sup>2</sup>; Stavros Vourekas<sup>2</sup>; Constantinos Constantinides<sup>2</sup>; <sup>1</sup>Biomedical Research of the Academy of Athens, Athens, Greece; <sup>2</sup>LAIKO Hospital of Athens, Urology Dept., Athens, Greece; <sup>3</sup>Eastern Virginia Medical School, Pathology Dept., VA; <sup>4</sup>Univ. of Athens Medical School, Pathoanatomy Dept., Athens, Greece
- MP 638 **Proteomics of Astrocytic Neoplasms: The Search for Tumor-Vascular/Matrix Interactions;** Uros Rajcevic<sup>1</sup>; Simone Niclou<sup>1</sup>; Dominique Revets<sup>2</sup>; Fred Fack<sup>2</sup>; Jorge Terzis<sup>3</sup>; Rolf Bjerkvig<sup>4</sup>; <sup>1</sup>NorLux - Neuro Oncology, CRP - Sante, Luxembourg, Luxembourg; <sup>2</sup>Institute of Immunology, LNS, Luxembourg, Luxembourg; <sup>3</sup>NorLux - Neuro Oncology, CHL, CRP - Sante, Luxembourg, Luxembourg; <sup>4</sup>NorLux - Neuro Oncology, University of Bergen, Bergen, Norway
- MP 639 **Proteomic Investigation of the Pathway of L-Asparaginase Drug Resistance in MOLT-4 Leukemia Cells;** Susan E Abbatiello<sup>1</sup>; Brian L Hood<sup>2</sup>; David A Lucas<sup>2</sup>; King C Chan<sup>2</sup>; Nan Su<sup>3</sup>; YuanXiang Pan<sup>3</sup>; Michael S Kilberg<sup>3</sup>; Thomas P Conrads<sup>2</sup>; Timothy D Veenstra<sup>2</sup>; Nigel G J Richards<sup>1</sup>; John R Eyler<sup>1</sup>; <sup>1</sup>University of Florida, Department of Chemistry, Gainesville, FL; <sup>2</sup>SAIC-Frederick, Inc, Frederick, MD; <sup>3</sup>University of Florida, Department of Biochemistry, Gainesville, FL
- MP 640 **A Proteomic Signature of Relapse-Related Death Predicting Clinical Outcome in Human Non-Small Cell Lung Cancer (NSCLC);** Kiyoshi Yanagisawa<sup>1</sup>; Shuta Tomida<sup>1</sup>; Yasushi Yatabe<sup>2</sup>; Tetsuya Mitsudomi<sup>2</sup>; Takashi Takahashi<sup>1</sup>; <sup>1</sup>Nagoya University Graduate School of Medicine, Nagoya, Aichi, Japan; <sup>2</sup>Aichi Cancer Center Hospital, Nagoya, Aichi, Japan
- MP 641 **Determination of Biomarkers of Disease Status in Saliva by HPLC-MS/MS;** Byoung Joon Ko<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; Craig S. Miller<sup>2</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX; <sup>2</sup>University of Kentucky, Lexington, KY
- MP 642 **Differential Lectin Capture of Serum Glycoproteins Combined with Pre-Fractionation Methods for Prostatic Disease Biomarker Discovery;** Ellen Schwegler<sup>1</sup>; Gunjan Malik<sup>1</sup>; Michael Ward<sup>1</sup>; Shamina Mitchell<sup>1</sup>; Oliver J Semmes<sup>1</sup>; Richard R Drake<sup>1</sup>; <sup>1</sup>Eastern Virginia Medical School, Norfolk, VA

## POSTER SPACE

- PROTEOMICS: METHODS FOR PHOSPHO PROTEINS**
- MP 643 **Absolute Quantification (AQUA) of Phosphorylation Levels in Biological Samples using Immobilized Metal Affinity Chromatography Enrichment (IMAC);** Jeffrey L. Turner<sup>1</sup>; John G. Dapron<sup>1</sup>; Justin Wildsmith<sup>1</sup>; Jessica M. Moeller<sup>1</sup>; Kevin Ray<sup>1</sup>; Graham B. I. Scott<sup>1</sup>; <sup>1</sup>Sigma-Aldrich Corporation, St. Louis, MO
- MP 644 **Selective Enrichment of Phosphopeptides from Peptide Mixtures by Isoelectric Focusing after Methyl-Esterification;** ChongFeng Xu<sup>1</sup>; Thomas A. Neubert<sup>1</sup>; <sup>1</sup>New York University School of Medicine, New York, NY
- MP 645 **Ion Mapping Tandem Mass Spectrometry Using either a vMALDI or Nanospray Source Detects More Phosphopeptides than Neutral Loss Experiments;** Dawn Z Chen<sup>1</sup>; Tatiana N. Boronina<sup>1</sup>; Rosa Viner<sup>2</sup>; Robert N. Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins University, School of Medicine, Baltimore, MD; <sup>2</sup>Thermo Electron Co., San Jose, CA
- MP 646 **Separation and Detection of Protein Post-Translational Modifications by Liquid Chromatography Coupled with a Novel Ion Mobility Mass Spectrometer;** Ole N. Jensen<sup>1</sup>; Martin R. Larsen<sup>1</sup>; Jason Wildgoose<sup>2</sup>; Robert H. Bateman<sup>2</sup>; Kevin Giles<sup>2</sup>; Steven Pringle<sup>2</sup>; Chris Hughes<sup>2</sup>; Jim Langridge<sup>2</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Waters Corp. MS Technologies Centre, Manchester, UK
- MP 647 **Proteomics Analysis of Effect of Casein Phosphopeptides on Metal Ion Binding;** Jiaxi Wang<sup>1</sup>; Kirk Green<sup>1</sup>; Graham McGibbon<sup>1</sup>; Brain McCarry<sup>1</sup>; <sup>1</sup>McMaster University, Hamilton, Canada
- MP 648 **Complementary Analysis of Phosphorylated Proteins by MALDI and nano ESI-MS/MS;** Rosa Viner<sup>1</sup>; Terry Zhang<sup>1</sup>; Ken Miller<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA
- MP 649 **Identification and Quantification of Focal Adhesion Kinase Phosphorylation Sites using Stable Isotope Dilution Nanospray LC/MS and MRM-Initiated Detection and Sequencing;** Eugene Ciccimaro<sup>1</sup>; John M. Hevko Hevko<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>Center for Cancer Pharmacology, University of Penn, Philadelphia, PA; <sup>2</sup>Applied Biosystems, Foster City, CA
- MP 650 **Identification of Insulin Receptor Phosphorylation Sites using a Novel PhosphoTip Purification Protocol;** Clifford Bolinger<sup>1</sup>; Jamie Graham<sup>1</sup>; Leslie M Frost<sup>1</sup>; <sup>1</sup>Marshall University, Huntington, WV
- MP 651 **From the Comparison of Phosphoproteomes to a Global Phosphoproteome Database;** Søren Schandorff<sup>1</sup>; Ole Vorm<sup>1</sup>; Hans Jespersen<sup>1</sup>; Alexandre Podtelejnikov<sup>1</sup>; <sup>1</sup>Proxeon, Odense, Denmark
- MP 652 **Insulin Induced-Changes of the Tyrosine Phosphoproteomes of Brown Preadipocytes and Adipocytes;** Marcus Krueger<sup>1</sup>; Irina Kratchmarova<sup>2</sup>; Blagoy Blagoev<sup>2</sup>; Yu-Hua Tseng<sup>3</sup>; C. Ronald Kahn<sup>3</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Munich, Germany; <sup>2</sup>University of Southern Denmark, Odense, Denmark; <sup>3</sup>Joslin Diabetes Center, Harvard Medical School, Boston, MA
- MP 653 **Data Dependent Electron Capture Dissociation (ECD) of Phosphorylated Proteins;** Andrew J. Creese<sup>1</sup>; C. Logan Mackay<sup>2</sup>; Stefan K. Weidt<sup>2</sup>; Pat Langridge-Smith<sup>2</sup>; Nick Morrice<sup>3</sup>; Helen J. Cooper<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>University of Edinburgh, Edinburgh, UK; <sup>3</sup>University of Dundee, Dundee, UK
- MP 654 **Dephosphorylation Induced Chromatographic Shift and Isobaric Tagging: an Exquisitely selective and**

- sensitive method for quantitative phosphopeptide profiling;** Duncan L. Smith<sup>1</sup>; Andrew JK Williamson<sup>1</sup>; Anthony D Whetton<sup>1</sup>; <sup>1</sup>*University of Manchester, Manchester, UK*
- MP 655 **High Probability MS Identification of Phosphopeptides by their Mass Defect;** Erol E. Gulcicek<sup>1</sup>; Mark A. Shifman<sup>1</sup>; Perry Miller<sup>1</sup>; Christopher M. Colangelo<sup>1</sup>; Kathryn L. Stone<sup>1</sup>; TuKiet T. Lam<sup>1</sup>; Can Bruce<sup>1</sup>; <sup>1</sup>*Yale University, New Haven, CT*
- MP 656 **Dynamics of in vivo Tyrosine Phosphorylation Events to Elucidate Growth Factor Induced Pathways by High-Accuracy Orbitrap Tandem Mass Spectrometry;** Jesper V. Olsen<sup>1</sup>; Blagoy Blagoev<sup>2</sup>; Sonja Krueger<sup>1</sup>; Florian Gnad<sup>1</sup>; Boris Macek<sup>1</sup>; Peter Mortensen<sup>2</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>*Max-Planck-Institute of Biochemistry, Martinsried, Germany*; <sup>2</sup>*CEBI - University of Southern Denmark, Odense, Denmark*
- MP 657 **Mining Phosphopeptides in LC-MS Data for Protein Phosphorylation Site Determination;** Hsin-Yi Wu<sup>1</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>*Medical College, National Cheng Kung University, Tainan, Taiwan*
- MP 658 **Shotgun<sup>2</sup> Tandem Collision-Induced Dissociation Mass Spectrometry of Phosphotyrosine Peptides;** Yu Shi<sup>1</sup>; Lauren Rosen<sup>1</sup>; Alexis Ramos<sup>1</sup>; Xudong Yao<sup>1</sup>; <sup>1</sup>*University of Connecticut, Storrs, CT*
- MP 659 **Discerning Phosphorylation from Tyrosine Sulfation in a Single Polypeptide Using Nanoelectrospray Ionization Tandem Mass Spectrometry;** Lisa A. Marzilli<sup>1</sup>; Erin E. Wiswall<sup>1</sup>; Himakshi K. Patel<sup>1</sup>; Mike A. Jankowski<sup>1</sup>; Jason C. Rouse<sup>1</sup>; <sup>1</sup>*Wyeth BioPharma, Andover, MA*
- MP 660 **Enhancement of Ionization Efficiency and Selective Enrichment of Phosphorylated Peptides using Polyhistidine-Tags;** Pegah R Jalili<sup>1</sup>; Deepti Sharma<sup>1</sup>; Haydn Ball<sup>1</sup>; <sup>1</sup>*University of Texas Southwestern Medical Center, Dallas, TX*
- MP 661 **Direct Determination of Dialkyl Phosphates (DAPs) by Strong Anion Exchange Atmospheric Pressure Chemical Ionization (APCI) LC-MS-MS;** W. M. Draper; P. Behniwal; D. Wijekoon; *Sanitation and Radiation Laboratory Branch, California Department of Health Services, 850 Marina Bay Parkway, Richmond, CA*
- MP 662 **Substrate and Functional Diversity of Lysine Acetylation Revealed by a Proteomics Survey;** Sung Chan Kim<sup>1</sup>, Robert Sprung<sup>1</sup>, Yue Chen<sup>1</sup>, Yingda Xu<sup>1</sup>, Haydn Ball<sup>1</sup>, Jimin Pei<sup>1</sup>, Nick V. Grishin<sup>1,2</sup>, Yingming Zhao<sup>1</sup> <sup>1</sup>*Department of Biochemistry, UT Southwestern Medical Center, Dallas, Texas* <sup>2</sup>*Howard Hughes Medical Institute and Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX*
- MP 663 **Proteomic Analysis of Lysine Acetylation in E. coli;** Junmei Zhang, Sungchan Kim, Robert Sprung, and Yingming Zhao; *Department of Biochemistry, UT Southwestern Medical Center, Dallas, Texas*

## TUESDAY POSTERS

### POSTER SPACE

### TUESDAY POSTERS

These posters should be set up at 7:30 am on Tuesday and removed at 7:30 pm. Be sure to use the poster space number next to the title.

#### ISOTOPE RATIO MS

- TP 9 **Determination of High-Precision Isotope Ratios from Experimental Isotopic Distributions;** Parminder Kaur<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA
- TP 10 **The 13C/12C Ratio Analyses of CO<sub>2</sub> in Human Breath of Suspected Helicobacter pylori Infection using Continuous Flow GC/IRMS;** Chul-Min Shin<sup>1</sup>; Won-Gi An<sup>1</sup>; Jong-Jin Lee<sup>1</sup>; Yoon-Jin Lee<sup>1</sup>; Hae-Seon Nam<sup>1</sup>; Sung-Ho Kim<sup>1</sup>; <sup>1</sup>Soonchunhyang University, Asan, South Korea
- TP 11 **Simultaneous Pulse Counting Detection of Isotopic Ion Beams using a Microchannelplate Array;** Peter J. Todd<sup>1</sup>; Henry S. McKown<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN

TP 12

#### PARTICLE ANALYSIS

- TP 13 **Exploration of the Laser Desorption and Ionization Process of Individual Aerosol Particles;** Erica L. McJimpsey<sup>1</sup>; Paul T. Steele<sup>2</sup>; George R. Farquar<sup>2</sup>; David P. Fergenson<sup>2</sup>; Sue I. Martin<sup>2</sup>; Matthias Frank<sup>2</sup>; Eric E. Gard<sup>2</sup>; Herbert J. Tobias<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California-Davis, Davis, CA; <sup>2</sup>Lawrence Livermore National Laboratory, Livermore, CA
- TP 14 **Lithium Ion Attachment as a Soft Ionization Approach for Detection of Organic Species in the Aerodyne AMS;** Achim M Trimborn<sup>1</sup>; John Jayne<sup>1</sup>; Megan Northway<sup>1</sup>; Doug Worsnop<sup>1</sup>; <sup>1</sup>Aerodyne Research Inc., Billerica, MA
- TP 15 **Spectra Analysis for Aerosol Particles Measured in Parallel with Two Online TOF Laser Mass Spectrometers LAMPAS 2 and SPASS;** Klaus-Peter Hinz<sup>1</sup>; Nicole Erdmann<sup>2</sup>; Carsten Grüning<sup>3</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>University of Giessen, Giessen, Germany; <sup>2</sup>University of Mainz, Mainz, Germany; <sup>3</sup>Joint Research Center Ispra, Ispra, Italy
- TP 16 **Application of Non-Resonant Laser Ablation Mass Spectrometry for Fast Isotope Analysis of Metal Microparticles;** Kyuseok Song<sup>1</sup>; Bowha Ahn<sup>1</sup>; Sunho Han<sup>1</sup>; Yongjoon Park<sup>1</sup>; Wonho Kim<sup>1</sup>; <sup>1</sup>Korea Atomic Energy Research Institute, Taejeon, Korea

#### HYDROCARBONS AND PETROCHEMICALS BY FTMS

- TP 17 **Automated Field Desorption FT-ICR MS for Petroleum Analysis;** Donald F. Smith<sup>1</sup>; Tanner M. Schaub<sup>2</sup>; Christopher L. Hendrickson<sup>2</sup>; Ryan P. Rodgers<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Tallahassee, FL; <sup>2</sup>Ion Cyclotron Resonance Program, NHMFL, FSU, Tallahassee, FL
- TP 18 **Analysis of High Boiling Petroleum Products by LC/MS;** Jennifer Huang<sup>1</sup>; Charlie Van Wandelen<sup>1</sup>; Ray Chen<sup>1</sup>; Chris Loran<sup>1</sup>; <sup>1</sup>Thermo Electron Corp., San Jose, California
- TP 19 **Detailed Compositional Comparison of Acidic NSO Compounds Before and After Bioremediation of Crude Oil-Contaminated Soil;** Samantha A. Galasso<sup>1</sup>; Christine A. Hughey<sup>1</sup>; <sup>1</sup>Chapman University, Orange, CA
- TP 20 **A Comprehensive Comparison of the Polar NSO Compounds in a Suite of Biodegraded Oils by ESI FT-ICR MS;** Geoffrey C Klein<sup>1</sup>; Ryan P. Rodgers<sup>1</sup>; Barry Bennett<sup>2</sup>; Steve R Larter<sup>2</sup>; Alan G Marshall<sup>1</sup>; <sup>1</sup>NHMFL, Tallahassee, FL; <sup>2</sup>University of Calgary, Calgary, Canada

### POSTER SPACE

- TP 21 **Isolation and Characterization of Crude Oil Asphaltenes and Coprecipitants by Negative-Ion Electrospray Ionization FT-ICR Mass Spectrometry;** Do-Gyun Kim<sup>1</sup>; Jeremiah M. Purcell<sup>2</sup>; Ryan P. Rodgers<sup>1</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, FSU, Tallahassee, Florida; <sup>2</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, Florida

TP 22

- TP 23 **Detailed Compositional Characterization of Water-in-Oil Emulsion Stabilizers in Canadian Bitumens by ESI FT-ICR MS;** Lateefah A Stanford<sup>1</sup>; Don Smith<sup>1</sup>; Jan Czarnecki<sup>2</sup>; Alex Wu<sup>2</sup>; Ryan P Rodgers<sup>1</sup>; Alan G Marshall<sup>1</sup>; <sup>1</sup>NHMFL-FSU, Tallahassee, FL; <sup>2</sup>SynCrude Research, Edmonton, Canada

#### METABOLITE PROFILING AND IDENTIFICATION: APPLICATIONS

- TP 24 **Identification of An Unusual Defluorination-GSH Conjugate Using Linear Ion Trap Mass Spectrometer;** Ji Ma<sup>1</sup>; Robert Cho<sup>1</sup>; Jianxia Shi<sup>1</sup>; Shichang Miao<sup>1</sup>; Chun Li<sup>2</sup>; Craig Uyeda<sup>1</sup>; Monica Sweany<sup>1</sup>; Meghan Canfield<sup>1</sup>; George Tonn<sup>1</sup>; <sup>1</sup>Amgen Inc, South San Francisco, USA; <sup>2</sup>Amgen, Thousand Oaks, USA
- TP 25 **Metabolite Identification using LC/LTQ/Orbitrap with Accurate Mass Measurement at 60,000 Resolution of Precursor/Product Ions from Data-Dependent Mass Analysis;** H.K. Lim<sup>1</sup>; Carlo Sensenhauser<sup>1</sup>; Jie Chen<sup>1</sup>; Kevin L. Cook<sup>1</sup>; Vangala Subrahmanyam<sup>1</sup>; <sup>1</sup>J&J Pharmaceutical Research & Development, Raritan, NJ
- TP 26 **Metabolic Interspecies Comparison, by LCMS and Principle Component Analysis;** Elliott Jones<sup>1</sup>; Ji Ma<sup>2</sup>; Sasaki Tania<sup>1</sup>; Robert Cho<sup>2</sup>; <sup>1</sup>Appliedbiosystems, Foster City, CA; <sup>2</sup>Amgen, South San Francisco, CA
- TP 27 **A Novel DynamicFlow System for Sensitive Radioisotope Detection and Structural Elucidation;** Dian Y. Lee<sup>1</sup>; Kevin Hsu<sup>1</sup>; <sup>1</sup>AIM Research Co., Hockessin, DE
- TP 28 **MS/MS Characterization of New Sulfate Metabolites of Aristolochic Acid I;** Robert A. Rieger<sup>1</sup>; Horacio Priestap<sup>1</sup>; Tomoko Freshwater<sup>2</sup>; David R. Taft<sup>2</sup>; M.Cecilia Torres<sup>1</sup>; Charles R. Iden<sup>1</sup>; <sup>1</sup>State University of New York at Stony Brook, Stony Brook, NY; <sup>2</sup>Long Island University, Brooklyn, NY
- TP 29 **Investigation of Metabolic Pathways in Desulfobivrio v. by ESI FT-ICR;** Francesco Pingitore<sup>1</sup>; Yinjie Tang<sup>1</sup>; Aindrila Mukhopadhyay<sup>1</sup>; Jay Keasling<sup>1</sup>; <sup>1</sup>University of California, Berkeley, Berkeley, CA
- TP 30 **Analysis of Ceramides in Body Fluids by Electrospray LC/MS/MS;** Jie Chen<sup>1</sup>; Srinivas B. Narayan<sup>1</sup>; Michael J. Bennett<sup>1</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA
- TP 31 **Profiling of Urinary Metabolites;** Vladimir V. Tolstikov<sup>1</sup>; Kindra D. Brooks<sup>1</sup>; Robert H. Weiss<sup>2</sup>; <sup>1</sup>UC Davis Genome Center, Davis, CA; <sup>2</sup>Div. Of Nephrology, UC Davis, Davis, CA
- TP 32 **Stereoselective metabolism of methadone by human liver microsomes and cDNA-expressed P450s;** Yan Chang<sup>1</sup>; Shen-Nan Lin<sup>1</sup>; David E Moody<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT
- TP 33 **Chiral and Achiral LC/MS for Studies on the Formation of Hydroxylated Metabolites of Ketamine;** Joelle Onorato<sup>1</sup>; Peter Bullock<sup>2</sup>; Maria E. Rodriguez-Rosas<sup>1</sup>; Irving Wainer<sup>1</sup>; <sup>1</sup>NIH/NIA, Baltimore, MD; <sup>2</sup>Panacos, Rockville, MD
- TP 34 **Identification of a metabolite of atrazine, N-ethyl-6-methoxy-N'- (1-methylethyl)-1,3,5-triazine-2, 4-**

## TUESDAY POSTERS

### POSTER SPACE

- TP 35 **diamine, upon incubation with rat liver microsomes; Aiqun Li<sup>1</sup>; Matthew P. May<sup>1</sup>; James C Bigelow<sup>1</sup>; <sup>1</sup>Idaho State University, College of Pharmacy, Pocatello, Idaho**  
**High Performance Liquid Chromatography followed by Post Source Decay Laser Desorption Ionization Mass Spectrometry for Retinoid Characterization from Retinol Metabolism; Moo-Jin Suh<sup>1</sup>; Xiaohan Tang<sup>1</sup>; Lorraine J Gudis<sup>1</sup>; <sup>1</sup>Weill Medical College of Cornell University, New York, NY**
- TP 36 **Metabolite Detection and Characterization by High-Resolution Orbitrap Mass Spectrometry: Application of Mass Defect and Product Ion Filtering Techniques; Qian Ruan<sup>1</sup>; Scott Peterman<sup>2</sup>; Mark A. Szewc<sup>2</sup>; Li Ma<sup>1</sup>; Dan Cui<sup>1</sup>; W. Griffith Humphreys<sup>1</sup>; Mingshe Zhu<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ ; <sup>2</sup>Thermo Electron Corp, Somerset, NJ**
- TP 37 **LC-FTMS for High-Throughput Analysis of Oxidative Stress Biomarkers in Human Plasma; Jennifer M. Johnson<sup>1</sup>; Frederick H Strobel<sup>1</sup>; Dean P. Jones<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA**
- TP 38 **Characterization of Microsomal Metabolism of BML-190, a CB2 Selective Agonist by HPLC-MS/MS; Qiang Zhang<sup>1</sup>; Peng Ma<sup>1</sup>; Richard B Cole<sup>2</sup>; Guangdi Wang<sup>1</sup>; <sup>1</sup>Xavier University of LA, New Orleans, LA ; <sup>2</sup>University of New Orleans, New Orleans, LA**
- TP 39 **Qualitative Reaction Phenotyping of P450 Isozymes involved in the Metabolism of Selegiline to Desmethylselegiline and Methamphetamine; Salete Benetton<sup>1</sup>; Che Fang<sup>1</sup>; Yanou Yang<sup>1</sup>; Ramya Alok<sup>1</sup>; Mey Year<sup>1</sup>; Chin-Chung Lin<sup>1</sup>; Li-Tain Yeh<sup>1</sup>; <sup>1</sup>Valeant Research & Development, Costa Mesa, CA**
- TP 40 **Combining MDF and PeakMatch Techniques for Comprehensive and Selective Detection of Drug Metabolites in Vivo; Haiying Zhang<sup>1</sup>; Mingshe Zhu<sup>1</sup>; Li Ma<sup>1</sup>; Kan He<sup>1</sup>; W. Griffith Humphreys<sup>1</sup>; Mark Sanders<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ**
- TP 41 **Drug Metabolism of Curcumin by Liquid Chromatography Tandem Mass Spectrometry (LC-MS-MS) on a hybrid quadrupole linear ion trap system; Constantin Tamvakopoulos<sup>1</sup>; Zacharias D. Sofianos<sup>1</sup>; Spiros D. Garbis<sup>1</sup>; James Wyche<sup>2</sup>; Zhiyong Han<sup>2</sup>; Panayotis Pantazis<sup>1</sup>; <sup>1</sup>Biomedical Research of the Academy of Athens, Athens, Greece; <sup>2</sup>Oklahoma University Health Sciences Center, Oklahoma City, OK**
- TP 42 **In vitro Metabolism of Abyssinone II, a Potential Anticancer Agent from *Broussonetia papyrifera* (L.); Yan Pang<sup>1</sup>; John M. Pezzuto<sup>2</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, Illinois; <sup>2</sup>Purdue University School of Pharmacy, West Lafayette, Indiana**
- TP 43 **Metabolite Identification of Ac-CHAVC-NH2 in Human Plasma using LC-MS/MS; Qiao Zhan<sup>1</sup>; Mark Bednarcik<sup>2</sup>; Jonathan Green<sup>1</sup>; <sup>1</sup>Research Triangle Institute, International, RTP, NC; <sup>2</sup>Adherex Technologies Inc., Durham, NC**
- TP 44 **The Power of Hyphenated Technologies Combined with Traditional Approaches in Degradation Chemistry Investigation: A Case Study on Vitamin D; Fa Zhang<sup>1</sup>; <sup>1</sup>Johnson & Johnson CPWW, Skillman, NJ**
- TP 45 **Identification of in vitro and in vivo Metabolites of Degarelix, a GnRH (Gonadotropin-Releasing Hormone) Receptor Blocker, by LC-MS; Anders Sonesson<sup>1</sup>; Birgitte Buur Rasmussen<sup>1</sup>; <sup>1</sup>Ferring Pharmaceuticals A/S, Copenhagen, Denmark**

### POSTER SPACE

- |       | METABOLITE PROFILING AND IDENTIFICATION METHODS                                                                                                                                                                                                                                                                                                                                                                     |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| TP 46 | <b>A High Throughput Approach for Metabolite Profiling and Characterization Using a Linear Ion Trap Mass Spectrometer; <u>Min He</u><sup>1</sup>; Alicia Du<sup>1</sup>; Gargi Choudhary<sup>1</sup>; Diane Cho<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA</b>                                                                                                                                          |
| TP 47 | <b>Metabolomics: Using Electrochemistry / MS to Investigate Biological Metabolite Identification; <u>David F. Meyer</u><sup>1</sup>; Michael C. Granger<sup>1</sup>; Qi Zhang<sup>1</sup>; Milind P. Nagale<sup>1</sup>; Ian Acworth<sup>1</sup>; Paul H. Gamache<sup>1</sup>; <sup>1</sup>ESA Biosciences, Chelmsford, MA</b>                                                                                      |
| TP 48 | <b>Identification of in vivo Metabolites: Challenges and Solutions using an LTQ Orbitrap; <u>Young G. Shin</u><sup>1</sup>; Teresa Dong<sup>1</sup>; Alica Du<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Yan Chen<sup>2</sup>; Patrick J. Rudewicz<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Thermo Electron, San Jose, CA</b>                                                        |
| TP 49 | <b>Custom Software to Expedite Qualitative and Quantitative Profiling of Drug Metabolites; <u>Robert Langish</u><sup>1</sup>; Jonathan Josephs<sup>1</sup>; Mary Grubb<sup>1</sup>; Petia Shipkova<sup>1</sup>; Mark Sanders<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, Hopewell, NJ; <sup>2</sup>Bristol-Myers Squibb, Lawrenceville, NJ</b>                                                                   |
| TP 50 | <b>Withdrawn</b>                                                                                                                                                                                                                                                                                                                                                                                                    |
| TP 51 | <b>Accurate Mass Measurements of Product Ions for Metabolite Identification on Unit Mass Resolution Mass Spectrometers; <u>Jianyao Wang</u><sup>1</sup>; Ming Gu<sup>2</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>Wyeth Pharmaceuticals, Collegeville, PA; <sup>2</sup>Cerno Bioscience, Monmouth Junction, NJ</b>                                                                                               |
| TP 52 | <b>The Impact of the "Reversed Energy Ramp" Scan Function on Metabolite Identification at or Below 1uM on a Triple Quadrupole; <u>Louis Maljers</u><sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA</b>                                                                                                                                                                                                      |
| TP 53 | <b>Semiquantitation of Diclofenac Metabolites using a Triversa Nanospray Source Interface and Comparison with a Conventional Electrospray Interface; <u>Mary F. Grubb</u><sup>1</sup>; Jonathan Josephs<sup>1</sup>; Gary A. Schultz<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, Pennington, NJ; <sup>2</sup>Advion BioSystems, Inc., Ithaca, NY</b>                                                             |
| TP 54 | <b>Binding Affinity of the Immobilized &amp;beta;-Cyclodextrin with Urinary Androgens and Estrogens; Ju-Yeon Moon<sup>1</sup>; <u>Man Ho Choi</u><sup>1</sup>; <sup>1</sup>Korea Institute of Science and Technology, Seoul, Korea</b>                                                                                                                                                                              |
| TP 55 | <b>Withdrawn</b>                                                                                                                                                                                                                                                                                                                                                                                                    |
| TP 56 | <b>Online Class-based HPLC Separation/Time-of-flight Mass Spectrometry for Profiling of Structural Lipids and Oxylipins of <i>Arabidopsis thaliana</i>; <u>Michael C. Stagliano</u><sup>1</sup>; A. Daniel Jones<sup>1</sup>; Heidi Appel<sup>2</sup>; Jack C. Schultz<sup>2</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>The Pennsylvania State University, University Park, PA</b> |
| TP 57 | <b>Detection and Enhanced Characterization of Low-Level Metabolites by Peak Parking And LC-MSn; <u>Miao Zhuang</u><sup>1</sup>; Prakash Chandra<sup>1</sup>; <sup>1</sup>Pfizer Global Reserach &amp; Development, Groton, CT</b>                                                                                                                                                                                   |
| TP 58 | <b>Identification of Metabolites from Phosphate Based HPLC Systems using 96 Well Fraction Collection, Off Line Counting and LC/MSn; <u>Richard Clayton</u><sup>1</sup>; Brian Morrison<sup>1</sup>; <sup>1</sup>Covance Laboratories, Harrogate, United Kingdom</b>                                                                                                                                                 |
| TP 59 | <b>Biosynthesis, Isolation and Stability of Retigabine N-Glucuronide by HPLC and LC-MS/MS; <u>Hong Kim</u><sup>1</sup>; Nanqun Zhu<sup>1</sup>; Chin-Chung Lin<sup>1</sup>; Li-Tain Yeh<sup>1</sup>; <sup>1</sup>Valeant Pharmaceutical, Costa Mesa, CA</b>                                                                                                                                                         |
| TP 60 | <b>Automated Data Dependent<sup>TM</sup> Precursor Ion MS<sup>3</sup> for Identification of Biotransformations using an Ion Trap Mass Spectrometer; <u>Marta Kozak</u><sup>1</sup>; Gargi Choudhary<sup>1</sup>; Diane Cho<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA</b>                                                                                                                               |

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#### METABOLISM XENOBIOTICS

- TP 61 **A Novel Approach to Metabolite Detection and Identification by the Use of UPLC-Hybrid Quadrupole-Travelling Wave-IMS-oaToF**; Jose Castro-Perez<sup>1</sup>; John Shockcor<sup>1</sup>; Kevin Giles<sup>2</sup>; Steve Pringle<sup>2</sup>; Robert Bateman<sup>2</sup>; Alan Millar<sup>2</sup>; Iain Beattie<sup>3</sup>; Jason Wildgoose<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters MS Technology, Manchester, UK; <sup>3</sup>AstraZeneca, Loughborough, UK
- TP 62 **Complete Characterization of ML3403 Metabolites from Liver Microsomes using ESI-Qq-TOF-MS and LC-SPE-cryo NMR/MS**; Holger Scheible<sup>1</sup>; Stefan Laufer<sup>1</sup>; Wolfgang Albrecht<sup>2</sup>; Gabriela Zurek<sup>3</sup>; Manfred Spraul<sup>4</sup>; Markus Godejohann<sup>4</sup>; Bernd Kammerer<sup>1</sup>; <sup>1</sup>University of Tübingen, Tuebingen, Germany; <sup>2</sup>Merckle GmbH, Ulm, Germany; <sup>3</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>4</sup>Bruker BioSpin GmbH, Rheinstetten, Germany
- TP 63 **Automated on-Line Column-Switching HPLC-MS/MS Method for the Determination of Five Parabens in Urine**; Xiaoyun Ye<sup>1</sup>; Amber Bishop<sup>1</sup>; Larry L. Needham<sup>1</sup>; Antonia M. Calafat<sup>1</sup>; <sup>1</sup>Centers for disease control and prevention, Atlanta, GA
- TP 64 **Systematic Approaches in Phytochemical Determination using Mass Spectrometry**; Qingguo Tian<sup>1</sup>; Mark Failla<sup>1</sup>; Gary Stoner<sup>1</sup>; Steven Schwartz<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- TP 65 **Structure Elucidation of M15, a Motexafin Gadolinium (MGd) Metabolite**; Purvi Jejurkar<sup>1</sup>; Wenchen Luo<sup>1</sup>; Alice Lin<sup>1</sup>; Chitra Mani<sup>1</sup>; Garry Boswell<sup>1</sup>; Dale Miles<sup>1</sup>; <sup>1</sup>Pharmacyclics, Inc., Sunnyvale, CA
- TP 66 **Simultaneous Measurement of Multiple Hemoglobin Adducts of Environmental Chemicals by HPLC/MS/MS**; Maria P. Ospina<sup>1</sup>; Enada Archibold<sup>1</sup>; Tunde Meyers<sup>1</sup>; Antoinette Smith<sup>1</sup>; Leigha Ingham<sup>1</sup>; Gary L. Myers<sup>1</sup>; Hubert Vesper<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA
- TP 67 **Etoposide Glucuronidation is Specifically Catalyzed by Human UGT1A1: Structural Characterization of Glucuronide Conjugates and Estimation of Enzyme Kinetics by LC-ESI-MS**; Zhiming Wen<sup>1</sup>; Melanie N. Tallman<sup>1</sup>; Shazia Y. Ali<sup>1</sup>; Philip C. Smith<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 68 **Identification of Plant Metabolites Using Accurate Mass, MS/MS, and MSn Data**; Sara J. Linder<sup>1</sup>; Jeffrey R. Gilbert<sup>1</sup>; Roobina I. Baloch<sup>1</sup>; Jesse L. Balcer<sup>1</sup>; Carla N. Yerkes<sup>1</sup>; Gerrit J. Deboer<sup>1</sup>; <sup>1</sup>Dow AgroSciences, Indianapolis, IN
- TP 69 **Development of Automated Software for Creation of Metabolite LC/MS Methods for a QQQ/LIT Hybrid Mass Spectrometer**; Claire J Bramwell-German<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Elliott Jones<sup>1</sup>; Robert Campbell<sup>3</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Sciex, Concord, ON, Canada; <sup>3</sup>Theravance, South San Francisco, CA
- TP 70 **The Use of Liquid Chromatography Tandem Mass Spectrometry to Identify Drug Metabolites Produced by *Cunninghamella elegans***; Annica Tevell<sup>1</sup>; Marina Lushnikova<sup>2</sup>; Ulf Bondesson<sup>3</sup>; Mikael Hedeland<sup>3</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>HFL, Fordham, United Kingdom; <sup>3</sup>National Veterinary Institute, Uppsala, Sweden
- TP 71 **On-Line Solid-Phase ESI-MS/MS Analyses Revealed the Association between Glutathione S-Transferase Genetic Polymorphism and the Urinary Metabolic Profile of Benzene Exposure**; Lung-Cheng Lin<sup>1</sup>; Yin-Mei Chiung<sup>2</sup>; Wan-Jou Cheng<sup>1</sup>; Tung-Sheng Shih<sup>2</sup>; Pao-

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- Chi Liao<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan; <sup>2</sup>Institute of Occupational Safety and Health, Taipei, Taiwan
- TP 72 **Optimization of a Linear Ion Trap Mass Spectrometer for Structural Elucidation of Metabolites**; Jim M Schmidt<sup>1</sup>; Aixia Sun<sup>1</sup>; Charles P Cruz<sup>1</sup>; Ling Li<sup>1</sup>; Liam B. Moran<sup>1</sup>; <sup>1</sup>Lexicon Genetics, The Woodlands, TX
- TP 73 **Increased Sensitivity of the Altrenogest Glucuronide in Liquid Chromatography Tandem Mass Spectrometry by Chemical Derivatization**; Matilda Lampinen Salomonsson<sup>1</sup>; Elin Beckman<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 74 **In Vitro Metabolism of Vorinostat (Suberoylanilide Hydroxamic Acid), a Novel Anticancer Agent**; Natasa D. Pajkovic<sup>1</sup>; Kenneth A. Koeplinger<sup>1</sup>; Maribeth P. Baker<sup>1</sup>; Eric D. Soli<sup>2</sup>; Scott E. Fauty<sup>1</sup>; Punam Sandhu<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA; <sup>2</sup>Merck Research Laboratories, Rahway, NJ
- TP 75 **Collision-Induced Dissociation of Metal Complexes to Identify Isomeric Flavonoid Glucuronide Metabolites**; Barry D. Davis<sup>1</sup>; Paul W. Needs<sup>2</sup>; Paul A. Kroon<sup>2</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>The University of Texas at Austin, Austin, TX; <sup>2</sup>The Institute of Food Research, Norwich, United Kingdom

#### QUANTITATIVE ANALYSIS OF DRUGS AND METABOLITES II

- TP 76 **A Highly Sensitive and Specific LC/MS/MS Method for Quantitation of Methotrexate and Its 7-Hydroxy Metabolite in Human Plasma**; Yong-Xi Li<sup>1</sup>; Dawei Zhou<sup>1</sup>; <sup>1</sup>XenoBiotic Laboratories, Inc., Plainsboro, NJ
- TP 77 **Study of Atmospheric Pressure Chemical Ionization and Electrospray Ionization Mass Spectrometric Quantitative Analysis for Lopinavir and Ritonavir**; Jun Zhang<sup>1</sup>; Qin Ji<sup>1</sup>; Tawakol El-Shourbagy<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
- TP 78 **LC/MS/MS Determination of Fluoxetine and Norfluoxetine in Equine Biological Fluids**; Jhoana A. Mendoza<sup>1</sup>; Keith D. Zientek<sup>2</sup>; Patrick T. Colahan<sup>3</sup>; Cynthia A. Cole<sup>2</sup>; John R. Eyster<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>UF, College of Vet. Med., Racing Laboratory, Gainesville, FL; <sup>3</sup>UF, College of Veterinary Medicine, Gainesville, FL
- TP 79 **Simultaneous Determination of Ribavirin and Ribavirin Base in Monkey Plasma Using Liquid Chromatography with Tandem Mass Spectrometry**; Wenkui Li<sup>1</sup>; Suyi Luo<sup>1</sup>; Shaoyong Li<sup>1</sup>; Lawrence Athill<sup>1</sup>; Amy Wu<sup>1</sup>; Tapan Ray<sup>1</sup>; Wei Zhou<sup>1</sup>; June Ke<sup>1</sup>; Francis Tse<sup>1</sup>; <sup>1</sup>Novartis Pharmaceuticals Corporation, East Hanover, NJ
- TP 80 **Quantitation of Norelgestromin in Human Plasma via HPLC with MS/MS Detection**; Moucun Yuan<sup>1</sup>; Jingdian Chi<sup>1</sup>; Rand Jenkins<sup>1</sup>; Bruce Hidy<sup>1</sup>; <sup>1</sup>PPD, Richmond, VA
- TP 81 **Solving the Plasma Mycophenolic Acid Analytical Challenges: A Validated Liquid Chromatography/Tandem Mass Spectrometry Quantitation Method**; Ling Zhu<sup>1</sup>; Andrew Cooper<sup>1</sup>; J.J. Thiessen<sup>2</sup>; <sup>1</sup>Allied Research International, Mississauga, Canada; <sup>2</sup>School of Pharmacy, University of Waterloo, Waterloo, Canada
- TP 82 **A Novel APCI LC-MS/MS Method for the Determination of Finasteride in Human Plasma**; Michael Deng<sup>1</sup>; Heather Wan<sup>1</sup>; Andrew Cooper<sup>1</sup>; J.J. Thiessen<sup>2</sup>; <sup>1</sup>Allied Research International, Mississauga,

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- Canada; <sup>2</sup>School of Pharmacy, University of Waterloo, Waterloo, Canada
- TP 83 **High Performance Liquid Chromatography-Tandem Mass Spectrometric Determination of N-methyl-4-isoleucine-cyclosporin (NIM811) in Human Whole Blood;** Suyi Luo<sup>1</sup>; Lawrence Athill<sup>1</sup>; Wenkui Li<sup>1</sup>; Michael Hayes<sup>1</sup>; Handan He<sup>1</sup>; Francis Tse<sup>1</sup>; <sup>1</sup>Novartis Pharmaceuticals Corporation, East Hanover, NJ
- TP 84 **Withdrawn**
- TP 85 **Determination of Chlorpromazine in Rat Plasma and Brain Tissue by LC MS/MS;** Guodong Zhang<sup>1</sup>; Alvin V. Terry<sup>1</sup>; Michael G. Bartlett<sup>1</sup>; <sup>1</sup>Department of PBS, School of Pharmacy, UGA, Athens, GA
- TP 86 **Stability Studies of Vorinostat and Its Two Metabolites in Human Plasma, Serum and Urine;** Lihong Du<sup>1</sup>; Donald Musson<sup>1</sup>; Amy Wang<sup>2</sup>; <sup>1</sup>Merck Research Lab, west point, PA; <sup>2</sup>GlaxoSmithKline Pharmaceutical, King of Prussia, PA
- TP 87 **Single Mass Spectrometry Method for the Determination of Nevirapine in Human EDTA K<sub>2</sub> Plasma using Automated SPE Extraction;** Jean Couture<sup>1</sup>; Nadia Smith<sup>1</sup>; Marie-Claude Th  berge<sup>1</sup>; Fran  ois Vall  e<sup>1</sup>; <sup>1</sup>SFBC Anapharm, Ste-Foy, QC, Canada
- TP 88 **Quantitative Analysis of Valacyclovir Following Automated Protein Precipitation;** Matthew Amundson<sup>1</sup>; Melissa Meyer<sup>1</sup>; Darren Hoffman<sup>1</sup>; Laura Baum<sup>1</sup>; Andrew Osenga<sup>1</sup>; Dan Aufman<sup>1</sup>; Ardeshir Khadang<sup>1</sup>; <sup>1</sup>PRACS Institute, Fargo, ND
- TP 89 **Advantages of using Tetrahydrofuran-Water Mobile Phases in Quantitative Determination of Cyclosporin A in Monkey Plasma;** Yinghe Li<sup>1</sup>; Austin C. Li<sup>1</sup>; Wilson Z. Shou<sup>1</sup>; Xiangyu Jiang<sup>1</sup>; <sup>1</sup>Covance Laboratories, Inc., Madison, WI
- TP 90 **Simultaneous Quantification of Tenofovir Diphosphate and Emtricitabine Triphosphate in Human and Macaque Primary Lymphocytes;** David C Delinsky<sup>1</sup>; Brenda I Hernandez-Santiago<sup>1</sup>; Raymond F Schinazi<sup>1</sup>; <sup>1</sup>Emory University / VA Medical Center, Decatur, GA
- TP 91 **Overcome Selectivity Issues in Developing a Rugged LC-MS/MS Method for Dextromethorphan and Dextrorphan in Human Plasma;** Ernest YK Wong<sup>1</sup>; Dezhong Liu<sup>1</sup>; Anita Towers<sup>1</sup>; Nicola Hughes<sup>1</sup>; <sup>1</sup>Biovail Contract Research, Toronto, Ontario, Canada
- TP 92 **Determination of Stevioside in Mouse Plasma by Use of Automated 96-Well SPE and LC/MS/MS;** Seung Kwon Yang<sup>1</sup>; Moon-Sun Jang<sup>1</sup>; Kyung Ryul Lee<sup>2</sup>; Hee Joo Lee<sup>1</sup>; Seungwoo Kang<sup>1</sup>; <sup>1</sup>BioCore Co., Ltd, Seoul, Korea; <sup>2</sup>Seoul Medical Science Institute, Seoul, Korea
- TP 93 **High-Throughput LC-MS/MS Analysis of Sirolimus in Whole Blood by Automated Protein Precipitation and Solid-Phase Extraction;** Aimin Tan<sup>1</sup>; Peter Hang<sup>1</sup>; Rajah Uthaya<sup>1</sup>; Jean Couture<sup>2</sup>; Saleh Hussain<sup>1</sup>; Francois Vallee<sup>2</sup>; <sup>1</sup>SFBC Anapharm (Richmond Hill), Richmond Hill, ON, Canada; <sup>2</sup>SFBC Anapharm (Quebec), Ste-Foy, QC, Canada
- TP 94 **Determination of an Immunosuppressant Mycophenolic Acid and Its Prodrug Mycophenolate Mofetil in Human Plasma by A High Throughput LC/MS-MS Platform;** V Srivatsan<sup>1</sup>; A K Dasgupta<sup>1</sup>; Prashant Kale<sup>1</sup>; Sandeep Sharma<sup>1</sup>; Gunjan Soni<sup>1</sup>; <sup>1</sup>Lambda Therapeutic Research Ltd., Ahmedabad, INDIA
- TP 95 **A Novel Approach to Quantify Unbound Cisplatin, Carboplatin and Oxaliplatin in Human Plasma Ultrafiltrate by Measuring Platinum-DDTC Complex Using LC/MS/MS;** Min Meng<sup>1</sup>; Ryan Kuntz<sup>1</sup>; Al

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- Fontanet<sup>1</sup>; Patrick K. Bennett<sup>1</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT
- TP 96 **Withdrawn**
- TP 97 **An Unusual High Percentage of Aqueous Mobile Phase to Achieve Maximum Sensitivity in LC-MS Bioanalysis of Penciclovir;** Guy Th  riault<sup>1</sup>; Vincent Moreau<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval (Montreal), Canada
- TP 98 **Exploring Different Ionization Techniques in LC-MS/MS to Optimize the Sensitivity of Tacrolimus;** Marie-Pierre Taillon<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval (Montreal), Canada
- QUANTITATIVE ANALYSIS OF DRUGS: METHOD DEVELOPMENT II**
- TP 99 **A General Strategy Using Mass Spectrometry as a Powerful Tool to Handle Metabolite Issues from the Drug Biotransformation;** V  ronique Gauvreau<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval (Montreal), Canada
- TP 100 **Significantly Improving Quantitative LC-MSMS Analysis for Large Number of Analytes (>500) with Scheduled-MRM;** Nic Bloomfield<sup>1</sup>; J.C. Yves Le Blanc<sup>1</sup>; Byron Kieser<sup>1</sup>; Andre Schreiber<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- TP 101 **Accelerator Mass Spectrometry (AMS) in Early Drug Development: An Ultrasensitive ADME/PK Study of a Diabetes Compound in Mice;** Ali Arjomand<sup>1</sup>; Ugo Zoppi<sup>1</sup>; Michael Chansler<sup>1</sup>; <sup>1</sup>Accium BioSciences, Seattle, WA
- TP 102 **The Application of High Resolution MRM in Routine Quantitative Bioanalysis;** Mike J Redrup<sup>1</sup>; Caroline Clegg<sup>1</sup>; Derek Lewis<sup>1</sup>; Kun N Cheng<sup>1</sup>; <sup>1</sup>BioDynamics Research Ltd, Rushden, Northants, United Kingdom
- TP 103 **Development of a Bioanalytical LC/MS/MS Method for the Selective Quantitation of Small Organic Acids In Plasma;** Michael G. Ma<sup>1</sup>; Salma Sarwary<sup>1</sup>; Kyung Kwon<sup>1</sup>; Michael B. Martin<sup>1</sup>; <sup>1</sup>Arena Pharmaceuticals Inc., San Diego, CA
- TP 104 **Ultra Low Limits of Quantitation Utilizing LC-MS/MS with a Novel High Throughput Autosampler Technology;** Mauro Aiello<sup>1</sup>; Thomas Londo<sup>2</sup>; Thomas Covey<sup>1</sup>; Peter Kovarik<sup>1</sup>; Byron Kieser<sup>3</sup>; <sup>1</sup>MDS Sciex, Concord, Canada; <sup>2</sup>Parker Life Sciences, Hollis, NH; <sup>3</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- TP 105 **Automated Column/Mobile Phase Screening System to Achieve Optimum Chromatographic Separation and Sensitivity during LC-MS/MS Bioanalytical Method Development;** Yuan-Qing Xia<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Mohammed Jemal<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ
- TP 106 **Validation of an LC-MS/MS Method for a Schering-Plough Development Compound using the Symbiosis Pharma with Direct Addition of Internal Standard;** James E. Schiller<sup>1</sup>; Hui Lin<sup>1</sup>; Roger N. Hayes, Ph.D.<sup>1</sup>; Dirk Hiemstra<sup>2</sup>; Steven Eendhuizen<sup>2</sup>; Valerie Cloutier<sup>2</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, NJ; <sup>2</sup>Spark Holland, Plainsboro, NJ
- TP 107 **Elimination of Carryover in Determination of a Cyclic Hexapeptide using LC/MS;** Michael H. Wang<sup>1</sup>; Kimberly Algayer<sup>1</sup>; Kimberly Manser<sup>1</sup>; Danielle Euler<sup>1</sup>; Henry Wu<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA
- TP 108 **Comparison of UPLC, TFC, and Conventional HPLC for Bioanalytical Quantitation of Preclinical Drug Candidates in the Presence of Interfering Metabolites;**

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- Marc Browning<sup>1</sup>; Michael Donegan<sup>1</sup>; Daniel Morgan<sup>1</sup>;  
<sup>1</sup>Bristol-Myers Squibb, Wallingford, CT
- TP 109 **Quantitative Analysis of HIV-1 Protease Inhibitors in Biological Matrices by MALDI-TOF Mass Spectrometry**; Jeroen J.A. van Kampen<sup>1</sup>; Peter C. Burgers<sup>1</sup>; Ronald de Groot<sup>2</sup>; Theo M. Luider<sup>1</sup>; <sup>1</sup>Erasmus Medical Center, Rotterdam, The Netherlands; <sup>2</sup>UMC st. Radboud, Nijmegen, The Netherlands
- TP 110 **Quantitative Determination of Hydrophilic Ionic Compounds Using Gradient Chromatofocusing-Cation-Exchange LC-ESI-MS/MS**; Jianhua Tang<sup>1</sup>; Lian Shan<sup>2</sup>; Xiang Zhou<sup>1</sup>; Anderson J. David<sup>1</sup>; <sup>1</sup>Cleveland State University, Cleveland, OH; <sup>2</sup>Frantz BioMarkers, Cleveland, OH
- TP 111 **Speed vs. Sensitivity? The Influence of Peakwidth and Flow Rate on Sensitivity in UHPLC-MS for Bioanalytical Quantitation**; Gunter Boehm<sup>1</sup>; Michel Wagner<sup>1</sup>; Paul-Gerhard Lassahn<sup>2</sup>; <sup>1</sup>Flux Instruments AG, Basel, Switzerland; <sup>2</sup>Spectronex AG, Basel, Switzerland
- TP 112 **Selected Techniques for Increasing Sensitivity in Quantitative LC-MS/MS**; Mike Larson<sup>1</sup>; Mary Pelzer<sup>1</sup>; Tom Addison<sup>1</sup>; Xiangyu Jiang<sup>1</sup>; <sup>1</sup>Covance Laboratories, Inc., Madison, WI
- TP 113 **Better Understanding of MALDI-MS/MS for Quantitative Analysis**; Emily D Adarayan<sup>1</sup>; <sup>1</sup>Merck Research Labs, West Point, PA
- TP 114 **Automated and Parameter-Free Peak Integration for LC/MS/MS Quantitation**; Ming Gu<sup>1</sup>; Dawei Zhou<sup>2</sup>; Zheming Gu<sup>2</sup>; Yongdong Wang<sup>1</sup>; <sup>1</sup>Cerno Bioscience, Monmouth Junction, NJ; <sup>2</sup>XenoBiotic Laboratories, Plainsboro, NJ
- TP 115 **Optimized High Resolution SRM Quantitative Analysis using a Calibration Correction Method on a Triple Quadrupole System**; Ya-Mei Liu<sup>1</sup>; Kristi Akervik<sup>1</sup>; Louis Maljers<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA
- TP 116 **Performance of a Novel Parameter-Less Integrator with Built-In Peak Quality Validation for Reliable Unsupervised Integration of Triple Quadrupole MRM Data**; Lee H. Altmayer<sup>1</sup>; Frank E. Kuhlmann<sup>1</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, CA
- TP 117 **Method Development of Minimizing Carry Over in LC/MS/MS - Novel Cleaning Technique and Device**; Jun Watanabe<sup>1</sup>; Hiroshi Hike<sup>2</sup>; Yoshifumi Kogure<sup>1</sup>; Hansjoerg Cueni<sup>3</sup>; Yasuhiko Bando<sup>2</sup>; <sup>1</sup>TAKARA BIO INC., Shiga, Japan; <sup>2</sup>AMR, Inc., Tokyo, Japan; <sup>3</sup>CTC Analytics AG, Zwingen, Switzerland
- TP 118 **Chemometric Optimization of LC-MS-MS Assay for Quantification of Candidate Drug and Three Metabolites in Plasma**; Margret Thorsteinsdottir<sup>1</sup>; Baldur B Sigurdsson<sup>1</sup>; Gisli Bragason<sup>1</sup>; Thorkell Andresson<sup>1</sup>; <sup>1</sup>deCODE Genetics, Reykjavik, Iceland
- TP 119 **Quantitation of Nipride (Sodium Nitroprusside Dihydrate) in Human Plasma by ICP-MS**; Jing Ke<sup>1</sup>; Qian Liu<sup>1</sup>; Allan Xu<sup>1</sup>; <sup>1</sup>SFBC Analytical Laboratories, Inc., North Wales, PA
- TP 120 **MALDI TOF/TOF MS and MS/MS Analysis of Fluorescently Tagged Peptides with the Fluorogenic Agent 3-(2-furoyl)-quinoline-2-carboxaldehyde**; David A. Michels<sup>1</sup>; <sup>1</sup>Amgen Inc, Seattle, WA
- TP 121 **Guidelines for Non-Linear Regression in LC-MS Analysis**; Stephanie F. Baldrey<sup>1</sup>; John L. Burrows<sup>1</sup>; Tony A. Bates<sup>1</sup>; Graeme T. Smith<sup>1</sup>; Ian Flack<sup>1</sup>; Timothy P. Sangster<sup>2</sup>; <sup>1</sup>Huntingdon Life Sciences, Alconbury,

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- Huntingdon, United Kingdom; <sup>2</sup>Huntingdon Life sciences, Princeton, New Jersey*
- TP 122 **Experimental Factors Affecting Accuracy and Precision in Quantitative MS Analyses**; Michael S. Alexander<sup>1</sup>; <sup>1</sup>BASi Northwest Laboratory, McMinnville, Oregon

### REACTION INTERMEDIATES

- TP 123 **Development and Application of Mass Spectrometric Methods for the Investigation of Organocatalytic Reactions**; Wolfgang Schrader<sup>1</sup>; Peni Handayani<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Kohlenforschung, Mülheim / Ruhr, Germany
- TP 124 **Novel Carbon-Nitrogen (CN) ortho-Benzynes**; Michael J. Yurkovich<sup>1</sup>; Karinna Campbell<sup>1</sup>; John J. Nash<sup>1</sup>; Hilkka I. Kenttamaa<sup>1</sup>; <sup>1</sup>Purdue University, IN
- TP 125 **A d,d,d-Triradical Cation: The 2,4,6-Tridehydropyridinium Ion**; Nelson R. Vinuesa<sup>1</sup>; Bartłomiej J. Jankiewicz<sup>1</sup>; Anthony Adeuya<sup>1</sup>; Michael J. Yurkovich<sup>1</sup>; John J. Nash<sup>1</sup>; Hilkka I. Kenttamaa<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, Indiana
- TP 126 **Characterization of an Exception to the "Even Electron Rule" in Negative Ion Electrospray Mass Spectrometry**; Yang Cai<sup>1</sup>; Zhenzhen Mo<sup>1</sup>; Bruce C. Gibb<sup>2</sup>; Bing Guan<sup>2</sup>; Richard B. Cole<sup>2</sup>; <sup>1</sup>The Research Institute for Children, New Orleans, LA; <sup>2</sup>University of New Orleans, New Orleans, LA
- TP 127 **FT-ICR Studies on the Reactivity of Aromatic Biradicals toward Amino Acid**; George O. Pates<sup>1</sup>; Hilkka Kenttamaa<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, Indiana
- TP 128 **A Neutralization-Reionization Mass Spectrometric and Computational Study of Arginine Amide Radicals**; Xiaohong Chen<sup>1</sup>; František Tureček<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, Washington
- TP 129 **Mass Spectrometric Elucidation of The Free Radical Nitric Oxide-Mediated Ras Guanine Nucleotide Dissociation Mechanism using Mass Spectrometric Analyses**; Jongyun Heo<sup>1</sup>; Viorel Mocanu<sup>1</sup>; Kirk C. Prutzman<sup>1</sup>; Sharon L. Campbell<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- TP 130 **Singlet-Triplet Splittings of Substituted Chlorinated Phenyl Nitrene: Negative Ion Photoelectron Spectroscopy**; Maria C Da Fonte<sup>1</sup>; Paul G Wenthold<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN

### ION STRUCTURES AND ENERGETICS

- TP 131 **Low-Energy Resonant Reactions of Free Electrons and Glycine Oligomers**; Yury V Vasil'ev<sup>1</sup>; Benjamin J Figard<sup>1</sup>; Jeffrey Morré<sup>1</sup>; Valery G Voinov<sup>1</sup>; Douglas F Barofsky<sup>1</sup>; Max L Deinzer<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- TP 132 **Structure Determination by Surface-Enhanced Raman Scattering of Subzeptomole Quantities of Gas-Phase Ions after Soft Landing on Dry Metal Surfaces**; Michael Voln&vacute;<sup>1</sup>; Atanu Sengupta<sup>1</sup>; Christopher B. Wilson<sup>1</sup>; E. James Davis<sup>1</sup>; František Tureček<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 133 **Ab Initio Studies of Nitramine Radical Anion Fragmentation**; M. Paul Chiarelli<sup>1</sup>; Jan Florian<sup>1</sup>; Denise K. MacMillan<sup>2</sup>; Lan Gao<sup>1</sup>; Vladimir Zhukhovskyy<sup>1</sup>; <sup>1</sup>Loyola University, Chicago, IL; <sup>2</sup>USACE, Omaha, NE
- TP 134 **Collisionally-Induced Dissociation of Famotidine, Folic Acid and Azithromycin: Mechanisms of Ion Formation Using Hydrogen/Deuterium Exchange and**

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- Electrospray Ionization Mass Spectrometry;** Kevin Colizza<sup>1</sup>; Patrick Jeanville<sup>2</sup>; Amin, M. Kamel<sup>1</sup>; <sup>1</sup>Pfizer Global Research and Development, Groton, CT; <sup>2</sup>Thermo Electron Corporation, West Palm Beach, FL
- TP 135 **Studies on Facile McLafferty-type Rearrangements Shown by Certain Substituted Carboxylate Anions;** J. Stuart Grossert<sup>1</sup>; Matthew C. Cook<sup>1</sup>; Robert L. White<sup>1</sup>; <sup>1</sup>Dalhousie University, Halifax, NS, Canada
- TP 136 **Density Functional Theory Examinations of the Fragmentation Reactions of Amino-Acid Radical-Cations Containing Aromatic Side-Chains (Phenylalanine<sup>&bull;+</sup>, Tyrosine<sup>&bull;+</sup>, and Tryptophan<sup>&bull;+</sup>);** Chi-Kit Siu<sup>1</sup>; Yuyong Ke<sup>1</sup>; Junfang Zhao<sup>1</sup>; Alan C. Hopkinson<sup>1</sup>; K. W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- TP 137 **Sodium Ion Affinities of Commonly Used MALDI Matrices Determined by Guided Ion Beam Tandem Mass Spectrometry and Theoretical Studies;** S.D.M. Chinthaka<sup>1</sup>; M.T. Rodgers<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI
- TP 138 **TPEICO Investigation of the Acetone Radical;** Emma E. Rennie<sup>1</sup>; Anne-Marie Boulanger<sup>1</sup>; Paul M. Mayer<sup>1</sup>; David M. P. Holland<sup>2</sup>; David A. Shaw<sup>2</sup>; Louise Cooper<sup>3</sup>; Christopher A. F. Johnson<sup>3</sup>; John E. Parker<sup>3</sup>; <sup>1</sup>University of Ottawa, Ottawa, Canada; <sup>2</sup>Daresbury Laboratory, Daresbury, Warrington, England; <sup>3</sup>Heriot-Watt University, Edinburgh, Scotland
- TP 139 **Relative Ca<sup>2+</sup> Affinities of Amino Acids Determined by Using the Kinetic Method;** Ming-Wei Yang<sup>1</sup>; Yen-Peng Ho<sup>1</sup>; <sup>1</sup>National Dong Hwa University, Hualien, Taiwan, R.O.C.
- TP 140 **Generation and Fragmentation Mechanisms of Two Isomeric Histidine Radical Cations in the Gas Phase;** Junfang Zhao<sup>1</sup>; Yuyong Ke<sup>1</sup>; Udo H. Verkerk<sup>1</sup>; Alan C. Hopkinson<sup>1</sup>; K. W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- TP 141 **Theoretical and Experimental Investigation of the Energetics of Cis-Trans Proline Isomerization in Peptide Models;** Jennifer L. Poutsma<sup>1</sup>; Olivia E. Schroeder<sup>2</sup>; Emily Carper<sup>2</sup>; Joshua J. Wind<sup>2</sup>; Felicia A. Etzkorn<sup>3</sup>; John C. Poutsma<sup>2</sup>; <sup>1</sup>Old Dominion University, Norfolk, VA; <sup>2</sup>College of William and Mary, Williamsburg, VA; <sup>3</sup>Virginia Tech, Blacksburg, VA
- TP 142 **Thermochemical Studies of o-, m- and p-quinomethane;** Silvi A. Chacko<sup>1</sup>; Paul G. Wenthold<sup>1</sup>; <sup>1</sup>Department of Chemistry, Purdue University, West Lafayette, IN
- TP 143 **Anion Photoelectron Spectroscopy of Collision Cooling Negative Ions;** Xue-Bin Wang<sup>1</sup>; Hin-Koon Woo<sup>1</sup>; Lai-Sheng Wang<sup>1</sup>; <sup>1</sup>Washington State University, Richland, WA
- TP 144 **Uranyl Nitrate Interactions with Formamide and Acetamide Ligands Studied by Electrospray Ionization Ion Trap Mass Spectrometry;** Garold L. Gresham<sup>1</sup>; Tate R. Crain<sup>1</sup>; Amy Custer<sup>1</sup>; J. Sigrid Barklund<sup>1</sup>; Michael J. Van Stipdonk<sup>2</sup>; Gary S. Groenewold<sup>1</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>2</sup>Wichita State University, Wichita, KS
- TP 145 **Gas Phase Acidities of the 20 Protein Amino Acids from the Extended Kinetic Method;** Kathryn E. Colyer<sup>1</sup>; Christopher M. Jones<sup>1</sup>; Rachel A. Metz<sup>1</sup>; Anna K. Pawlow<sup>1</sup>; Emily D. Wischow<sup>1</sup>; John C. Poutsma<sup>1</sup>; <sup>1</sup>College of William and Mary, Williamsburg, VA
- TP 146 **Collision-Induced Dissociation of Silver(I)Amide Complexes;** Vladimir A. Romanov<sup>1</sup>; Junfang Zhao<sup>1</sup>;

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- Houssain El Aribi<sup>2</sup>; Alan C. Hopkinson<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada; <sup>2</sup>MDS SCIEX, Concord, Canada
- TP 147 **Electron Affinities of Polynuclear Aromatic Hydrocarbons and Chlorinated Hydrocarbons and Their Analysis by Negative Ion Chemical Ionization Mass Spectrometry;** Leon D. Betowski<sup>1</sup>; Mark A. Enlow<sup>2</sup>; Donald H. Aue<sup>3</sup>; <sup>1</sup>U.S. Environmental Protection Agency, Las Vegas, NV; <sup>2</sup>Applied Research Associates, Inc, Tyndall AFB, FL; <sup>3</sup>University of California at Santa Barbara, Santa Barbara, CA
- TP 148 **Structure and Reactivity of Organolithium Compounds;** Zhixin Tian<sup>1</sup>; Steven R. Kass<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN
- TP 149 **Influence of Solvents (Water, Methanol, Acetone, and Acetonitrile) on the Binding of Copper Ions to Imidazole and Pyridine;** Nalaka S. Rannulu<sup>1</sup>; M.T. Rodgers<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI
- TP 150 **Correlation of Bond Dissociation Energies in Ten-Electron Hypervalent Systems to Atomic Properties;** Changtong Hao<sup>1</sup>; Lee S. Sunderlin<sup>1</sup>; <sup>1</sup>Northern Illinois University, DeKalb, IL
- TP 151 **Experimental and Computational Study of the Formation of Boron Cage Cluster Ions from BBr<sub>3</sub> in a Pulsed Discharge Ion Source;** David A Hales<sup>1</sup>; Jay S VanDenbos<sup>1</sup>; Shawna M Riggsby<sup>1</sup>; Catrin M Mills<sup>1</sup>; R Bret Yarbrow<sup>1</sup>; Tony P Tauer<sup>1</sup>; <sup>1</sup>Hendrix College, Conway, AR
- TP 152 **Examination of the Gas-Phase Ion Structure of Cationized Arginine (Na<sup>+</sup>, K<sup>+</sup>) by Infrared Multi Photon Dissociation Spectroscopy and Computational Modelling;** Mathias Schäfer<sup>1</sup>; Nick C. Polfer<sup>2</sup>; Jos Oomens<sup>2</sup>; Dirk Blunk<sup>1</sup>; Rebecca A. Jockusch<sup>3</sup>; <sup>1</sup>Institute for Organic Chemistry University Cologne, Cologne, Germany; <sup>2</sup>FOM Institute for Plasmaphysics Rijnhuizen, Nieuwegein, the Netherlands; <sup>3</sup>Department of Chemistry, University of Toronto, Toronto, Canada
- TP 153 **O-Alkylated Nitroalkane Cations in the Gas Phase: Selective Preparation of C<sub>3</sub>H<sub>8</sub>NO<sub>2</sub><sup>+</sup> Isomers and Elucidation of their Unimolecular Chemistry;** Miroslav Polášek<sup>1</sup>; Jiri Kubišta<sup>1</sup>; <sup>1</sup>J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
- TP 154 **Structural Investigation of an Unexpected Impurity Originating from a Polyester Filter Cloth;** John A. Castoro<sup>1</sup>; Albert J. DelMonte<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, New Brunswick, NJ
- TP 155 **Collisionally-Induced Dissociation of Methimazole and Acetylsalicylic Acid: Mechanisms of Ion Formation Using Hydrogen/Deuterium Exchange and Electrospray Ionization Mass Spectrometry;** Patrick Jeanville<sup>2</sup>; Kevin Colizza<sup>1</sup>; Amin, M. Kamel<sup>1</sup>; <sup>1</sup>Pfizer Global Research and Development, Groton, CT; <sup>2</sup>Thermo Electron Corporation, West Palm Beach, FL
- TP 156 **Simple Computational Method for Converting Gas-Phase Ion Heats of Formation into Energetics of Ionic Solids;** Lee S. Sunderlin<sup>1</sup>; Nathaniel A. Fulton<sup>1</sup>; Paul Weber<sup>1</sup>; Changtong Hao<sup>1</sup>; <sup>1</sup>Northern Illinois University, DeKalb, IL
- TP 157 **Monitoring Prenucleation in Solid State Formation of Silicates using ESI-MS;** Stefan Pelster<sup>1</sup>; Ferdi Schüth<sup>1</sup>; Wolfgang Schrader<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Kohlenforschung, Mülheim / Ruhr, Germany
- TP 158 **Evidence for Ring-size Controlled Competitive Channels in &alpha; vs.&omega;-Hydrogen Migration in N-(5-Phenylvaleryl)azacycloalkan-2-thiones Probed by Isotope Labeling and Charge Inversion;** Hiroshi



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Yamaoka<sup>1</sup>; Kei Shiono<sup>1</sup>; Shigeo Hayakawa<sup>1</sup>; Kimio Isa<sup>2</sup>; Naoto Dougawa<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

- TP 159 **Experimental and Computational Study of the Gas-Phase Reactivity of Lead(II) Ions Towards D-Glucosamine, N-Ac-D-Glucosamine and Uronic Acids;** Jean-Yves Salpin<sup>1</sup>; Ahlam El Firdoussi<sup>2</sup>; Jeanine Tortajada<sup>1</sup>; <sup>1</sup>LAMBE - UMR 8587 CNRS/CEA/UEVE, Evry, France; <sup>2</sup>Cadi Ayyad University, Marrakech, Morocco

### ENVIRONMENTAL ANALYSIS: WATER

- TP 160 **Determination of Acrylamide in Drinking Water using Direct Injection into LC-ESI/MS/MS;** Daniel Temponi Lebre<sup>1</sup>; Helio Alves Martins-Júnior<sup>1</sup>; Alexandre Yautin Wang<sup>1</sup>; Valéria Chiérice Rodrigues<sup>2</sup>; <sup>1</sup>Applied Biosystems, Sao Paulo, Brazil; <sup>2</sup>Nestlé Brasil Ltda, Sao Paulo, Brazil
- TP 161 **Investigation of Chlorotetracycline Isomerization using LC-MS/MS;** Jonathan Bailey<sup>1</sup>; Kerry M. Peru<sup>1</sup>; Allan J. Cessna<sup>1</sup>; John V. Headley<sup>1</sup>; <sup>1</sup>Environment Canada, Saskatoon, Canada
- TP 162 **Analysis of Hydroxylated Metabolites of PCBs and PBDEs in Fish using GC/MS and LC/MS;** Fatin Samara<sup>1</sup>; Diana S. Aga<sup>1</sup>; <sup>1</sup>State University of New York-University at Buffalo, Buffalo, NY
- TP 163 **Direct Aqueous Injection/Gas Chromatography-High Resolution Mass Spectrometry (DAI/GC-HRMS) of Water Soluble Organic Compounds;** Vince Y Taguchi<sup>1</sup>; Angelina So<sup>1</sup>; Moschoula A Trikoupi<sup>1</sup>; <sup>1</sup>Ministry of the Environment, Toronto, Canada
- TP 164 **Withdrawn**
- TP 165 **From Mass to Structure: Analysis of Aromaticity of Suwannee River Fulvic Acid by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Boris Koch<sup>1</sup>; Matthias Witt<sup>2</sup>; Thorsten Dittmar<sup>3</sup>; <sup>1</sup>Alfred-Wegener-Institut, Bremerhaven, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Florida State University, Tallahassee, FL
- TP 166 **Analysis of Natural Organic Matter by FTMS: Effect of Ionization Techniques for the Analysis of Suwannee River Fulvic Acid;** Matthias Witt<sup>1</sup>; Philippe Schmitt-Kopplin<sup>2</sup>; Moritz Frommberger<sup>2</sup>; Norbert Hertkorn<sup>2</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>GSF - National Research Center, Neuherberg, Germany
- TP 167 **Synthesis and Determination of Dicarboxylic Degradation Products of Nonylphenol Polyethoxylates by Gas Chromatography-Mass Spectrometry;** Wang-Hsien Ding<sup>1</sup>; Chin-Yuan Cheng<sup>1</sup>; Wen-Ren Li<sup>1</sup>; <sup>1</sup>Dept. Chemistry, National Central University, Chung-Li, Taiwan
- TP 168 **Experimental and Theoretical Approaches: Identification of Disinfection Byproducts in Drinking Water with Multidimensional GC/FT-ICR MS;** Touradj Solouki<sup>1</sup>; Indira Silwal<sup>1</sup>; Caleb Heffner<sup>1</sup>; <sup>1</sup>University of Maine, Orono, ME
- TP 169 **SELDI-TOF-MS Analysis of Circadian Expression of Proteins from *Karenia brevis*, a Harmful Algal Bloom Causing Dinoflagellate;** Brian P. Gregson<sup>1</sup>; Bill Richardson<sup>2</sup>; David P. Fries<sup>1</sup>; <sup>1</sup>University of South Florida, St. Petersburg, FL; <sup>2</sup>Florida Fish & Wildlife Conservation Commission, St. Petersburg, FL
- TP 170 **Withdrawn**

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- TP 171 **Mass Spectrometric Identification of Biodegradates of Pharmaceuticals in Wastewater Treatment Systems;** Diana S. Aga<sup>1</sup>; Peter Eichhorn<sup>1</sup>; Sandra Perez<sup>1</sup>; Dawn Celiz<sup>1</sup>; <sup>1</sup>Univeristy at Buffalo, Buffalo, NY
- TP 172 **Direct injection Detection using LC/MS/MS for the Analysis of Dissociated Organo-Phosphorus Pesticides and their Degradation Products in Water;** Friedrich Werres<sup>1</sup>; Jens Dahlmann<sup>2</sup>; Kristin von Czapiewski<sup>2</sup>; André Schreiber<sup>2</sup>; <sup>1</sup>Rhenish-Westfalian Institute for Water Research, Mülheim/Ruhr, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- TP 173 **Determination of 100 Endocrine Disrupting Compounds in River Water Using LC/MS/MS with a combination of APCI and ESI ionization;** Christopher D Borton<sup>1</sup>; Hesham Ghobarah<sup>1</sup>; Elliott B Jones<sup>1</sup>; Loren Y Olson<sup>1</sup>; André Schreiber<sup>2</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Applied Biosystems/MDS Sciex, Toronto, Canada
- TP 174 **Quantitative Analysis of POPs Plastic Debris in the Ocean;** Urja V. Narayan<sup>1</sup>; Lorena M. Rios<sup>1</sup>; Charles Moore<sup>2</sup>; Patrick R. Jones<sup>1</sup>; O. David Sparkman<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA; <sup>2</sup>Algalita Marine Research Foundation, Long Beach, CA
- TP 175 **Behavior and Presence of Antidepressant Pharmaceuticals and Their Degradates in Municipal Wastewater;** Melissa M. Schultz<sup>1</sup>; Edward T. Furlong<sup>1</sup>; <sup>1</sup>U.S. Geological Survey, Denver, CO
- TP 176 **Determination of Antibiotics within Various Wastewater Treatment Plants and their Impact on Surrounding Surface Waters;** Angela L. Batt<sup>1</sup>; Sungpyo Kim<sup>1</sup>; Ian B. Bruce<sup>2</sup>; Diana S. Aga<sup>1</sup>; <sup>1</sup>State University of New York at Buffalo, Buffalo, NY; <sup>2</sup>Buffalo State College, Buffalo, NY
- TP 177 **Direct Injection Detection using the API 5000 LC/MS/MS for Analysis of Residual Amounts of Various Phenoxy Acid Herbicides in Water;** Wolfram Seitz<sup>1</sup>; Jens Dahlmann<sup>2</sup>; Axel Besa<sup>2</sup>; Walter Weber<sup>1</sup>; <sup>1</sup>Zweckverband Landeswasserversorgung, Langenau, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- TP 178 **Ultra Performance Liquid Chromatography-Tandem Mass Spectrometry (UPLC-LC-MS/MS) for Low ng/L Determination of Quinolone and Macrolide Antibiotics in Wastewater;** Lidija Požar Frketic<sup>2</sup>; Mira Petrovic<sup>3</sup>; Damia Barcelo<sup>3</sup>; Francesc Ventura<sup>1</sup>; <sup>1</sup>AGBAR, Barcelona, Spain; <sup>2</sup>PLIVA, Zagreb, Croatia; <sup>3</sup>IIQAB CSIC, Barcelona, Spain
- TP 179 **Development of an Electrospray LC/MS Library Identification Protocol for the Screening of Organic Contaminants in Drinking Water;** Lawrence B. Zintek<sup>1</sup>; Joshua D. Neukom<sup>1</sup>; Dennis J. Wesolowski<sup>1</sup>; Jim Krol<sup>2</sup>; <sup>1</sup>US EPA, Chicago, IL; <sup>2</sup>Waters Corporation, Milford, MA
- TP 180 **Withdrawn**
- TP 181 **Hybrid Quadrupole Time of Flight (Q-TOF) for Screening and Confirmation of Pharmaceuticals in Wastewaters;** Damia Barcelo<sup>1</sup>; Mira Petrovic<sup>1</sup>; <sup>1</sup>IIQAB-CSIC, Department of Environmental Chemistry, Barcelona, Spain

### ENVIRONMENTAL ANALYSIS: AIR

- TP 182 **Mass Spectrometry and Electronic Nose. A Complementary Approach in Environmental Odor Characterization and Measurement;** Enrico Davoli<sup>1</sup>; Giancarlo Bianchi<sup>1</sup>; Roberto Fanelli<sup>1</sup>; Laura Capelli<sup>2</sup>; Selena Sironi<sup>2</sup>; <sup>1</sup>Istituto Mario Negri, Milano, Italy; <sup>2</sup>Politecnico di Milano, Milano, Italy

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- TP 183 **Mass Spectral Identification of Bioaerosols Through a Novel Capturing and Detection System;** Charlene W. Bayer<sup>1</sup>; Danielle E. Bayer<sup>1</sup>; Victor R. De Jesus<sup>1</sup>; <sup>1</sup>Georgia Tech Research Institute, Atlanta, GA
- TP 184 **Distinguishing Environmentally-Relevant Isomers using Selected Ion Chemical Ionization in a Quadrupole Ion Trap Mass Spectrometer;** Karen S. Wendling<sup>1</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>The University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 185 **A Fast and Reliable Method for the Analysis of Respiratory Quinones from Environmental Samples using LC/APCI/MS/MS;** Sung-Chan Jo<sup>1</sup>; Margaret Gan<sup>1</sup>; James M. Cantu<sup>1</sup>; David C. White<sup>1</sup>; <sup>1</sup>Center for Biomarker Analysis, Knoxville, TN
- TP 186 **Mass Spectrometry Identification of VOCs in the Atmosphere by a Combination of Cartridge Adsorption and SPME;** Alessandro Saba<sup>1</sup>; Andrea Raffaelli<sup>1</sup>; Marco Tumbiolo<sup>2</sup>; Piero Salvadori<sup>2</sup>; <sup>1</sup>CNR-ICCOM, Pisa, Italy; <sup>2</sup>Dipartimento di Chimica e Chimica Industriale, Pisa, Italy
- TP 187 **Determination of Chlorophenols in Aqueous Solution via Headspace Ionic Liquid Coating Solid-Phase Microextraction Coupled with Gas Chromatography-mass spectrometry;** Tse-Tsung Ho<sup>1</sup>; Maw-Rong Lee<sup>1</sup>; <sup>1</sup>National Chung-Hsing University, Taichung, Taiwan, ROC
- TP 188 **Field Evaluation of a BTEX Analyzer Using a Mobile TAGA MS/MS System;** Andy Ng<sup>1</sup>; Natalie Stacey<sup>1</sup>; Qing-Feng Chen<sup>1</sup>; Nicholas Karellas<sup>1</sup>; <sup>1</sup>Ontario Ministry of the Environment, Toronto, Ontario, Canada
- TP 189 **Derivatization Procedures and Determination of Monosaccharide Anhydrides in Atmospheric Aerosols by Gas Chromatography-Mass Spectrometry;** Jia-Lin Wang<sup>1</sup>; Ching-Lin Hsu<sup>1</sup>; Wang-Hsien Ding<sup>1</sup>; <sup>1</sup>Dept. Chemistry, National Central University, Chung-Li, Taiwan
- TP 190 **The First Parts Per Trillion Detection with SIFT-MS;** Daniel B. Milligan<sup>1</sup>; Barry J. Prince<sup>1</sup>; Gregory J. Francis<sup>2</sup>; Murray J. McEwan<sup>2</sup>; <sup>1</sup>Syft Technologies Limited, Christchurch, New Zealand; <sup>2</sup>University of Canterbury, Christchurch, New Zealand
- TP 191 **Novel High Sensitivity HPLC/ESI-MS/MS Methodology for the Analysis of Amines in Ambient Air;** Mathieu Fournier<sup>1</sup>; Jacques Lesage<sup>2</sup>; Claude Ostiguy<sup>2</sup>; Huu van Tra<sup>1</sup>; <sup>1</sup>UQAM, Montreal, Canada; <sup>2</sup>IRSST, Montreal, Canada
- TP 192 **Determination of Urea Thermal Decomposition Products in Diesel Engine Emissions Using High Performance Liquid Chromatography with Mass Spectrometry Detection;** Valbona Celo<sup>1</sup>; Ewa Dabek-Zlotorzynska<sup>1</sup>; <sup>1</sup>Environment Canada, ETC, AAQD, Ottawa, ON, K1A 0H3, Canada
- TP 193 **Trace Level Determination of Trichloroethylene in Biological Samples by Headspace Solid Phase Microextraction Gas Chromatography-Mass Spectrometry;** Yongzhen Liu<sup>1</sup>; James V. Bruckner<sup>1</sup>; Michael G. Bartlett<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 194 **Environmental Proteomics Study of Elemental Sulfur Oxidation in Anaerobic Conditions;** Ann M Snellinger-O'Brien<sup>1</sup>; Rachael Morgan-Kiss<sup>2</sup>; Thomas Hanson<sup>2</sup>; Murray V Johnston<sup>1</sup>; <sup>1</sup>University of Delaware, Newark, DE; <sup>2</sup>Delaware Biotechnology Institute, Newark, DE
- TP 195 **Real Time Measurement of Environmental Pollutants by Ion Attachment Mass Spectrometry;** Megumi Nakamura<sup>1</sup>; Harumi Maruyama<sup>1</sup>; Masko Inoue<sup>1</sup>; Yoshiki

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- Hirano<sup>1</sup>; Yasuyuki Taneda<sup>1</sup>; Yoshiro Shiokawa<sup>1</sup>; <sup>1</sup>Canon ANELVA Technix Corporation, Fuchu-shi, Tokyo, Japan
- SAMPLE PREPARATION FOR LC/MS II**
- TP 196 **Evaporation-Free Automated Solid Phase Extraction Approach for Faster Bioanalysis by LC/MS/MS in Support of Toxicokinetic and Pharmacokinetic Studies;** Naiyu Zheng<sup>1</sup>; Jianing Zeng<sup>1</sup>; Zheng Ouyang<sup>2</sup>; Stephanie Pasasfarmer<sup>1</sup>; Deborah M. Parker<sup>1</sup>; Adela Buzescu<sup>1</sup>; John Lute<sup>1</sup>; Mohammed Jemal<sup>2</sup>; Mark E. Arnold<sup>1</sup>; Steve E. Unger<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, New Brunswick, NJ; <sup>2</sup>Bristol-Myers Squibb Company, Princeton, NJ
- TP 197 **Automated, High-Throughput Method Development for HTLC-MS;** Lisa A. Ford<sup>1</sup>; Michael Zhou<sup>1</sup>; <sup>1</sup>Scynexis, Inc., RTP, NC
- TP 198 **Novel Derivatization Technique for the LC/MS/MS Analysis of Neurosteroids;** Farooq Azam<sup>1</sup>; Neal Simon<sup>2</sup>; Ray Bakhtiar<sup>1</sup>; Rasmy Talaat<sup>1</sup>; <sup>1</sup>wyeth Research, Collegeville, PA; <sup>2</sup>Lehigh University, Bethlehem, PA
- TP 199 **Dealing with Detergents and Dosing Vehicles in Samples Submitted for LC-MS Analysis;** Kathryn Black<sup>1</sup>; Halil Erol<sup>1</sup>; Joseph M. Di Bussolo<sup>2</sup>; <sup>1</sup>West Chester University of Pennsylvania, West Chester, PA; <sup>2</sup>Cohesive Technologies, Franklin, MA
- TP 200 **Semi-Automated Solid Phase Extraction Procedure for high throughput Bioanalytical Assays;** Jianbo Zhang<sup>1</sup>; Hong Gao<sup>1</sup>; Andrew Jayaraj<sup>1</sup>; <sup>1</sup>Vertex Pharm. Inc., Cambridge, MA
- TP 201 **A Case Study: Adsorptive Losses in a Bioanalytical LC/MS/MS Urine Assay;** Brian T. Hoffman<sup>1</sup>; Sanjeev Bhadresa<sup>1</sup>; Limian Zhao<sup>1</sup>; George Hade<sup>1</sup>; Erika Moore<sup>1</sup>; Stephanie Nowak<sup>1</sup>; Sara Heit<sup>1</sup>; Daniel Mulvana<sup>1</sup>; Mike-Qingtao Huang<sup>2</sup>; Naidong Weng<sup>2</sup>; Steve Unger<sup>2</sup>; <sup>1</sup>Advion BioServices, Ithaca, NY; <sup>2</sup>Bristol Myers Squibb Company, New Brunswick, NJ
- TP 202 **Evaluation of Cartridge-Saturation versus OTC Drugs Interference When Using Cation-Exchange SPE for Bioanalytical Method Development in LC-MS/MS;** Jean-Nicholas Mess<sup>1</sup>; Audrey Tousignant<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval (Montreal), Canada
- TP 203 **Comparison of Oasis HLB Extraction to Cohesive Turbulent Flow Online Analysis;** Adlai E. Niggebrugge<sup>1</sup>; Angela Shen<sup>1</sup>; <sup>1</sup>Charles River Laboratories, Worcester, MA
- TP 204 **A Novel Approach for Tissue Sample Preparation: Enzymatic Disruption of Drug-Receptor Interactions for LC-MS/MS Bioanalysis of RU-486;** Yuhui Yang<sup>1</sup>; Tuyen Ngyuen<sup>1</sup>; Xin Zhang<sup>1</sup>; Jakal Amin<sup>1</sup>; <sup>1</sup>Charles River Labs, Bioanalytical Chemistry, Worcester, MA
- TP 205 **On-line SPE-LC-MS/MS Method Development: A New Simple and Fast Clean-Up Approach to Improve Sample Throughput;** Emile Koster<sup>1</sup>; <sup>1</sup>Spark Holland Inc., Plainsboro, NJ
- TP 206 **Evaluation of iTRAQ™ Reagents for Quantitative Amino Acid Analysis of Peptide and Protein Hydrolysates by LC/MS/MS;** Elizabeth S. Ingle<sup>1</sup>; Jennie R. Lill<sup>1</sup>; Claire Bramwell<sup>3</sup>; Scott Daniels<sup>2</sup>; Subodh Nimkar<sup>3</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA; <sup>2</sup>Applied Biosystems, Framingham, MA; <sup>3</sup>Applied Biosystems, Foster City, CA
- TP 207 **Fractionation of the Human Plasma Proteome Prior to Analysis by LC/MS/MS;** Susanne Moyer<sup>1</sup>; Hongbin Liu<sup>1</sup>; Nina Zolotarjova<sup>1</sup>; James Martosella<sup>1</sup>; Peter Mrozinski<sup>1</sup>;

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- TP 208 **Therapeutic Drug Monitoring of Antiretroviral Drugs by Automated Fast Online XLC-MS/MS as Gold-Standard Technique;** Therese Koal<sup>1</sup>; Alex Berhiti<sup>2</sup>; Emile Koster<sup>2</sup>; Martin Sibum<sup>2</sup>; Volkhard Kaever<sup>1</sup>; <sup>1</sup>Medical School Hannover Institute for Pharmacology, Hannover, Germany; <sup>2</sup>Spark Holland Inc., Plainsboro, NJ
- TP 209 **Improving Biological Sample Handling and Analyte Response with SPE Technologies for LC/MS/MS Assay;** Raymond J Gonzalez<sup>1</sup>; Irina Miksa<sup>1</sup>; Juan Chen<sup>1</sup>; Michelle Schreier<sup>1</sup>; Denny Christian<sup>1</sup>; <sup>1</sup>Merck & Co., West Point, PA
- TP 210 **Determination of Lercanidipine in Human Plasma using Automated Online Solid Phase Extraction Combined with Electro Spray Ionization Tandem Mass Spectrometry;** Kwang-Youl Kim<sup>1</sup>; Sang-Man Han<sup>1</sup>; Kwang-Hyeon Kim<sup>1</sup>; John Crutchfield<sup>2</sup>; Robert Mensen<sup>2</sup>; Heon-Soo Lee<sup>1</sup>; <sup>1</sup>Bio-Medieng, Seoul, Korea; <sup>2</sup>Spark Holland Inc., Plainsboro, NJ
- TP 211 **Novel LC/MS Method of IgG1 Fragments Through Limited Proteolysis and Low Ph Reduction for Identification and Quantification of Post-Translational Modifications;** Gary D Pipes<sup>1</sup>; <sup>1</sup>Amgen Inc, Thousand Oaks, CA
- TP 212 **LC-MS Analysis of Tricyclic Antidepressants in Human Plasma Using Supported Liquid Extraction Sample Preparation;** Matthew Cleeve<sup>1</sup>; Lee Williams<sup>1</sup>; Scott Merriman<sup>1</sup>; Helen Lodder<sup>1</sup>; Anne Howells<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Richard Calverley<sup>1</sup>; <sup>1</sup>Argonaut Technologies, now a Biotage company, Hengoed, UK
- TP 213 **Tandem On-line Extraction LC-MS/MS for Monitoring Drug Levels in Combination Therapy;** Otto Halmingh<sup>1</sup>; Martin Sibum<sup>1</sup>; Emile Koster<sup>1</sup>; <sup>1</sup>Spark Holland Inc., Plainsboro, NJ
- TP 214 **Reduced Sample Preparation Complexity for the Analysis of Irinotecan and Metabolite SN-38 Utilizing the Sensitivity Gains of the API 5000;** Alexandre Pimenov<sup>1</sup>; Jeff Plomley<sup>1</sup>; Tim Samuels<sup>1</sup>; <sup>1</sup>Charles River Laboratories, Preclinical Services, Montreal, Canada
- TP 215 **Online and Offline Nanoelectrospray Analysis of Phosphopeptides Purified by TiO<sub>2</sub>, ZrO<sub>2</sub>, and Carbon Wall-Coated Pipette Tips;** Christopher J. Toher<sup>1</sup>; Adam W. Perala<sup>1</sup>; Carla J. Marshall-Waggett<sup>1</sup>; Gary A. Valaskovic<sup>1</sup>; Ashok K. Shukla<sup>2</sup>; A.A. Oetting<sup>2</sup>; M.M. Shukla<sup>2</sup>; N. Manohar<sup>2</sup>; <sup>1</sup>New Objective, Inc., Woburn, MA; <sup>2</sup>Glygen, Inc., Columbia, MD
- TP 216 **A New Method for the Determination of Free Drugs in Mouse Brains By Acoustic Homogenization, Ultracentrifugation and LC-MS/MS;** Philip Wong<sup>1</sup>; Bernd Bruenner<sup>1</sup>; Dean Hickman<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA
- TP 217 **Automated Reversed-Phase Solid-Phase Extraction Optimization of Plasma Samples for LC-MS/MS Bioanalysis of Drugs and Metabolites;** Zheng Ouyang<sup>1</sup>; Yuan-Qing Xia<sup>1</sup>; Mohammed Jemal<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ
- TP 218 **Stabilization of Reduced Glutathione in Whole Blood and Quantitation of Reduced and Oxidized Glutathione in Human Plasma by LC/MS/MS;** Henry H. Li<sup>1</sup>; Hongzhuan Chen<sup>1</sup>; Yongdong Zhu<sup>1</sup>; Yuan-Shek Chen<sup>1</sup>; Jamie Zhao<sup>1</sup>; Benjamin Chien<sup>1</sup>; Christopher J. Pazoles<sup>2</sup>; <sup>1</sup>Quest Pharmaceutical Services, Newark, DE; <sup>2</sup>Novelos Therapeutics, Inc., Newton, MA

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- TP 219 **Improving the MS Detection of Aflatoxins using a LC/MS system with Automated On-line Solid Phase Extraction and Derivatization;** Juergen Wendt<sup>1</sup>; Norbert Helle<sup>2</sup>; Dirk Bremer<sup>3</sup>; <sup>1</sup>Agilent Technologies LSCA Sales & Service GmbH, Waldbronn, Germany; <sup>2</sup>TeLA Techn.Lebensmittel- und Umweltanalytik GmbH, Bremerhaven, Germany; <sup>3</sup>Gerstel GmbH & CoKG, Muelheim an der Ruhr, Germany
- TP 220 **Does Column Switching Reduce Phospholipid Ion Suppression in the Analysis of Rapamycin Using HPLC-ESI-MS/MS?** Cory A. Hawkins<sup>1</sup>; Melissa M. Kiser<sup>1</sup>; Lori D. Payne<sup>1</sup>; <sup>1</sup>Bioanalytical Systems, Inc. Northwest Laboratory, McMinnville, OR

### CLINICAL CHEMISTRY II

- TP 221 **A Rapid UPLC-MS/MS Method for Determining Specific Amino Acids Associated with Maple Syrup Urine Disease and Phenylketonuria Management;** Scott M. Freeto<sup>1</sup>; Donald Mason<sup>1</sup>; Jie Chen<sup>2</sup>; Robert Scott<sup>2</sup>; Srinivas Narayan<sup>2</sup>; Michael Bennett<sup>2</sup>; <sup>1</sup>Waters Corporation, Beverly, MA; <sup>2</sup>Children's Hospital of Philadelphia, Philadelphia, PA
- TP 222 **Enrichment of Cardiac and Skeletal Muscle Glycogen and Glucose Tetrasaccharide Pools with [<sup>13</sup>C]<sub>6</sub>glucose in Pompe Disease Knock-out Mice;** Haoyue Zhang<sup>1</sup>; Sarah P. Young<sup>1</sup>; Baodong Sun<sup>2</sup>; Dwight D. Koeberl<sup>2</sup>; David S. Millington<sup>1</sup>; <sup>1</sup>Duke University Medical Center, Research Triangle Park, NC; <sup>2</sup>Duke University Medical Center, Durham, NC
- TP 223 **Rapid Quantitation of Steroids from Dried Plasma Spots Using Electrospray Ionization LC-MS/MS;** Susan C. Leonard<sup>1</sup>; Jeffrey D. Miller<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA
- TP 224 **Identification and Quantitation of  $\beta$ -Lactam Antibiotics in Human by LC/MS/MS Identification and Quantitation of  $\beta$ -Lactam Antibiotics in Human Urine by LC/MS/MS;** Anh Pham<sup>1</sup>; David Simons<sup>1</sup>; Gary Myers<sup>1</sup>; Hubert Vesper<sup>1</sup>; <sup>1</sup>Center for Disease Control, Atlanta, GA
- TP 225 **High Throughput Analysis of Testosterone and Immunosuppressants by Elevated Temperature LC with MS/MS detection;** Bingfang Yue<sup>1</sup>; Mark M. Kushnir<sup>1</sup>; Gwen McMillin<sup>2</sup>; A. Wayne Meikle<sup>2</sup>; Alan L. Rockwood<sup>2</sup>; Stephanie J. Marin<sup>3</sup>; W. Dale Felix<sup>3</sup>; <sup>1</sup>ARUP Laboratories, Salt Lake City, UT; <sup>2</sup>University of Utah, Salt Lake City, UT; <sup>3</sup>Selerity Technologies, Salt Lake City, UT
- TP 226 **An On-Line Extraction Assay for the Diagnosis of Congenital Adrenal Hyperplasia in Human Serum by LC-MS/MS;** James L. Bruton<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN
- TP 227 **Withdrawn**
- TP 228 **Method Development for the Determination of 19-Norandrosterone in Human Urine Using Isotope-Dilution Liquid Chromatography-Tandem Mass Spectrometry;** Susan S. Tai<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- TP 229 **On-Line Analysis of Opiates and Opioid Analgesics in Urine;** Francois A. Espourteille<sup>1</sup>; <sup>1</sup>Cohesive Technologies, Inc., Franklin, MA
- TP 230 **An Assay for Simultaneous Quantification of Seven Vitamin D Derivatives including D<sub>2</sub>, D<sub>3</sub>, Mono-Hydroxy Metabolites and Dihydroxy Metabolites in Human Serum;** Yan Ling Zhang<sup>1</sup>; Valerie Burns<sup>1</sup>; Leah Swanson<sup>1</sup>; Michol Rothman<sup>1</sup>; Margaret Wierman<sup>1</sup>; Chester Ridgeway<sup>1</sup>; Uwe Christians<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, CO

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- TP 231 **Biomarker Discovery for Renal Clear Cell Carcinoma Using a Two-dimensional (2D) LC-MS Peptidomic Differential Profiling Assay;** Hua Lin<sup>1</sup>; Thomas A. Shaler<sup>1</sup>; Brad Brown<sup>1</sup>; Melissa Chen<sup>1</sup>; Praveen Kumar<sup>1</sup>; Ted Jones<sup>1</sup>; Christopher H Becker<sup>1</sup>; <sup>1</sup>*Biomarker Discovery Sciences, PPD, Inc., Menlo Park, CA*
- TP 232 **Measurement of Serum Dihydrotestosterone by LC-MS/MS;** Robert E. Nelson<sup>1</sup>; Ravinder J. Singh<sup>1</sup>; Stefan K. Grebe<sup>1</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*
- TP 233 **Detection of DNA Methylation in Human Epithelial Cancer Cells Using Electrospray Ionization Mass Spectrometry;** Yun Jiang<sup>1</sup>; Raymond Ranken<sup>1</sup>; Cristina Agasino Ivy<sup>1</sup>; Steven Hofstadler<sup>1</sup>; <sup>1</sup>*Ibis Division, A Division of Isis Pharmaceuticals, Carlsbad, CA*
- TP 234 **Simultaneous Measurement of Serum/Plasma Oxcarbazepine and 10-Hydroxycarbazepine by On-line High Turbulence Liquid Chromatography-Tandem Mass Spectrometry;** Qibo Jiang<sup>1</sup>; Sum Chan<sup>1</sup>; Richard E. Reitz<sup>1</sup>; <sup>1</sup>*Quest Diagnostics Nichols Institute, San Juan Capistrano, CA*
- TP 235 **A Sensitive, Automated Assay for the Quantification of Bilirubin A9 in Blood after Eluting from Coronary Stents: Pushing the Limits;** Yan Ling Zhang<sup>1</sup>; Jamie Bendrick-Pearl<sup>1</sup>; Ron Betts<sup>2</sup>; Uwe Christians<sup>1</sup>; <sup>1</sup>*University of Colorado Health Sciences Center, Denver, CO;* <sup>2</sup>*Biosensors International-USA, Newport Beach, CA*
- TP 236 **Quantitative LC-MS/MS Analysis of Endogenous Biomarkers for Clinical Diagnosis in Endocrinology;** Mary K Mor<sup>1</sup>; Andrew D Wagner<sup>1</sup>; Milan Patel<sup>1</sup>; Russell P Grant<sup>1</sup>; <sup>1</sup>*Esoterix inc, 4301 Lost Hills Rd, Calabasas Hills, CA*
- TP 237 **Quantitative Measurement of Potential Biomarkers in Schizophrenia: Analysis of D-Serine, L-Serine and Glycine in Biological Matrices using LC-MS/MS;** Thomas J. McLellan<sup>1</sup>; Francis Sweeney<sup>1</sup>; Maria Rosario<sup>1</sup>; Richard O'Sullivan<sup>1</sup>; Holly Soares<sup>1</sup>; <sup>1</sup>*Pfizer Global Research and Development, Groton, CT*
- TP 238 **Contribution of LC-Tandem Mass Spectrometry for the Determination of Dansylated Polyamines;** Daniel RUFFIEUX<sup>1</sup>; Hélène BELVA-BESNET<sup>2</sup>; Florence DE FRAIPONT<sup>1</sup>; Véronique DUCROS<sup>1</sup>; <sup>1</sup>*Département de Biologie Intégrée, CHU, GRENOBLE, FRANCE;* <sup>2</sup>*Appliedbiosystems, Courtaboeuf, FRANCE*
- TP 239 **Catecholamine Concentration Determination: iTRAQ<sup>®</sup> and Derivatization and LC-MS/MS Quantitation;** Peter G. Lodenguai<sup>1</sup>; Susan C. Leonard<sup>1</sup>; Johnnie C. Brown<sup>1</sup>; David R. Dupont<sup>1</sup>; Subodh Nimkar<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Foster City, CA*
- TP 240 **Multivariate Statistics of LC/UV and LC/MS Data from Urinary Nucleoside Profiles;** Antje Frickenschmidt<sup>1</sup>; Gabriela Zurek<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Jim Cunningham<sup>3</sup>; Hartmut Liebich<sup>4</sup>; Christoph Gleiter<sup>1</sup>; Holger Fröhlich<sup>5</sup>; Andreas Zell<sup>5</sup>; Bernd Kammerer<sup>1</sup>; <sup>1</sup>*Tuebingen University, Tuebingen, Germany;* <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany;* <sup>3</sup>*Bruker Daltonics, Billerica, MA;* <sup>4</sup>*University Hospital Tuebingen, Tuebingen, Germany;* <sup>5</sup>*Centre for Bioinformatics Tuebingen, Tuebingen, Germany*
- TP 241 **Comparison of Fenopropfen and Deuterated Ketoprofen as Internal Standards for Ketoprofen Analysis in Microdialysis and Open Flow Microperfusion Samples;** Karin Pickl<sup>1</sup>; Christoph Magnes<sup>1</sup>; Manfred Bodenlenz<sup>1</sup>; Günther Fauler<sup>2</sup>; Thomas R. Pieber<sup>1</sup>; Frank M. Sinner<sup>1</sup>; <sup>1</sup>*Inst. of Medical Technologies a. Health M., Graz, Austria;* <sup>2</sup>*CIMCL, Medical University Graz, Graz, Austria*

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- TP 242 **Differentiation of Triiodothyronines by Electrospray Ionization Tandem Mass Spectrometry;** Yuntao Zhang<sup>1</sup>; Abigail H. Conrad<sup>1</sup>; Gary W. Conrad<sup>1</sup>; <sup>1</sup>*Kansas State University, Manhattan, KS*
- TP 243 **Simultaneous LC-ESI-MS-MS Determination of Cyclosporine A, Tacrolimus, and Sirolimus in Blood and Mycophenolic Acid in Plasma, using Common Pretreatment Procedure;** Maciej Bogusz<sup>1</sup>; Jamil Abdel-Jawwad<sup>1</sup>; Eid Al-Enazi<sup>1</sup>; Huda Hassan<sup>1</sup>; Mohammed Al-Tufail<sup>1</sup>; <sup>1</sup>*King Faisal Specialist Hospital and Research Centr, Riyadh, Saudi Arabia*
- TP 244 **Mass Spectrometric Single Eye Analysis and Contralateral Eye Comparison in a Dry Eye Model;** Bryan M. Ham<sup>1</sup>; Jean T. Jacob<sup>2</sup>; Richard B. Cole<sup>1</sup>; <sup>1</sup>*University of New Orleans, New Orleans, LA;* <sup>2</sup>*Louisiana State University-Health Sciences Center, New Orleans, LA*
- TP 245 **Detection of the Causative Agents of Bacteremia in the Presence of Large Human DNA Background by Electrospray Ionization Mass Spectrometry;** Raymond Ranken<sup>1</sup>; Yun Jiang<sup>1</sup>; Cristina Agasino Ivy<sup>1</sup>; Steven Hofstadler<sup>1</sup>; <sup>1</sup>*Ibis Division, A Division of Isis Pharmaceuticals, Carlsbad, CA*
- TP 246 **Enhancing the Limit of Quantitation of Testosterone at Clinically Relevant Levels Using FAIMS;** Jonathan C. McNally<sup>1</sup>; Barbara Ellis<sup>1</sup>; James Kapron<sup>1</sup>; <sup>1</sup>*ThermoElectron, San Jose, CA*
- TP 247 **Online Glu-C Digestion and Measurement of Hemoglobin A1C and A0 Peptides Using LC/MS;** Kheng B. Lim<sup>1</sup>; Joshua Pengson<sup>1</sup>; Daniel B Kassel<sup>1</sup>; <sup>1</sup>*Takeda San Diego, Inc, San Diego, CA*

### IMMUNOLOGY

- TP 248 **Identification of Brugia Adult Worm Proteins;** Tiffany Weinkopff<sup>1</sup>; Michael Nold<sup>2</sup>; Jeffrey Silva<sup>2</sup>; James Atwood<sup>1</sup>; George Punkosdy<sup>3</sup>; Brent Weatherly<sup>1</sup>; Ronald Orlando<sup>1</sup>; Patrick Lammie<sup>3</sup>; <sup>1</sup>*University of Georgia, Athens, GA;* <sup>2</sup>*Waters Corporation, Milford, MA;* <sup>3</sup>*Centers for Disease Control and Prevention, Atlanta, GA*
- TP 249 **Flu Fighters - Proteomics Surveillance of the Influenza Virus with Mass Spectrometry;** Bethny Morrissey<sup>1</sup>; Margaret Streamer<sup>1</sup>; Kevin Downard<sup>1</sup>; <sup>1</sup>*The University of Sydney, Sydney, AUSTRALIA*
- TP 250 **Comprehensive Immunopectome Display of Normal and Leukemic Cells using Multi-Dimensional Nanolc-MS-MS;** Marie-Hélène Fortier<sup>1</sup>; Chantal Baron<sup>1</sup>; Vincent Rineau<sup>1</sup>; Claude Perreault<sup>1</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*IRIC, Université de Montréal, Montréal, Canada*
- TP 251 **De Novo Sequencing of a Monoclonal Antibody Using LTQ-FTMS-MS/MS Analysis and Edman Degradation;** Victoria C. Pham<sup>1</sup>; David Arnott<sup>1</sup>; Jennie R. Lill<sup>1</sup>; <sup>1</sup>*Genentech Inc., South San Francisco, CA*
- TP 252 **Withdrawn**
- TP 253 **Identification of Infection-Related Antigenic Peptides Bound to MHC Class I or Class II Molecules Utilizing Dedicated Metabolic Labeling Strategies;** Hugo D. Meiring<sup>1</sup>; Rachel M. Stenger<sup>1</sup>; Betsy Kuipers<sup>1</sup>; Martien C.M. Poelen<sup>1</sup>; Jacqueline A.M. van Gaans-van den Brink<sup>1</sup>; Hans Timmermans<sup>1</sup>; Ad P.J.M. de Jong<sup>1</sup>; Ernst C. Soethout<sup>1</sup>; Cecile A.C.M. van Els<sup>1</sup>; <sup>1</sup>*Netherlands Vaccine Institute, Bilthoven, The Netherlands*
- TP 254 **Full length Sequencing of Monoclonal Antibody Light Chains using Nano-LC/MS/MS;** Yan Chen<sup>1</sup>; Jun Lu<sup>1</sup>; Huaiqin Wu<sup>1</sup>; <sup>1</sup>*Abbott Laboratories, Abbott Park, IL*
- TP 255 **Mass Spectrometric Characterization of a Discontinuous Epitope of the Hepatitis C Virus (HCV) E2 Protein by Differential Chemical Modification;**

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- Roxana E. Iacob<sup>1</sup>; Steven Fount<sup>2</sup>; Kenneth B. Tomer<sup>1</sup>;  
<sup>1</sup>National Institute of Environmental Health Science, RTP, NC; <sup>2</sup>Department of Pathology, Stanford University, Stanford, CA
- TP 256 **Analysis of HLA-DR4 Restricted Peptides by Electron transfer Dissociation (ETD) Mass Spectrometry;** Jie Qian<sup>1</sup>; Valentina Robila<sup>1</sup>; Dina Bai<sup>1</sup>; Joy M. Polefrone<sup>1</sup>; Lewis Y. Geer<sup>2</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>National Center for Biotechnology Information, NIH, Bethesda, MD
- TP 257 **Comparing Apples to Pears: Quantitative Comparison Between MHC-Ligand- and mRNA-Ratios Shows Only Faint Correlation;** Andreas Weinzierl<sup>1</sup>; Margret IJ Mueller<sup>1</sup>; <sup>1</sup>Institute for Cell Biology, Tuebingen, Germany
- TP 258 **Unexpected Abundance of HLA Class II Presented Peptides in Primary Renal Cell Carcinomas;** Joern Dengel<sup>1</sup>; Maria-Dorothea Nastke<sup>1</sup>; Gitsios Gitsioudis<sup>1</sup>; Oliver Schoor<sup>1</sup>; Florian Altenberend<sup>1</sup>; Margret Müller<sup>1</sup>; Björn Krämer<sup>1</sup>; Anna Missiou<sup>1</sup>; Martina Sauter<sup>2</sup>; Jörg Hennenlotter<sup>3</sup>; Arnulf Stenzl<sup>3</sup>; Hans-Georg Rammensee<sup>1</sup>; Karin Klingel<sup>2</sup>; Stefan Stevanovic<sup>1</sup>; <sup>1</sup>Immunology, University of Tuebingen, Tuebingen, Germany; <sup>2</sup>Molecular Pathology, University of Tuebingen, Tuebingen, Germany; <sup>3</sup>Urology, University of Tuebingen, Tuebingen, Germany
- TP 259 **Determination of Interleukin-4 Induced Expression within the Nuclear Proteome of CD4+ Cells using Isotope Tagged Relative and Absolute Quantitation Reagents;** Robert Moulder<sup>1</sup>; Jan-Jonas Filén<sup>1</sup>; Laura Elo<sup>1</sup>; Petri Kouvonen<sup>1</sup>; Tero Aittokallio<sup>2</sup>; Riitta Lahesmaa<sup>1</sup>; Tuula Nyman<sup>3</sup>; <sup>1</sup>Turku Centre for Biotechnology, Turku, Finland; <sup>2</sup>Department of Mathematics, University of Turku, Turku, Finland; <sup>3</sup>National Public Health Institute, Helsinki, Finland
- TP 260 **Proteomics-Based Development and Testing of Aspergillus Fumigatus Vaccine Candidates;** Teresa B. Hong<sup>1</sup>; Joseph M. Lyons<sup>1</sup>; Yunan Miao<sup>1</sup>; Terry D. Lee<sup>1</sup>; James I. Ito<sup>1</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope National Medical Center, Duarte, CA
- TP 261 **Combining SILAC and iTRAQ for Large Scale Identification of MHC Peptides;** Eilon Barnea<sup>1</sup>; Ilan Beer<sup>2</sup>; Yifat Yanku<sup>1</sup>; Elena Milner<sup>1</sup>; Arie Admon<sup>1</sup>; <sup>1</sup>Technion-Israel Inst. of Technology, Haifa, Israel; <sup>2</sup>IBM Haifa Research Laboratory, Haifa, Israel
- TP 262 **Using NanoLC and HPLC Chip to Identify Novel Membrane Proteins Associated with MHC Class II;** Karen R. Jonscher<sup>2</sup>; Lei Jin<sup>1</sup>; Nichole A. Reisdorph<sup>2</sup>; John Cambier<sup>1</sup>; <sup>1</sup>National Jewish Medical and Research Ctr, UCHSC, Denver, CO; <sup>2</sup>University of Colorado Health Sciences Center, Denver, CO
- TP 263 **Interaction Between Designed Ankyrin Repeat Proteins and CD4 Studied at the Molecular Level by Combined Cross-Linking Chemistry and Mass Spectrometry;** Tatiana Pimenova<sup>1</sup>; Andreas Schweizer<sup>2</sup>; Alexis Nazabal<sup>1</sup>; Patrick Amstutz<sup>3</sup>; Alexandra Trkola<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>University Hospital Zurich, Zurich, Switzerland; <sup>3</sup>Molecular Partners, Zürich, Switzerland
- TP 264 **Detection of Acetylated-N-Terminal Peptide Hormones Released from the Human MOLT-4 T-Cell Line;** Colette J Rudd<sup>1</sup>; Carol L Soppe<sup>1</sup>; Robert J Barkovich<sup>1</sup>; James H Shofstahl<sup>1</sup>; Diether Recktenwald<sup>2</sup>; <sup>1</sup>Thermo Electron, San Jose, CA; <sup>2</sup>BD BioSciences, San Jose, CA

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#### MALDI TANDEM MS

- TP 265 **Characterization of a Microbial SGNH-Lipase and its Inhibitor-Complexes by MALDI-TOF, ESI-IT, MALDI-IT/TOF and MALDI-TOF/TOF Mass Spectrometry;** Martin Zehl<sup>1</sup>; Ivana Lescic-Asler<sup>2</sup>; Filip Kovacic<sup>2</sup>; Marija Abramic<sup>2</sup>; Biserka Kojic-Prodic<sup>2</sup>; Emmanuel Raptakis<sup>3</sup>; Guenter Allmaier<sup>1</sup>; <sup>1</sup>Vienna University of Technology, Vienna, Austria; <sup>2</sup>Ruder Boskovic Institute, Zagreb, Croatia; <sup>3</sup>Shimadzu Biotech-Kratos Analytical, Manchester, United Kingdom
- TP 266 **Extending Protein Sequence Information Using a Combination of MALDI in-Source Decay and High Energy CID Fragmentation;** Rachel L. Martin<sup>1</sup>; Emmanuel Raptakis<sup>1</sup>; <sup>1</sup>Shimadzu Biotech, Manchester, UK
- TP 267 **Structural Characterization of Pyridylaminated Oligosaccharides and Peptides by Atmospheric Pressure MALDI-QIT-TOF Mass Spectrometry;** Emi Ito<sup>1</sup>; Akio Tominaga<sup>2</sup>; Hiroto Itoi<sup>2</sup>; Shuichi Shinma<sup>3</sup>; Mitsutoshi Setou<sup>3</sup>; Kozo Miseki<sup>2</sup>; Akemi Suzuki<sup>1</sup>; Minoru Suzuki<sup>1</sup>; <sup>1</sup>RIKEN Frontier, Saitama, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Okazaki National Research Institutes, Okazaki, Japan
- TP 268 **The Correlation of Milk Peptide and Protein Profiling with the Acute Inflammatory Stage in Cows Affected by Mastitis;** Anna Napoli<sup>1</sup>; Donatella Aiello<sup>1</sup>; Leonardo Di Donna<sup>1</sup>; Dora Spina<sup>1</sup>; Giovanni Sindona<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Calabria, Rende, Italy
- TP 269 **Top-Down and Middle-Down Proteome Analysis by MALDI TOF/TOF;** Angela K. Walker<sup>1</sup>; John R. Strahler<sup>1</sup>; Hasand Ghandi<sup>2</sup>; Peggy H. Ostrom<sup>2</sup>; P.C. Andrews<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Michigan State University, Lansing, MI
- TP 270 **Increased Sensitivity and Resolution of Low Mass Fragment Ions on a MALDI TOF-TOF via Low Mass Zoom Analysis Mode;** Joanne B. Connolly<sup>1</sup>; Andrew R. Bowdler<sup>2</sup>; Stuart J. McLarnon<sup>3</sup>; <sup>1</sup>Shimadzu Biotech, Manchester, UK; <sup>2</sup>Kratos Analytical, Manchester, UK; <sup>3</sup>University of Manchester, Manchester, UK

#### METAL IONS IN BIOLOGY

- TP 271 **Electron Capture Dissociation of Biological Molecules Complexed with Metal Ions;** Kristina Hakansson<sup>1</sup>; Haichuan Liu<sup>1</sup>; Jiong Yang<sup>1</sup>; Julie T. Adamson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- TP 272 **Characterization of the Zinc-Binding Properties of Prothymosin- $\alpha$ ;** William B. Monteith<sup>1</sup>; Chris L. Wilson<sup>1</sup>; Colin S. Burns<sup>1</sup>; Allison S. Danell<sup>1</sup>; <sup>1</sup>East Carolina University, Greenville, NC
- TP 273 **Proteomic Analysis of Calcium- and Phosphorylation-dependent Calmodulin Complexes in Mammalian Cells;** Daojing Wang<sup>1</sup>; Deok-Jin Jang<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA
- TP 274 **Sequencing of Biological Chromium Peptides by Mass Spectrometry;** Carolyn J. Cassidy<sup>1</sup>; Jungie Gao<sup>1</sup>; Zhong Li<sup>1</sup>; Dan Pu<sup>1</sup>; <sup>1</sup>The University of Alabama, Tuscaloosa, AL
- TP 275 **Search for Proteins Involved in Transport of Low-Molecular-Mass Iron;** Petr Pompach<sup>1</sup>; Petr Man<sup>1</sup>; Karel Valis<sup>2</sup>; Jaroslav Truksa<sup>2</sup>; Jan Kovar<sup>2</sup>; <sup>1</sup>Institute of Microbiology, Prague, Czech Republic; <sup>2</sup>Institute of Molecular Genetics, Prague, Czech Republic
- TP 276 **Top-Down Probing of Protein: Metal and Protein:Nucleic Acid Complexes Via Slow-heating Fragmentation Methods in FTMS;** Katherine A. Kellersberger<sup>1</sup>; Danielle A. Fabris<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore County, Baltimore, MD

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- TP 277 **Copper Binding of the Prion Protein Studied by Metal-Catalyzed Oxidation Reactions and Mass Spectrometry;** R Srikanth<sup>1</sup>; Juma D Bridgewater<sup>1</sup>; Richard W Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA

### NATURAL PRODUCTS

- TP 291 **Development of a Mass Spectrometry-Based Assay for the Evaluation of Inhibitors of the Cyclooxygenases COX-1 and COX-2;** Yi Tao<sup>1</sup>; Dejan Nikolic<sup>1</sup>; Wenkui Li<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL
- TP 292 **The Role of the Hybrid Linear Ion Trap - FTMS in Natural Product Discovery;** Jeffrey R Gilbert<sup>1</sup>; Dennis O Duebelbeis<sup>1</sup>; Paul Lewer<sup>1</sup>; Don R Hahn<sup>1</sup>; <sup>1</sup>Dow AgroSciences, Indianapolis, IN
- TP 293 **Sequencing Hop (HUMULUS LUPULUS L.) Proanthocyanidin Oligomers by LC/ Electrospray Tandem Mass Spectrometry;** hui-jing Li<sup>1</sup>; Brian Arbogast<sup>1</sup>; Max L. Deinzer<sup>1</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR
- TP 294 **Withdrawn**
- TP 295 **Determination of Urinary Phytoestrogens by HPLC-MS/MS: A Comparison of Atmospheric Pressure Chemical Ionization (APCI) and Electrospray Ionization (ESI);** Michael E. Rybak<sup>1</sup>; Daniel L. Parker<sup>1</sup>; Christine M. Pfeiffer<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA
- TP 296 **Identification of Nitrogen-Containing Compounds in Black Cohosh (Actaea racemosa L.) by Mass Spectrometric Dereplication;** Dejan Nikolic<sup>1</sup>; David Lankin<sup>1</sup>; Shao Nong Chen<sup>1</sup>; Guido F. Pauli<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL
- TP 297 **The Structural Characterisation of Flavonoids by Negative Ion Chip-Based Nanospray Tandem Mass Spectrometry;** Clare Stewart<sup>1</sup>; Mark H Allen<sup>2</sup>; Alistair Sterling<sup>2</sup>; Norberto P Lopes<sup>3</sup>; Paul J Gates<sup>1</sup>; <sup>1</sup>University of Bristol, Bristol, United Kingdom; <sup>2</sup>Advion BioSciences Ltd., Norwich, United Kingdom; <sup>3</sup>FCFRP-University of Sao Paulo, Ribeirao Preto, Brazil
- TP 298 **Selective Analytical Determination of Phenolic Compounds in Natural Products by ESI-MS/MS Precursor Ion analysis;** Claudio Medana<sup>1</sup>; Claudio Baiocchi<sup>1</sup>; Francesco Carbone<sup>1</sup>; <sup>1</sup>Università di Torino, Torino, Italy
- TP 299 **Chemical Profiling and Quantification of Isoflavone Phytoestrogens in Kudzu Using LC/UV/MSD;** Qing-Li Wu<sup>1</sup>; Yong-Hong Yang<sup>2</sup>; James E. Simon<sup>1</sup>; <sup>1</sup>Rutgers University, New Brunswick, NJ; <sup>2</sup>Yunnan Agricultural University, Kunming, Yunnan, China
- TP 300 **Natural Product Analysis Utilizing an Ion Trap - Time-of-Flight (IT-TOF) Mass Spectrometer;** Joy M. Ginter<sup>1</sup>; Holly M. Shackman<sup>1</sup>; Joseph P. Fox<sup>1</sup>; Masayuki Nishimura<sup>1</sup>; Masahiko Taniguchi<sup>2</sup>; Yoshihide Usami<sup>2</sup>; Kuo-Hsiung Lee<sup>2</sup>; <sup>1</sup>Shimadzu, Columbia, MD; <sup>2</sup>University of North Carolina, Chapel Hill, NC
- TP 301 **Structure Elucidation of Key Polyphenols in Rosemary Extract by Liquid Chromatography Tandem Mass Spectrometry;** Alun W Davies<sup>1</sup>; Craig S Newby<sup>1</sup>; <sup>1</sup>GlaxoSmithKline Consumer Healthcare R&D, Weybridge, United Kingdom
- TP 302 **Computer Aided LC/MS or TOF Analysis Of Complex Pharmaceutical Natural Product Extracts For Structure Elucidation And Ingredient Comparison In Different Subspecies;** Edgar Nägele<sup>1</sup>; <sup>1</sup>Agilent

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- Technologies R&D and Marketing GmbH & Co., Waldbronn, Germany*
- TP 303 **Identification and Structural Characterization of Chlorophyll Catabolites in Senescent Plants using NanoLC-ESI Mass Spectrometry;** Thomas Mueller<sup>1</sup>; Kathrin Breuker<sup>1</sup>; Bernhard Kraeutler<sup>1</sup>; <sup>1</sup>Inst. of Organic Chemistry, Univ. of Innsbruck, Innsbruck, Austria
- TP 304 **Method Development for Determinations of Two Anti Cancer Bioactive Compounds Isolated from Chinese Herbal Medicine by LC-MS/MS;** Yan Ling Zhang<sup>1</sup>; Zheng Jie Liu<sup>2</sup>; Dale Leitman<sup>2</sup>; Richard Staub<sup>2</sup>; Jenny Jackson<sup>2</sup>; Sylvia Chow<sup>2</sup>; Isaac Cohen<sup>2</sup>; Uwe Christians<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, CO; <sup>2</sup>Bionovo, Inc., Emeryville, CA
- TP 305 **LC-MS/MS Analysis of Novel Isoflavone C-Glucosides in Pueraria lobata In Vitro Cultures;** Jeevan K Prasain<sup>1</sup>; Adam Reppert<sup>2</sup>; Ray Moore<sup>1</sup>; Stephen Barnes<sup>1</sup>; Mary A Lila<sup>2</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Illinois Urbana-Champaign, Urbana-Champaign, IL
- TP 306 **Determination of Gibberellic Acid in Plants by Liquid Chromatography – Mass Spectrometry;** Maw-Rong Lee<sup>1</sup>; Jie-Hong Huang<sup>1</sup>; Zu-Guang Li<sup>1</sup>; Shune-Fang Lo<sup>1</sup>; Liang-Jwa Chen<sup>1</sup>; <sup>1</sup>National Chung-Hsing University, Taichung, Taiwan, ROC
- TP 307 **Protein identification in Pollination Drop of Three Cupressaceous Conifers;** Rebecca E. Wagner<sup>1</sup>; Serena Mugnaini<sup>3</sup>; Darryl Hardie<sup>2</sup>; Patrick von Aderkas<sup>1</sup>; <sup>1</sup>University of Victoria, Victoria, Canada; <sup>2</sup>UVic-Genome BC Proteomics Centre, Victoria, Canada; <sup>3</sup>University of Siena, Siena, Italy
- TP 308 **Substrate and Activity Screening of NRPS and PKS Systems by Large Molecule Mass Spectrometry;** Pieter C. Dorrestein<sup>1</sup>; Jonathan Blackhall<sup>1</sup>; Steven van Lanen<sup>3</sup>; Paul Straight<sup>2</sup>; Daniel Edwards<sup>5</sup>; Zachary D. Aron<sup>2</sup>; William H. Gerwick<sup>4</sup>; Roberto Kolter<sup>2</sup>; Ben Shen<sup>3</sup>; Christopher Walsh<sup>2</sup>; Neil Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL; <sup>2</sup>Harvard Medical School, Boston, Ma; <sup>3</sup>University of Wisconsin, Madison, WI; <sup>4</sup>Scripps Institution of Oceanography, San Diego, Ca; <sup>5</sup>California State University, Chico, Ca
- TP 309 **Structural Determination of Glycerolipids Isolated from Marine Sponge by FAB Tandem Mass Spectrometry;** Jongki Hong<sup>1</sup>; Min-Sun Kim<sup>1</sup>; Ji-Hye Gil<sup>3</sup>; Jee H. Jung<sup>2</sup>; <sup>1</sup>College of Pharmacy, Kyung Hee University, Seoul, South Korea; <sup>2</sup>College of Pharmacy, Pusan National University, Pusan, South Korea; <sup>3</sup>Korea Basic Science Institute, Seoul, South Korea
- TP 310 **Characterization of Iridoids by Metal Complexation using Electrospray-Mass Spectrometry and/or Liquid Chromatography-Electrospray-Mass Spectrometry;** Mathew M Nindi<sup>1</sup>; Andrew Muzila<sup>1</sup>; Moses N. Munkombwe<sup>1</sup>; Titus A. M. Msagati<sup>1</sup>; <sup>1</sup>University of Botswana, Department of Chemistry, Gaborone, Botswana
- TP 311 **A Combined MS/MS, NMR, and ab initio Computational Study of Flavonoids and Flavonoid Glycosides;** Raymond E. March<sup>1</sup>; Darcy C. Burns<sup>1</sup>; Errol G. Lewars<sup>1</sup>; Hongxia Li<sup>1</sup>; David A. Ellis<sup>1</sup>; <sup>1</sup>Trent University, Peterborough, ON, Canada
- TP 312 **An LC/MS/MS Approach for Characterization of Silybin, Isosilybin, Silydianin and Silychristin in Milk Thistle Standardized Extract and Human Plasma;** James I. Lee<sup>1</sup>; Di Wu<sup>1</sup>; Bih Hsu<sup>2</sup>; Jeffrey S. Barrett<sup>1</sup>; <sup>1</sup>The

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- Children's Hospital of Philadelphia, Philadelphia, PA;  
<sup>2</sup>Exelixis, Inc., South San Francisco, CA
- TP 313 **The Use of Exact Mass Measurements at High Resolution to Probe Structural Diversity in Complex Natural Products Mixtures;** Deborah Zink<sup>1</sup>; Scott Campbell<sup>2</sup>; <sup>1</sup>Merck Research Laboratories, Rahway, NJ; <sup>2</sup>Sierra Analytics, Inc., Modesto, CA
- TP 314 **LC-MS/MS Analysis of Glucosinolates and their Enzymatic Degradation Products in Meadowfoam Seed Meal;** Nicholas G. Kesinger<sup>1</sup>; Jeffrey Morré<sup>1</sup>; Stephen Machado<sup>1</sup>; Jan F. Stevens<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, Or
- TP 315 **Structural Analysis of Sepia Melanin Degradation Products by Liquid Chromatography- Tandem Mass Spectrometry;** Weslyn C. Ward<sup>1</sup>; William S. Lee<sup>1</sup>; Lian Hong<sup>1</sup>; John D. Simon<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- TP 316 **Determination of Ginkgolides and Flavonols in Ginkgo Biloba Products and NIST Ginkgo Reference Standard by LC/UV/MS;** Mustafa Ozcan<sup>1</sup>; Pei Chen<sup>1</sup>; <sup>1</sup>USDA,, Beltsville Hhuman Nutrition Resarch Center, Beltsville, MD
- TP 317 **Rapid Determination of Catechins in Tea and Chocolate using Ultra Performance Liquid Chromatography-Tandem Mass Spectrometry;** Joseph J. Dalluge<sup>1</sup>; Keri L. Ross<sup>1</sup>; Travis T. Tu<sup>1</sup>; <sup>1</sup>Cargill Incorporated, Minneapolis, MN
- TP 318 **Accurate Mass Quantitation of Ginsenosides in Dietary Supplements using Simultaneous MSn Confirmation;** Helmüt Muenster<sup>1</sup>; Mary Blackburn<sup>1</sup>; <sup>1</sup>Thermo Electron, Somersset, NJ
- TP 319 **Lycopene Uptake and Sub-Cellular Localization in Prostate Cancer Cells;** Ang Liu<sup>1</sup>; Yan Pang<sup>1</sup>; Dongwei Zhu<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL

### GLYCOPROTEINS I

- TP 320 **Towards Automated Glycoanalysis of Proteomes: Partial Fractionation and Limited Database Deployment;** Lewis K Pannell<sup>1</sup>; Julio C Ruiz<sup>1</sup>; Amra Zuzo<sup>1</sup>; Nathan E Jones<sup>2</sup>; Tina R Hubler<sup>1</sup>; <sup>1</sup>Cancer Research Institute, USA, Mobile, AL; <sup>2</sup>Penn State University, University Park, PA
- TP 321 **Sequencing of N-Linked Glycans of 1-D SDS-PAGE Separated Glycoprotein: Fragmentation of 3-Aminophthalic Hydrazide-Derivatized Oligosaccharides with MALDI-TOF/TOF;** So Young Jang<sup>1</sup>; Seung Il Kim<sup>1</sup>; Jong-Soon Choi<sup>1</sup>; Young Hwan Kim<sup>1</sup>; <sup>1</sup>Proteomics Team, Korea Basic Science Institute, Taejeon, South Korea
- TP 322 **Structural Analysis of Rat Epididymal Cysteine Rich Secretory Protein CRISP1;** Joseph L Wothers<sup>1</sup>; Chee-Keng Ng<sup>1</sup>; Mike Nolan<sup>1</sup>; Kenneth Roberts<sup>2</sup>; Kathy Ensrud<sup>2</sup>; David Hamilton<sup>2</sup>; Daniel Johnston<sup>1</sup>; Qiu Yongchang<sup>1</sup>; <sup>1</sup>Wyeth Research, Cambridge, MA; <sup>2</sup>University of Minnesota, Minneapolis, MN
- TP 323 **Development of Reversed Phase HPLC Methods for Monitoring Fragments and Oxidized Species in Humanized Monoclonal Antibodies;** Jinhua Feng<sup>1</sup>; Mingyan Cao<sup>1</sup>; Ziping Wei<sup>1</sup>; Mark A. Schenerman<sup>1</sup>; <sup>1</sup>Medimmune, Gaithersburg, MD
- TP 324 **Comparative Serum Glycoproteomics using Lectin Selected Glycoproteins with Glycan Structure Analysis by QIT MS: Application to Pancreatic Cancer Serum;** Jia Zhao<sup>1</sup>; Diane M. Simeone<sup>1</sup>; Daivd M. Lubman<sup>1</sup>; <sup>2</sup>Fan Xiang; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Shimadzu Biotech, Pleasanton, CA

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- TP 325 **Microwave Assisted Deglycosylation of Antibodies for Accurate Intact Molecular Weight Determination;** Jennie Lill<sup>1</sup>; Wendy Sandoval<sup>1</sup>; Helga Raab<sup>1</sup>; Fred Arellano<sup>1</sup>; David Arnott<sup>1</sup>; Richard Vanden<sup>1</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA
- TP 326 **Glycosylation of Porcine Seminal Plasma Proteins: Selective Enrichment and Characterization;** David S. Selby<sup>1</sup>; Martin R. Larsen<sup>1</sup>; Gareth Evans<sup>2</sup>; Peter Roepstorff<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>The University of Sydney, Sydney, Australia
- TP 327 **Glycosylation Profiling of a Therapeutic Recombinant Monoclonal Antibody with Two Glycosylation Sites by Liquid Chromatography/Mass Spectrometry;** Amareth Lim<sup>1</sup>; Angelia Reed-Bogan<sup>1</sup>; Bryan J. Harmon<sup>1</sup>; <sup>1</sup>Eli Lilly and Company, Indianapolis, Indiana
- TP 328 **A Method for Peptide Identification during Glycopeptide Analysis using a Prediction Table and Collision Induced Dissociation Mass Spectrometry;** Janet W. Irungu<sup>1</sup>; Dilusha S Dalpathado<sup>1</sup>; Hy-Vy Ha<sup>2</sup>; George R Bousfield<sup>2</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS; <sup>2</sup>Wichita State University, Wichita, KS
- TP 329 **On-line Nano-LC-ECD FT-ICR Mass spectrometry for Determination of O-Linked Glycosylation in MUC1 Mucin Reveals Two Variants of Site Occupancy;** Carina Sihlbom<sup>1</sup>; Malin Baeckstroem<sup>1</sup>; Hasse Karlsson<sup>1</sup>; Carol L Nilsson<sup>2</sup>; Gunnar C Hansson<sup>1</sup>; <sup>1</sup>Institute of Biomedicine, Goteburg University, Goteburg, Sweden; <sup>2</sup>NHMF and Florida State University, Tallahassee, FL
- TP 330 **ESI-FTICR Studies of a Metalloprotein Laccase: Copper Depletion and Glycoforms;** Asse Marjasvaara<sup>1</sup>; Kristiina Kruus<sup>2</sup>; Pirjo Vainiotalo<sup>1</sup>; <sup>1</sup>University of Joensuu, Joensuu, Finland; <sup>2</sup>VTT Biotechnology, Espoo, Finland
- TP 331 **Structural Characterization of a Recombinant Antibody Produced in Yeast;** P. Clayton Gough<sup>1</sup>; <sup>1</sup>Eli Lilly and Company, Indianapolis, IN
- TP 332 **Data-Dependent Neutral Loss Analysis of Glycans and Glycoprotein Digests;** Patrick D. Perkins<sup>1</sup>; Bryan D. Miller<sup>1</sup>; Ning Tang<sup>1</sup>; Christine A. Miller<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- TP 333 **Automated LC-MALDI Analysis of Glycopeptides from Glycoprotein Digests using DHB as Matrix;** Arndt Asperger<sup>1</sup>; Anja Resemann<sup>1</sup>; Katrin Spabier<sup>1</sup>; Detlef Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany
- TP 334 **Structural Determination of the N- and C-Terminus in gp41, the Predominant Glycoprotein in the Vitelline Envelope of Xenopus laevis Eggs;** Haiqiang Yu<sup>1</sup>; Ruben T. Almaraz<sup>2</sup>; Kenji Murata<sup>2</sup>; Jerry L. Hedrick<sup>2</sup>; Fan Xiang<sup>3</sup>; Andreas H. Franz<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA; <sup>2</sup>University of California, Davis, CA; <sup>3</sup>Shimadzu Biotech Corporation, Pleasanton, CA
- TP 335 **Purification and Characterization of a Therapeutic Monoclonal Antibody from Preclinical Serum Samples;** Camille N. Strachan<sup>1</sup>; Michael Lewis<sup>1</sup>; Michael Bond<sup>1</sup>; Qing Mike Tang<sup>1</sup>; <sup>1</sup>Centocor R&D, Inc., Radnor, PA
- TP 336 **Molecular Basis for Glycoprotein P0 Dimer in Native Membranes of Xenopus laevis Peripheral Nerve -Non-covalent Equilibrium Between Dimer and Monomer;** Bo Xie<sup>1</sup>; Xiaoyang Luo<sup>2</sup>; Daniel A. Kirschner<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston College, Chestnut Hill, MA
- TP 337 **Analysis of Glycopeptides with ESI Liner Ion Trap FT MS;** Shohei Shioyama<sup>1</sup>; Tomonori Takami<sup>1</sup>; Yasuhiro



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- Yamashita<sup>1</sup>; Rieko Goto<sup>1</sup>; Naoe Yamane<sup>1</sup>; Hisami Murai<sup>1</sup>; Zenzaburo Tozuka<sup>1</sup>; <sup>1</sup>JCL Bioassay, Nishiwaki, Japan
- TP 338 **Use of High Performance Boronate Affinity Chromatography Combined with LC-MS in Isolation and Identification of Glycoproteins from Human Serum;** Chen Li<sup>1</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- TP 339 **N-linked Glycosylation in Non-Consensus Sequence;** Zhuchun Wu<sup>1</sup>; Luke Bergerud<sup>1</sup>; Angie Deng<sup>1</sup>; Michael Lemar<sup>1</sup>; Mark Hesselberg<sup>1</sup>; Thomas Spitznagel<sup>1</sup>; Michael Byrne<sup>1</sup>; <sup>1</sup>Human Genome Sciences, Inc., Rockville, MD
- TP 340 **Structural Assignments of N-Glycans and Identification of Peptide Sequence of N-Glycopeptides Using na NonESI/Linear-IT-TOF MS and MS<sup>n</sup> Spectral Matching;** Hiroki Ito<sup>1</sup>; Yasuhiro Takegawa<sup>1</sup>; Kisaburo Deguchi<sup>1</sup>; Shinji Nagai<sup>2</sup>; Shinji Yoshioka<sup>2</sup>; Hiroaki Nakagawa<sup>1</sup>; Yasuro Shinohara<sup>1</sup>; Shin-Ichiro Nishimura<sup>1</sup>; <sup>1</sup>Hokkaido University, Sapporo, Japan; <sup>2</sup>Hitachi High-Technologies Corporation, Tokyo, Japan

### MODIFIED PROTEINS II

- TP 341 **Identification and Characterization of a New Ubiquitin-Like Protein Modification-Neddylolation using a Targeted Proteomic Approach;** Jeffrey Jones<sup>1</sup>; Yinying Yang<sup>1</sup>; Kenneth Wu<sup>2</sup>; Cortnie Guerrero<sup>1</sup>; Nadinath Nillegoda<sup>2</sup>; Pan Zhen-Qiang<sup>2</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California Irvine, Irvine, CA; <sup>2</sup>Mount Sinai School of Medicine, New York, NY
- TP 342 **Intact Protein LC-FTICR MS Identifies Calmodulin as a Substrate for Putative Denitrase in Macrophages;** Natacha M. Lourette<sup>1</sup>; Heather S. Smallwood<sup>1</sup>; Seema Sharma<sup>1</sup>; Curt B. Boschek<sup>1</sup>; David C. Simpson<sup>1</sup>; Thomas C. Squier<sup>1</sup>; Richard D. Smith<sup>1</sup>; Ljiljana Pasa-Tolic<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 343 **Endogenously Nitrated Proteins in Mouse Brain: Links To Neurodegenerative Disease;** Colette A. Sacksteder<sup>1</sup>; Wei-jun Qian<sup>1</sup>; Tatyana V. Knyushko<sup>1</sup>; Haixing Wang<sup>1</sup>; Mark H. Chin<sup>2</sup>; Goran Lacan<sup>2</sup>; William P. Melega<sup>2</sup>; David G. Camp II<sup>1</sup>; Richard D. Smith<sup>1</sup>; Desmond J. Smith<sup>2</sup>; Thomas C. Squier<sup>1</sup>; Diana J. Bigelow<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>David Geffen School of Medicine at UCLA, Los Angeles, CA
- TP 344 **Integrated Strategy for Proteomic Analysis of Acetylated Lysine using Tandem Mass Spectrometry;** Morten Beck Trelle<sup>1</sup>; Hye Ryung Jung<sup>1</sup>; Saverio Minucci<sup>2</sup>; Ole Nørregaard Jensen<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>European Institute of Oncology, Milan, Italy
- TP 345 **Homocysteine Thiolactone Modification of Fibrinogen Analyzed by Mass Spectrometry and its Implication to Impaired Fibrinolysis;** Maria E. Warren<sup>1</sup>; Derrick L. Sauls<sup>2</sup>; Carol E. Parker<sup>1</sup>; Maureane Hoffman<sup>3</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Durham Veterans Affairs Medical Center, Durham, NC; <sup>3</sup>Duke University, Durham, NC
- TP 346 **Withdrawn**
- TP 347 **Seyting Histone Lysine Methyltransferases and Heterochromatin Straight;** Tara L. Muratore<sup>1</sup>; Yifan Liu<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
- TP 348 **Screening for Chemoprevention Agents in the Botanical Dietary Supplement *Angelica sinensis* using Mass Spectrometry;** Dongting Liu<sup>1</sup>; Yan Luo<sup>1</sup>; Birgit M. Dietz<sup>1</sup>; Aimee L. Egger<sup>1</sup>; Judy L. Bolton<sup>1</sup>; Guido F.

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- Pauli<sup>1</sup>; Andrew D. Mesecar<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL
- TP 349 **Extensive Age-Related Deamidation of Human  $\gamma$ S Crystallin at a Single Site Determined Quantitatively by Top Down Mass Spectrometry;** Vlad Zabrouskov<sup>1</sup>; Noah E. Robinson<sup>2</sup>; Jennifer Zhang<sup>1</sup>; Kirsten J. Lampi<sup>3</sup>; Arthur B. Robinson<sup>2</sup>; <sup>1</sup>Thermo Electron, San Jose, CA; <sup>2</sup>Oregon Institute of Science and Medicine, Cave Junction, OR; <sup>3</sup>Oregon Health and Science University, Portland, OR
- TP 350 **Reprogramming of Post-translational modifications on Histones H3 and H4 by Egg Extracts from *Xenopus* Laevis;** Raghu K. Chitta<sup>1</sup>; David F. Shechter<sup>2</sup>; Benjamin A. Garcia<sup>1</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>Rockefeller University, New York, NY
- TP 351 **Improving Dynamic Range on the LTQ-FT Instrument using Hypothesis-Driven Mass Spectrometry;** Nadezhda A. Galeva<sup>1</sup>; Yakov M. Koen<sup>1</sup>; Viktor S. Sharov<sup>1</sup>; Christian Schöneich<sup>1</sup>; Robert B. Hanzlik<sup>1</sup>; Todd D. Williams<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS
- TP 352 **Characterization and Quantitation of Glycated Hemoglobins;** Brian Imai<sup>1</sup>; Xianglin Yuan<sup>1</sup>; Nagarajan Chandramouli<sup>1</sup>; Haiteng Deng<sup>1</sup>; <sup>1</sup>Rockefeller University, New York, NY
- TP 353 **Top Down Mass Spectrometric Analyses of Human Histone H4: Determination of Cancer-Specific and Cell-cycle Correlated Modification Profiles;** James J. Pesavento<sup>1</sup>; Craig A. Mizzen<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois - Urbana, Urbana, IL
- TP 354 **Identification and Structure Determination of Tyrosine Nitration in Human Eosinophils using High Resolution Mass Spectrometry in Combination with Immunoanalytical Methods;** Alina Petre<sup>1</sup>; Reinhold Weber<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>University of Tübingen, Tübingen, Germany

### NEUROPEPTIDES

- TP 355 **Application of MALDI-FTMS to Determine Variations in Peptide Isoforms Between Individuals using Single Tissues or Organs from Decapod Crustaceans;** Christopher R. Cashman<sup>1</sup>; Yun-Wei A. Hsu<sup>2</sup>; Daniel I. Messinger<sup>2</sup>; Patsy S. Dickinson<sup>1</sup>; Andrew E. Christie<sup>2</sup>; Elizabeth A. Stemmler<sup>1</sup>; <sup>1</sup>Bowdoin College, Brunswick, ME; <sup>2</sup>University of Washington, Seattle, WA
- TP 356 **Identification of Potential Biomarkers for Multiple Sclerosis in Cerebrospinal Fluid using SELDI and MALDI-TOF MS;** Ashley S. Beasley<sup>1</sup>; David Wheeler<sup>1</sup>; Avindra Nath<sup>1</sup>; David Irani<sup>1</sup>; Douglas Kerr<sup>1</sup>; Peter Calabresi<sup>1</sup>; Robert J. Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- TP 357 **Qualitative and Quantitative *in situ* Analysis of Neuropeptides Involved in Feeding;** Stephanie S. DeKeyser<sup>1</sup>; Kimberly K. Kutz-Naber<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of WI, Madison, WI
- TP 358 **Mass Spectrometric Measurements from Neurons Cultured in Microfluidic Devices;** Michael L. Heien<sup>1</sup>; Lucas B. Thompson<sup>1</sup>; Ralph G. Nuzzo<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana-Champaign, IL
- TP 359 **Characterizing Cell-to-Cell Signaling Molecules in the Mammalian Brain;** Suresh P. Annangudi<sup>1</sup>; Nathan G. Hatcher<sup>1</sup>; Elena V. Romanova<sup>1</sup>; Stanislav S. Rubakhin<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana-Champaign, IL



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- TP 360 **On-Target Reduction and Alkylation of Disulfide-Bond Containing Peptides;** Kimberly K. Kutz-Naber<sup>1</sup>; Shelly K. Heinzelman<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI
- TP 361 **Rat Neuropeptidomics by LC/MS/MS and MALDI-FTMS: Enhanced Extraction Techniques Coupled with 2D RP-RP HPLC Separation;** James Dowell<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin, Madison, WI
- TP 362 **Capillary LC-MALDI-TOF-MS at the Attomole Level for Discovering Endogenous Peptides in Rat Brain;** Hui Wei<sup>1</sup>; Kerstin Nolkrantz<sup>1</sup>; Kristin Schultz<sup>1</sup>; Minshan Shou<sup>1</sup>; Robert T. Kennedy<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- TP 363 **The Effect of Reserpine on the Levels of Striatal Neuropeptides - A Time Course Study;** Anna Nilsson<sup>1</sup>; Karl Sköld<sup>1</sup>; Maria Fälth<sup>1</sup>; Marcus Svensson<sup>1</sup>; Per Svenningsson<sup>2</sup>; Per E. Andrén<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institute, Stockholm, Sweden
- TP 364 **Accurate Mass Mapping and Sequencing of Corpus Cardiacum Neuropeptides by Means of LC-MALDI-TOF MS/MS and UPLC-TOF MS;** Peter D. Verhaert<sup>1</sup>; Gerold Schwarz<sup>2</sup>; Arthur R. Kroon<sup>1</sup>; James L. Langridge<sup>2</sup>; Johannes P.C. Vissers<sup>2</sup>; <sup>1</sup>Delft University of Technology, Delft, Netherlands; <sup>2</sup>Waters Corporation - MS Technologies Centre, Manchester, UK
- TP 365 **Coupling Microdialysis to NanoLC-MS for In Vivo Monitoring of Neuropeptides;** Heidi L. Behrens<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- TP 366 **Optimization of Peptide Extraction Conditions for Peptidomic Studies;** Fa-Yun Che<sup>1</sup>; Lloyd D Fricker<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, New York
- TP 367 **Mass Spectrometric Approaches for the Analysis of Biomarkers of Cocaine Addiction-Related Behaviors;** Elena V. Romanova<sup>1</sup>; Jessica Stanis<sup>1</sup>; Joshua M. Gulley<sup>1</sup>; Stanislav S. Rubakhin<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL
- TP 368 **Immunoaffinity-Based Mass Spectrometric Characterization of the RFamide Neuropeptide Family in the Pericardial Organ of Cancer borealis;** Mingming Ma<sup>1</sup>; Kimberly K. Kutz-Naber<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin, Madison, WI

### PROTEIN CONFORMATION I: HYDROGEN EXCHANGE

- TP 369 **Conformational Studies on the Tachykinin and Related Peptides using Hydrogen/Deuterium Exchange Coupled with Mass Spectrometry;** Tarun Ghevi<sup>1</sup>; Chhabil Dass<sup>1</sup>; <sup>1</sup>The University of Memphis, Memphis, TN
- TP 370 **Conformational Properties of Full Length HIV and SIV Nef by Mass Spectrometry;** James M. Hochrein<sup>1</sup>; Thomas E. Wales<sup>1</sup>; Edwina C. Lerner<sup>2</sup>; Anthony P. Schiavone<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA
- TP 371 **Hydrogen Exchange FT-ICR Mass Spectrometry Study on Intact Human SOD1;** Murat Karabacak<sup>1</sup>; Mike Aguiar<sup>2</sup>; Jeffrey Agar<sup>1</sup>; Bernard F. Gibbs<sup>2</sup>; <sup>1</sup>Brandeis University, Waltham, MA; <sup>2</sup>McGill University, Montreal, Canada
- TP 372 **Activator Binding Site of Arp2/3 Complex Probed by Hydrogen Exchange and Mass spectrometry;** Wendy Zenccheck<sup>1</sup>; Hui Xiao<sup>1</sup>; Steven Almo<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY

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- TP 373 **Ligand-Induced Conformational Changes in Human Serum Transferrin probed by SUPREX;** Petra L. Roullhac<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- TP 374 **Novel Application of Supercritical Fluid Chromatography to Eliminate Back Exchange after Solution-Phase Hydrogen/Deuterium Exchange;** Mark R. Emmett<sup>1</sup>; Sasa Kazazic<sup>1</sup>; Alan G. Marshall<sup>1</sup>; Wei Chen<sup>2</sup>; Stone D.-H Shi<sup>2</sup>; Ben Bolanos<sup>2</sup>; Michael J. Greig<sup>2</sup>; <sup>1</sup>Ion Cyclotron Resonance Program, NHMFL-FSU, Tallahassee, FL; <sup>2</sup>Global Research & Development, Pfizer Inc., San Diego, CA
- TP 375 **H/D Exchange MS Study of Peroxiredoxin;** Ji-Eun Yi<sup>1</sup>; Leslie B. Poole<sup>2</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon state university, Corvallis, OR; <sup>2</sup>Wake Forest university, winston-salem, NC
- TP 376 **Time Resolved H/D Exchange of Gas-Phase Protein Ions in a Linear Ion Trap;** P. John Wright<sup>1</sup>; D.J. Douglas<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC
- TP 377 **The Interaction of Thrombin and its DNA Ligand Investigated by PLIMSTEX;** J. Micah Wilcox<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, Saint Louis, MO 63130
- TP 378 **Investigation of Various Ligands Interactions with Human RXR $\alpha$  Ligand Binding Domain by Hydrogen/Deuterium Exchange and Mass Spectrometry;** Xuguang Yan<sup>1</sup>; David Broderick<sup>1</sup>; Jeff Morre<sup>1</sup>; Michael Schimerlik<sup>1</sup>; Max Deinzer<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- TP 379 **Site Specific H/D Exchange Analysis of Protein by Mass Spectrometry Coupled with Carboxypeptidase Digestion;** Tatsuya Yamamoto<sup>1</sup>; Shunsuke Izumi<sup>1</sup>; Jorge Fernandez-de-Cossio<sup>2</sup>; Toshifumi Takao<sup>3</sup>; Kunihiro Gekko<sup>1</sup>; <sup>1</sup>Hiroshima University, Higashi-Hiroshima, Japan; <sup>2</sup>Center for Genetic Engineering and Biotechnology, Havana, Cuba; <sup>3</sup>Institute for Protein Research, Osaka University, Suita, Japan
- TP 380 **Conformational Analysis of  $\alpha$ - and  $\beta$ -Neo-Endorphins in Membrane-Mimetic Environments by Hydrogen/Deuterium Exchange and ESI-MS/MS;** Hari Kosanam<sup>1</sup>; Chhabil Dass<sup>1</sup>; <sup>1</sup>The University of Memphis, Memphis, TN
- TP 381 **Toward Conformer-Specific Characterization of Protein Structure and Dynamics: Combination of Hydrogen Exchange and Tandem Mass Spectrometry;** Rinat Abzalimov<sup>1</sup>; Igor Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts at Amherst, Amherst, MA
- TP 382 **Structural Analysis of a Metal-Binding Protein Domain by Hydrogen/Deuterium Exchange and ESI-MS/MS;** Peter L. Ferguson<sup>1</sup>; Jingxi Pan<sup>1</sup>; Brian R Dempsey<sup>1</sup>; Gilles A Lajoie<sup>1</sup>; Brian H Shilton<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, ON CANADA
- TP 383 **Non-Covalent Small Heat Shock Protein Complex Studied by Hydroxyl radical Modification, H/D Exchange and Native Nanospray;** Guilong Cheng<sup>1</sup>; David Hambly<sup>2</sup>; Christopher M. Jones<sup>1</sup>; Elizabeth Vierling<sup>1</sup>; Michael L. Gross<sup>2</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Washington University in St. Louis, St. Louis, MO
- TP 384 **Hydrogen/Deuterium Exchange (HDX) is an Indispensable Tool in determining Regions of Destabilization in ALS-Causing SOD1 Mutant proteins;** Armando Durazo<sup>1</sup>; Bryan F. Shaw<sup>1</sup>; Kym F.

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- Faull<sup>1</sup>; Julian P. Whitelegge<sup>1</sup>; Joan S. Valentine<sup>1</sup>;  
<sup>1</sup>University of California, Los Angeles, CA
- TP 385 **Local H/D Exchange Kinetics of Calmodulin and Human Centrin 2 Reveal Differences in Calcium Binding;** Justin Sperry<sup>1</sup>; Michael L. Gross<sup>1</sup>; Rajiv Kumar<sup>2</sup>; <sup>1</sup>Washington University in St. Louis, Saint Louis, MO; <sup>2</sup>Mayo Clinic, Rochester, MN
- TP 386 **Use of Two Different Proteases to Improve the Spatial Resolution in the H/D Exchange Study of the Creatine Kinase Dynamics;** Hortense Mazon<sup>2</sup>; Christian Vial<sup>2</sup>; Eric Forest<sup>1</sup>; <sup>1</sup>Institute of Structural Biology, Grenoble, France; <sup>2</sup>University Claude Bernard, Lyon, France
- TP 387 **Identification and Characterization of EX1 Kinetics in H/D Exchange Mass Spectrometry by Peak Width Analysis;** Matthew Hotchko<sup>1</sup>; David D. Weis<sup>2</sup>; Lynn F. Ten Eyck<sup>1</sup>; John R. Engen<sup>2</sup>; <sup>1</sup>University of California - San Diego, La Jolla, CA; <sup>2</sup>University of New Mexico, Albuquerque, NM
- TP 388 **Conformational Dynamics of Enzymes during Catalysis Studied by Hydrogen-Deuterium Exchange and ESI-MS;** Yuhong Liu<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>The University of Western Ontario, London, Canada
- TP 389 **Conformational Analysis of the Tip Protein from Herpesvirus Saimiri with Hydrogen Exchange and Mass Spectrometry;** Jennifer M. Carter<sup>1</sup>; R. P. Triple<sup>2</sup>; Lori A. Emert-Sedlak<sup>2</sup>; Edwina C. Lerner<sup>2</sup>; Jeremy J. Applen<sup>1</sup>; Daniel F. Cimino<sup>1</sup>; David D. Weis<sup>1</sup>; Bartholomew M. Sefton<sup>3</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA; <sup>3</sup>The Salk Institute for Biological Studies, La Jolla, CA
- TP 390 **Mapping the Interaction Between Human Chorionic Gonadotropin and its Receptor by Hydrogen Exchange and Mass Spectrometry;** Yongsheng Li<sup>1</sup>; Ron Orlando<sup>1</sup>; David Puett<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 391 **Conformational Analysis of Type III Secretion Pilins by HDX and Mass Spectrometry;** Olivia Guerre<sup>1</sup>; Jason M. Criscione<sup>1</sup>; Michael D. Stein<sup>1</sup>; Joel S. Lwande<sup>1</sup>; J. Throck Watson<sup>1</sup>; William J. Wedemeyer<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- TP 392 **Binding Induced Changes in Backbone Dynamics for the Hck YEEI:HIV Nef Protein Complex Observed by HX MS;** Thomas E. Wales<sup>1</sup>; James M. Hochrein<sup>1</sup>; Edwina C. Lerner<sup>2</sup>; Anthony P. Schiavone<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA
- TP 393 **HXMS Reveals Phosphorylation-Dependent Conformational Changes in the catalytic Domain of Lymphocytic Cell Kinase;** David D. Weis<sup>1</sup>; Lori A. Emert-Sedlak<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA
- TP 394 **Automated Hydrogen Deuterium Exchange with High Resolution FT-ICR MS Analysis and Enhanced Automated Data Reduction;** Saša Kazazic<sup>1</sup>; Mark R. Emmett<sup>1</sup>; Gregory T. Blakney<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>ICR Program, NIMFL, Florida State University, Tallahassee, FL

### PEPTIDES: FRAGMENTATION AND SEQUENCING II

- TP 395 **Abundant B-Type Ions produced in Electron Capture Dissociation (ECD) of Peptides Without Basic Amino Acid Residues;** Haichuan Liu<sup>1</sup>; Kristina Hakansson<sup>1</sup>;

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- <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, MI
- TP 396 **The CID and ECD Behavior of Sulfur-Containing Peptides;** Robert J. Chalkley<sup>1</sup>; Katalin F. Medzihradsky<sup>1</sup>; Al L. Burlingame<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA
- TP 397 **B-Ions and Other Odd Fragments in Electron Capture Dissociation;** Kim F. Haselmann<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark
- TP 398 **Differentiating between Y-ions and B-ions in a CID Spectrum using Positive to Negative Charge Inversion;** Joshua F. Emory<sup>1</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, Indiana
- TP 399 **Electron Capture Dissociation (ECD) of Bipyridine Capped Peptides and Metal Directed Protein Bundles;** Jace W. Jones<sup>1</sup>; Frank Turecek<sup>1</sup>; David R. Goodlett<sup>1</sup>; Tomikazu Sasaki<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 400 **Comparison of Electron Capture Dissociation (ECD) Behaviors of Alanine-Rich Peptides that Contain Lysine Homologues;** Sunyoung Lee<sup>1</sup>; Soojin Park<sup>1</sup>; Han Bin Oh<sup>1</sup>; <sup>1</sup>Sogang University, Seoul, South Korea
- TP 401 **A Comparison of Electron-Transfer Dissociation to Collision-Activated Dissociation Tandem Mass Spectrometry for Peptide (1 – 5 kDa) Sequencing;** David M. Good<sup>1</sup>; Matthew Wirtala<sup>1</sup>; Graeme C. McAlister<sup>1</sup>; Danielle L. Swaney<sup>1</sup>; Jae C. Schwartz<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- TP 402 **Electron Capture Dissociation Proceeds With a Low Degree of Intramolecular Migration of Amide Hydrogens;** Thomas J.D. Jorgensen<sup>1</sup>; Jesper V. Olsen<sup>3</sup>; Matthias Mann<sup>3</sup>; Peter Roepstorff<sup>1</sup>; Henrik Gardsvoll<sup>2</sup>; Michael Ploug<sup>2</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Finsen Laboratory, Rigshospitalet, Copenhagen, Denmark; <sup>3</sup>Max-Planck-Institute of Biochemistry, Martinsried, Germany
- TP 403 **Generation of b-/y- and Atypical Internal Fragment Ions in Electron Capture Dissociation of Peptides;** Eva Yi Man Fung<sup>1</sup>; Kelly Wai Yi Chan<sup>1</sup>; Dominic Tak-Wah Chan<sup>1</sup>; <sup>1</sup>The Chinese University of Hong Kong, HK SAR, China
- TP 404 **Tryptic Peptide Fragmentation Using Time-Delayed Fragmentation For Specific Y-ion Series Generation;** Alan Morrish<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- TP 405 **Electron Transfer Dissociation of Disulfide Linked Polypeptides: Effect of Charge State and Charge Site;** Harsha P. Gunawardena<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 406 **A Novel SID/TOF Source for MALDI-IM-SID-oTOF MS;** Wenjian Sun<sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- TP 407 **Phospho-peptide Fragmentation with Electron Transfer Dissociation Mass Spectrometry;** An Chi<sup>1</sup>; Dina Bai<sup>1</sup>; Lewis Y. Geer<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>National Center for Biotechnology Information, Bethesda, MD
- TP 408 **Thermally-Induced Fragmentation of Peptide and Protein Ions at Atmospheric Pressure;** Hao Chen<sup>1</sup>; Livia Eberlin<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 409 **Mechanisms of Electron Capture Dissociation and Collision-Activated Dissociation are truly Complementary;** Frank Kjeldsen<sup>1</sup>; Mikhail M. Savitski<sup>1</sup>;

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- Michael L. Nielsen<sup>1</sup>; Roman A. Zubarev<sup>1</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*
- TP 410 **Electron Transfer Dissociation of Multiply Charged Peptides: Investigation of the Z. + 33Da Adduct;** David E. Erickson<sup>1</sup>; Yu Xia<sup>1</sup>; Paul Chrisman<sup>1</sup>; Sharon Pitteri<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- TP 411 **Dissociation Induced by Electron Transfer of Multiply Charged Ions on Collision with Rare Gas and Alkali Metal Targets;** Shigeo Hayakawa<sup>1</sup>; Akihiro Kitaguchi<sup>1</sup>; Satoko Kameoka<sup>1</sup>; Michisato Toyoda<sup>2</sup>; Toshio Ichihara<sup>2</sup>; <sup>1</sup>*Osaka Prefecture University, Sakai, Osaka, Japan*; <sup>2</sup>*Osaka University, Toyonaka, Osaka, Japan*
- TP 412 **Improved Sequencing of Oxidized Peptides Using Electron Transfer Dissociation in a 3-D Quadrupole Ion Trap;** Richard W. Vachet<sup>1</sup>; Juma D. Bridgewater<sup>1</sup>; Jonathan Wilson<sup>2</sup>; Ali Kettani<sup>2</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*Bruker Daltonics, Inc., Billerica, MA*
- TP 413 **Comparison of Collision-Induced Dissociation (CID) Fragmentation with Electron Capture Dissociation (ECD) fragmentation of the phospho peptide;** Tomonori Takami<sup>1</sup>; Shohei Shiroyama<sup>1</sup>; Rieko Goto<sup>1</sup>; Naoe Yamane<sup>1</sup>; Hisami Murai<sup>1</sup>; Zenzaburo Tozuka<sup>1</sup>; <sup>1</sup>*JCL Bioassay, Nishiwaki, Japan*
- TP 414 **Electron Transfer Dissociation for Sequence Characterization of Larger Peptides and Small Proteins;** Jonathan Wilson<sup>1</sup>; Andreas Brekenfeld<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Ralf Hartmer<sup>2</sup>; <sup>1</sup>*Bruker Daltonics, Billerica, MA*; <sup>2</sup>*Bruker Daltonik, Bremen, Germany*
- TP 415 **Mechanistic Elements on the Hydrogen Transfers Occuring during the Electron Capture Dissociation (ECD) of Peptides;** Guillaume van der Rest<sup>1</sup>; Julia Chamot-Rooke<sup>1</sup>; <sup>1</sup>*Ecole Polytechnique, Palaiseau, France*
- TP 416 **The Effect of Collision Gas Pressure on the STEP Analysis for Two Mass Spectrometers- Triple quadrupole and Ion Trap;** Dilusha S Dalpathado<sup>1</sup>; Qing Chang<sup>1</sup>; Colleen M Burkett<sup>1</sup>; Mary Bandu<sup>1</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>*University of Kansas, Lawrence, KS*
- TP 417 **Probing the Long-lived Radical Intermediates in Electron Capture Dissociation with a Double Resonance Experiment;** Cheng Lin<sup>1</sup>; Jason J. Cournoyer<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; <sup>1</sup>*Boston University, School of Medicine, Boston, MA*
- TP 418 **Electron-Transfer Ion/Ion Reactions of Triply and Doubly Protonated Peptides: Effect of Cooling Gas Pressure;** Hongling Han<sup>1</sup>; Xiaorong Liang<sup>1</sup>; Harsha Gunawardena<sup>1</sup>; Yu Xia<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*

### PEPTIDES: QUANTITATION

- TP 419 **High throughput Quantitative Analysis of Hematide dimer by LC/MS/MS;** JooSoo Hyun<sup>1</sup>; Xun Cheng<sup>1</sup>; Douglas L. Cole<sup>1</sup>; Jing J. Zhang<sup>1</sup>; <sup>1</sup>*Affymax, Inc, Palo Alto, CA*
- TP 420 **Identification and Quantitation of Proteins in Plasma and Serum using a Non-Isobaric Labeling Technique;** James E Carlson<sup>1</sup>; Margorie S Minkoff<sup>1</sup>; Scott N Daniels<sup>1</sup>; Brian L Williamson<sup>1</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*
- TP 421 **Accomplishing Trace Level Quantitation During Bioanalytical Method Development of a Large Peptide;** Greg Rahn<sup>12</sup>; Gene Miller<sup>12</sup>; Todd Branch<sup>12</sup>; Larry Davey<sup>12</sup>; Tom Parish<sup>12</sup>; <sup>1</sup>*Procter & Gamble Pharmaceuticals, Norwich, NY*; <sup>2</sup>*Procter & Gamble Pharmaceuticals, Mason, OH*

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- TP 422 **Withdrawn**
- TP 423 **Fast and Accurate Protein Quantitation in Biological Samples - an Alternative of ELISA;** Judit Krenyacz<sup>1</sup>; Laszlo Drahos<sup>1</sup>; Zoltan Takats<sup>1</sup>; Karoly Vekey<sup>1</sup>; <sup>1</sup>*Chemical Research Center Hung. Acad. Sci., Budapest, Hungary*
- TP 424 **A Method for the Determination of Terlipressin and the Monitoring of Lys8-Vasopressin (analogs of ADH) in Human Plasma via LC-MS/MS;** Lee Winchester<sup>1</sup>; Yousef Basir<sup>1</sup>; Alan Dzerk<sup>1</sup>; Chad Briscoe<sup>1</sup>; Curtis Sheldon<sup>1</sup>; <sup>1</sup>*MDS Pharma Services, Lincoln, NE*
- TP 425 **Sensitive Quantification of the Disease Associated Prion Protein PrPSc Using Standard Peptides and Selected Reaction Monitoring;** Dorothea Rutishauser<sup>1</sup>; Erich Brunner<sup>2</sup>; Ralph Schlapbach<sup>1</sup>; Adriano Aguzzi<sup>3</sup>; <sup>1</sup>*Functional Genomics Center Zurich, Zurich, Switzerland*; <sup>2</sup>*Institute of Zoology, Zurich, Switzerland*; <sup>3</sup>*Institute of Neuropathology, University Hospital, Zurich, Switzerland*
- TP 426 **Quantitation of PYY [3-36] in Human plasma by On-line SPE LC/MS/MS;** Miryam Kadkhodayan<sup>1</sup>; Kevin McCowen<sup>1</sup>; Deirdre Hauser<sup>1</sup>; <sup>1</sup>*Amylin Pharmaceuticals Inc., San Diego, CA*
- TP 427 **Online-LC GLAD for Partition Coefficient Determination of Tau-Related Peptides;** Jessica Bereszczak<sup>1</sup>; Federico A. Rojas Quijano<sup>2</sup>; Warren J. Goux<sup>2</sup>; Francesco L. Brancia<sup>1</sup>; <sup>1</sup>*Shimadzu Research Laboratory, Manchester, UK*; <sup>2</sup>*The University of Texas at Dallas, Richardson, Texas*
- TP 428 **Quantitation of Hepcidin in Urine using Deuterated and Non-Deuterated Vinylpyridine Alkylation and SELDI;** Kenyon M Evans-Nguyen<sup>1</sup>; Amanda Ray<sup>1</sup>; Richard D Semba<sup>1</sup>; Luigi Ferrucci<sup>2</sup>; Robert J Cotter<sup>1</sup>; <sup>1</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*; <sup>2</sup>*National Institute on Aging, Baltimore, MD*
- TP 429 **Determination of the Relative and Absolute Stoichiometry of Proteins in Mixtures using Quantitative Mass Spectrometry of Fluorescent Concatenated Peptide Standards;** Dhaval Nanavati<sup>1</sup>; Marjan Gucek<sup>1</sup>; Melinda McFarland<sup>1</sup>; Jacqueline Milne<sup>2</sup>; Sriram Subramaniam<sup>2</sup>; Sanford P. Markey<sup>1</sup>; <sup>1</sup>*National Institute of Mental Health, Bethesda, MD*; <sup>2</sup>*National Cancer Institute, Bethesda, MD*
- TP 430 **Quantitation of Low Abundance Proteins in Human Plasma using Stable Isotope Standards and Capture by Anti-Peptide Antibodies (SISCAPA);** Angela M Jackson<sup>1</sup>; Derek S Smith<sup>1</sup>; Terry W Pearson<sup>1</sup>; Jamie M Thomas<sup>1</sup>; Leigh N Anderson<sup>2</sup>; <sup>1</sup>*University of Victoria, Victoria, Canada*; <sup>2</sup>*Plasma Proteome Institute, Washington, DC*
- TP 431 **Quantification of Voltage Dependant Anion Channel (VDAC) Protein in Human Alzheimer's disease Brain Mitochondrial Sample by Immunoaffinity Purification and LC-MS/MS;** Anup P. Thakur<sup>1</sup>; Mark A. Lovell<sup>1</sup>; Bert C. Lynn<sup>1</sup>; <sup>1</sup>*University of Kentucky, Lexington, KY*
- TP 432 **Quantitative Determination of Methionine Oxidation Product Levels in PEGylated Peptides by LC-MS;** Xun Cheng<sup>1</sup>; JongSoo Hyun<sup>1</sup>; Pallavi Golla<sup>1</sup>; Shan Lin<sup>1</sup>; Douglas L. Cole<sup>1</sup>; Jing J. Zhang<sup>1</sup>; <sup>1</sup>*Affymax, Inc, Palo Alto, CA*
- TP 433 **Quantification of Intermediate Abundance Proteins in Serum by Multiple-Reaction-Monitoring (MRM) Mass Spectrometry In a Single-Quadrupole Ion Trap;** Shanhua Lin<sup>1</sup>; Thomas Shaler<sup>1</sup>; Christopher Becker<sup>1</sup>; <sup>1</sup>*PPD, Menlo Park, CA*

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- TP 434 **Quantitation of Antimicrobial Peptides in Human Saliva;** Michael S. Gardner<sup>1</sup>; Yinfai Amy Siu<sup>1</sup>; James L. Stephenson<sup>1</sup>; <sup>1</sup>RTI International, Research Triangle Park, NC
- TP 435 **Targeted Protein Absolute Quantification using Isotopic Dilution with Heavy Peptides;** Stéphanie Kirsch<sup>1</sup>; Joëlle Widart<sup>1</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>University of Liege, Liege, Belgium
- TP 436 **Quantitation of Substance P in Biofluids by LC/ESI, LC/MALDI and Elisa - a Comparative Study;** Klaus C Rumpel<sup>1</sup>; Hendrik Neubert<sup>1</sup>; Marina Lumberras<sup>1</sup>; Andrew D Scott<sup>1</sup>; <sup>1</sup>Pfizer Global R&D, Sandwich, Kent, UK
- TP 437 **Stable Isotope Dilution LC-Negative ESI/MS/MS and Immunoaffinity Purification for Analysis of Amyloid Beta Peptides in Alzheimer's Disease;** Tomoyuki Oe<sup>1</sup>; Koichi Inoue<sup>1</sup>; Carlos Garner<sup>2</sup>; Brad L. Ackermann<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>Center for Cancer Pharmacology, University of Penn, Philadelphia, PA; <sup>2</sup>Drug Disposition, Eli Lilly and Company, Indianapolis, IN

### PEPTIDES: POST-TRANSLATIONAL MODIFICATIONS I

- TP 438 **Using Complementary Hydrazide Chemistry Based Methods with Precursor-Ion Scanning to Characterize Potential in Vivo Sites of HNE Modification;** Mikel R. Roe<sup>1</sup>; Hongwei Xie<sup>1</sup>; Sricharan Bandhakavi<sup>1</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>University of Minnesota, St. Paul, MN
- TP 439 **Characterization Of Human Growth Hormone Oxidation Using LC/MS and Peptide Mapping;** Charles Pan<sup>1</sup>; Jane Pepper<sup>1</sup>; Frances Liu<sup>1</sup>; Rosario LoBrutto<sup>1</sup>; Hans Wallny<sup>2</sup>; Alan Jones<sup>1</sup>; Richard Vivilecchia<sup>1</sup>; <sup>1</sup>Novartis Pharmaceuticals Corporation, East Hanover, New Jersey; <sup>2</sup>Novartis AG, Basel, Switzerland
- TP 440 **Hybrid Linear Ion Trap-FTICR Mass Spectrometer-Based Examination of Histone Post-Translational Modifications in Neurospora Crassa;** D. C. Anderson<sup>1</sup>; Kristina Smith<sup>1</sup>; Ray Green<sup>2</sup>; Eric U. Selker<sup>1</sup>; <sup>1</sup>Institute of Molecular Biology, Univ. of Oregon, Eugene, OR; <sup>2</sup>Mercer University, Atlanta, GA
- TP 441 **In vitro Model of Muscle Aging: Functional, Structural and Chemical Effects of Hydrogen Peroxide Oxidation on Skinned Muscle Fibers;** Daniel J. Spakowicz<sup>1</sup>; Ewa Prochniewicz<sup>1</sup>; Dawn A. Lowe<sup>1</sup>; LeeAnn Higgins<sup>1</sup>; Deborah A. Ferrington<sup>1</sup>; LaDora V. Thompson<sup>1</sup>; David D. Thomas<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN
- TP 442 **Defining Specificity for Four Previously Uncharacterized Histone Acetyltransferases (HATs) in Arabidopsis;** Rachel A. Reuther<sup>1</sup>; Keith W. Earley<sup>1</sup>; Craig S. Pikkard<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO
- TP 443 **Improved Methods for Comprehensive Sample Analysis Using Protein Prospector;** Peter R Baker<sup>1</sup>; Robert J Chalkley<sup>1</sup>; Katalin F Medzihradszky<sup>1</sup>; June O Snedecor<sup>1</sup>; Alma L Burlingame<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA
- TP 444 **Characterisation, Identification and Prediction of n-Terminus Acetylated Proteins;** Samuel Kanor<sup>1</sup>; Ioannis Xenarios<sup>3</sup>; Anne Estreicher<sup>4</sup>; Manfredo Quadroni<sup>1</sup>; Willy V Bienvenut<sup>2</sup>; <sup>1</sup>Protein Analysis Facility, University of Lausanne, Epalinges, Switzerland; <sup>2</sup>The Beatson Institute for Cancer Research, Glasgow, United-Kingdom; <sup>3</sup>Serono pharmaceutical research institute, Plan-les-Ouates, Switzerland; <sup>4</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland
- TP 445 **Mapping Sites of Asparagine Deamidation in Recombinant Proteins by MALDI TOF and MALDI tandem TOF mass spectrometry;** Peter S. Backlund<sup>1</sup>;

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- Pradeep Gupta<sup>2</sup>; Stephen H. Leppla<sup>2</sup>; Alfred L. Yergey<sup>1</sup>; <sup>1</sup>NICHD, National Institutes of Health, Bethesda, MD; <sup>2</sup>NIAD, National Institutes of Health, Bethesda, MD
- TP 446 **Specific Modification of Citrulline Containing Peptides and their Characterization by MALDI- and ESI Mass Spectrometry;** Anders Holm<sup>1</sup>; Nicole Sessler<sup>1</sup>; Frode Rise<sup>2</sup>; Ludvig M Sollid<sup>1</sup>; Kjell Undheim<sup>2</sup>; Burkhard Fleckenstein<sup>1</sup>; <sup>1</sup>University of Oslo, Institute of Immunology, Oslo, Norway; <sup>2</sup>University of Oslo, Department of Chemistry, Oslo, Norway
- TP 447 **Modification of Peptides by Lipid Peroxidation Products Studied by MALDI-MS/MS using a TOF/TOF Instrument;** Jianyong Wu<sup>1</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- TP 448 **Direct Detection of Covalent Lipidations of Mammalian Plasma ApoA-I;** Frederic J. Halgand<sup>1</sup>; Lang Yam<sup>1</sup>; Sara Bassilian<sup>1</sup>; Pedram Ghasri<sup>1</sup>; Puneet Souda<sup>1</sup>; Kym F. Faul<sup>1</sup>; Verne Schumaker<sup>1</sup>; Don Puppione<sup>1</sup>; Julian P. Whitelegge<sup>1</sup>; <sup>1</sup>The Pasarow Mass Spectrometry Laboratory, UCLA, Los Angeles, CA
- TP 449 **Comprehensive Analysis of Aldehyde Modifications by LC-ESI LTQ-FT MS Methods;** Erin M Shonsey<sup>1</sup>; Shannon M Eliuk<sup>1</sup>; Marion Kirk<sup>1</sup>; Helen Kim<sup>1</sup>; Matthew Renfrow<sup>1</sup>; Stephen Barnes<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL
- TP 450 **Two-Pass Searches Using Protein-Specific Custom Databases to Determine Protein Truncation Sites;** Jason C. Rogalski<sup>1</sup>; Matthew J. Sniatynski<sup>1</sup>; Sebastian G.B. Furness<sup>1</sup>; Kelly M. McNaghy<sup>1</sup>; Juergen Kast<sup>1</sup>; <sup>1</sup>The Biomedical Research Centre, Vancouver, Canada
- TP 451 **Identification and Characterization of Deamidation in anti-EGFR Monoclonal Antibody Cetuximab;** Li Yang<sup>1</sup>; Tun Liu<sup>1</sup>; Jay Charlebois<sup>1</sup>; Yuemei Ma<sup>1</sup>; Babita Saxena<sup>1</sup>; Ann Daus<sup>1</sup>; S.Joseph Tarnowski<sup>1</sup>; Qinwei Zhou<sup>1</sup>; <sup>1</sup>ImClone Systems Incorporated, Branchburg, NJ
- TP 452 **Electron Capture Dissociation and Electron Transfer Dissociation for Identification of p53 Dependent Histone Modifications Following Topoisomerase I Mediated DNA Damage;** C. Logan Mackay<sup>1</sup>; Stefan Weidt<sup>1</sup>; Emma Carrick<sup>2</sup>; Mike Lang<sup>2</sup>; J. Kenicer<sup>2</sup>; Yves Pommier<sup>3</sup>; Ted Hupp<sup>2</sup>; Pat Langridge-Smith<sup>1</sup>; R. Larry Hayward<sup>2</sup>; <sup>1</sup>SIRCAMS, University of Edinburgh, Edinburgh, UK; <sup>2</sup>Edinburgh Cancer Centre, Edinburgh, UK; <sup>3</sup>Laboratory of Molecular Pharmacology, Bethesda, MD
- TP 453 **LC/MS/MS Characterization of Oxidized Amyloid Beta Peptides as Potential Biomarkers of Alzheimer's Disease;** Koichi Inoue<sup>1</sup>; Carlos Garner<sup>2</sup>; Brad L. Ackermann<sup>2</sup>; Tomoyuki Oe<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Lilly Corporate Center, Indianapolis, IN
- TP 454 **Reliable Identification of Deamidations from Tandem Mass Spectrometry Data Using Corrected Parent Ion Masses and Chromatographic Time Differences;** Surendra Dasari<sup>1</sup>; Phillip A. Wilmarth<sup>2</sup>; D. Leif Rustvold<sup>2</sup>; Larry L. David<sup>2</sup>; Srinivasa R. Nagalla<sup>1</sup>; <sup>1</sup>School of Medicine, Oregon Health & Science Univ., Portland, OR; <sup>2</sup>School of Dentistry, Oregon Health & Science Univ., Portland, OR
- TP 455 **Characterization of Stable Cysteine Sulfenic Acid in a Synthetic Peptide PRCGVPDVA of Pro-Matrix Metalloproteinase-7 (Pro-MMP-7);** Vivekananda Shetty<sup>1</sup>; Thomas A Neubert<sup>1</sup>; <sup>1</sup>New York UniVersity School of Medicine, New York, NY

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- TP 456 **Analysis of Dynamic Changes in Post-Translational Modifications of Human Histone During Cell Cycle by Mass Spectrometry;** Débora Bonenfant<sup>1</sup>; Harry Towbin<sup>1</sup>; Michèle Coulot<sup>1</sup>; Adrian Salathé<sup>1</sup>; Patrick Schindler<sup>1</sup>; Jan Van Oostrum<sup>1</sup>; <sup>1</sup>Novartis Institutes of Biomedical Research, Basel, Switzerland
- TP 457 **Histone Post-translational Modification Analysis Using High Energy Collisions on a Tandem TOF/TOF Mass Spectrometer with a Curved Field Reflectron;** Robert Cotter<sup>1</sup>; Omar Belgacem<sup>2</sup>; Wendell Griffith<sup>1</sup>; Rachel Martin<sup>2</sup>; Emmanuel Raptakis<sup>2</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Shimadzu Biotech, Manchester, United Kingdom

#### PHOSPHOPEPTIDE ENRICHMENT

- TP 458 **Cell Cycle-Defined Phosphoproteome Analysis of Cancer Cells by Titanium Dioxide Enrichment and Mass Spectrometry;** Li-Rong Yu<sup>1</sup>; Zhongyu Zhu<sup>2</sup>; King C. Chan<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; Haleem J. Issaq<sup>1</sup>; Dimiter S. Dimitrov<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>National Cancer Institute at Frederick, Frederick, MD
- TP 459 **Selective Zirconium Dioxide-Based Enrichment of Phosphorylated Peptides for Mass Spectrometric Analysis;** Hye Kyong Kweon<sup>1</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- TP 460 **Phosphoproteome analysis of Human Stem Cell Plasma Membranes using TiO<sub>2</sub> Columns and Mass Spectrometry;** Tine E. Thingholm<sup>1</sup>; Martin R. Larsen<sup>1</sup>; Leonard J. Foster<sup>2</sup>; Moustapha Kassem<sup>3</sup>; Ole N. Jensen<sup>1</sup>; <sup>1</sup>Biochemistry and Molecular Biology, Odense, Denmark; <sup>2</sup>Biochemistry and Molecular Biology, BC, Vancouver, Canada; <sup>3</sup>Clinic of Endocrinology Treatment, Odense, Denmark
- TP 461 **Evaluation of the Titanium Oxide-Based Phosphopeptide Enrichment in Phosphoproteomics;** Clementine Klemm<sup>1</sup>; Sebastian Otto<sup>1</sup>; Constanze Wolf<sup>1</sup>; Michael Beyermann<sup>1</sup>; Eberhard Krause<sup>1</sup>; <sup>1</sup>Institute of Molecular Pharmacology, Berlin, Germany
- TP 462 **Profiling the Phosphoproteome of Endometrial Carcinoma;** Adrian M. Taylor<sup>1</sup>; Leroi DeSouza<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, ON, Canada
- TP 463 **Withdrawn**
- TP 464 **Comparison Between the Behavior of Different Sorbents Commonly Used for the Selective Isolation of Phosphopeptides from Complex Peptide Mixtures;** Stefano Gotta<sup>1</sup>; Georg C. Terstappen<sup>1</sup>; Roberto Raggiaschi<sup>1</sup>; <sup>1</sup>Sienabiotec S.p.A. Discovery Research, Siena, Italy
- TP 465 **A Novel Mixed Mode Chromatography Method for the Isolation and Separation of Phosphopeptides;** Ying Qing Yu<sup>1</sup>; Jennifer Fournier<sup>1</sup>; Petra Olivova<sup>1</sup>; Martin Gilar<sup>1</sup>; John Gebler<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- TP 466 **Analysis of Phosphopeptides using Off-line TiO<sub>2</sub> Microcolumns Followed by Nano-HPLC Coupled to ESI Ion Trap;** JUAN CASADO-VELA<sup>1</sup>; Antonio Núñez<sup>1</sup>; Jose Ignacio CASAL<sup>1</sup>; <sup>1</sup>CNIO. Spanish National Cancer Centre, MADRID, SPAIN
- TP 467 **Phosphopeptide Enrichment for Mass Spectrometry Analysis Using Micro Scale Titanium Dioxide Solid Phase Extraction;** Jennifer Fournier<sup>1</sup>; Ying Qing Yu<sup>1</sup>; Martin Gilar<sup>1</sup>; Grace M. Credo<sup>1</sup>; Weibin Chen<sup>1</sup>; John C. Gebler<sup>1</sup>; <sup>1</sup>Life Science R&D, Waters Corporation, Milford, MA
- TP 468 **Optimization of IMAC and TiO<sub>2</sub> Chromatography for Phosphoproteomics;** Susumu Imanishi<sup>1</sup>; Hanna-Mari

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- Pallari<sup>1</sup>; Vitaly Kochin<sup>1</sup>; John E. Eriksson<sup>1</sup>; <sup>1</sup>Turku Centre for Biotechnology, Turku, Finland
- TP 469 **Unraveling the Phosphoproteome by Combinations of SCX, TiO<sub>2</sub> Phosphopeptide Enrichment, Chip Based LC and Electron Transfer Induced Dissociation;** Shabaz Mohammed<sup>1</sup>; Martijn Pinkse<sup>1</sup>; Joris Benschoop<sup>1</sup>; Albert JR Heck<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands
- TP 470 **Metal Affinity Capture Tandem Mass Spectrometry for the Selective Detection of Phosphopeptides;** Grady R. Blacken<sup>1</sup>; Michael H. Gelb<sup>1</sup>; František Tureček<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 471 **Using Titanium Dioxide to Selective Enrich and Fractionate Phosphorylated Peptides from Complex Mixtures;** David R. Craft<sup>1</sup>; Kenneth A. Chisholm<sup>1</sup>; Devanand M. Pinto<sup>1</sup>; <sup>1</sup>National Research Council - IMB, Halifax, Canada
- TP 472 **Comparison of IMAC and TiO<sub>2</sub> Methodologies for Phosphopeptide Enrichment before MALDI-TOF Analysis;** Eliandre Oliveira<sup>1</sup>; Oscar Blanco<sup>2</sup>; Maria Antonia Odena<sup>1</sup>; <sup>1</sup>Barcelona Science Park - University of Barcelona, Barcelona, Spain; <sup>2</sup>IRB\_Biomedical Research Institute, Barcelona Scien, Barcelona, Spain
- TP 473 **Label-free Comparative Study of Phosphatase Inhibitor Induced Phosphoproteomics Using Data-directed Analysis;** feng yang<sup>1</sup>; Navdeep Jaitly<sup>1</sup>; Hemalatha Jayachandran<sup>2</sup>; quanzhou luo<sup>1</sup>; Marina Gristenko<sup>1</sup>; David J. Anderson<sup>1</sup>; rui zhang<sup>1</sup>; Samuel O. Purvine<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Heather M. Mottaz<sup>1</sup>; Mary S. Lipton<sup>1</sup>; David G. Camp, II<sup>1</sup>; Harold R. Udseth<sup>1</sup>; Sandra Rossie<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Department of Biochemistry, Purdue University, West Lafayette, IN
- TP 474 **Global Phosphoproteome Analysis by Combining Highly Selective TiO<sub>2</sub> Enrichment and EDTA-Enhanced Detection by LC-MS;** Cunjie Zhang<sup>1</sup>; Suyu Liu<sup>1</sup>; John Lenehan<sup>1</sup>; David W. Litchfield<sup>1</sup>; Gilles A. Lajoie<sup>1</sup>; <sup>1</sup>The University of Western Ontario, London, Canada

#### PROTEOMICS: FUNDAMENTAL STUDIES

- TP 475 **Analysis of the Extracellular Matrix and Vesicle Proteomes in Osteoblasts;** Zhen Xiao<sup>1</sup>; Corinne E. Camalier<sup>2</sup>; Kunio Nagashima<sup>1</sup>; King C. Chan<sup>1</sup>; David A. Lucas<sup>1</sup>; Stephen Lockett<sup>1</sup>; Haleem J. Issaq<sup>1</sup>; Timothy D. Veenstra<sup>1</sup>; George R. Beck, Jr.<sup>2</sup>; Thomas P. Conrads<sup>2</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>Emory University, Atlanta, GA
- TP 476 **Enzymes Screening with Enzymatic Proteomics;** Chao-Lin Liu<sup>1</sup>; Yu-Sheng Chen<sup>1</sup>; Jeen-Kuan Chen<sup>3</sup>; Long-Chung Wu<sup>1</sup>; Chia-Rui Shen<sup>2</sup>; <sup>1</sup>MingChi University of Technology, Taishan, Taiwan; <sup>2</sup>Chang Gung University, Kweishan, Taiwan; <sup>3</sup>Chinese Petroleum Company, Chiayi, Taiwan
- TP 477 **Evaluation of Methionine Oxidation State on the Efficacy of MS/MS based Database Search Analysis Strategies;** Jennifer M. Froelich<sup>1</sup>; Gavin E. Reid<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- TP 478 **Efficient detection of fragment ions and its utilization for protein identification using Curved Field Reflectron-based High Energy CID MS/MS;** Yuzo Yamazaki<sup>1</sup>; Masaki Yamada<sup>1</sup>; Hiroki Nakajima<sup>1</sup>; Hiroyuki Fukuda<sup>1</sup>; <sup>1</sup>Life Science Laboratory, Shimadzu Corporation, Kyoto, Japan
- TP 479 **Altering Electrospray Responses of Peptides via Zwitterionic Additives;** Tegafaw T. Mekecha<sup>1</sup>; Harsha P.

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- Gunawardena<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 480 **Stable Isotope Labelling Strategies to Measure the Dynamics of Protein Turnover on a Proteome-Wide Scale in Intact Animals;** Ian J Edwards<sup>1</sup>; Mary K Doherty<sup>1</sup>; Rob J Beynon<sup>1</sup>; Dominique Rocha<sup>2</sup>; Heather McCormack<sup>3</sup>; Colin Whitehead<sup>3</sup>; <sup>1</sup>University of Liverpool, Liverpool, United Kingdom; <sup>2</sup>Genus Plc, Cambridge, United Kingdom; <sup>3</sup>Roslin Institute, Edinburgh, Scotland
- TP 481 **Cooperative Effect of Factors Governing Molecular Ion Yield in Desorption/ionization Mass Spectrometry;** Takashi Nishikaze<sup>1</sup>; Mitsuo Takayama<sup>1</sup>; <sup>1</sup>Yokohama City University, Yokohama, Japan
- TP 482 **Building Cotyledon Proteome Map in Arabidopsis thaliana using Two Dimensional Gel Electrophoresis and Multi dimensional Protein Identification;** Brahmananda Reddy Chitteti<sup>1</sup>; Zhaohua Peng<sup>1</sup>; <sup>1</sup>Mississippi State University, Starkville, MS
- TP 483 **Reproducible and Specially Designed Internal Process Performance Standards for in-Gel Protein Identification using LC/MS/MS;** D. Eric Anderson<sup>1</sup>; <sup>1</sup>PMSF/NIDDK/NIH, Bethesda, Maryland
- TP 484 **Improving Top Down Sequencing of Proteins on a Quadrupole Ion Trap Mass Spectrometer Using Heavy Gases;** Angela M. Fahey<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA
- TP 485 **Tsg101 Gene Knock Down using siRNA, and its Effect on Protein Expression in 293 Mammalian Cells using SILAC Technology;** Mahbod Hajivandi<sup>1</sup>; Xiquan Liang<sup>1</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>Invitrogen, Carlsbad, California
- TP 486 **Global Survey of Organ and Organelle Protein Expression in Mouse through Combined Proteomic and Transcriptomic Profiling;** Thomas Kislinger<sup>1</sup>; Brian Cox<sup>2</sup>; Anitha Kannan<sup>1</sup>; Clement Chung<sup>1</sup>; Pingzhao Hu<sup>1</sup>; Alexandr Ignatchenko<sup>1</sup>; Michelle S. Scott<sup>3</sup>; Anthony O. Gramolini<sup>1</sup>; Quaid Morris<sup>1</sup>; Michael T. Hallett<sup>3</sup>; Janet Rossant<sup>2</sup>; Timothy R. Hughes<sup>1</sup>; Brendan Frey<sup>1</sup>; Andrew Emili<sup>1</sup>; <sup>1</sup>University of Toronto, Toronto, ONT Canada; <sup>2</sup>Hospital for Sick Children, Toronto, ONT Canada; <sup>3</sup>McGill University, Montreal, QC Canada
- TP 487 **New strategies for a "Peptide Mass Fingerprint" Database Search using Less Specific Proteolytic Enzymes;** Björn Meyer<sup>1</sup>; Bernd Ludwig<sup>1</sup>; Michael Karas<sup>1</sup>; <sup>1</sup>J.W. Goethe University, Frankfurt am Main, Germany
- TP 488 **Bath Gas Pressure Effects on Protein Charge State Distribution and Intensity;** Brittany L. Butler<sup>1</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>The University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 489 **Bioinformatic Analysis of Body Fluid Proteomes;** Søren Schandorff<sup>1</sup>; Jun Adachi<sup>2</sup>; Bartosz Pilch<sup>2</sup>; Gustavo De Souza<sup>2</sup>; Matthias Mann<sup>2</sup>; Alexandre Podtelejnikov<sup>1</sup>; <sup>1</sup>Proxeon, Odense, Denmark; <sup>2</sup>Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 490 **The Study of the Effect of MicroRNA on Protein Expression in Cultured Cells;** Haibo Qiu<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA

### PROTEOMICS: NEW METHODS II

- TP 491 **Automated Ultra-high Pressure Multidimensional Protein Identification Technology (MudPIT) for Improved Peptide Identification of Proteomic Samples;** Akira Motoyama<sup>1</sup>; John D. Venable<sup>1</sup>; Cristian I. Ruse<sup>1</sup>; John R. Yates, III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA
- TP 492 **Proteomic Analysis of Ubiquitinated Proteins from Human MCF-7 Cells Using a Novel Gel-Free**

### POSTER SPACE

- Approach;** Julian Vasilescu<sup>1</sup>; Nicholas Denis<sup>1</sup>; Martin Ethier<sup>1</sup>; Daniel Figey<sup>1</sup>; <sup>1</sup>Ottawa Institute of Systems Biology, Ottawa, Canada
- TP 493 **Low Pressure Liquid Chromatographic (LPLC) Peptide Separation Allows for Fast and Accurate Protein Identification by Online ESI MS/MS;** Ole Hørning<sup>1</sup>; Ole Nørregaard Jensen<sup>1</sup>; Ole Vorm<sup>2</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Proxeon Biosystems A/S, Odense, Denmark
- TP 494 **Comprehensive Characterization of Post-Translational Modifications In Vivo Using NanoLC-ESI-q-TOF Tandem Mass Spectrometry: Selectively Excluded Mass Screening Analysis (SEMSA);** Jawon Seo<sup>1</sup>; Jaeho Jeong<sup>1</sup>; Kong-Joo Lee<sup>1</sup>; <sup>1</sup>Center for Cell Signaling Research, SEOUL, Korea
- TP 495 **Processing ESI-MS1 Data Obtained on a Q-TOF Mass Spectrometer to Improve the Results of Protein Analysis;** Nadezhda A Galeva<sup>1</sup>; Lei Jiang<sup>1</sup>; Asma Zaidi<sup>1</sup>; Mary L. Michaelis<sup>1</sup>; Todd D Williams<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS
- TP 496 **Proteomic Approach for Characterization of Lipid Modified Proteins;** Chie Murata<sup>1</sup>; Yoshiya Oda<sup>1</sup>; Moonjin Ra<sup>1</sup>; Kazutaka Ikeda<sup>1</sup>; Takao Shimizu<sup>1</sup>; Ryo Taguchi<sup>1</sup>; <sup>1</sup>The University of Tokyo, Tokyo, Japan
- TP 497 **Fast LC-MS strategies for protein identification and modification characterization of a gel-free Ash1 immunoprecipitation;** David M Cox<sup>1</sup>; Brett Larsen<sup>2</sup>; Chris Lock<sup>1</sup>; Nic Bloomfield<sup>1</sup>; QuinQuan Liu<sup>2</sup>; Marcia Roy<sup>2</sup>; Mike Tyers<sup>2</sup>; <sup>1</sup>Applied Biosystems / MDS Sciex, Concord, Canada; <sup>2</sup>Samuel Lunenfeld Research Institute, Toronto, Canada
- TP 498 **ppTime-of-Flight Mass Spectrometry for the Identification of c-type Cytochromes from Geobacter Species;** Angela J. Ahrendt<sup>1</sup>; Carl Lindberg<sup>1</sup>; Gyorgy Babnigg<sup>1</sup>; Kelly P. Nevin<sup>2</sup>; Derek R. Lovley<sup>2</sup>; Carol S. Giometti<sup>1</sup>; <sup>1</sup>Argonne National Laboratory, Argonne, IL; <sup>2</sup>University of Massachusetts, Amherst, MA
- TP 499 **Digitized Nanobore LC-MS Control System with Integrated Emitter Divert and Rinse for Improved Nanospray Performance;** James L. Stephenson<sup>1</sup>; Jonathan L. Bundy<sup>1</sup>; Gary A. Valaskovic<sup>2</sup>; Mike S. Lee<sup>3</sup>; <sup>1</sup>RTI International, Research Triangle Park, NC; <sup>2</sup>New Objective Inc., Woburn, MA; <sup>3</sup>Milestone Development Services Inc., New Town, PA
- TP 500 **Miniaturized Multi-dimensional LC-MS Platform Using 20 µm ID Monolithic Columns and Novel Microfluidic Connectors for Enhancing Proteomic Dynamic Range;** Eileen Yue<sup>1</sup>; Shiao-Lin Wu<sup>1</sup>; Gary Valaskovic<sup>2</sup>; Barry Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>New Objective, Woburn, MA
- TP 501 **The Impact of High Efficiency Peptide Separations on Dissecting the Human Serum Proteome;** Koen Sandra<sup>1</sup>; Christine Labeur<sup>1</sup>; Gregoire Thomas<sup>1</sup>; Lies Vanneste<sup>1</sup>; Filip D'Hondt<sup>1</sup>; Koen De Cremer<sup>1</sup>; Koen Kas<sup>1</sup>; Pat Sandra<sup>2</sup>; Kathleen Verleysen<sup>1</sup>; <sup>1</sup>Peakadilly N.V., Zwijnaarde, Belgium; <sup>2</sup>Research Institute for Chromatography (RIC), Kortrijk, Belgium
- TP 502 **Protein Identification in Human Plasma by Integrated Multidimensional Liquid Chromatography (IMDL) Coupled with Mass Spectrometry;** Jie Dai<sup>1</sup>; Chia-Hui Shieh<sup>1</sup>; Rong Zeng<sup>1</sup>; <sup>1</sup>Shanghai Institutes for Biological Sciences, Shanghai, China
- TP 503 **High Dynamic Range Protein Mapping by Automated Nanoelectrospray Combined with an Orbitrap;** Ai-Ping Lu<sup>1</sup>; Reinaldo Almeida<sup>2</sup>; Jesper V. Olsen<sup>1</sup>; Guoqing Li<sup>1</sup>;

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- Matthias Mann<sup>1</sup>; <sup>1</sup>Max-Planck Institute for Biochemistry, Munich, Germany; <sup>2</sup>Advion Biosciences Limited, Norfolk, UK
- TP 504 **Increased Sequence Coverage in Protein Analysis using Automated Nanofraction Collection in Combination with Nanospray MS/MS Infusion;** Maria Eugenia Soria-Diaz<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Gerard Hopfgartner<sup>1</sup>; <sup>1</sup>LSMS, EPGL-University of Geneva, Geneva, Switzerland
- TP 505 **Effect of Guanidination-Dimethylation Labeling for Membrane Proteome Analysis Using Nano-LC-ESI QTOF;** Chengjie Ji<sup>1</sup>; Andy Lo<sup>1</sup>; Sandra L. Marcus<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada
- TP 506 **Fully Automated Top-Down Protein Identification using pLC-MSn on a Linear Ion Trap Mass Spectrometer;** Jesse D. Canterbury<sup>1</sup>; Peter Brzovic<sup>1</sup>; Rachel E. Klevitt<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 507 **Effects of LC-ESI QTOF MS/MS Data Acquisition Methods on Proteome Analysis of Tissue Samples;** Nan Wang<sup>1</sup>; Jing Zheng<sup>1</sup>; Randy Whittall<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada
- TP 508 **HPLC Elution Shifts Reflecting Protein-Protein Interactions and Post-Translational Modifications detected by Mass Spectrometry;** Samuel L. Perkins<sup>1</sup>; Lili Niu<sup>2</sup>; William K. Russell<sup>1</sup>; Neil Sharma<sup>3</sup>; Issa Isaac<sup>3</sup>; Matthew M. Champion<sup>4</sup>; Deborah A. Siegle<sup>5</sup>; James C. Hu<sup>2</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Chemistry Department, Texas A&M University, College Station, TX; <sup>2</sup>Biochemistry Department, Texas A&M University, College Station, TX; <sup>3</sup>Genomic Solutions, Ann Arbor, MI; <sup>4</sup>Applied Biosystems, Foster City, CA; <sup>5</sup>Biology Department, Texas A&M University, College Station, TX
- TP 509 **Improved Hydrophobic Peptide Recovery during Online 2D Nano LC/MS/MS for Proteomic Analysis;** Hongji Liu<sup>1</sup>; Jeffrey W. Finch<sup>1</sup>; John C. Gebler<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- TP 510 **Automated capillary HPLC Systems for Mass Spectrometric Analyses of Proteomic and Metabolomic Samples;** Eric A. Livesay<sup>1</sup>; Rui Zhao<sup>1</sup>; Keqi Tang<sup>1</sup>; Yufeng Shen<sup>1</sup>; Daniel J. Orton<sup>1</sup>; Tom O. Metz<sup>1</sup>; Michael A. Buschbach<sup>1</sup>; Beverley K. Taylor<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Gordon A. Anderson<sup>1</sup>; Harold R. Udseth<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 511 **Improved Protein Separation and Identification from Mass Spectrometry-Based Proteomics Experiments by use of 2D Liquid Protein Fractionation;** Konstantinos Thalassinos<sup>1</sup>; Susan E. Slade<sup>1</sup>; Martha M. Clokie<sup>1</sup>; Nicholas H. Mann<sup>1</sup>; James H. Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, United Kingdom
- TP 512 **Utilization of Temperature to Improve LC/MS Performance in Proteomics;** Kerry Nugent<sup>1</sup>; Peter Kent<sup>1</sup>; Eric Kemp<sup>1</sup>; Lori Ann Upton<sup>1</sup>; <sup>1</sup>Michrom Bioresources, Inc., Auburn, CA
- TP 513 **Reversed-Phase Separation, on-Line Digestion, and Automated MS Identification of Proteins at Picogram Levels;** Gordon W. Slysz<sup>1</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, Canada
- TP 514 **Rapid Determination of Disulfide Bonds in Large Proteins by Top Down Liquid Chromatography Mass Spectrometry;** Ying Ge<sup>1</sup>; Dong S. Zhao<sup>1</sup>; Andy S. Lemoff<sup>1</sup>; Xuelin Gu<sup>1</sup>; Derek M. Wood<sup>1</sup>; Xiaoya Ding<sup>1</sup>; <sup>1</sup>PPD, Inc., Madison, WI

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- TP 515 **Improved Matching of Methionine Oxide-containing Peptides by Including Neutral Loss from Methionine Oxide Residues;** Andrew J Thompson<sup>1</sup>; Ritchie Williamson<sup>1</sup>; Helen L. Byers<sup>2</sup>; James Campbell<sup>2</sup>; Malcolm Ward<sup>2</sup>; Brian Anderton<sup>1</sup>; <sup>1</sup>MRC Centre for Neurodegeneration Research KCL, IOP, London, UK; <sup>2</sup>Proteome Sciences plc, London, UK
- TP 516 **Protein Sequence Coverage Optimization by HPLC Separation and Consecutive Enzymatic Digestion;** Pavel Metalnikov<sup>1</sup>; Andrei Starostine<sup>1</sup>; Vivian Nguyen<sup>1</sup>; <sup>1</sup>Samuel Lunenfeld Research Institute, Toronto, Canada
- TP 517 **Rapid Determination of a Protein's Optimal MRM Transition for Sensitive Detection in Complex mixtures;** Michael A. Kuzyk<sup>1</sup>; S.-W. Grace Cheng<sup>1</sup>; Gregg B. Morin<sup>1</sup>; <sup>1</sup>Genome Sciences Centre, B.C. Cancer Agency, Vancouver, Canada
- TP 518 **Novel Strategies for Expression Profiling of Low Abundance Proteins in Human Serum;** Lining Qi<sup>1</sup>; Lifang Yang<sup>1</sup>; Rebecca Pitts<sup>2</sup>; Xiangming Fang<sup>3</sup>; O. John Semmes<sup>1</sup>; <sup>1</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA; <sup>3</sup>GenWay Biotech, Inc., San Diego, CA
- TP 519 **Investigation of Atypical Peptides Found via Thorough Database Search;** Alpesh A Patel<sup>1</sup>; Wilfred H Tang<sup>1</sup>; Sean L Seymour<sup>1</sup>; Ignat V Shilov<sup>1</sup>; Daniel A Schaeffer<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Foster City, CA
- TP 520 **Intact Protein Separation and Identification by non-Porous Reversed Phase Liquid Chromatography and Mass Spectrometry;** Claire Daully<sup>1</sup>; David H. Perlman<sup>1</sup>; Hua Huang<sup>1</sup>; Mark E. McComb<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- TP 521 **Digging Deeper into the Plant Proteome with Monolithic LC-MS/MS;** David P Sumpton<sup>1</sup>; Emma Edwards<sup>1</sup>; James Ault<sup>1</sup>; João Rodrigues<sup>1</sup>; Clara Diaz<sup>2</sup>; Herman P Spaink<sup>2</sup>; Jerry R Thomas<sup>1</sup>; Jane Thomas-Oates<sup>1</sup>; <sup>1</sup>University of York, York, UK; <sup>2</sup>Leiden University, Leiden, Netherlands
- TP 522 **Highly Specific Enrichment of Phosphorylated Peptides from Peptides Mixtures utilizing Magnetic Nanoparticles;** He-Hsuan Hsiao<sup>1</sup>; Hsin-Yu Hsieh<sup>1</sup>; Shu-Yu Lin<sup>1</sup>; Chi-Chi Chou<sup>1</sup>; Andrew H.-J. Wang<sup>2</sup>; Kay-Hooi Khoo<sup>2</sup>; <sup>1</sup>Core Facilities for Proteomic Research, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan
- TP 523 **Purification and Characterization of the Human 26S Proteasome using a New Tandem Affinity Purification Strategy and Quantitative Mass Spectrometry;** Xiaorong Wang<sup>1</sup>; Chi-Fen Chen<sup>2</sup>; Cortnie Guerrero<sup>1</sup>; Peter Baker<sup>3</sup>; Phang-lang Chen<sup>2</sup>; Peter Kaiser<sup>2</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>Dept of Physiology & Biophysics, UC Irvine, Irvine, CA; <sup>2</sup>Dept of Biological Chemistry, UC-irvine, Irvine, CA; <sup>3</sup>Dept of Pharmaceutical Chemistry, UCSF, San Francisco, CA
- TP 524 **Comparison of an Affinity MALDI Plate and Magnetic beads Conjugated with Phenylboronic acid for Direct Detection of Glycoproteins;** Jeong Heon Lee<sup>1</sup>; Moonkwon Lee<sup>2</sup>; Jungsuk Park<sup>3</sup>; Hyoung Soon Park<sup>4</sup>; Yongsun Kim<sup>1</sup>; <sup>1</sup>Proteonik, INC, Ansan, Korea; <sup>2</sup>Microbiochip Ct., Ansan, Korea; <sup>3</sup>Korea Polytechnic University, Siheung, Korea; <sup>4</sup>ProBiond,co,ltd, Seoul, Korea
- TP 525 **Analysis of BCL2 Proteins Interactions by Tandem Mass Spectrometry;** David K. Crockett<sup>1</sup>; Amit R. Phansalkar<sup>1</sup>; Megan S. Lim<sup>2</sup>; Kojo S.J. Elenitoba-Johnson<sup>2</sup>; <sup>1</sup>ARUP Laboratories, Salt Lake City, UT;

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- <sup>2</sup>University of Utah School of Medicine, Salt Lake City, UT
- TP 526 **Use of Ethylenediaminetetraacetic Acid (EDTA) - Magnetic Bead Complex in Protein Isolation and Detection by MALDI-TOF Mass Spectrometry;** Mohammad Abul Farah<sup>1</sup>; Jeong Heon Lee<sup>1</sup>; Yangsun Kim<sup>1</sup>; <sup>1</sup>Proteonik Inc., Ansan City, South Korea
- TP 527 **Proteomic Mapping of the Vascular Endothelium Luminal Surface for Tissue Specific Target Identification;** Eric Sousa<sup>1</sup>; Xiang-Yang Tan<sup>1</sup>; Wei Liu<sup>1</sup>; Vasu Maganti<sup>1</sup>; Yongchang Qiu<sup>1</sup>; Debra Pittman<sup>1</sup>; Jeffrey Feldman<sup>1</sup>; Robert Schaub<sup>1</sup>; James Keith<sup>1</sup>; Davinder Gill<sup>1</sup>; Steve Herrmann<sup>1</sup>; Jiang Wu<sup>1</sup>; <sup>1</sup>Wyeth Research, Cambridge, MA
- TP 528 **Analysis of cGMP/cAMP Signaling Pathways Using a Chemical Proteomics Approach in Heart Tissue;** Arjen Scholten<sup>1</sup>; Mee Kian-Poh<sup>1</sup>; Toon van Veen<sup>1</sup>; Marc Vos<sup>1</sup>; Albert J R Heck<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands
- TP 529 **A New Tandem Affinity Tag to Study Proteome-Wide Ubiquitination and ULP modification Profiles;** Christian Tagwerker<sup>1</sup>; <sup>1</sup>UC Irvine, Irvine, CA
- TP 530 **Proteomic Analysis of Human Blood Serum using Peptide Library Beads;** Lau Sennels<sup>1</sup>; Mogjiborahman Salek<sup>2</sup>; Lee Lomas<sup>3</sup>; Egisto Boschetti<sup>3</sup>; Pier G. Righetti<sup>4</sup>; Juri Rappsilber<sup>1</sup>; <sup>1</sup>The Wellcome Trust Center, University of Edinburgh, Edinburgh, United Kingdom; <sup>2</sup>FIRC Institute for Molecular Oncology Foundation, Milan, Italy; <sup>3</sup>Ciphergen Biosystems Inc, Fremont, CA; <sup>4</sup>Polytechnic of Milano, Milan, Italy
- TP 531 **Pathogen derived MHC-Binding Peptides – A Proteomics Approach to their Identification;** Karin M Green<sup>1</sup>; Iwona Strug<sup>1</sup>; Jinal Patel<sup>1</sup>; Shibani Mitra-Kaushik<sup>1</sup>; Lawrence J Stern<sup>1</sup>; James E Evans<sup>1</sup>; <sup>1</sup>University of Massachusetts Medical School, Worcester, MA
- TP 532 **Peptide and Protein Analysis by MALDI-TOF MS using Magnetic Bead Based Metal Ion Affinity Chromatography;** Katja Blaesing<sup>1</sup>; Thomas Ellsner<sup>2</sup>; Markus Kostrzewa<sup>2</sup>; <sup>1</sup>Hochschule Anhalt, Köthen, Germany; <sup>2</sup>Bruker Daltonik GmbH, Leipzig, Germany
- TP 533 **High Throughput Mass Spectrometric Immunoassays in Human Plasma Profiling and Targeted Protein Analysis;** Randall W Nelson<sup>1</sup>; Urban A Kiernan<sup>1</sup>; Dobrin Nedelkov<sup>1</sup>; Kemmons Tubbs<sup>1</sup>; Eric E Niederkofer<sup>1</sup>; <sup>1</sup>Intrinsic Bioprobes, Inc., Tempe, AZ
- TP 534 **Targeted Proteomic Analysis of Active Transcription Factor Complexes using Oligoprecipitation;** Zhaojing Meng<sup>1</sup>; Corinne E. Camalier<sup>2</sup>; David A. Lucas<sup>1</sup>; Timothy D. Veenstra<sup>1</sup>; George R. Beck, Jr.<sup>2</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>Emory University School of Medicine, Atlanta, GA

### PROTEOMICS: SAMPLE PREPARATION AND FRACTIONATION II

- TP 535 **Temporal Separation of Endocytotic Pathway Vesicles by Magnetic Fractionation and Subsequent Proteomic Analysis;** Gregg A Czerwieniec<sup>1</sup>; Georgia Dolios<sup>1</sup>; Fannie W Chen<sup>1</sup>; Yiannis A Ioannou<sup>1</sup>; Rong Wang<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY
- TP 536 **Multi dimensional Chromatography Coupled with MALDI-TOF/TOF for Proteomic Analysis of Complex Samples;** Stephanie Hahner<sup>1</sup>; Urs Lewandrowski<sup>2</sup>; Albert Sickmann<sup>2</sup>; Sven Brand<sup>1</sup>; Jörg Glandorf<sup>1</sup>; Wolfgang Jabs<sup>1</sup>; Sergei Dikler<sup>3</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, D; <sup>2</sup>Rudolf-Virchow-Zentrum, University Würzburg, Würzburg, D; <sup>3</sup>Bruker Daltonics, Billerica, MA

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- TP 537 **Negative-Pressure Liquid Chromatography (nPLC): Design and Performance of a Novel Off-Line Separation-Deposition Interface for MALDI-Mass Spectrometry;** Vincent C. Chen<sup>1</sup>; Vlad-Andre Ionescu<sup>1</sup>; James I. Nagy<sup>1</sup>; Helene Perreault<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada
- TP 538 **Sequential Extraction of E. coli Outer Membrane Proteins for Bottom-up Proteomic Analysis of Low Abundance Proteins at Different Growth Phases;** Leon H.Y. Lau<sup>1</sup>; Andy Lo<sup>1</sup>; Chengjie Ji<sup>1</sup>; Monica M. Palcic<sup>2</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, Canada; <sup>2</sup>Carlsberg Research Center, Copenhagen, Denmark
- TP 539 **Removal of High Abundance Proteins for Proteomic Analysis of Cerebrospinal Fluid (CSF) using Molecular Weight Cutoff Filters;** Kevin S. Shores<sup>1</sup>; Daniel R. Knapp<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, South Carolina
- TP 540 **WAX-RPLC/FTICR-MS for Profiling Intact Proteins;** Seema Sharma<sup>1</sup>; David C. Simpson<sup>1</sup>; Nikola Tolic<sup>1</sup>; Natacha Lourette<sup>1</sup>; Richard D. Smith<sup>1</sup>; Ljiljana Pasa-Tolic<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 541 **Protein pre-Fractionation to Enhance Differential Expression Analysis with LC-MS;** Johan Axelman<sup>1</sup>; Caroline Berg<sup>1</sup>; Daniel Haid<sup>1</sup>; Daniel Ivansson<sup>1</sup>; Staffan Renlund<sup>1</sup>; <sup>1</sup>GE Healthcare, Uppsala, Sweden
- TP 542 **Divide and Conquer: Fractionating Salivary Proteins;** Pinmanee Boonthueung<sup>1</sup>; Prasanna Ramachandran<sup>1</sup>; Yongming Xie<sup>1</sup>; Shen Hu<sup>1</sup>; David T. Wong<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California-Los Angeles, Los Angeles, CA
- TP 543 **Fractionation of Complex Proteomic Samples for Low Abundant Biomarker Discovery by MS;** Tony J. Tegeler<sup>1</sup>; Dariusz J. Janecki<sup>1</sup>; <sup>1</sup>Indiana Centers for Applied Protein Sciences, Indianapolis, IN
- TP 544 **Application of Micro-scale Solution Isoelectrofocusing for Proteomic Analysis of Urines from Sodium Fluoride Treated Rats;** Charlotte C. Yu Ip<sup>1</sup>; Raymond J. Gonzalez<sup>1</sup>; Frank D. Sistare<sup>1</sup>; William H. Schaefer<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- TP 545 **Development of a Proteomic Reactor for Efficient Protein Digestion and Mass Spectrometric Preparation;** Martin Ethier<sup>1</sup>; Weimin Hou<sup>1</sup>; Daniel Figeys<sup>1</sup>; <sup>1</sup>Ottawa Institute of Systems Biology, Ottawa, Canada
- TP 546 **Characterizing an Albumin Enriched Fraction of Human Serum via Chromatography, MALDI-TOF MS and LC-MS/MS;** Rebekah L Gundry<sup>1</sup>; Christine A Jelinek<sup>1</sup>; Qin Fu<sup>1</sup>; Jennifer E Van Eyk<sup>1</sup>; Robert J Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- TP 547 **Off-Gel Electrophoretic Fractionation of Proteins and Peptides to Improve Protein Identification in Complex Samples;** Patric Hoerth<sup>1</sup>; Christine A. Miller<sup>2</sup>; Christian Wenz<sup>1</sup>; <sup>1</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 548 **Reversed-phase LC/LC Separation of Immunodepleted Human Blood Serum, with Subsequent Characterization by MALDI TOF/TOF/MS and ESI/MS;** William R. Alley<sup>1</sup>; Milan Madera<sup>1</sup>; Iveta Klouckova<sup>1</sup>; Yehia Mechref<sup>2</sup>; Milos V. Novotny<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>METACyt Biochemical Analysis Center, Bloomington, IN
- TP 549 **Feasibility of Multi-lectin Glycoprotein Capture Combined with Free-Flow Electrophoreses (FFE)**



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- Separation prior to LC-MS/MS Bottom-Up Identification of Plasma Glycoproteins;** Daniel Eikel<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>National Institutes of Health - NIDDK, Bethesda, MD
- TP 550 **Investigation of Non-Specific Protein:Protein Interactions Following Removal of Twenty High Abundance Proteins From Human Plasma;** Graham B.I. Scott<sup>1</sup>; Chris D. Melm<sup>1</sup>; Angela S. Crawford<sup>1</sup>; Holly A. Chapman<sup>1</sup>; Justin Wildsmith<sup>1</sup>; Kevin B. Ray<sup>1</sup>; Dian Er Chen<sup>1</sup>; Mark D. Schuchard<sup>1</sup>; <sup>1</sup>Sigma-Aldrich, Life Science and Technology Center, St. Louis, MO
- TP 551 **Comparison of Multiple Liquid Partition Chromatography to Fractionate Human Serum for LC-MALDI Mass Spectrometry and LC-ESI Tandem Mass Spectrometry;** Monika Tucholska<sup>1</sup>; Peihong Zhu<sup>1</sup>; Catherine Stacey<sup>2</sup>; John Marshall<sup>1</sup>; <sup>1</sup>Ryerson University, Toronto, Canada; <sup>2</sup>Bruker Daltonics, Ballerica, MA

### PROTEOMICS: QUANTITATIVE TECHNIQUES II

- TP 552 **Quantification and Identification in Protein Biomarker Discovery Using Hybrid Ion Trap and TOF Mass Spectrometer Combining with Stable Isotope Coding;** Fan Xiang<sup>1</sup>; Joseph Fox<sup>1</sup>; Jia Zhao<sup>2</sup>; Willard Bankert<sup>1</sup>; David M Lubman<sup>2</sup>; <sup>1</sup>Shimadzu Biotech, Pleasanton, CA; <sup>2</sup>The University of Michigan, Ann Arbor, MI
- TP 553 **Quantitative Proteomics of Fruit Fly Development by Metabolic Labeling;** Joost W. Gouw<sup>1</sup>; Martijn W.H. Pinkse<sup>1</sup>; Tokameh Mahmoudi<sup>2</sup>; Maria Monti<sup>1</sup>; C. Peter Verrijzer<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; Jeroen Krijgsveld<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Erasmus Medical Center, Rotterdam, The Netherlands
- TP 554 **Absolute Quantification of Multiple Proteins in Biological Systems using Artificial QconCAT Proteins as Internal Standards for Mass Spectrometry;** Jenny Rivers<sup>1</sup>; Mary K Doherty<sup>1</sup>; Deborah M Simpson<sup>1</sup>; Simon J Gaskell<sup>2</sup>; Dominique Rocha<sup>3</sup>; Robert J Beynon<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, U.K.; <sup>2</sup>University of Manchester, Manchester, U.K.; <sup>3</sup>Genus Cambridge Research Laboratory, Cambridge, U.K.
- TP 555 **Quantification of Cell Surface Proteins and Plasma Proteins between Normal and Malignant Breast Cells;** Xiquan Liang<sup>1</sup>; Mahbod Hajivandi<sup>1</sup>; Erlend Ragnhildstveit<sup>2</sup>; Geir Fonnum<sup>2</sup>; Marie Bosnes<sup>2</sup>; David Gillooly<sup>2</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>Invitrogen, Carlsbad, California; <sup>2</sup>Dynal Biotech ASA, Oslo, Norway
- TP 556 **Identification and Quantification of Different Protein Species by using the ICPL (isotope-coded protein labelling) Technology;** Thomas M. Halder<sup>1</sup>; Conny Ciosto<sup>2</sup>; Josef Kellermann<sup>2</sup>; Friedrich Lottspeich<sup>2</sup>; <sup>1</sup>TopLab, Martinsried, Germany; <sup>2</sup>Max-Planck-Institute for Biochemistry, Martinsried, Germany
- TP 557 **Novel Approach to Identify Peroxin Interacting Proteins using Metabolic Labeling and Quantitative Mass Spectrometry;** Silke Oeljeklaus<sup>1</sup>; Christine David<sup>2</sup>; Ralf Erdmann<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Bettina Warscheid<sup>1</sup>; <sup>1</sup>Medical Proteom-Center, Ruhr-University, Bochum, Germany; <sup>2</sup>Department for Systems Biochemistry, Bochum, Germany
- TP 558 **Quantitative Proteomic Identification of &Alpha-Synuclein- and DJ-1-Associated Proteins using Stable Isotope Labeling with Amino Acids in Cell Culture (SILAC);** Jinghua Jin<sup>1</sup>; Yan Wang<sup>1</sup>; Catherine Pan<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>University of Washington School of Medicine, Seattle, WA

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- TP 559 **Non-Isobaric Triplex-Labeling Strategies for Proteome Analyses are Compatible with Protein Pre-fractionation;** Josef Kellermann<sup>1</sup>; Friedrich Lottspeich<sup>1</sup>; Eva Keidel<sup>1</sup>; W Jabs<sup>2</sup>; S Hahner<sup>2</sup>; S Brand<sup>2</sup>; Detlef Suckau<sup>2</sup>; <sup>1</sup>Max-Planck-Institute for Biochemistry, Martinsried, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany
- TP 560 **Stable Isotopic Labeling of Amino Acids in Cultured Primary Neurons for the Study of Protein Turnover and Neuronal Signal Transduction;** Daniel S. Spellman<sup>1</sup>; Rithwick Rajagopal<sup>1</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
- TP 561 **Use of N-15 Metabolic Labeling for Biomarker Discovery in the Apc<sup>min</sup> Mouse Model for Colorectal Cancer;** Edward L. Huttlin<sup>1</sup>; Adrian D. Hegeman<sup>1</sup>; Xiaodi Chen<sup>1</sup>; Greg Barret-Wilt<sup>1</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
- TP 562 **Quantitative Proteomics Analysis using Stable Isotope Dilution Nanospray LC/MS after Inhibition of Endothelial Cell Dihydrofolate Reductase;** Colin G. Barry<sup>1</sup>; Alexander S. Whitehead<sup>1</sup>; Anastasia K. Yocum<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- TP 563 **Quantitative Profiling of Tumor Cell Lines Using Isotope Coded Protein Labeling (ICPL) and Liquid Chromatography-Tandem Mass Spectrometry;** Yang Shi<sup>1</sup>; Chun-Ming Huang<sup>2</sup>; Gongyi Shi<sup>3</sup>; Wenhong Zhu<sup>1</sup>; Jeffrey Smith<sup>1</sup>; Yuliang Ma<sup>1</sup>; <sup>1</sup>The Burnham Institute for Medical Research, La Jolla, CA; <sup>2</sup>La Jolla Institute for Molecular Medicine, San Diego, CA; <sup>3</sup>Bruker Daltonics Inc., Fremont, CA
- TP 564 **Determination of Quantitative Proteomics Changes in Mixed Lineage Leukemia By Stable Isotope Dilution Nanospray LC/MS;** Anastasia K. Yocum<sup>1</sup>; Carolyn A. Felix<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>The Children's Hospital of Philadelphia, Philadelphia, PA
- TP 565 **Quantification of Secreted Proteins between Normal and Malignant Breast Cells;** Xiquan Liang<sup>1</sup>; Jarkko Huuskonen<sup>1</sup>; Mahbod Hajivandi<sup>1</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>Invitrogen, Carlsbad, California
- TP 566 **Comparison of Three Methods of Quantitative Proteomics by Mass Spectrometry;** Qiangwei Xia<sup>1</sup>; Tiansong Wang<sup>1</sup>; Fred Taub<sup>1</sup>; Erik L. Hendrickson<sup>1</sup>; John A. Leigh<sup>1</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 567 **Quantitative Proteomic Comparison of Wild-type and Adenylyl Cyclase VII Transgenic Mouse Synaptic Membranes Utilizing <sup>15</sup>N Metabolic Labeling and MudPIT;** Kathleen J. Grant<sup>1</sup>; Boris Tabakoff<sup>1</sup>; Christine C. Wu<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Aurora, CO
- TP 568 **Comprehensive Identification of Proteome Changes Associated With Metastatic Melanoma By Combining SILAC and 3-D Protein Profiling;** Huan Wang<sup>1</sup>; Logan J Everett<sup>2</sup>; Mee-Jung Han<sup>1</sup>; David Speicher<sup>1</sup>; <sup>1</sup>The Wistar Institute, Philadelphia, PA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- TP 569 **Mass Spectrometric analysis of Associated Proteins of rab11a in the Endocytosis Process of a-Synuclein Into Microglia;** Jun Liu<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>University of Washington School of Medicine, Seattle, USA

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- TP 570 **Quantifying Proteomic ICPL Samples by ESI Ion Trap MS**; Ulrike Schweiger-Hufnagel<sup>1</sup>; Marina Behrens<sup>1</sup>; Ali Kettani<sup>1</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany
- TP 571 **Comparing <sup>15</sup>N-Metabolic Labeling Relative Quantification Strategies with Light or Dark Grown Arabidopsis: As Clear as Night and Day?**; Adrian D. Hegeman<sup>1</sup>; Edward L. Huttlin<sup>1</sup>; Amy C. Harms<sup>1</sup>; Michael R. Sussman<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI
- TP 572 **Use of QconCAT Multiplexed Quantification for Polymorphism Mapping by Stable Isotope Dilution Mass Spectrometry**; Stuart D. Armstrong<sup>1</sup>; Deborah M. Simpson<sup>1</sup>; Jane L. Hurst<sup>1</sup>; Simon J. Gaskell<sup>2</sup>; Robert J. Beynon<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, UK; <sup>2</sup>University of Manchester, Manchester, UK
- TP 573 **Study of Stable Isotope Labeling with Amino Acids in cell culture (SILAC) in combination with 1DE and 2DE**; Annika Dahl<sup>1</sup>; Erik Portelius<sup>1</sup>; Kristina Hedberg-Fogel<sup>1</sup>; Kaj Blennow<sup>1</sup>; Ann Westman-Brinkmalm<sup>1</sup>; <sup>1</sup>Inst of Neuroscience and physiology, Mölndal, Sweden
- TP 574 **Evaluation of a Stable Isotope Labeled Whole Protein for Absolute Protein Quantitation Using LC/MS/MS and Multiple Reaction Monitoring**; Zhaoyan Jin<sup>1</sup>; <sup>1</sup>Eli Lilly and Company, Greenfield, IN; <sup>2</sup>Roche Protein Expression Group, Indianapolis, IN
- TP 575 **Subtle Modification of Isotope-Ratio Proteomics (SMIRP) in Multicellular Organisms: <sup>15</sup>N/<sup>14</sup>N Alteration in Plants**; Andrew J. Norris<sup>1</sup>; Arthur Laganowsky<sup>2</sup>; John Nishio<sup>2</sup>; Sara Bassilian<sup>1</sup>; Frederic Halgand<sup>1</sup>; Puneet Souda<sup>1</sup>; Kym F. Faull<sup>1</sup>; Jonathan Katz<sup>1</sup>; Julian P. Whitelegge<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, CA; <sup>2</sup>California State University, Chico, CA
- TP 576 **Comparative Secretomics in RPE Cells from Normal and Age Related Macular Degeneration Donors**; Eunkyung An<sup>1</sup>; Xiaoning Lu<sup>1</sup>; Jessica Flippin<sup>1</sup>; Joe Devaney<sup>1</sup>; Brian Halligan<sup>2</sup>; Karl Csaky<sup>3</sup>; Yetrib Hathout<sup>1</sup>; <sup>1</sup>Children's National Medical Center, Washington, DC; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>3</sup>NEI/NIH, Bethesda, MD
- TP 577 **Identification of Endogenous Protein-Protein Interactions by RNAi and Quantitative Proteomics**; Matthias Selbach<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Munich, Germany
- TP 578 **Double Stable Isotope Labeling with Amino Acids in Cell Culture: Quantitation and Dynamics of Acetylation and Methylation In Cancer Cells**; Chen Ren<sup>1</sup>; Shujun Liu<sup>1</sup>; Guido Marcucci<sup>1</sup>; Kalpana Ghoshal<sup>1</sup>; Samson T. Jacob<sup>1</sup>; Michael A. Freitas<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- TP 579 **A Mass Spectrometry-Based Approach to Absolute Quantitation of mRNA Capping Enzyme in Mammalian Total Cell Lysate**; Haiyan Zheng<sup>1</sup>; Chun Chu<sup>1</sup>; Aaron J Shatkin<sup>1</sup>; <sup>1</sup>University of Medicine and Dentistry of New Jersey, Piscataway, NJ

### PROTEOMICS: BIOCHEMISTRY: NON-MAMMALIAN

- TP 580 **Characterization of Polyglutamine aggregates by Mass Spectrometry**; Yan Wang<sup>1</sup>; Anatoli B. Meriin<sup>1</sup>; Michael Y. Sherman<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA
- TP 581 **Identification and Molecular Characterisation of Centrosomal Proteins in Drosophila Melanogaster**; Johan Gobom<sup>1</sup>; Hanna Mueller<sup>1</sup>; Verena Lehmann<sup>1</sup>; Gustavsson Niklas<sup>2</sup>; Lehrach Hans<sup>1</sup>; Lange Bodo<sup>1</sup>; Mirgorodskaya Ekaterina<sup>1</sup>; <sup>1</sup>Max Planck Institute for

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- Molecular Genetics, Berlin, Germany; <sup>2</sup>Lund University, Lund, Sweden
- TP 582 **Hemagglutinating Activity and Protein Characterization of Curcuma Plants in Thailand**; Polkit Sangvanich<sup>1</sup>; Sophon Kaeothip<sup>1</sup>; Chantagan Phiphobmongkol<sup>2</sup>; Jisnusun Svasti<sup>2</sup>; Pornpimon Thiptara<sup>1</sup>; Amorn Petsom<sup>1</sup>; <sup>1</sup>Faculty of Science, Chulalongkorn University, Bangkok, Thailand; <sup>2</sup>Chulabhorn Research Institute, Bangkok, Thailand
- TP 583 **Mass Spectrometry Based Proteomic Analysis of Bacterial Cold Adaptation in Exiguobacterium sp. Strain 255-15**; Yinghua Qiu<sup>1</sup>; Sophia Kathariou<sup>2</sup>; Fan Xiang<sup>3</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>North Carolina State University, Raleigh, NC; <sup>3</sup>Shimadzu Biotech, Pleasanton, CA
- TP 584 **Mapping the 26S Proteasome Interaction Network in Saccharomyces Cerevisiae using QTAX**; Cortnie M. Guerrero<sup>1</sup>; Christian Tagwerker<sup>1</sup>; Peter Kaiser<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA
- TP 585 **Post-Translational Modifications of Caulobacter Crescentus Ribosomal Proteins**; William E. Running<sup>1</sup>; James P. Reilly<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- TP 586 **Examining Aspergillus Niger Morphology Control by Global Proteome Analysis**; Ellen A. Panisko<sup>1</sup>; Laura J Hubbard<sup>1</sup>; Linda L. Lasure<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 587 **Differential Protein Expression Analysis of Drosophila melanogaster Embryogenesis using Liquid Chromatography with Ion-Mobility and Ion-Trap Mass Spectrometry**; Ruwan T. Kurulugama<sup>1</sup>; Stephen J. Valentine<sup>1</sup>; Thomas C. Kaufman<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- TP 588 **Identification of Immune Induced Peptides in the Hemolymph of the Fruitfly**; Geert Baggerman<sup>1</sup>; Peter Verleyen<sup>1</sup>; Wannes D'Hertog<sup>1</sup>; Evy Vierstraete<sup>1</sup>; Steven Husson<sup>1</sup>; Liliane Schoofs<sup>1</sup>; <sup>1</sup>K.U.Leuven, Leuven, Belgium
- TP 589 **Iron-Regulated Protein Expression Profiling in B. Anthracis using Amine Specific Labeling and LC MS/MS analysis**; Andrew Koppisch<sup>2</sup>; Sanjeev Bhardwaj<sup>1</sup>; Christy Ruggiero<sup>2</sup>; Srinivas Iyer<sup>2</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>Los Alamos National Laboratory, Los Alamos, NM
- TP 590 **Tandem LC-MS/MS Comparison of COP9/Signalosome Interactions Across Various Species**; Marcia M Roy<sup>1</sup>; Lionel Pintard<sup>1</sup>; Danielle Dewar<sup>1</sup>; Brett Larsen<sup>1</sup>; Mike Tyers<sup>1</sup>; <sup>1</sup>Samuel Lunenfeld Research Institute, Toronto, Ontario, CANADA
- TP 591 **Automated High Throughput Microfluidics nano-LC/MS/MS of Transient Protein Assemblies in Bacteria**; William R. Wikoff<sup>1</sup>; Sunia Trauger<sup>1</sup>; Junefredo Apon<sup>1</sup>; Angeli Menon<sup>2</sup>; Michael Adams<sup>2</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>University of Georgia, Athens, GA
- TP 592 **Mapping The Stimulus-specific Signaling Pathways Involved in THP-1 Cells Exposed to Porphyromonas gingivalis LPS vs. Fimbria vs. Live P.g**; Julian A. Saba<sup>1</sup>; David H. Perlman<sup>2</sup>; Hua Huang<sup>2</sup>; Mark E. McComb<sup>2</sup>; Catherine E. Costello<sup>2</sup>; Salomon Amar<sup>1</sup>; <sup>1</sup>BU Goldman School of Dental Medicine, Boston, MA; <sup>2</sup>Boston University School of Medicine, Boston, MA
- TP 593 **Characterization of Novel Ubiquitin-Specific Protease Interacting Proteins by Mass Spectrometry and Genetic Experiments**; Jeroen A.A. Demmers<sup>1</sup>; B.R. Prashanth Kumar<sup>1</sup>; Jan A. van der Knaap<sup>1</sup>; Karel

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- Bestarosti<sup>1</sup>; C. Peter Verrijzer<sup>1</sup>; <sup>1</sup>Erasmus University Medical Center, Rotterdam, The Netherlands
- TP 594 **Time-Resolved Proteomic Characterization of Distinct States of the Eukaryotic Pre-Initiation Complex of the DNA Replication Cycle;** Matthew D Sekedat<sup>1</sup>; Alan J Tackett<sup>1</sup>; Brian T Chait<sup>1</sup>; <sup>1</sup>The Rockefeller University, New York, New York
- TP 595 **Studies on the Mitochondrial Proteome of *Tetrahymena thermophila* using LC/LC-MS/MS;** Daryl G.S. Smith<sup>1</sup>; David F. Spencer<sup>2</sup>; Michael W. Gray<sup>2</sup>; Ronald E. Pearlman<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada; <sup>2</sup>Dalhousie University, Halifax, Canada
- TP 596 **Shotgun Proteomic Analysis of Lrp regulated Proteins of *Methanococcus maripaludis* Using Accurate Mass Measurement and <sup>15</sup>N-Metabolic Labeling;** Li Jing<sup>1</sup>; Yuchen Liu<sup>1</sup>; William B. Whitman<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 597 **Serum proteomics of honeybee castes;** Queenie WT Chan<sup>1</sup>; Leonard J Foster<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada
- TP 598 **Quantitative Protein Profiling and Genetic Analysis of TOR-inhibition in Yeast Reveal Novel Insights into Connections Between Cellular Growth and Stress;** Sricharan Bandhakavi<sup>1</sup>; Hongwei Xie<sup>1</sup>; DoHyung Kim<sup>1</sup>; Timothy J Griffin<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN
- TP 599 **Mass Spectrometric Identification of Cellular Proteins Targeting the N-termini of KSHV-LANA Homologs;** Donna L Potts<sup>1</sup>; Brenna K Kelley-Clarke<sup>2</sup>; Andrew Barbera<sup>2</sup>; Kenneth M Kaye<sup>2</sup>; Catherine E Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Brigham and Women's Hospital, Boston, MA
- TP 600 **Characterization of Aromatic Compound Degradation Pathways and Their Regulation in *Rhodopseudomonas palustris* Using Stable Isotope Labeling Quantitative Proteomics;** Chongle Pan<sup>1</sup>; Patricia K. Lankford<sup>1</sup>; Bing Zhang<sup>1</sup>; Yasuhiro Oda<sup>2</sup>; Nagiza F. Samatova<sup>1</sup>; Caroline S. Harwood<sup>2</sup>; Dale A. Pelletier<sup>1</sup>; Robert L. Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Washington, Seattle, WA

### PROTEOMICS: BIOMARKERS IN TISSUE AND SERUM

- TP 601 **Serum Glycan Profiling as a Diagnostic Aid in Breast Cancer;** Suzanne Miyamoto<sup>1</sup>; Crystal Kirmiz<sup>2</sup>; Bensheng Li<sup>2</sup>; Hyun Joo An<sup>2</sup>; Robert Alecio<sup>3</sup>; Anthony Ferrige<sup>3</sup>; Carlito Lebrilla<sup>2</sup>; <sup>1</sup>UC Davis Cancer Center, Sacramento, CA; <sup>2</sup>UC Davis, Davis, CA; <sup>3</sup>Positive Probability Limited, Isleham, UK, CB7 5RX
- TP 602 **Using IMS-MS for Human Plasma Proteome Profiling;** Xiaoyun Liu<sup>1</sup>; Manolo Plasencia<sup>1</sup>; Stephen Valentine<sup>2</sup>; David Clemmer<sup>1</sup>; <sup>1</sup>Department of Chemistry, Indiana University, Bloomington, IN; <sup>2</sup>Predictive Physiology and Medicine (PPM), Bloomington, IN
- TP 603 **Proteomic Analysis of Rat's Cerebrospinal Fluid Changes Following Lipopolysaccharide-induced CNS Inflammation by Liquid Chromatography Tandem Mass Spectrometry;** Yun-Han Wang<sup>1</sup>; Yu-Chang Tyan<sup>1</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan
- TP 604 **A Comparison of the Protein Expression Lists from Mass Spectrometry of Human Blood Fluids Using Peptide Sequences and BLAST;** Peihong Zhu<sup>1</sup>; Peter Bowden<sup>1</sup>; Voitek Pendrak<sup>1</sup>; Ken Kupfer<sup>1</sup>; Ken Evans<sup>2</sup>; Terry Sills<sup>2</sup>; Herbert Thiele<sup>1</sup>; KW Siu<sup>2</sup>; Eleftherios P Diamandis<sup>2</sup>; Marshall John<sup>1</sup>; <sup>1</sup>Ryerson University,

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- Toronto, Canada; <sup>2</sup>Ontario Cancer Biomarker Network, Toronto, Canada; <sup>3</sup>Bruker Daltonics, Bremen, Germany
- TP 605 **The Proteomic Responses in Mouse Plasma to Sepsis Generated from CLP Model;** Yan Ren<sup>1</sup>; Jiandong Wang<sup>2</sup>; Ji Xia<sup>1</sup>; Ning Ning<sup>2</sup>; Kang Zhao<sup>1</sup>; Ningzhi Xu<sup>1</sup>; Yingxin Xu<sup>2</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>Beijing Genomics Institute, CAS, Beijing, China; <sup>2</sup>The General Hospital of Military, Beijing, China
- TP 606 **Quantitative Proteomic Analysis of Fibrosis Progression in Human Liver Biopsies from Hepatitis C Virus (HCV)-Infected Patients;** Deborah L. Diamond<sup>1</sup>; Jon M. Jacobs<sup>2</sup>; Zachary Caldwell<sup>1</sup>; Marina A. Gritsenko<sup>2</sup>; David G. Camp II<sup>2</sup>; Anne M. Larson<sup>3</sup>; Richard D. Smith<sup>2</sup>; Michael G. Katze<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Hepatology Section, University of Washington, Seattle, WA
- TP 607 **New Serum Biomarkers for Gastric Cancer Discovered using SELDI Protein Chip Technology;** Wenjing Wang<sup>1</sup>; Liang Zhu<sup>2</sup>; Zhiwen Luo<sup>2</sup>; Ping Liao<sup>1</sup>; Weifen Xie<sup>2</sup>; Wei Lu<sup>1</sup>; <sup>1</sup>Shanghai Center for Disease Control and Prevention, Shanghai, CHINA; <sup>2</sup>Chang-zheng Hospital, Shanghai, CHINA
- TP 608 **Large-Scale Identification of Protein in Human Urine Proteome by Gel-Free Proteomic Approach;** Yu-Chang Tyan<sup>1</sup>; How-Ran Guo<sup>1</sup>; Chia-Yuan Liu<sup>1</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan
- TP 609 **A Proteomic Approach to the Discovery of Biomarkers in the Urine of Cachectic Cancer Patients;** Andrew, David Cronshaw<sup>1</sup>; Alan R. Millar<sup>1</sup>; Robert Wakefield<sup>1</sup>; Alastair Aitken<sup>1</sup>; Christopher Deans<sup>1</sup>; Alastair Lowrie<sup>1</sup>; Kenneth C.H. Fearon<sup>1</sup>; James A. Ross<sup>1</sup>; <sup>1</sup>University of Edinburgh, Edinburgh, Scotland
- TP 610 **An Integrated Approach for Profiling Potential Biomarkers in Human Plasma for Detection of Non-small Cell Lung Cancer;** Valeriy E. Shevchenko<sup>1</sup>; Irina B. Zborovskaya<sup>1</sup>; Natalia E. Arnotskaya<sup>1</sup>; Oxana P. Trifonova<sup>1</sup>; Valentina A. Yurchenko<sup>1</sup>; Maria E. Kochetkova<sup>1</sup>; David G. Zaridze<sup>1</sup>; <sup>1</sup>N. N. Blokhin Russian Cancer Research Center, Moscow, Russia
- TP 611 **Mass Spectrometric Assay for Specific Subtypes of Low Abundance Cytokine in Human Serum;** Anita Izrael-Tomasevic<sup>1</sup>; Qui Phung<sup>1</sup>; David Arnott<sup>1</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, California
- TP 612 **Fast LC/MS Separations: Improved Platform for Discovery and Identification of Plasma Protein Biomarkers;** Michael Schirm<sup>1</sup>; Kevin Eng<sup>1</sup>; Kossi Lekpor<sup>1</sup>; Sylvain Tessier<sup>1</sup>; Greg Opitck<sup>1</sup>; Paul Kearney<sup>1</sup>; Joanna Hunter<sup>1</sup>; <sup>1</sup>Caprion Pharmaceuticals, Montreal, Canada
- TP 613 **Developing a Procedure for Specific and Efficient Isolation of N-linked Glycopeptides for Serum Profiling;** Yong Zhou<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA
- TP 614 **A Protein Identification Strategy by Combining Accurate MS and MS/MS Data and Plasma Proteome Analysis;** Jin Young Kim<sup>1</sup>; Kyung-Hoon Kwon<sup>1</sup>; Gun Wook Park<sup>1</sup>; Jeong Hwa Lee<sup>1</sup>; Ju Yeon Lee<sup>1</sup>; Kun Cho<sup>1</sup>; Young Ki Paik<sup>2</sup>; Jong Shin Yoo<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Daejeon, South Korea; <sup>2</sup>Yonsei University, Seoul, South Korea
- TP 615 **Applying Protein Microarrays and Mass Spectrometry to the Study of Pancreatic Cancer Signatures in Patient Serum;** Tasneem H. Patwa<sup>1</sup>; Diane Simeone<sup>1</sup>;

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- David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- TP 616 **A Global Proteome Investigation of Inter and Intra Variability of Human Serum Samples;** Nicolas A. Stewart<sup>1</sup>; DaRue A. Prieto<sup>1</sup>; David A. Lucas<sup>1</sup>; Louis M. Cosentino<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD
- TP 617 **Histone Deacetylase Inhibitor SAHA Arrests Cancer Cell Growth – A Proteomics Based Study for Screening Posttranslational Modifications by Acetylation;** Christian Scharf<sup>1</sup>; Le Thi Thu Hong<sup>1</sup>; Jürgen Sonnemann<sup>1</sup>; Elke Hammer<sup>1</sup>; Karanam Narasimha Kumar<sup>1</sup>; James F. Beck<sup>1</sup>; Uwe Völker<sup>1</sup>; <sup>1</sup>Ernst-Moritz-Drndt-University, Medical School, Greifswald, Germany
- TP 618 **LC-MS-based Proteomic Analysis of Plasma from Sled Dogs for Potential Biomarkers of Exertion-Induced Muscle Injury;** Fanyu Meng<sup>1</sup>; Xuemei Zhao<sup>1</sup>; J. Greg Slatter<sup>2</sup>; Nathan Yates<sup>1</sup>; Kenneth Hinchcliff<sup>3</sup>; Roger G. Ulrich<sup>2</sup>; Ronald Hendrickson<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Rahway, NJ; <sup>2</sup>Rosetta Inpharmatics LLC, Merck & Co., Inc., Seattle, WA; <sup>3</sup>Ohio State University, Columbus, OH
- TP 619 **Development of Nanoprobe-Based Affinity Mass Spectrometry for Plasma Protein Profiling;** Po-Hung Chou<sup>2</sup>; Shu-Hua Chen<sup>2</sup>; Hsin-Kai Laio<sup>1</sup>; Po-Chaio Lin<sup>1</sup>; Gour-Rong Her<sup>2</sup>; Chun-Chen Lin<sup>1</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of Chemistry and Genomic Research Center, Taipei, TAIWAN; <sup>2</sup>Department of Chemistry, National Taiwan University, Taipei, TAIWAN
- TP 620 **Proteome-Wide Analysis of Formalin-Fixed Paraffin Embedded Head and Neck Cancer Tissues Using Laser Capture Microdissection and Mass Spectrometry;** Brian L. Hood<sup>1</sup>; Vyomesh Patel<sup>2</sup>; David A. Lucas<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; Alfredo Molinolo<sup>2</sup>; J. Silvio Gutkind<sup>2</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>National Institutes of Health, Bethesda, MD
- TP 621 **Quantitative Proteomic Research on Different Stage of HCC;** Heyi Yang<sup>1</sup>; Yezhou Sun<sup>1</sup>; Gregg Czerwieniec<sup>1</sup>; Weijia zhang<sup>1</sup>; Rong Wang<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY
- TP 622 **Proteomic Analysis of Serum for the Discovery of Biomarkers for Head and Neck Carcinomas;** Lisa J. Zimmerman<sup>1</sup>; Robert J. Slebos<sup>1</sup>; Amy N. Evjen<sup>1</sup>; David L. Tabb<sup>1</sup>; Daniel C. Liebler<sup>1</sup>; Wendell G. Yarbrough<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 623 **Searching for Proteomic Predictors of Disease Progression in a Subpopulation of African American Subjects with Kidney Disease Using SELDI/TOF/MS;** Victor Anbalagan<sup>1</sup>; John Roboz<sup>1</sup>; Michael S. Lipkowitz<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY
- TP 624 **Detection of Oxidatively-Modified Proteins in Human Cerebrospinal Fluid (CSF) using an Aldehyde Reactive Probe;** Woon-Gye Chung<sup>1</sup>; Cristobal L. Miranda<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- TP 625 **Plasma Protein Profile Changes from Adolescence to Adulthood;** Yan Zhang<sup>1</sup>; Alan Sinaiko<sup>1</sup>; Gary Lee Nelsestuen<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, Minnesota
- TP 626 **Identification of Expression Changes and Biomarkers in Mucinous and Serous Pancreatic Cystic Neoplasms;** Babak Hassanzadeh<sup>1</sup>; Puneet Souda<sup>1</sup>; James Farrell<sup>1</sup>; Julian P Whitelegge<sup>1</sup>; Kym F Faull<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA

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- TP 627 **A Two-Step Proteomic Strategy for Rapid Identification of Potential Plasma Biomarkers;** Tatiana Plavina<sup>1</sup>; Marina Hincapie<sup>1</sup>; Eric Wakshull<sup>2</sup>; William S. Hancock<sup>1</sup>; <sup>1</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>2</sup>Biogen Idec, Inc., Cambridge, MA
- TP 628 **Annexin-I as a Target Protein for Green Tea Extract (GTE) Induced Actin Remodeling;** Gary Guishan Xiao<sup>1</sup>; Yu-Sheng Jin<sup>2</sup>; Zuo-Feng Zhang<sup>2</sup>; Arie Beldegrun<sup>2</sup>; Robert Figlin<sup>2</sup>; Qing-Yi Lu<sup>2</sup>; Allan Pantuck<sup>2</sup>; Yun Yen<sup>3</sup>; JianYu Rao<sup>2</sup>; <sup>1</sup>University of California Irvine, Irvine, CA; <sup>2</sup>UCLA, Los Angeles, CA; <sup>3</sup>City of Hope National Medical Center, Duarte, CA
- TP 629 **Proteomic Analysis of Modified ApoB100 Formed by Lipid Peroxidation of LDL in Human Blood Plasma;** Hye-Young H. Kim<sup>1</sup>; Keri A. Tallman<sup>1</sup>; Jianxin Ji<sup>1</sup>; Daniel C. Liebler<sup>1</sup>; Ned A. Porter<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 630 **Development of a Reference Method for the Quantitation of B-type Natriuretic Peptide in Serum by Liquid Chromatography-Mass Spectrometry;** Johanna E Camara<sup>1</sup>; David M Bunk<sup>1</sup>; Michael J Welch<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- TP 631 **Serum Protein Profiling for Detection of Pancreatic Cancer;** Jianzhong Chen<sup>1</sup>; Diane M Simeone<sup>1</sup>; David M Lubman<sup>1</sup>; <sup>1</sup>University of Michigan-Ann Arbor, Ann Arbor, MI
- TP 632 **Pancreatic Cancer Biomarker Discovery - Comparative Analysis of the Low Molecular Fraction from Case/Control Plasma Samples Analyzed by LC/MS TOF;** Michael W. Holmes<sup>1</sup>; Kenneth L. Johnson<sup>1</sup>; H. Robert Bergen III<sup>1</sup>; Douglas W. Mahoney<sup>1</sup>; Ann L. Oberg<sup>1</sup>; David A. Weil<sup>2</sup>; David C. Muddiman<sup>3</sup>; <sup>1</sup>Mayo Clinic College of Medicine, Rochester, MN; <sup>2</sup>Agilent Technologies, Schaumburg, IL; <sup>3</sup>North Carolina State University, Raleigh, NC
- TP 633 **Determination of Beta-Amyloid Peptide Signatures in Cerebrospinal Fluid using Immunoprecipitation-Mass Spectrometry;** Erik Portelius<sup>1</sup>; Henrik Zetterberg<sup>1</sup>; Kaj Blennow<sup>1</sup>; Ann Westman-Brinkmalm<sup>1</sup>; <sup>1</sup>Institute of Clinical Neuroscience and Physiology, Göteborg, Sweden
- TP 634 **Multidimensional Separations for Improved Protein Identification for Proteomes of Human Serum and Rat Liver Tissues;** Iveta Klouckova<sup>1</sup>; Yehia Mechref<sup>2</sup>; Milan Madera<sup>1</sup>; Milos V Novotny<sup>3</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>National Center of Glycomics and Glycoproteomic, Bloomington, IN; <sup>3</sup>METACyt Biochemical Analysis Center, Bloomington, IN
- TP 635 **Identification of Glycoproteins from Human Cerebrospinal Fluid Using Mass Spectrometry Based Proteomics;** Yan Wang<sup>1</sup>; Jinghua Jin<sup>1</sup>; Catherine Pan<sup>1</sup>; Jane Li<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>University of Washington School of Medicine, Seattle, WA
- TP 636 **Differentiating Various Anti-Hypertensives Based on Clinical Response and Plasma Profiling;** Sylvain Tessier<sup>1</sup>; Heather Butler<sup>1</sup>; Nathan Currier<sup>1</sup>; Joanna Hunter<sup>1</sup>; Paul Kearney<sup>1</sup>; Gregory J. Opitck<sup>1</sup>; <sup>1</sup>Caprion Pharmaceuticals, Montreal, Canada
- TP 637 **Expression Profiling in Rat Serum after Carcinogen Administration for Liver Cancer Biomarker Discovery;** Jihyeon Lim<sup>1</sup>; Anuradha Menthena<sup>1</sup>; Linda Siconolfi-Baez<sup>1</sup>; Peicheng Du<sup>1</sup>; Phyllis M. Novikoff<sup>1</sup>; Ruth H. Angeletti<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY

## TUESDAY POSTERS

### POSTER SPACE

#### BIOINFORMATICS II

- TP 638 **Reducing False Positive Rates in MS/MS Sequence Searching and Incorporating Intensity into Match Based Statistics**; Lewis Y. Geer<sup>1</sup>; Dina L. Bai<sup>2</sup>; Jeffrey Kowalak<sup>3</sup>; An Chi<sup>2</sup>; Ming Xu<sup>1</sup>; Jeffrey Shabanowitz<sup>2</sup>; Sanford P. Markey<sup>3</sup>; Donald F. Hunt<sup>2</sup>; Stephen H. Bryant<sup>1</sup>; <sup>1</sup>National Library of Medicine, Bethesda, MD; <sup>2</sup>University of Virginia, Charlottesville, VA; <sup>3</sup>National Institute for Mental Health, Bethesda, MD
- TP 639 **Human Plasma Peptide Atlas**; Eric Deutsch<sup>1</sup>; Nichole King<sup>1</sup>; Jimmy Eng<sup>2</sup>; Alexey Nesvizhskii<sup>3</sup>; Olga Vitek<sup>1</sup>; Ruedi Aebersold<sup>4</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 Michigan Medical School, Ann Arbor, MI; <sup>4</sup>Institute for Molecular Systems Biology, ETH Zurich, Zurich, Switzerland
- TP 640 **DTASelect 2.0: Improving the Confidence of Peptide and Protein Identifications**; Daniel Cociorva<sup>1</sup>; John R Yates<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA
- TP 641 **Processing Raw Mass Spectral Data for High Mass Accuracy**; Yongdong Wang<sup>1</sup>; Ming Gu<sup>1</sup>; <sup>1</sup>Cerno Bioscience, Danbury, CT
- TP 642 **Improved Fragment Assignment by Visual Assistance (FAVA) program**; Shenheng Guan<sup>1</sup>; Alma L. Burlingame<sup>1</sup>; <sup>1</sup>University of California, San Francisco, CA
- TP 643 **Protein Extractor – from Peptide ID to Protein ID**; Martin Blueggel<sup>1</sup>; Gerhard Koerting<sup>1</sup>; Katrin Marcus<sup>3</sup>; Daniel Chamrad<sup>1</sup>; Ulrike Schweiger-Hufnagel<sup>2</sup>; Jörg Glandorf<sup>2</sup>; Meyer Helmut E. <sup>3</sup>; Herbert Thiele<sup>2</sup>; <sup>1</sup>Protagen AG, Dortmund, Germany; <sup>2</sup>Bruker Daltonics GmbH, Bremen, Germany; <sup>3</sup>Medizinisches Proteom Center, Bochum, Germany
- TP 644 **Seeking Effective Combinations of Library Search Methods for Peptide Identifications: A study Using Two Enzymes, Three Concentrations and Five Methods**; Gelio Alves<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>NCBI/NLM/NIH, Bethesda, Maryland; <sup>2</sup>NHLBI/NIH, Bethesda, Maryland
- TP 645 **Clustering Precursors and Associated Products Data Across Multiple Samples**; Guo-Zhong Li<sup>1</sup>; Marc V Gorenstein<sup>1</sup>; Dan Golick<sup>1</sup>; Richard Denny<sup>1</sup>; Craig A. Dorschel<sup>1</sup>; Jeffrey C. Silva<sup>1</sup>; Scott J. Geromanos<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- TP 646 **Models Utilizing Randomized Databases and Peptide Frequency Information from MS/MS for Protein Identification and Relative Expression**; Roger S. Higdon<sup>1</sup>; Jason M. Hogan<sup>1</sup>; Eugene Kolker<sup>1</sup>; <sup>1</sup>The BIATECH Institute, Bothell, WA
- TP 647 **False positive assessment in database search**; Wilfred H. Tang<sup>1</sup>; Sean L. Seymour<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Foster City, CA
- TP 648 **A Next Generation Search Engine that Substantially Improves Peptide Identification by Using Sequence Temperatures and Feature Probabilities**; Sean L. Seymour<sup>1</sup>; Ignat V. Shilov<sup>1</sup>; Alpesh A. Patel<sup>1</sup>; Alex Loboda<sup>1</sup>; Wilfred H. Tang<sup>1</sup>; Sean P. Keating<sup>1</sup>; Daniel A. Schaeffer<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Foster City, CA
- TP 649 **Strategies for achieving high confidence peptide identifications from tandem MS data without losing low abundance components in complex proteomes**; Glenn C. Tan<sup>1</sup>; Hsin-Yao Tang<sup>1</sup>; David W. Speicher<sup>1</sup>; <sup>1</sup>The Wistar Institute, Philadelphia, PA

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- TP 650 **Integrated Top-Down and Bottom-Up Protein Identification Software - PTMSearch Plus**; Heather M. Connelly<sup>1</sup>; Vilmos Kertesz<sup>2</sup>; Robert L. Hettich<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
- TP 651 **A Support Vector Machine Classifier to Reduce False Positive Peptide Spectrum Matches by Identifying Poor Quality Spectra**; Barbara E Frewen<sup>1</sup>; Aaron A Klammer<sup>1</sup>; William Stafford Noble<sup>1</sup>; Michael J MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 652 **Protein Panorama: Probability and Parsimony-based Software for Assessing Proteins Assembled from Peptides Inferred from MS/MS Data**; Jian Feng<sup>2</sup>; Bret Cooper<sup>1</sup>; Daniel Q. Naiman<sup>2</sup>; <sup>1</sup>Soybean Genomics and Improvement Laboratory, USDA, Beltsville, MD; <sup>2</sup>The Johns Hopkins University, Baltimore, MD
- TP 653 **Genome Annotation via Mass Spectrometry**; Stephen Tanner<sup>1</sup>; Francisco Camara<sup>3</sup>; Liliana Florea<sup>2</sup>; Roderic Guigo<sup>3</sup>; Pavel Pevzner<sup>1</sup>; Vineet Bafna<sup>1</sup>; <sup>1</sup>Univ. Cal. San Diego, San Diego, CA; <sup>2</sup>George Washington Univ, Washington, D.C.; <sup>3</sup>Univ. Barcelona, Barcelona, Spain
- TP 654 **Comparing Methods of Associating Precursor and Fragment Ions using Chromatographic Elution Profiles from Data Independent Tandem Mass Spectrometry**; Gregory K. Taylor<sup>1</sup>; Catalin E. Doneanu<sup>1</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 655 **An Open-Source Framework for Evaluating MS/MS Score Functions: “Pluggable Scoring” in X! Tandem**; Brendan MacLean<sup>1</sup>; Jimmy Eng<sup>2</sup>; Martin McIntosh<sup>2</sup>; <sup>1</sup>LabKey Software, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- TP 656 **Cross Correlation Algorithm for Calculation of Peptide Molecular Weight from Tandem Mass Spectra**; John Venable<sup>1</sup>; Tao Xu<sup>1</sup>; Daniel Cociorva<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA
- TP 657 **Contribution of Proteomics Data to the Analysis of the Genome of Francisella tularensis Ssp. Novicida Strain U112**; Laurence Rohmer<sup>1</sup>; Mitch Brittnacher<sup>1</sup>; Jinzhi Chen<sup>1</sup>; Tina Guina<sup>1</sup>; Mike Wasnick<sup>1</sup>; Christie Fong<sup>1</sup>; Ted Larson Freeman<sup>1</sup>; Rajinder Kaul<sup>1</sup>; Scott Shaffer<sup>1</sup>; Byron Gallis<sup>1</sup>; Greg Taylor<sup>1</sup>; David R. Goodlett<sup>1</sup>; Samuel I. Miller<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- TP 658 **Incorporating Predicted Peptide Fragmentation Patterns into MASPIC Scoring Scheme**; Chandra Narasimhan<sup>1</sup>; Robert L. Hettich<sup>3</sup>; Edward C. Uberbacher<sup>2</sup>; <sup>1</sup>UT-ORNL Genome Science & Tech., Oak Ridge, TN; <sup>2</sup>Life Science Division, Oak Ridge National Lab, Oak Ridge, TN; <sup>3</sup>Chemical Science Division, Oak Ridge National Lab, Oak Ridge, TN
- TP 659 **Principle and Applications of a new Algorithm for Monoisotopic Mass Determination**; Jens Decker<sup>1</sup>; Michael Easterling<sup>2</sup>; Christian B. Berg<sup>2</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA
- TP 660 **Intensity-Based Scoring for Peptide Identification using Tandem Mass Spectra**; Randy J. Arnold<sup>1</sup>; Divya Aggarwal<sup>1</sup>; David E. Clemmer<sup>1</sup>; Narmada Jayasankar<sup>1</sup>; Predrag Radivojac<sup>1</sup>; Zhiyin Xun<sup>1</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- TP 661 **Automated Reprocessing Pipeline for Analysing Heterogenic Data of the HUPO Brain Proteome Project Pilot Phase**; Christian Stephan<sup>1</sup>; Martin Blüggel<sup>4</sup>; Kai A. Reidegeld<sup>1</sup>; Gerhard Körting<sup>4</sup>; Daniel Chamrad<sup>4</sup>; Michael Hamacher<sup>1</sup>; Katrin Marcus<sup>1</sup>; Rolf Apweiler<sup>2</sup>;

## TUESDAY POSTERS

### POSTER SPACE

Henning Hermjakob<sup>2</sup>; Michael Müller<sup>2</sup>; Lennart Martens<sup>3</sup>; Herbert Thiele<sup>5</sup>; David Parkinson<sup>6</sup>; Andre Dowsey<sup>7</sup>; Michael Dunn<sup>8</sup>; Helmut E. Meyer<sup>1</sup>; <sup>1</sup>*Medical Proteom-Center, Bochum, Germany*; <sup>2</sup>*European Bioinformatics Institute, Hinxton, United Kingdom*; <sup>3</sup>*Department of Medical Protein Research, Ghent, Belgium*; <sup>4</sup>*Protagen AG, Dortmund, Germany*; <sup>5</sup>*Bruker Daltonics GmbH, Bremen, Germany*; <sup>6</sup>*Biomedical Research Centre, Sheffield, United Kingdom*; <sup>7</sup>*Imperial College, London, United Kingdom*; <sup>8</sup>*Proteomics Department, Conway Institute, Dublin, Ireland*

- TP 662 **De novo Algorithm Significantly Outperform Database Search in Coverage of "Normal" Proteins;** Andrey Gorin<sup>1</sup>; Robert M. Day<sup>1</sup>; Nikita D. Arnold<sup>1</sup>; Tema Fridman<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*

### RECOMBINANT PROTEINS

- TP 663 **Characterization of Monoclonal Antibody Degradants;** Qing (Mike) Tang<sup>1</sup>; Maggie Huang<sup>1</sup>; Weijun Ren<sup>1</sup>; Michael J. Lewis<sup>1</sup>; Michael D. Bond<sup>1</sup>; <sup>1</sup>*Centocor, Inc., Radnor, PA*
- TP 664 **Evaluating the Disulfide Map of A Recombinant Membrane Protein by LC/MS/MS;** Marc Wenger<sup>1</sup>; Peter A. DePhillips<sup>1</sup>; Lorenzo H. Chen<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*
- TP 665 **High-Throughput Identification of Recombinant Protein Phosphorylation Sites using ESI Q-TOF Mass Spectrometry;** Matthew R. Stump<sup>1</sup>; Mark T. Cancilla<sup>1</sup>; <sup>1</sup>*Sunesis Pharmaceuticals, South San Francisco, CA*
- TP 666 **Rapid Removal of Non-ionic Detergents From Monoclonal Antibodies and Other Proteins for Mass Spectrometry Analysis Using Centrifugal Ultrafiltration;** Gary W Lange<sup>1</sup>; Joseph W Leone<sup>1</sup>; Barrett R Thiele<sup>1</sup>; Megan A Danielewicz<sup>2</sup>; Stone D-H Shi<sup>2</sup>; <sup>1</sup>*Pfizer Inc, St. Louis, MO*; <sup>2</sup>*Pfizer Inc, La Jolla, CA*
- TP 667 **Characterization of Antibody-Drug Conjugates by ESI/LC/MS;** Galahad U Deperalta<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*
- TP 668 **Characterization and Investigation of N-terminal Cyclization of Monoclonal Antibodies in the Formulation Products;** Bryan L. Yu<sup>1</sup>; Alona Vizel<sup>1</sup>; Richard L. Remmele Jr.<sup>1</sup>; Bing He<sup>1</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*
- TP 669 **Rapid Identification of Therapeutic Proteins by Peptide Mass Fingerprinting;** Mary Zhu<sup>1</sup>; William E. Haskins<sup>1</sup>; Viswanatham Katta<sup>1</sup>; <sup>1</sup>*Genentech, Inc., South San Francisco, CA*
- TP 670 **Characterization of Inter-Capsomeric Disulfide Bonding in Human Papillomavirus Recombinant Virus-Like Particles Using LC/MS;** Colleen E. Price<sup>1</sup>; Marc Wenger<sup>1</sup>; Pete DePhillips<sup>1</sup>; Lorenzo Chen<sup>1</sup>; <sup>1</sup>*Merck and Co., Inc., West Point, PA*
- TP 671 **Determination of Minor Variants in Recombinant Proteins by Hydrophobic Interaction Chromatography Combined with High Resolution Mass Spectrometry;** Terry D. Cyr<sup>1</sup>; Diane Bertrand<sup>1</sup>; Susan Pozzobon<sup>1</sup>; Barry Lorbetskie<sup>1</sup>; Sean Li<sup>1</sup>; Mary Alice Hefford<sup>1</sup>; Michel Girard<sup>1</sup>; <sup>1</sup>*Centre for Biologics Research, Health Canada, Ottawa, Canada*
- TP 672 **Structural Characterization of an Extracellular Domain of a Recombinant Human Respiratory Syncytial Virus Fusion (RSV F) Protein;** Steven C Pomerantz<sup>1</sup>; Nicole D. Day<sup>1</sup>; Changbao Liu<sup>1</sup>; Lester L. Gutshall<sup>1</sup>; Patrick J. Branigan<sup>1</sup>; Robert T. Sarisky<sup>1</sup>; Alfred

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M. Del Vecchio<sup>1</sup>; Jennifer F. Nemeth<sup>1</sup>; <sup>1</sup>*Centocor Research and Development, Radnor, PA*

- TP 673 **Rapid Characterization of an IgG2 Monoclonal Antibody utilizing UPLC/MS (Ultraperformance Liquid Chromatography/Mass Spectrometry);** Robert L. Dufield<sup>1</sup>; James A. Carroll<sup>1</sup>; <sup>1</sup>*Pfizer, Chesterfield, MO*

# WEDNESDAY POSTERS

## POSTER SPACE

### WEDNESDAY POSTERS

These posters should be set up at 7:30 am on Wednesday and removed at 7:30 pm.

Be sure to use the poster space number next to the title.

#### ION MOLECULE REACTIONS

- WP 9 **Inter- & Intraligand Reactions in Cu(II)/Amino Acid and Peptide Complexes;** Ping Wang<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH
- WP 10 **New Ion/Molecule Reactions with Novel Implementations for the Selective Detection of Nitroaromatic Explosives;** Yishu Song<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 11 **H/D Exchange Reactions of Arginine and Arginine-Containing Peptides;** Yiqun Huang<sup>1,2,3,4</sup>; Shane Tichy<sup>1,2,3,4</sup>; Joe Marini<sup>1,2,3,4</sup>; John Mclean<sup>1,2,3,4</sup>; David Russell<sup>1,2,3,4</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Texas A&M University, College Station, TX; <sup>3</sup>Texas A&M University, College Station, TX; <sup>4</sup>Texas A&M University, College Station, TX
- WP 12 **Reaction of Furan, Thiophene and Pyrrole Radical Cations with Simple Alkynes in the Gas Phase;** Daryl Giblin<sup>1</sup>; Chang-fu Cheng<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University, St. Louis, MO
- WP 13 **An Unprecedented Rearrangement in Collision-Induced Mass Spectrometric Fragmentation of Protonated Benzylamines;** Jason B. Bialecki<sup>1</sup>; <sup>1</sup>Stevens Institute of Technology, Hoboken, NJ
- WP 14 **Identification of Ion Isomers Produced in Ion-Molecule Reactions;** Pavel Vinogradov<sup>1</sup>; Alexander Misharin<sup>1</sup>; <sup>1</sup>Institute of Energy Problems of Chemical Physics, Moscow, Russia
- WP 15 **Gas-Phase Reactions of Bare and Oxo-Ligated Actinide Cations with Alkanes and Alkenes Studied by FTICR-MS;** Marta Santos<sup>1</sup>; Joaquim Marçalo<sup>1</sup>; António Pires de Matos<sup>1</sup>; John K. Gibson<sup>2</sup>; Richard G. Haire<sup>2</sup>; <sup>1</sup>Instituto Tecnológico e Nuclear, Sacavém, Portugal; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- WP 16 **Gas-Phase Oxidation of Atomic Lanthanide Cations: Trends in Reactivity and New Insights into Controlling Factors;** Michael J. Y. Jarvis<sup>1</sup>; Gregory K. Koyanagi<sup>1</sup>; Voislav Blagojevic<sup>1</sup>; Ping Cheng<sup>1</sup>; Diethard K. Bohme<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada
- WP 17 **Interface of Liquid Chromatography - Mass Spectrometry with Ion-Molecule Reactions in the Quadrupole Ion Trap;** Yuriy Pyatkivskyy<sup>1</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>Northern Illinois University, DeKalb, IL
- WP 18 **Sodium Binding Affinity of Adenine;** Bethany L. Subel<sup>1</sup>; Ping Wang<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH
- WP 19 **Mass Spectrometric Fingerprints of Novel Synthetic Cholesteryl Neoglycolipids: The Presence of a Unique C Glycoside Species;** Anas El-Aneel<sup>1</sup>; Joseph Banoub<sup>2</sup>; Paul Boullanger<sup>3</sup>; Dominique Lafont<sup>3</sup>; Mariano Koehn-Alonso<sup>2</sup>; <sup>1</sup>Memorial University of Newfoundland, St. John's, NL; <sup>2</sup>Department of Fisheries and Oceans, St. John's, NL; <sup>3</sup>Université Claude Bernard, Villeurbanne, France
- WP 20 **Reduction of Nitriles to Amines in Positive Ion Electrospray Ionization Mass Spectrometry;** Jiyuan Ma<sup>1</sup>; Zhe-ming Gu<sup>1</sup>; <sup>1</sup>XenoBiotic Laboratories, Inc., Plainsboro, NJ
- WP 21 **Ion-Dipole Effects on the Binding in Cation- $\pi$  Complexes: Absolute Bond Dissociation Energies of Alkali Metal Cation-Methylated Aniline Complexes;**

## POSTER SPACE

Nuwan Hallowita<sup>1</sup>; M.T. Rodgers<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI

- WP 22 **Identification of the Tertiary N-Oxide Functionality via Ion-Molecule Reactions in a Fourier Transform Ion Cyclotron Resonance (FT-ICR) Mass Spectrometer;** Penggao Duan<sup>1</sup>; Todd A. Gillespie<sup>2</sup>; Brian E. Winger<sup>2</sup>; Hilkka I. Kenttämä<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Eli Lilly and Company, Indianapolis, IN
- WP 23 **Acidity and Proton Affinity of Hypoxanthine, a Potentially Mutagenic Nucleobase;** Xuejun Sun<sup>1</sup>; Jeehiun K. Lee<sup>1</sup>; <sup>1</sup>Rutgers University-New Brunswick, Piscataway, NJ

#### IONIZATION MECHANISMS

- WP 24 **Microchannel Plate Detection Efficiencies of Large Biomolecules;** Ling-Chu Lora Huang<sup>1</sup>; Yi-Sheng Wang<sup>1</sup>; Chung-Hsuan Winston Chen<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan
- WP 25 **Kinematic Investigation of Electrosprayed Droplets for Mechanistic Studies of Desorption Electrospray Ionization;** Andre Venter<sup>1</sup>; Paul E. Sojka<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, Indiana
- WP 26 **Theoretical Investigation of the (PA) and (GB) of Neutral x,y-Dihydroxybenzoic (DHB) Acid and its Derivatives;** Mario E Gomez<sup>1</sup>; Sajid Bashir<sup>1</sup>; Nichollas Beller<sup>1</sup>; Brandon Rebber<sup>2</sup>; Kyle Beran<sup>2</sup>; <sup>1</sup>Texas A&M University-Kingsville, Kingsville, Texas; <sup>2</sup>University of Texas at The Permian Basin, Odessa, Texas
- WP 27 **Particle Formation in MALDI;** Xing Fan<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- WP 28 **Dependencies on Pressure and Wavelength in Ablation During UV-MALDI;** Dirk Walbrodt<sup>1</sup>; Tassilo Muskat<sup>1</sup>; Juergen Grotemeyer<sup>1</sup>; <sup>1</sup>Inst. f. Phys. Chem., CAU, Kiel, Germany
- WP 29 **Solid Phase Protonation/Deprotonation Model for MALDI Mechanism;** C.H.(Winston) Chen<sup>1</sup>; Wei-Chao Chang<sup>1</sup>; L.C.(Lora) Huang<sup>1</sup>; Yi-Sheng Wang<sup>1</sup>; Wen-Ping Peng<sup>1</sup>; Nien-Yeen Hsu<sup>2</sup>; Wen-Bin Yang<sup>1</sup>; Huan-Cheng Chang<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan; <sup>2</sup>National Taiwan University, Taipei, Taiwan
- WP 30 **Electrospray Ions in Statu Nascendi or a Chemical View on the Last Steps of the Birth of Electrosprayed Ions;** Michael Karas<sup>1</sup>; Ute Bahr<sup>1</sup>; <sup>1</sup>J.W. Goethe University, Frankfurt, Germany
- WP 31 **Origin of Peptide/Matrix Adduct Ions Generated under AP-MALDI;** Jessie Naban-Maillet<sup>1</sup>; Carlos Afonso<sup>1</sup>; Anne Bossée<sup>2</sup>; Françoise Fournier<sup>1</sup>; Bruno Bellier<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris 6, UMR 7613, Paris, France; <sup>2</sup>CEB/DGA, Vert-le-Petit, France
- WP 32 **Ionization Pathways for Arylboronic Acids under Electrospray Conditions;** Siming L Wang<sup>12</sup>; Binghe Wang<sup>12</sup>; <sup>1</sup>Department of Chemistry, Georgia State University, Atlanta, GA; <sup>2</sup>Department of Chemistry, Georgia State University, Atlanta, GA
- WP 33 **Current Mapping Within the Electrospray Emitter;** Boguslaw P. Pozniak<sup>1</sup>; Richard B. Cole<sup>1</sup>; <sup>1</sup>University of New Orleans, New Orleans, LA
- WP 34 **Electron Transfer MALDI: Thermodynamic and Kinetic Factors Affecting Ion Intensities;** Richard Knochenmuss<sup>1</sup>; Andrew Hotelling<sup>2</sup>; William Nichols<sup>2</sup>; David Giesen<sup>2</sup>; Jerome Lenhard<sup>2</sup>; <sup>1</sup>Novartis Inst. of Biomedical Research, Basel, Switzerland; <sup>2</sup>Research & Development, Eastman Kodak, Rochester, NY
- WP 35 **Resonant Electron Capture of Peptides Desorbed by In-Beam Technique;** Benjamin J. Figard<sup>1</sup>; Yuri V.

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- Vasil'ev<sup>1</sup>; Max L. Deinzer<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- WP 36 **Correlation of Thermodynamic and (photo)physical Properties of MALDI Matrices with Analyte Ionization Efficiencies**; Ganga S. Fernando<sup>1</sup>; Gary R. Kinsel<sup>1</sup>; <sup>1</sup>Southern Illinois University, Carbondale, IL

### DIRECT IONIZATION TECHNIQUES

- WP 37 **Observing Droplet Electrospray ionization Processes in Desorption Electrospray Ionization (DESI) Mass Spectrometry**; Hsiu-Jung Hsu<sup>1</sup>; Yu-Xiang Lin<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan
- WP 38 **Evaluation of the Use of Desorption Ionisation Techniques for the Analysis of Formulated Products**; Abigale J Marcus<sup>1</sup>; Anthony P. New<sup>2</sup>; <sup>1</sup>GlaxoSmithKline, King of Prussia, PA; <sup>2</sup>GlaxoSmithKline, Ware, UK
- WP 39 **Forensic Applications with a Direct Analysis in Real Time (DART) Mass Spectrometer**; Eshwar Jagerdeo<sup>1</sup>; Jeffrey N. Leibowitz<sup>1</sup>; Robert B. Cody<sup>2</sup>; Jay Clark<sup>1</sup>; Lisa Schumacher<sup>1</sup>; Marc LeBeau<sup>1</sup>; <sup>1</sup>FBI Laboratory, Quantico, VA; <sup>2</sup>JEOL USA Inc., Peabody, MA
- WP 40 **Direct Identification of API in Expired Medicines and the Pfizer Drugs Separated by TLC with DART AccuTOF System**; Zhongli Zhang<sup>1</sup>; Ronald Morris<sup>1</sup>; Eugene Kadar<sup>1</sup>; Robert Cody<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>JEOL USA, Peabody, MA
- WP 41 **New Surfaces for Desorption Electrospray-Mass Spectrometry: Porous Silicon Chips and Ultra-Thin Layer Chromatography Plates**; Tiina J. Kauppila<sup>1</sup>; Nari N. Talaty<sup>2</sup>; Piia K. Salo<sup>1</sup>; Tapio Kotiaho<sup>1</sup>; Risto Kostiaainen<sup>1</sup>; R. Graham Cooks<sup>2</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland; <sup>2</sup>Purdue University, West Lafayette, IN
- WP 42 **Direct Analysis of S9 Fractions without Sample Preparation**; Matthew I Lochansky<sup>1</sup>; <sup>1</sup>GlaxoSmithKline, Research Triangle Park, NC
- WP 43 **Desorption Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry of Self-Assembling Phloroglucinol Derivative Inclusion Complexes**; Joanna E. Barbara<sup>1</sup>; David H. Powell<sup>1</sup>; John R. Eyler<sup>1</sup>; Ronald R. Castellano<sup>1</sup>; Andrew J. Lampkins<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- WP 44 **Plume/Sample Interaction with Desorption-Electrospray Ionization (DESI) Mass Spectrometry: Impact on Surface Imaging and Nanospray Formats**; Gary A. Valaskovic<sup>1</sup>; Mike S. Lee<sup>2</sup>; <sup>1</sup>New Objective, Inc., Woburn, MA; <sup>2</sup>Milestone Development, Inc., New Town, PA
- WP 45 **Direct Analysis of Phospholipids from Tissue Sections by DESI and MALDI MS**; Satu M. Puolitaival<sup>1</sup>; Justin M. Wiseman<sup>2</sup>; Zoltán Takáts<sup>3</sup>; R. Graham Cooks<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Department of Chemistry, Nashville, TN; <sup>2</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>3</sup>Hungarian Academy of Sciences, Budapest, Hungary
- WP 46 **High Throughput Direct Probe-Based Identification of Chemicals with DART**; Douglas H. Simmons<sup>1</sup>; Brian D. Musselman<sup>1</sup>; <sup>1</sup>IonSense, Inc., Danvers, MA
- WP 47 **"Out in the Open": Direct Analysis in Real Time (DART) One Year Later**; Robert B. Cody<sup>1</sup>; James A. Laramée<sup>2</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA; <sup>2</sup>ECBC, Aberdeen, MD
- WP 48 **On-Surface Eberlin Reactions Via Desorption Electrospray Ionization Mass Spectrometry**; Marcos N Eberlin<sup>1</sup>; Livia S Eberlin<sup>1</sup>; Regina Sparrapan<sup>1</sup>; Renato Haddad<sup>1</sup>; Rodinei Augusti<sup>2</sup>; R. Graham Cooks<sup>3</sup>; <sup>1</sup>State

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- University of Campinas, Campinas, Brazil; <sup>2</sup>Federal University of Minas Gerais, Belo Horizonte, Brazil; <sup>3</sup>Purdue University, West Lafayette, IN
- WP 49 **Desorption Electrospray Ionization Mass Spectrometry of Blood Samples**; Luc Alexis Leuthold<sup>1</sup>; Jean-François Mandscheff<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Life Sciences Mass Spectrom., Geneva, Switzerland
- WP 50 **DESI-MS: A New Tool for Forensic Chemistry Laboratories**; Sandra E. Rodriguez-Cruz<sup>1</sup>; <sup>1</sup>Drug Enforcement Administration - SWL, Vista, CA
- WP 51 **The use of Tandem Mass Spectrometry and Ion Mobility Approaches to Increase the Information Content of Direct Ionisation Methods**; James H Scrivens<sup>1</sup>; Jonathan P Williams<sup>1</sup>; Richard J Holland<sup>1</sup>; Vibhuti J Patel<sup>1</sup>; Susan E Slade<sup>1</sup>; Robert H Bateman<sup>2</sup>; Kevin Giles<sup>2</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Micromass MS Technologies Waters UK, Manchester, UK

### COMPUTER APPLICATIONS

- WP 52 **An Affordable LIMS System Designed for an Academic Environment and Customized for Both Open-Access and Service Labs**; Dana Reed<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN
- WP 53 **Rapid Development of Automated Instrument Control using Python Script Language**; Kenji Nagatomo<sup>1</sup>; Toshinobu Hondo<sup>1</sup>; Jun Tamura<sup>1</sup>; Robert Cody<sup>2</sup>; <sup>1</sup>JEOL Ltd., Akishima, Tokyo, Japan; <sup>2</sup>JEOL USA Inc., Peabody, MA
- WP 54 **Calculation of Key Characteristics for Ion Ensembles in Quadrupole Ion Traps Without Using Trajectory Simulations**; Douglas E. Goeringer<sup>1</sup>; Larry A. Viehland<sup>2</sup>; Daniel M. Danailov<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>Chatham College, Pittsburgh, PA
- WP 55 **A Novel Adaptive Background Subtraction Algorithm for Reduction of Chemical Noise in Mass Spectra**; Martin R Green<sup>1</sup>; Keith Richardson<sup>1</sup>; Martin Palmer<sup>1</sup>; Richard Denny<sup>1</sup>; Iain Campuzano<sup>1</sup>; John Skilling<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, England; <sup>2</sup>Maximum Entropy Data Consultants Ltd, Kenmare, Ireland
- WP 56 **Peak Shape Self-Modelling for Low Abundance Analytes in Complex Mixtures**; Anthony Ferrige<sup>1</sup>; Robert Alecio<sup>1</sup>; Peter Leopold<sup>2</sup>; <sup>1</sup>Positive Probability Ltd, Isleham, UK; <sup>2</sup>BioAnalyte Inc., Portland, ME
- WP 57 **Molecular Weight Determination of Large Molecules by Maximum Entropy Charge Deconvolution of ESI-FTMS Analyses**; Peter Sander<sup>1</sup>; Thomas Roemer<sup>1</sup>; Michael Easterling<sup>2</sup>; Linda DeNoyer<sup>3</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Spectrum Square Associates, Ithaca, NY
- WP 58 **Systematic Investigation of Lycopene Mechanism in Prostate Cancer using Novel Large-Scale Proteomic Analysis Software**; Young Ah Goo<sup>1</sup>; Zheng Li<sup>2</sup>; Natasa Pajkovic<sup>3</sup>; Greg Taylor<sup>1</sup>; Larry Arnstein<sup>2</sup>; Scott Shaffer<sup>1</sup>; Richard van Breemen<sup>3</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Teranode Corporation, Seattle, WA; <sup>3</sup>University of Illinois, Chicago, IL
- WP 59 **Software Applications for Integration and Analysis of Mass Spectroscopy Data**; Bindu Nanduri<sup>1</sup>; Shane C Burgess<sup>1</sup>; Edward B Allen<sup>1</sup>; <sup>1</sup>Mississippi State University, Mississippi State, MS
- WP 60 **Extensible Cross-Platform FileMaker Pro-Based Software Tools for Proteomic Calculations**; Fred J Taub<sup>1</sup>; Qiangwei Xia<sup>1</sup>; Tiansong "Tony" Wang<sup>1</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA



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- WP 61 **Comparison of Methods for Detecting and Deisotoping Weak, High Charge Signals in Data;** Tony G Ferrige<sup>1</sup>; Robert Alecio<sup>1</sup>; Stuart Ray<sup>1</sup>; Lewis K Pannell<sup>2</sup>; <sup>1</sup>Positive Probability Limited, Isleham, UK; <sup>2</sup>Cancer Research Institute, Mobile, AL
- WP 62 **CRAM'ing Macromolecular Ions in an ICR;** David C Green<sup>1</sup>; Simin D Maleknia<sup>1</sup>; <sup>1</sup>Griffith University, Brisbane, Australia; <sup>2</sup>Sciformatics, Sydney, Australia
- WP 63 **PRISM - A New Computer Algorithm to Shed Light on Protein Interactions by Mass Spectrometry;** Joshua Ho<sup>1</sup>; Kevin Downard<sup>1</sup>; <sup>1</sup>The University of Sydney, Sydney, Australia
- WP 64 **NRPP MS Viewer: Full Featured Open Source Spectrum Viewing Annotation And Spectrum Processing Tool;** Panagiotis G Papoulias<sup>1</sup>; Philip C Andrews<sup>1</sup>; David H Lentz<sup>1</sup>; <sup>1</sup>University Of Michigan, Ann Arbor, MI
- WP 65 **Unambiguous Identification of Compounds in LC/MS<sup>n</sup> Analyses by Mass-Spectral Library Search;** Peter Sander<sup>1</sup>; Birgit Schneider<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany
- WP 66 **PRIME: Proteome Research Information Management Environment For High-Throughput Proteomics Laboratories;** David H. Lentz<sup>1</sup>; Panagiotis G Papoulias<sup>1</sup>; Philip C Andrews<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- WP 67 **Using MS Search Programs/EI Databases in Identification of Compounds that Generate Mass Spectra Regardless of Mass-Accuracy or Ionization Technique;** O. David Sparkman<sup>1</sup>; Patrick R. Jones<sup>1</sup>; Teresa Vail<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA
- WP 68 **PROXIMO - A New Docking Algorithm to Model Protein Complexes with Data from Radical Probe Mass Spectrometry;** Sebastien Gerega<sup>1</sup>; Kevin Downard<sup>1</sup>; <sup>1</sup>The University of Sydney, Sydney, Australia
- WP 69 **Comparison of Several Wavelet Techniques for Denoising and Enhancement of Fourier-Transform Ion Cyclotron Resonance Mass Spectral Data;** Paul D. Schnier<sup>1</sup>; Mikhail Toupikov<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA
- WP 70 **Why is Automating the Determination of Molecular Ion using Automated Approaches so Hard and How Might it be Used?;** Mark A. Bayliss<sup>1</sup>; Vitaly Lashin<sup>2</sup>; <sup>1</sup>Advanced Chemistry Development Inc, Toronto, ON; <sup>2</sup>Advanced Chemistry Development, Moscow, Russia
- WP 71 **MSPack - Mass Spectrometry Data Compression Software;** Mingjie Xie<sup>1</sup>; Bin Ma<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Canada
- WP 72 **GenoMass – An Automated Software Tool for Data Analysis of Complicated DNA and DNA-Adduct LC/MS Data;** Chang Shen<sup>1</sup>; Qing Liao<sup>2</sup>; Paul Vourou<sup>3</sup>; <sup>1</sup>Shenitech, Acton, MA; <sup>2</sup>Harvard University Mass Spec Facility, Cambridge, MA; <sup>3</sup>Northeastern University, Boston, MA
- WP 73 **A Software Application for MS Data Processing and Post Translational Modification Database Generation;** James West<sup>1</sup>; Hua Huang<sup>1</sup>; Weiwei Tong<sup>1</sup>; Yang Su<sup>1</sup>; David Perlman<sup>1</sup>; Mark E. McComb<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- WP 74 **IUPAC Standard Definitions of Terms Relating to Mass Spectrometry;** Kermit K. Murray<sup>1</sup>; Robert K. Boyd<sup>2</sup>; Marcos N. Eberlin<sup>3</sup>; G. John Langley<sup>4</sup>; Liang Li<sup>5</sup>; Yasuhide Naito<sup>6</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA; <sup>2</sup>National Research Council, Ottawa, Canada;

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- <sup>3</sup>State University of Campinas, Campinas, Brazil; <sup>4</sup>University of Southampton, Southampton, UK; <sup>5</sup>University of Alberta, Edmonton, Canada; <sup>6</sup>Graduate School Creat. New Photonics Industries, Hamamatsu, Japan
- WP 75 **New 3D Visualization Tools for Ion Trajectory Simulations in FTICR-MS;** Wojciech Burakiewicz<sup>2</sup>; Robert van Liere<sup>2</sup>; Eugene N. Nikolaev<sup>3</sup>; Alexander M. Popov<sup>4</sup>; Ioana M. Taban<sup>1</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM-insitute for Atomic and Molecular Physics, Amsterdam, The Netherlands; <sup>2</sup>Centre for Mathematics and Informatics, Amsterdam, The Netherlands; <sup>3</sup>The Institute for Energy Problems of Chem.Physics, Moscow, Russia; <sup>4</sup>Moscow State University, Moscow, Russia
- WP 76 **Use of a Novel Exact Mass Isotopic Matching Algorithm and Laser Desorption Ionisation for Rapid Identification of Dyes and Pigments;** Joanne Mather<sup>1</sup>; Jeff Goshawk<sup>1</sup>; Ramesh Rao<sup>1</sup>; Ronan O'Malley<sup>1</sup>; Dan McMillan<sup>1</sup>; <sup>1</sup>Waters MS Technologies Centre, Manchester, UK
- WP 77 **Modeling Experimental Designs in Proteomics to Improve the Dynamic Range;** Jan Eriksson<sup>1</sup>; David Fenyó<sup>2</sup>; <sup>1</sup>Swedish University of Agricultural Sciences, Uppsala, Sweden; <sup>2</sup>The Rockefeller University, New York, NY
- WP 78 **A Software Tool for Automated Molecular Composition Profiling of the Lipidome;** Eva Duchoslav<sup>1</sup>; Christer S. Ejsing<sup>2</sup>; Kim Ekroos<sup>3</sup>; Julie Wingate<sup>1</sup>; Ron Bonner<sup>1</sup>; Andrej Shevchenko<sup>2</sup>; <sup>1</sup>MDS Sciex, Concord, Canada; <sup>2</sup>MPI-CBG, Dresden, Germany; <sup>3</sup>AstraZeneca R&D, Molndal, Sweden
- WP 79 **A Diverse Dataset to Assist in the Production of Improved Peptide and Protein Identification Software;** John E. Klimek<sup>1</sup>; Laura J. Hohmann<sup>1</sup>; Jimmy K. Eng<sup>1</sup>; Jennifer Jackson<sup>1</sup>; Andrew B. Gemmill<sup>1</sup>; Daniel B. Martin<sup>1</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA
- WP 80 **Isotope Modeling Routines Applied to Empirical Formula Prediction;** Simon Ashton<sup>1</sup>; Richard Gallagher<sup>2</sup>; Neil Loftus<sup>1</sup>; John Warrander<sup>1</sup>; Ichiro Hirano<sup>3</sup>; Shinichi Yamaguchi<sup>3</sup>; Norio Mukai<sup>3</sup>; <sup>1</sup>Shimadzu ISS, Manchester, UK; <sup>2</sup>AstraZeneca, Alderley Park, Macclesfield, UK; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- WP 81 **Development of the Real-Time CID/ECD Switching and Control System Based on MS<sup>n</sup> spectra;** Toshiyuki Yokosuka<sup>1</sup>; Kiyomi Yoshinari<sup>1</sup>; Kinya Kobayashi<sup>1</sup>; Takashi Baba<sup>2</sup>; Hiroyuki Satake<sup>2</sup>; Atsumu Hirabayashi<sup>2</sup>; Yuichiro Hashimoto<sup>2</sup>; Izumi Waki<sup>2</sup>; <sup>1</sup>Hitachi, Ltd. Hitachi Research Laboratory, Hitachi, Japan; <sup>2</sup>Hitachi, Ltd. Central Research Laboratory, Kokubunji, Japan
- WP 82 **How to Manage a Large Jurisdiction of LC-MS/MS Users in a Typical Regulated Pharmaceutical Environment;** Björn Behrens<sup>1</sup>; Markus Mickel<sup>2</sup>; Axel Besa<sup>2</sup>; <sup>1</sup>Schering, Berlin, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- ENVIRONMENTAL ANALYSIS: FOOD AND PESTICIDES**
- WP 83 **Comparison of Different Ionization Techniques for the Determination of HBCD by LC-MS;** Sami Huhtala<sup>1</sup>; Gordia MacInnis<sup>2</sup>; Sean Backus<sup>2</sup>; Mark Hewitt<sup>2</sup>; Mehran Alaei<sup>2</sup>; Gregg Tomy<sup>3</sup>; Chris Marvin<sup>2</sup>; <sup>1</sup>Finnish Environment Institute, Helsinki, Finland; <sup>2</sup>Environment Canada, Burlington, ON, Canada; <sup>3</sup>Department of Fisheries and Oceans, Winnipeg, MA Canada
- WP 84 **Determination of Perchlorate in Soil by IC-MS using Accelerated Solvent Extraction with Integrated Clean-up: A Study of Time and Recoveries;** Rosanne W. Slingsby<sup>1</sup>; Sheldon E. Henderson<sup>2</sup>; Brett J. Murphy<sup>2</sup>;

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- Bruce E. Richter<sup>2</sup>; Douglas W. Later<sup>1</sup>; <sup>1</sup>Dionex Corporation, Sunnyvale, CA; <sup>2</sup>Dionex Corporation, Salt Lake City, UT
- WP 85 **Quantification and Verification of Aminoglycoside Antibiotics in Honey by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS-MS);** David Durden<sup>1</sup>; <sup>1</sup>Canadian Food Inspection Agency, Calgary, AB, Canada
- WP 86 **Analysis of Estrogens in Environmental Samples below 0.1 ng/L by LC/MS/MS using SPE with GPC for Enhanced Sample Preparation;** Stephen Lock<sup>1</sup>; Rakesh Kanda<sup>2</sup>; <sup>1</sup>Applied Biosystems, Warrington, UK; <sup>2</sup>Severn Trent Laboratories, Reading, UK
- WP 87 **DEP Metabolism;** James A. Campbell<sup>1</sup>; Andrea L. Busby<sup>1</sup>; Charles Timchalk<sup>1</sup>; Dana B. Barr<sup>2</sup>; Ralph D. Whitehead<sup>2</sup>; <sup>1</sup>Battelle, Pacific Northwest Division, Richland, WA; <sup>2</sup>Center for Disease Control and Prevention, Atlanta, Ga
- WP 88 **Photochemical Degradation of BDE-209 and GC-MS Study of the Products;** Xia Zeng<sup>1</sup>; Staci Simonich<sup>1</sup>; Douglas Barofsky<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- WP 89 **The Use of Red Wine as a Matrix to Test LC/MS System Robustness with Automated Sample Cleanup;** Jonathan R Beck<sup>1</sup>; Dipankar Ghosh<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA
- WP 90 **Quantitative LCMSMS Analysis of Disperse Dyes in Textile samples;** Matthew Grigg<sup>1</sup>; Andre Schreiber<sup>2</sup>; <sup>1</sup>Applied Biosystems, Singapore, Singapore; <sup>2</sup>MDS Sciex, Toronto, Canada
- WP 91 **Determination of Chlorophenols in Soils via Supercritical Fluid on Line with Solid-Phase Microextraction;** Wen-Hsin Li<sup>1</sup>; Maw-Rong Lee<sup>1</sup>; <sup>1</sup>National Chung-Hsing University, Taichung, Taiwan, ROC
- WP 92 **Comparison of Ion-Pairing and Solid-Phase Extraction Methods for LC-MS/MS Measurement of Perfluoroalkylated Substances in Human Serum;** Cariton Kubwabo<sup>1</sup>; Brian Stewart<sup>1</sup>; <sup>1</sup>Health Canada, Ottawa, Canada
- WP 93 **Applications of Imaging Matrix Assisted Laser Desorption Ionisation - Mass Spectrometry to the Study of Dermal Absorption of Isocyanates;** Brendan Prideaux<sup>1</sup>; Malcolm R Clench<sup>1</sup>; Vikki A Carolan<sup>1</sup>; Jackie Morton<sup>2</sup>; Bob Rajan-Sithamparanadarajah<sup>3</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>Health and Safety Laboratory, Buxton, UK; <sup>3</sup>Health and Safety Executive, Bootle, UK
- WP 94 **High Throughput Pesticide Screening: The Combination of Scheduled MRM Transitions and Fast Chromatography;** Sandra Chu<sup>1</sup>; Byron Kieser<sup>1</sup>; J.C.Yves Le Blanc<sup>1</sup>; Gary Impey<sup>1</sup>; <sup>1</sup>MDS Sciex, Concord, Canada
- WP 95 **Analysis of Perchlorate in Complex Matrices Utilizing LC/MS/MS;** Randy D Laubscher<sup>2</sup>; Denise K MacMillan<sup>1</sup>; <sup>1</sup>United States Army Corps of Engineers, Omaha, NE; <sup>2</sup>SpecPro Inc., Huntsville, AL
- WP 96 **Accuracy of Quantitation using External and Internal Calibration to Analyze 13 Azo-dyes in Extracts of Spices and Sauces;** Andre Schreiber<sup>1</sup>; Tanya Gamble<sup>1</sup>; Houssain El Aribi<sup>1</sup>; Steve Lock<sup>2</sup>; Jeremy Padfield<sup>3</sup>; Nick Byrd<sup>3</sup>; <sup>1</sup>MDS Sciex, Concord, Ontario, Canada; <sup>2</sup>Applied Biosystems, Warrington, UK; <sup>3</sup>Campden and Chorleywood Food Research, Chipping Campden, UK
- WP 97 **Analysis of Biogenic Amines by Ion Chromatography Coupled with Tandem Mass Spectrometry;** Houssain El

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- Aribi<sup>1</sup>; Stephen Antonsen<sup>2</sup>; Pearl Blay<sup>3</sup>; Takeo Sakuma<sup>1</sup>; Michael Quilliam<sup>3</sup>; <sup>1</sup>Applied Biosystems/MDS SCIEX, Concord, Ontario, Canada; <sup>2</sup>Dionex Canada Ltd, Oakville, Ontario, Canada; <sup>3</sup>NRC Institute for Marine Bioscience, Halifax, Nova Scotia, CA
- WP 98 **Biological Monitoring of Dicarboximide Fungicides in Human Urine using LC-MS/MS;** Christian H. Lindh<sup>1</sup>; Margareta Littorin<sup>1</sup>; Åsa Amilon<sup>1</sup>; Bo AG Jönsson<sup>1</sup>; <sup>1</sup>Dep. Occupational and Environmental Medicine, Lund, Sweden
- WP 99 **Determination of Natural and Synthetic Steroids and Their Conjugates in Environmental Samples by LC/MSMS;** Steve Cagampang<sup>1</sup>; Ed Sverko<sup>1</sup>; Mehran Alaei<sup>1</sup>; Josey Grabuski<sup>1</sup>; Takeo Sakuma<sup>2</sup>; Gordana Ivoev<sup>2</sup>; Mauro Aiello<sup>2</sup>; Robert Ellis<sup>2</sup>; Andre Schreiber<sup>2</sup>; Doina Caraiman<sup>2</sup>; Tanya Gamble<sup>2</sup>; Yves LeBlanc<sup>2</sup>; Nadia Pace<sup>2</sup>; <sup>1</sup>National Water Research Institute, Burlington, Canada; <sup>2</sup>Applied Biosystems-MDS-SCIEX, Concord, Canada
- WP 100 **Highly Sensitive and Selective Analysis of Peptides by MALDI-TOF Using Mixed Monolayer Protected Clusters (MMPC's) for Extraction and Concentration;** Benjamin N.Y. Vanderpuje<sup>1</sup>; Gang Han<sup>1</sup>; Vincent M. Rotello<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA
- WP 101 **Determination of Heterocyclic Amines in Food by  $\mu$ -LC/ESI-MS/MS;** Seung-Woon Myung<sup>1</sup>; <sup>1</sup>Kyonggi University, Suwon, Korea
- WP 102 **Evaluation of Unique Scan Functions of Triple Quadrupole and Linear Ion Trap Mass Spectrometers in Determining Chemical Species of Arsenic;** Robert Ellis<sup>1</sup>; Takeo Sakuma<sup>1</sup>; <sup>1</sup>MDS Sciex / Applied Biosystems, Toronto, Canada
- WP 103 **Quantitative Measurement of 19 Phthalate Metabolites in Human Meconium, Semen, Serum, and Breast Milk using Off-Line SPE- On-Line SPE- HPLC-MS/MS;** Kayoko Kato<sup>1</sup>; Manori J Silva<sup>1</sup>; Larry L Needham<sup>1</sup>; Antonia M Calafat<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA
- WP 104 **LC/MS/MS Analysis of Anti-infectives in Raw and Treated Sewage;** Pedro A. Segura<sup>1</sup>; Araceli Garcia Ac<sup>1</sup>; André Lajeunesse<sup>2</sup>; Dipankar Ghosh<sup>3</sup>; Christian Gagnon<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>Université de Montréal, Montréal, Canada; <sup>2</sup>Centre St-Laurent / Environnement Canada, Montréal, Canada; <sup>3</sup>Thermo Electron Corporation, San Jose, CA
- WP 105 **Validation of an JP-8 Fraction in Rat Liver and Whole Blood;** Shonetta D. Gregg<sup>1</sup>; Jeffrey W. Fisher<sup>1</sup>; Michael G. Bartlett<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, Ga
- WP 106 **A Multi-Residue LC-MS-MS Method for Evaluating Potato Pesticide Impacts in Atlantic Canada;** Suzanne Batchelor<sup>1</sup>; Herb Rees<sup>2</sup>; Lien Chow<sup>2</sup>; Linnell Edwards<sup>3</sup>; Allan Macrae<sup>3</sup>; Mark Hewitt<sup>1</sup>; <sup>1</sup>Environment Canada, Burlington, ON, Canada; <sup>2</sup>Agriculture and Agri-Food Canada (AAFC), Fredericton, NB, Canada; <sup>3</sup>AAFC, Charlottetown, PE, Canada

## AGRICULTURE AND PESTICIDE ANALYSIS

- WP 107 **Development, Validation and Performance of a Confirmatory LC/MS/MS Method for the Determination of Glyphosate Herbicide in Human Urine;** J. Mark Allan<sup>1</sup>; Ronald K. Beasley<sup>1</sup>; John D. Fuhrman<sup>1</sup>; <sup>1</sup>Monsanto Company, Saint Louis, MO
- WP 108 **Monitoring the Presence of Ergot Alkaloids in Forage Animal Samples;** Darrin L. Smith<sup>1</sup>; Wilson D. Shafer<sup>1</sup>; Lori L. Smith<sup>2</sup>; James L. Klotz<sup>2</sup>; James R. Strickland<sup>2</sup>; <sup>1</sup>Eastern Kentucky University, Richmond, KY; <sup>2</sup>Forage-

# WEDNESDAY POSTERS

## POSTER SPACE

- Animal Production Research Unit: USDA-ARS, Lexington, KY*
- WP 109 **Developing a Method for Investigating Beer Proteins Using Mass Spectrometry;** Yuwei Qian<sup>1</sup>; Werner Ens<sup>1</sup>; Marta Izydorczyk<sup>2</sup>; Sharon Bazin<sup>2</sup>; Ken Preston<sup>2</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Grain Research Laboratory, Winnipeg, Canada
- WP 110 **Identification of Photolytic Products by Fourier Transform Ion Cyclotron Mass Spectrometry and NMR Spectroscopy in Insecticide Research;** Ronald Shomo<sup>1</sup>; Shaaban ElNaggar<sup>1</sup>; Bill Creekmore<sup>1</sup>; Evon Bolessa<sup>1</sup>; Nikisha Joseph<sup>1</sup>; <sup>1</sup>FMC Corporation, Princeton, NJ
- WP 111 **Proteomic Analysis of Responses of Medicago truncatula to External Stimuli;** Zhentian Lei<sup>1</sup>; Satish Nagaraj<sup>1</sup>; Bonnie S. Watson<sup>1</sup>; Richard A. Dixon<sup>1</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>The Samuel Roberts Noble Foundation, Ardmore, OK
- WP 112 **The Development of a Method for Imaging the Distribution of Agrochemicals in Plants;** David M. G. Anderson<sup>1</sup>; Malcolm R. Clench<sup>1</sup>; Susan Crosland<sup>2</sup>; Susan Crosland<sup>2</sup>; Kate R. Sharples<sup>2</sup>; Vikki A. Carolan<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>Syngenta, Bracknell, UK
- WP 113 **Rapid Method for the Determination of 67 Pesticide Residues in Foods by Liquid Chromatography/Time-Of-Flight/Mass Spectrometry;** Masahiko Takino<sup>1</sup>; Douglas McIntyre<sup>2</sup>; Machiko Saka<sup>3</sup>; Kazuaki Iijima<sup>3</sup>; Yoshitsugu Odanaka<sup>3</sup>; <sup>1</sup>Yokogawa Analytical Systems, Inc., Tokyo, Japan; <sup>2</sup>Agilent technologies, Santa Clara, CA; <sup>3</sup>The Institute of Environmental Toxicology, Mitsuikado, Japan
- WP 114 **LC-MS-MS Determination of Malachite Green and Leucomalachite Green in Fish Product;** Tao Ding<sup>1</sup>; Jingzhong Xu<sup>1</sup>; Bing Wu<sup>1</sup>; Huilan Chen<sup>1</sup>; Chongyu Shen<sup>1</sup>; Fei Liu<sup>2</sup>; Paul Hendricks<sup>3</sup>; Kefei Wang<sup>3</sup>; <sup>1</sup>Jiangsu Entry-Exit Inspection & Quarantine Bureau, Nanjing, China; <sup>2</sup>Thermo Electron Corp, Shanghai, China; <sup>3</sup>Thermo Electron Corp, San Jose, CA
- WP 115 **A Fast and Sensitive Multiresidue Method for Pesticides Determination in Corn Grains using LC-MS/MS;** Helio Alves Martins-Júnior<sup>1</sup>; Daniel Temponi Lebre<sup>1</sup>; Tereza Atsuko Kussumi<sup>2</sup>; Maria Aparecida Faustino Pires<sup>2</sup>; Oscar Vega Bustillos<sup>2</sup>; <sup>1</sup>Applied Biosystems, Sao Paulo, Brazil; <sup>2</sup>Instituto de Pesquisas Energeticas e Nucleares, Sao Paulo, Brazil
- WP 116 **Mass Spectrometric Detection of Proteins in Non-Aqueous Media;** Michelle Douma<sup>1</sup>; Gina Kerr<sup>1</sup>; R. Stephen Brown<sup>1</sup>; Richard Oleschuk<sup>1</sup>; Bernd O. Keller<sup>1</sup>; <sup>1</sup>Queen's University, Kingston, Ontario
- WP 117 **Identification of Compounds in Three Species of False Rosemary (Conradina sp.) Native to Florida as Candidate Mosquito Repellents;** Brian P Quinn<sup>1</sup>; Ulrich R. Bernier<sup>1</sup>; Matthew M. Booth<sup>2</sup>; <sup>1</sup>USDA-ARS-CMAVE, Gainesville, FL; <sup>2</sup>University of Florida, Gainesville, Florida
- WP 118 **The Use of Dispersive SPE for the Analysis of Organophosphate Pesticides and Acidic Herbicides in Fruit and Vegetables by LC/MS/MS;** Nick Byrd<sup>1</sup>; Stephen Lock<sup>2</sup>; Neil Errington<sup>2</sup>; <sup>1</sup>Campden & Chorleywood Food Research Association, Chipping Campden, UK; <sup>2</sup>Applied Biosystems, Warrington, UK

## POSTER SPACE

- |        | LC/MS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| WP 119 | <b>Evaluation of Quantitative Accuracy for Chromatographic Peak Deconvolution on High-Throughput LC-TOFMS;</b> <u>Toshinobu Hondo</u> <sup>1</sup> ; Keiko Kaneda <sup>1</sup> ; Tetsuichiro Morita <sup>1</sup> ; Kenji Nagatomo <sup>1</sup> ; Jun Tamura <sup>1</sup> ; Zhanpin Wu <sup>2</sup> ; <sup>1</sup> JEOL Ltd., Tokyo, Japan; <sup>2</sup> JEOL USA Inc., Peabody, MA                                                                                                                        |
| WP 120 | <b>Evaluating the use of Phosphate Containing Mobile Phases with the 4000 Q TRAP®: Transitioning from LC-UV Stability Indicating Methods;</b> <u>Tom Bellman</u> <sup>2</sup> ; Gary Impey <sup>2</sup> ; Carmai Seto <sup>2</sup> ; Robert Papp <sup>1</sup> ; Wayne Mullett <sup>1</sup> ; Elizabeth Kwong <sup>1</sup> ; <sup>1</sup> Merck Frosst Canada & Co., Kirkland, Canada; <sup>2</sup> Applied Biosystems/MDS Sciex, Concord, Canada                                                          |
| WP 121 | <b>Acquity UPLC System for Discovery Bioanalytical Applications;</b> <u>Bogdan Slecza</u> <sup>1</sup> ; Hollie Booth <sup>1</sup> ; Celia D'Arienzo <sup>1</sup> ; Jian Wang <sup>1</sup> ; Timothy Olah <sup>1</sup> ; <sup>1</sup> Bristol-Myers Squibb, Princeton, NJ                                                                                                                                                                                                                                 |
| WP 122 | <b>Drug-HSA Binding Site Screening using Limited Digestion and LC-MS/MS;</b> <u>Min Bian</u> <sup>1</sup> ; David Hage <sup>1</sup> ; <sup>1</sup> University of Nebraska, Lincoln, Lincoln, NE                                                                                                                                                                                                                                                                                                           |
| WP 123 | <b>Comparison of Carryover Performance Between the Shimadzu SIL and CTC PAL Autosamplers Using Liquid Chromatography-Tandem Mass Spectrometry;</b> <u>Juan Chen</u> <sup>1,2,3</sup> ; Helengrace Schuck <sup>1,2,3</sup> ; Dina Goykhman <sup>1,2,3</sup> ; <sup>1</sup> Merck & Co., Inc., West Point, PA; <sup>2</sup> Merck & Co., Inc., West Point, PA; <sup>3</sup> Merck & Co., Inc., West Point, PA                                                                                               |
| WP 124 | <b>Assay of D-Amino Acid in Aplysia Californica's Central Nervous System by Capillary Liquid Chromatography-Tandem Mass Spectrometry;</b> <u>Yaru Song</u> <sup>1</sup> ; Fei Liang <sup>1</sup> ; Yiming Liu <sup>1</sup> ; <sup>1</sup> Jackson State University, Jackson, MS                                                                                                                                                                                                                           |
| WP 125 | <b>The Use of 1 mm i.d. Columns for Fast Generic Gradient Bioanalysis within Discovery;</b> <u>Anders Blomgren</u> <sup>1</sup> ; Margareta Maxe <sup>1</sup> ; <sup>1</sup> AstraZeneca R&D Lund, Lund, Sweden                                                                                                                                                                                                                                                                                           |
| WP 126 | <b>The Use of "Aqueous Normal Phase (ANP)" Chromatography for LC/MS on Silica-Hydride Based Bonded Stationary Phases;</b> <u>Joseph J. Pesek</u> <sup>1</sup> ; Maria T. Matyska <sup>1</sup> ; <sup>1</sup> San Jose State University, San Jose, CA                                                                                                                                                                                                                                                      |
| WP 127 | <b>Development of a New Column for The Measurement of Haloacetic Acids in Drinking Water by IC/MS and IC/MS/MS;</b> <u>Rida Al-Horri</u> <sup>1</sup> ; Charanjit Saini <sup>1</sup> ; Rosanne Slingsby <sup>1</sup> ; Christopher Pohl <sup>1</sup> ; <sup>1</sup> Dionex Corporation, Sunnyvale, CA                                                                                                                                                                                                     |
| WP 128 | <b>Elution and Characterization of Peptides Up to 40-mers in Length Using Supercritical Fluid Chromatography/Mass Spectrometry (SFC/MS);</b> Jun Zheng <sup>1</sup> ; <u>J. David Pinkston</u> <sup>2</sup> ; Paul Zoutendam <sup>2</sup> ; Larry Taylor <sup>1</sup> ; <sup>1</sup> Virginia Tech, Blacksburg, VA; <sup>2</sup> Procter & Gamble Pharmaceuticals, Mason, OH                                                                                                                              |
| WP 129 | <b>Surface Activated Chemical Ionization and High Flow Gradient Chromatography to Avoid Matrix Effect in Street Drugs Analysis;</b> <u>Simone Cristoni</u> <sup>1</sup> ; Luigi Rossi Bernardi <sup>2</sup> ; <sup>1</sup> ISB, Milan, Italy; <sup>2</sup> University of Milan, Milan, Italy                                                                                                                                                                                                              |
| WP 130 | <b>Electrochemical Assisted Electrospray Ionization Tandem Mass Spectrometry: Improving the Detection Limit of Electrochemically Active Species;</b> Robert Carr <sup>1</sup> ; <u>Jennifer (Binbin) Feng</u> <sup>2</sup> ; Kevin Kolodsick <sup>2</sup> ; Daphne Wang <sup>2</sup> ; Min Zhong <sup>2</sup> ; Christopher Holliman <sup>2</sup> ; Carol Kingsmill <sup>2</sup> ; <sup>1</sup> University of Michigan, Ann Arbor, MI; <sup>2</sup> Pfizer Global Research and Development, Ann Arbor, MI |

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- WP 131 **Structural Identification of Degradants and Impurities in Phospholipids in a Linear Ion Trap – Orbitrap Hybrid Mass Spectrometer;** Guodong Chen<sup>1</sup>; Ibrahim Daaro<sup>1</sup>; Birendra N. Pramanik<sup>1</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, NJ
- WP 132 **Screening of a Sulfonamides Library by Supercritical Fluid Chromatography Coupled to Mass Spectrometry (SFC-MS). Preliminary Properties-Retention Study;** Amaury Cazenave Gassiot<sup>1</sup>; G. John Langley<sup>1</sup>; Bob Boughtflower<sup>3</sup>; Mark Bradley<sup>8</sup>; Jeff Caldwell<sup>7</sup>; Steven Hoare<sup>2</sup>; Claire Holyoak<sup>3</sup>; Steve Lane<sup>4</sup>; Paul Oakley<sup>5</sup>; Frank Pullen<sup>6</sup>; Mark Taylor<sup>6</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>Evotec OAI Ltd., Abingdon, UK; <sup>3</sup>GlaxoSmithKline, CASS, Harlow, UK; <sup>4</sup>GlaxoSmithKline, Stevenage, UK; <sup>5</sup>Mettler-Toledo Autochem, Newark, DE; <sup>6</sup>Pfizer Global Research & Development, Sandwich, UK; <sup>7</sup>Princeton Chromatography Inc., Cranbury, NJ; <sup>8</sup>University of Edinburgh, Edinburgh, UK
- WP 133 **The Analysis of Basic Drugs by LC/MS/MS with High pH Mobile Phases;** Liming Peng<sup>1</sup>; Tivadar Farcas<sup>1</sup>; Ismail Rustamov<sup>1</sup>; <sup>1</sup>Phenomenex Inc, Torrance, California
- WP 134 **Evaluation of Porous Graphitic Carbon Column Coupled with Tandem Mass Spectrometry for Quantitation of Diastereomeric Drugs in Biological Samples;** Yuan-Qing Xia<sup>1</sup>; Mohammed Jemal<sup>1</sup>; Naiyu Zheng<sup>1</sup>; Xiaohang Shen<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ
- WP 135 **Simultaneously Probing and Identification of Radical-Scavenging Compounds in Biological Materials with Parallel Detection System;** Chang-Hsin Kuo<sup>1</sup>; Chen-Wei Liao<sup>1</sup>; Li-Lian Lin<sup>1</sup>; Kuo-Lung Ku<sup>1</sup>; <sup>1</sup>National Chiayi University, Chiayi City, Taiwan
- WP 136 **LC/MS-MS using UPLC and Superheated-Water Chromatography;** Richard Payne<sup>1</sup>; Dr Anthony Edge<sup>1</sup>; Dr Christopher Smith<sup>1</sup>; Dr Ian Wilson<sup>1</sup>; Stefanie Shillingford<sup>1</sup>; Elizabeth Thomas<sup>1</sup>; <sup>1</sup>AstraZeneca, Macclesfield, UK
- WP 137 **Simultaneous HPLC-MS-MS-UV Study of Solvent/Column Background;** Rajesh Dubey<sup>1</sup>; Karel Snoble<sup>2</sup>; Jim Przybytek<sup>2</sup>; Tony Kemperman<sup>2</sup>; John L. Welch<sup>1</sup>; <sup>1</sup>Honeywell International Inc., Buffalo, NY; <sup>2</sup>Honeywell Burdick & Jackson, Muskegon, MI

## GC/MS

- WP 139 **Analysis of Industrial Soil Contamination with Thermal Desorption/GC/MS;** Robert S. Frey<sup>1</sup>; <sup>1</sup>Scientific Instrument Services, Inc, Ringoes, NJ
- WP 140 **Hands-On GC/Tandem Mass Spectrometry in the Undergraduate Teaching Laboratory;** Bruce D. Allison<sup>1</sup>; Vincent Franco<sup>1</sup>; John W. Grossenbacher<sup>2</sup>; J. Mitchell Wells<sup>2</sup>; Garth E. Patterson<sup>2</sup>; Wendy J. Kramer<sup>2</sup>; Dennis J. Barket, Jr. <sup>2</sup>; <sup>1</sup>Rose-Hulman Institute of Technology, Terre Haute, IN; <sup>2</sup>Griffin Analytical Technologies, Inc., West Lafayette, IN
- WP 141 **Extending the Low Analyte Concentration Limit of Quantitation for GCMS using a Novel Maximum Aposteriori Probability (MAP) Algorithm;** Shahar Ben-Menahem<sup>1</sup>; James K. Breaux<sup>1</sup>; Sandeep Gulati<sup>1</sup>; Thomas George<sup>1</sup>; Bud Bromley<sup>1</sup>; Randy Roushall<sup>2</sup>; <sup>1</sup>ViaLog Corporation, Altadena, CA; <sup>2</sup>Agilent Corporation, Santa Clara, CA
- WP 142 **Biological Monitoring of Synthetic Pyrethroids, Organophosphates, and Carbamates in Human Blood Plasma Using Isotope Dilution Gas Chromatography-High Resolution Mass Spectrometry;** Jose J. Perez<sup>1</sup>; Kimberly Smith<sup>1</sup>; Gayanga Weerasekera<sup>1</sup>; Megan H.

## POSTER SPACE

- Williams<sup>2</sup>; Robin M. Whyatt<sup>2</sup>; Larry L. Needham<sup>1</sup>; Dana B. Barr<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>Mailman School of Public Health Columbia Univ., New York, NY
- WP 143 **GC-MS Sensitivity – Approaching OFN Limits with Difficult Compounds;** Aviv Amirav<sup>1</sup>; Alexander B. Fialkov<sup>1</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel
- WP 144 **Applications of Pyrolysis Gas Chromatography/Time-of-Flight Mass Spectrometry;** Masaaki Ubukata<sup>1</sup>; Kazuo Tanaka<sup>1</sup>; Jun Tamura<sup>1</sup>; Akihiko Kusai<sup>1</sup>; Robert Hertsens<sup>2</sup>; <sup>1</sup>JEOL Ltd., Akishima Tokyo, Japan; <sup>2</sup>JEOL (Europe) B.V., Zaventem, Belgium
- WP 145 **Elucidation of the Geometry and Double Bond Position of Long Chained Isomerized Olefin Mixtures using GC/MS with Electron Ionization;** Timothy P. McGinnis<sup>1</sup>; <sup>1</sup>Nalco Company, Naperville, IL
- WP 146 **Qualitative and Quantitative Evaluation of Volatile Extractables for Components of a Novel Inhalation Drug Delivery System by Headspace GC- MS;** Qiang Chen<sup>1</sup>; George Lin<sup>1</sup>; <sup>1</sup>Alexza Pharmaceuticals, Palo Alto, CA
- WP 147 **A Sensitive and Specific Methodology for CTAB Determination in a Novel Vaccine Using Liquid-Liquid Extraction with GC/MS;** Yieng-Hau R. Han<sup>1</sup>; Zhong Li<sup>1</sup>; Joyce A. Sweeney<sup>1</sup>; Pei-Kuo Tsai<sup>1</sup>; Brett S. Duersch<sup>1</sup>; William E. Bowen<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA

## METHODS FOR SMALL MOLECULE ANALYSIS

- WP 148 **Development and Validation of an LC-MS/MS Method for the Determination of FK330 in Human Plasma and Urine;** Yu-Luan Chen<sup>1</sup>; Shahzad Akhtar<sup>1</sup>; Hayato Kaneko<sup>2</sup>; Tsuyoshi Takaira<sup>2</sup>; Masakazu Kobayashi<sup>3</sup>; <sup>1</sup>Astellas Pharma US, Inc., Evanston, IL; <sup>2</sup>Astellas Pharma Inc., Tokyo, Japan; <sup>3</sup>Astellas Research Institute of America, Evanston, IL
- WP 149 **Translation of a Biomarker Panel - Validation of an LC/MS/MS Method for the Analysis of Endogenous 3-Methoxy-4-Hydroxyphenylglycol (MHPG) in Urine;** Wenlin (Wendy) Li<sup>1</sup>; Stephen Spindler<sup>2</sup>; Sandra Rojas-Caro<sup>2</sup>; Scott Fountain<sup>1</sup>; Gabriella Szekely-Klepser<sup>1</sup>; <sup>1</sup>Pfizer Inc. Biomarker Implementation Group, Ann Arbor, MI; <sup>2</sup>Pfizer Inc., Clinical R&D Operation, Ann Arbor, MI
- WP 150 **Stable Isotope Labeled Fatty Acid Analysis in Plasma using LC-FAIMS-SRM;** Kevin Bateman<sup>1</sup>; Sebastien Gagne<sup>1</sup>; Sheldon Crane<sup>1</sup>; Jean-Francois Levesque<sup>1</sup>; James Kapron<sup>2</sup>; <sup>1</sup>Merck Frosst Centre for Therapeutic Research, Kirkland, QC; <sup>2</sup>Thermo, Ottawa, ON
- WP 151 **A Fast and Economical MS/MS Procedure to Handle Glucuronidated Phase II Metabolites in the Development of Bioanalytical Methods;** Cynthia S. Côté<sup>1</sup>; Véronique Gauvreau<sup>1</sup>; Jean-Nicholas Mess<sup>1</sup>; Malika Madi<sup>1</sup>; Troy Bradley<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma, Laval (Montreal), Canada
- WP 152 **High Throughput UPLC/MS/MS Analysis of Underivatized Amino Acids;** Kate Yu<sup>1</sup>; Peter Alden<sup>1</sup>; Rob Plumb<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 153 **Comparison of Flow Injection-Electrospray MS, MS/MS, FAIMS-MS and FAIMS-MS/MS for the Determination of Underivatized Amino Acids in Yeast;** Margaret A. McCooey<sup>1</sup>; Zoltan Mester<sup>1</sup>; <sup>1</sup>National Research Council of Canada, Ottawa, Canada
- WP 154 **Withdrawn**
- WP 155 **An LC-MS/MS Method for the Quantification of Carbamazepine in Cerebrospinal Fluid Utilizing Methyl-Carbamazepine as an Internal Standard;**

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- Yingbo Yang<sup>1</sup>; Sophie Pan<sup>1</sup>; Lucy Liu<sup>1</sup>; Brad Gien<sup>1</sup>; Ines de Lannoy<sup>1</sup>; <sup>1</sup>NoAb BioDiscoveries, Mississauga, Canada
- WP 156 **Non-intuitive Strategies for Minimizing Matrix Effects in Development of Ultrasensitive Bioanalytical LC/MS/MS Methods;** Vladimir Capka<sup>1</sup>; Spencer J. Carter<sup>1</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT
- WP 157 **Chromatographic Separation and Quantitation of Gentamicin C1, C1a, C2 and C2a from a Gentamicin Sulfate Complex for Pharmacokinetics Studies;** G  rard Dussault<sup>1</sup>; Alain Arsenault<sup>1</sup>; Peter J. Roberts<sup>1</sup>; Manon Vranderick<sup>1</sup>; <sup>1</sup>MDS Pharma Services, Saint-Laurent (Montr  al), Canada
- WP 158 **A Simple Phase-Switching Method for the Direct LC-MS Analysis of Impurities in Pharmaceuticals with Non MS-Compatible Mobile Phases;** Eleftheria Galanaki<sup>1</sup>; Maria Altamura<sup>1</sup>; Antonio Triolo<sup>1</sup>; <sup>1</sup>Menarini Ricerche Spa, Firenze, Italy
- WP 159 **Bioanalytical Method Development and Validation of a LC-MS/MS Assay for Artesunic Acid and Dihydroartemisinin in Human Plasma;** B. O'Brien<sup>1</sup>; K. Thornton<sup>1</sup>; T. O'Neill<sup>1</sup>; L. Moody<sup>1</sup>; M. Smith<sup>1</sup>; L. Haney<sup>1</sup>; L. Siemann<sup>1</sup>; R. Harris<sup>1</sup>; K. S. Smith<sup>2</sup>; C. DiTusa<sup>2</sup>; <sup>1</sup>Midwest Research Institute, Kansas City, MO; <sup>2</sup>WRAIR-Division of Experimental Therapeutics, Silver Spring, MD
- WP 160 **Rapid UPLC/MS/MS Determination of Organic Acids in Cells and Fermentation Supernatants;** Keri L. Ross<sup>1</sup>; Joseph J Dalluge<sup>1</sup>; Travis T Tu<sup>1</sup>; <sup>1</sup>Cargill Incorporated, Minneapolis, MN
- WP 161 **Analysis of Pharmaceutical Drugs by HILIC and Reversed Phase;** Reno Nguyen<sup>1</sup>; Mark Jacyno<sup>1</sup>; Scott Anderson<sup>1</sup>; <sup>1</sup>Grace Davison, Deerfield, IL
- WP 162 **Advancing Single&minus;Photon Mass Spectrometry with Derivatization;** Jeannette Karczmariski<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- WP 163 **Complete Characterization of Impurities in Erythromycin A Oxime Using a Hybrid Ion Trap Fourier Transform Mass Spectrometer;** Shigeru Sakamoto<sup>1</sup>; Kazuyo Nakagawa<sup>1</sup>; Mihoko Yamaguchi<sup>1</sup>; Masayuki Kubota<sup>1</sup>; <sup>1</sup>Thermo Electron, Yokohama, Japan
- WP 164 **Comparison of Ion Source Sensitivity Capabilities for the Analysis of Low Molecular Weight Compounds in Rat Brain Samples;** Lisa M Buchholz<sup>1</sup>; Sarah Osgood<sup>1</sup>; Joe Palandra<sup>1</sup>; Lucinda Cohen<sup>1</sup>; <sup>1</sup>Pfizer Global Research & Development, Ann Arbor, MI
- WP 165 **An Automated, Rapid, LC-MS Method Development Approach Used for the Development of HPLC Methods for Active Pharmaceutical Ingredients (APIs);** Edward M Sheldon<sup>1</sup>; Andreas Kaerner<sup>1</sup>; <sup>1</sup>Eli Lilly Company, Indianapolis, IN
- WP 166 **Sub-ppb Multi-Residue Determination of Quinolone, Fluoroquinolone and Sulfonamides Antibacterials in Fish and Shrimp by LC-MSMS;** Guy L Dufresne<sup>1</sup>; <sup>1</sup>Health Canada-Food Directorate, Longueuil, Canada
- WP 167 **Overcoming the Interaction Between Fluticasone Propionate and Salmeterol in a Combined Validated Assay by LC/MS/MS;** Spencer J Carter<sup>1</sup>; Vladimir Capka<sup>1</sup>; Ed Brewer<sup>1</sup>; Patrick K Bennett<sup>1</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, UT
- WP 168 **A Sensitive and Selective Method for Quantification of Naturally-Occurring Foliates in Foods using Electrospray Tandem Mass Spectrometry;** Shyamala Vishnumohan<sup>1</sup>; Jayashree Arcot<sup>1</sup>; Russell Pickford<sup>1</sup>; <sup>1</sup>University of New South Wales, Sydney, Australia
- WP 169 **Quantification of the Biomarker 11-dehydro Thromboxane B2 in Human Urine by LC-MS/MS;**

## POSTER SPACE

- Yousef Basir<sup>1</sup>; Toby Julian<sup>1</sup>; Venjiman Lapko<sup>1</sup>; Kirk Newland<sup>1</sup>; <sup>1</sup>MDS Pharma Services, Lincoln, NE
- WP 170 **A Robust Method for Detection of Pregabalin at Micromolar Concentrations in Rat In Situ Brain Perfusion Samples;** Sarah Osgood<sup>1</sup>; Jeremy McFadden<sup>1</sup>; Julie Poe<sup>1</sup>; Cheryl Li<sup>1</sup>; Lisa Buchholz<sup>1</sup>; <sup>1</sup>Pfizer Global Research & Development, Ann Arbor, MI
- WP 171 **Sensitive LC-MS<sup>n</sup> Method for the Quantitation and Confirmation of Oxytocin in a Dilute IV Saline Solution;** Christine M. Karbiwnyk<sup>1</sup>; Kent C. Faul<sup>1</sup>; Sherri B. Turnipseed<sup>1</sup>; Keith E. Miller<sup>2</sup>; <sup>1</sup>U.S. Food & Drug Administration, Denver, CO; <sup>2</sup>University of Denver, Denver, CO
- WP 172 **Ion Suppression Comparisons of Micro Elution Style SPE Formats;** Raegan Goodell<sup>1</sup>; William Hudson<sup>1</sup>; <sup>1</sup>Varian Inc, Lake Forest, CA
- WP 173 **Automated HTLC/MS/MS Method Development Using a Cohesive TLX1 with MCM for TurboFlow and Analytical Column Optimization;** Chris Esposito<sup>1</sup>; Francois A. Espourteille<sup>1</sup>; <sup>1</sup>Cohesive Technologies, Inc., Franklin, MA
- WP 174 **Chemical Reactions Influencing Mass Spectral Responses in Electrospray Mass Spectrometry of Undiluted Ionic Liquids and Dissolved Analyte;** Yuchen Lu<sup>1</sup>; Douglas C Duckworth<sup>1</sup>; Gary J Van Berkel<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; Fred L King<sup>2</sup>; <sup>1</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>2</sup>West Virginia University, Morgantown, WV
- WP 175 **Hydrolysis Kinetics of Titan Tholin Analogues Determined by FT-ICR Mass Spectrometry;** Hiroshi Imanaka<sup>1</sup>; Katie Holso<sup>1</sup>; Arpad Somogyi<sup>1</sup>; Mark Smith<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- WP 176 **Analysis of Acrylamide in Food by LC/Time-of-Flight Mass Spectrometry;** Zhanpin Wu<sup>1</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA
- WP 177 **Small Molecule Analysis with Silicon Nanopowder-Assisted Laser Desorption/Ionization;** Shai Dagan<sup>1</sup>; Xiujuan Wen<sup>1</sup>; Dylan J. Boday<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- WP 178 **Improving Signal to Noise Ratio of Valproic Acid with Compromised MS/MS Conditions;** Saber H. Maleki<sup>1</sup>; Yong Q. Tang<sup>1</sup>; Xiangyu Jiang<sup>2</sup>; <sup>1</sup>Covance Analytical Services LLC, Indianapolis, IN; <sup>2</sup>Covance Laboratories Inc, Madison, WI

## DRUG METABOLISM: HIGH THROUGHPUT

- WP 179 **A Simple Generic High-Throughput LC-MS/MS Method for the Analysis of Biological Samples Generated in Drug Discovery;** Maria-A. Vindigni<sup>1</sup>; Olivier Meyer<sup>1</sup>; Julie Ducharme<sup>1</sup>; <sup>1</sup>AstraZeneca R&D Montreal, Montreal, Canada
- WP 180 **Investigation of Open Access Aria LC-MS/MS Systems: Variables that Contribute to Accuracy and Precision Problems during Quantitation of Pharmacokinetic Samples;** Laquisha E. Hamilton<sup>1</sup>; Rena Zhang<sup>1</sup>; W. Bart Emary<sup>1</sup>; <sup>1</sup>Merck & Co. Inc, West Point, PA
- WP 181 **Matrix Effects from Cofactors Commonly used in Microsome Stability Assays. A Study of NADPH and UDPGA Combined with Fast LC/MS/MS;** Sam Sperry<sup>1</sup>; Natalie Tran<sup>1</sup>; <sup>1</sup>SGX Pharmaceuticals, San Diego, CA
- WP 182 **An Intrinsically Two-Dimensional Approach to LC-MS Analysis Making Maximal Use of the LC-MS Method for Affinity Screening;** Jim Samuelsson<sup>1</sup>; Juergen Cox<sup>1</sup>; Marc Flesch<sup>1</sup>; Peter Haber<sup>1</sup>; Ruediger

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- Heidenblut<sup>1</sup>; Joe Shambaugh<sup>1</sup>; <sup>1</sup>Genedata, Martinsried, Germany
- WP 183 **A Rapid and Sensitive LC-MS/MS Method for the Determination of Cilazapril and its Active Metabolite in Human Plasma;** Heon-Woo Lee<sup>1</sup>; Ji-Hyung Seo<sup>1</sup>; Sung-Su Kim<sup>1</sup>; Yong-Won Kim<sup>1</sup>; Kyung-Tae Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Kyung Hee University, Seoul, Korea
- WP 184 **Early Metabolic Stability And Metabolite ID Profile Of Pharmaceuticals By A Two Column Fast And High Resolution LC/ESI oaTOF System;** Horst Lehmann<sup>1</sup>; Anabel Fandino<sup>1</sup>; Edgar Nägele<sup>1</sup>; <sup>1</sup>Agilent Technologies R&D and Marketing GmbH & Co., Waldbronn, Germany
- WP 185 **Extending the Polarity Range of Turbulent-Flow Liquid Chromatography Extractions;** Kimberly Navaline<sup>1</sup>; Kathryn Black<sup>2</sup>; Joseph Takarewski<sup>1</sup>; Joseph M. Di Bussolo<sup>1</sup>; <sup>1</sup>Cohesive Technologies, Franklin, MA; <sup>2</sup>West Chester University of Pennsylvania, West Chester, PA
- WP 186 **High Throughput Metabolic Stability Assay using a Linear Ion trap Mass Spectrometer;** Gargi Choudhary<sup>1</sup>; Marta Kozak<sup>1</sup>; Diane Cho<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA
- WP 187 **High Throughput Cytochrome P450 Inhibition Assay Using Laser Diode Thermal Desorption Mass Spectrometry (LDTD-MS);** Jin Wu<sup>1</sup>; Kevin P. Bateman<sup>1</sup>; Pierre Picard<sup>2</sup>; Sylvain Letarte<sup>2</sup>; Mireille Gaudreault<sup>1</sup>; Jean-Francois Levesque<sup>1</sup>; Deborah Nicoll-Griffith<sup>1</sup>; <sup>1</sup>Merck Frosst Center for Therapeutic Research, Kirkland, QC, Canada; <sup>2</sup>Phytronix Technologies Inc., Quebec, QC, Canada
- WP 188 **Cassette Plasma Protein Binding by Equilibrium Dialysis with 96-well Dialysis Plate;** Jingzhou Liu<sup>1</sup>; <sup>1</sup>AstraZeneca R&D Boston, Waltham, MA
- WP 189 **Quantitative Application of Up-Front Collision-Induced Dissociation for Direct Measurement of PEGylated Compounds in Dog Plasma;** Patrick Lin<sup>1</sup>; Dale Schoener<sup>1</sup>; Melanie Gee-Shihabi<sup>1</sup>; Richard Goodin<sup>23</sup>; Yuan Song<sup>23</sup>; Lida Antonian<sup>23</sup>; <sup>1</sup>Alta Analytical Laboratories, El Dorado Hills, CA; <sup>2</sup>Nektar Therapeutics, San Carlos, CA; <sup>3</sup>Nektar Therapeutics, Huntsville, AL
- WP 190 **Comparing Mass Defect Filtering and Accurate Mass Profile Extracted Ion Chromatogram (AMPXIC) for Metabolism Studies;** Don Kuehl<sup>1</sup>; Ming Gu<sup>1</sup>; Yongdong Wang<sup>1</sup>; <sup>1</sup>Cerno Bioscience, Danbury, CT
- WP 191 **Fast Bioanalytical Method for the Quantitative Analysis of Drugs in Plasma Using Dilute-and-Shoot Technique and Liquid Chromatography-Tandem Mass Spectrometry;** Helengrace A. Schuck<sup>1</sup>; Kari J Lynn<sup>1</sup>; Hale Barbara<sup>2</sup>; Danny W. Choo<sup>1</sup>; <sup>1</sup>Merck & Co. Inc., West Point, PA; <sup>2</sup>Ursinus College, Collegeville, PA
- WP 192 **Exploiting the High-Speed Capability of Ultra Performance Liquid Chromatography / Tandem Mass Spectrometry in Increasing Throughput in Metabolite Identification Studies;** Mary E. Lame<sup>1</sup>; Erin Chambers<sup>2</sup>; Marian Twohig<sup>2</sup>; Amit S. Kalgutkar<sup>1</sup>; <sup>1</sup>Pfizer Global Research and Development, Groton, CT; <sup>2</sup>Waters Corporation, Milford, MA
- WP 193 **Improving the Metabolite Identification Process with Efficiency and Speed;** Lorne M. Fell<sup>1</sup>; Carmai Seto<sup>1</sup>; Tom Bellman<sup>1</sup>; Gary Impey<sup>1</sup>; <sup>1</sup>Applied Biosystems/MDS Sciex, Concord, ON, Canada
- WP 194 **High Throughput Screening for Microsomal Stability of NCEs using LC-MS/MS with Sample Pooling, Automated Tuning and Automated Data Processing;**

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- Yongmin Li<sup>1</sup>; Krista Bellman<sup>1</sup>; Zhihua Liu<sup>1</sup>; Hongying Gao<sup>2</sup>; Licong Jiang<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals, Inc., San Diego, CA; <sup>2</sup>Vertex Pharmaceuticals, Inc., Cambridge, MA
- WP 195 **A High Throughput LC/MS/MS Method using an Eksigent Microfluidic Control System for Small Molecule Quantitation;** Bilin Chou<sup>1</sup>; Teresa Beaver<sup>2</sup>; Mark Atlas<sup>2</sup>; Young G. Shin<sup>1</sup>; Patrick J. Rudewicz<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Eksigent, Dublin, CA
- WP 196 **Rapid Identification and Structural Characterization for Drug Discovery Using a Linear Ion Trap Mass Spectrometer with Fast Polarity Switching;** Diane Cho<sup>1</sup>; Gargi Choudhary<sup>1</sup>; Laurance Lee<sup>1</sup>; Jonathan Josephs<sup>2</sup>; <sup>1</sup>Thermo Electron, San Jose, CA; <sup>2</sup>Bristol-Meyers Squibb, Hopewell, NJ
- WP 197 **An Automated High Throughput Approach to *in vitro* Metabolic Stability Screening and Simultaneous Metabolite Identification Data Acquisition using Capillary LC/MS/MS;** Robert Cho<sup>1</sup>; Loren Olson<sup>2</sup>; Ji Ma<sup>1</sup>; Shichang Miao<sup>1</sup>; Elliott B. Jones<sup>2</sup>; <sup>1</sup>Amgen, Inc, South San Francisco, CA; <sup>2</sup>Applied Biosystems, Foster City, CA
- WP 198 **Development of Cocktail-DDI Bioanalytical Methods: Quantification of 4'-Hydroxymephenytoin Across Multiple API-MS platforms (API-3000, API-3000(HSID), API-4000, API-5000);** Walter E. Mitchell<sup>1</sup>; John S. Janiszewski<sup>1</sup>; <sup>1</sup>Pfizer Inc., Groton, CT

## QUANTITATIVE ANALYSIS OF DRUGS AND METABOLITES III

- WP 199 **Determination of N-Acetyl Retigabine in Dog Plasma by LC/MS/MS Following Off-Line &mu;Elution 96-well Solid-Phase Extraction;** Wei Bu<sup>1</sup>; Mai Nguyen<sup>1</sup>; Chin-Chung Lin<sup>1</sup>; Li-Tain Yeh<sup>1</sup>; Virginia Borges<sup>1</sup>; <sup>1</sup>Valeant Pharmaceuticals International, Costa Mesa, CA
- WP 200 **Quantitative Analysis of Isradipine in Human Plasma by Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry;** Yun Young Lee<sup>1</sup>; Ye-Rie Lee<sup>1</sup>; Beom-Jin Lee<sup>3</sup>; Kyung Ryul Lee<sup>2</sup>; Seungwoo Kang<sup>1</sup>; Hee Joo Lee<sup>1</sup>; <sup>1</sup>BioCore co. Ltd., Seoul, Korea; <sup>2</sup>Seoul Medical Science Institute, Seoul, Korea; <sup>3</sup>Kangwon National University, Chuncheon, Korea
- WP 201 **Rapid Analysis of Donepezil in Human EDTA K<sub>2</sub> Plasma by LC/MS/MS using Automated SPE Extraction;** Myrian Coulombe<sup>1</sup>; Nadine Boudreau<sup>1</sup>; Jean Couture<sup>1</sup>; François Vallée<sup>1</sup>; <sup>1</sup>SFBC Anapharm, Ste-Foy, QC, Canada
- WP 202 **Validation of a LC-MS/MS Method for the Determination of Gefarnate and Its Metabolites in Rabbit Whole Blood;** Hidetoshi Mano<sup>1</sup>; Yoshihide Horibe<sup>1</sup>; Kouichi Kawazu<sup>1</sup>; <sup>1</sup>Santen Pharmaceutical, Ikoma, Nara, Japan
- WP 203 **Validation of an HPLC/MS/MS Bioanalytical Method for the Quantitative Analysis of Loxapine, Amoxapine, 7-OH-Loxapine and 8-OH-Loxapine in Human Plasma;** Jennifer S.D. Zimmer<sup>1</sup>; Chad D. Christianson<sup>1</sup>; Shane R. Needham<sup>1</sup>; <sup>1</sup>Alturas Analytics, Inc., Moscow, ID
- WP 204 **Validation of an HPLC/MS/MS Bioanalytical Method for the Quantitative Analysis of Alprazolam, &alpha;-OH-Alprazolam and 4-OH-Alprazolam in Human Plasma;** Chad D. Christianson<sup>1</sup>; Jennifer S.D. Zimmer<sup>1</sup>; Shane R. Needham<sup>1</sup>; <sup>1</sup>Alturas Analytics, Inc., Moscow, ID
- WP 205 **Validation of a Chiral HPLC/MS/MS Bioanalytical Method for Quantitative Analysis of the Enantiomers of Ketoconazole in Human and Dog Plasma;** Jennifer

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- S.D. Zimmer<sup>1</sup>; Chad D. Christianson<sup>1</sup>; Shane R. Needham<sup>1</sup>; <sup>1</sup>Alturas Analytics, Inc., Moscow, ID
- WP 206 **Development and Validation of An LC-MS/MS Method for the Determination of Atorvastatin in Human Plasma for Bioequivalence Study**; Zhongping John Lin<sup>2</sup>; Asiya Wufuer<sup>1</sup>; Weihua Ji<sup>1</sup>; Linyee Shum<sup>1</sup>; <sup>1</sup>Avantix Laboratories Inc., New Castle, DE; <sup>2</sup>AstraZeneca, DMPK, Wilmington, DE
- WP 207 **Determination of Simvastatin and Simvastatin acid in Human Plasma Using Liquid Chromatography-Tandem mass Spectrometry with Ionization Polarity Switch**; Jung Jin Park<sup>1</sup>; Sun Neo Lee<sup>1</sup>; Jong Soo Woo<sup>3</sup>; Kyung Ryul Lee<sup>2</sup>; Seungwoo Kang<sup>1</sup>; Hee Joo Lee<sup>1</sup>; <sup>1</sup>BioCore Co., Ltd., Seoul, Korea; <sup>2</sup>Seoul Medical Science Institute, Seoul, Korea; <sup>3</sup>Hanmi Pharm. Co.,Ltd., Seoul, Korea
- WP 208 **Validation of a Rugged, Sensitive and Selective LC-MS/MS Method for the Determination of Granisetron in Human Plasma**; Juan Fan<sup>1</sup>; Nada Kurt Stojkovic<sup>1</sup>; Anita Towers<sup>1</sup>; Iffat Balkhi<sup>1</sup>; Chrysantha Xavier<sup>1</sup>; Nicola Hughes<sup>1</sup>; <sup>1</sup>Biovail Contract Research, Toronto, Ontario, Canada
- WP 209 **Method Development and Validation for the Determination of Hyoscine Butylbromide (Buscopan) in Rat Plasma Using LC/MS/MS**; John Yu<sup>1</sup>; Helen Luo<sup>1</sup>; Jeffrey Duggan<sup>1</sup>; <sup>1</sup>Boehringer Ingelheim Pharmaceutical Co., Ridgefield, ct
- WP 210 **Determination of PT-100 in Human Urine by LC/MS/MS**; Bashir A. Mansoori<sup>1</sup>; Yongdong Zhu<sup>1</sup>; Vivek Tummala<sup>1</sup>; David Quirico<sup>1</sup>; Marva LoBlack<sup>1</sup>; Lee Anderson<sup>1</sup>; Benjamin Chien<sup>1</sup>; Margaret J. Uprichard<sup>2</sup>; John McCartney<sup>2</sup>; <sup>1</sup>Quest Pharmaceutical Services, Newark, DE; <sup>2</sup>Point Therapeutics, Boston, MA
- WP 211 **Rapid and Sensitive Determination of Fluvastatin in Rat Plasma by Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry**; Sang Beom Han<sup>1</sup>; Seungwoo Kang<sup>2</sup>; Kyung Ryul Lee<sup>2</sup>; Seok Park<sup>1</sup>; Jeong-Rok Youm<sup>1</sup>; <sup>1</sup>Chung-Ang University, Seoul, South Korea; <sup>2</sup>BioCore Co. Ltd, Seoul, South Korea
- WP 212 **A 96-Well Single-Pot Liquid-Liquid Extraction, Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry Method for the Determination of Muraglitazar in Human Plasma**; Jane Liu<sup>1</sup>; Steve Unger<sup>1</sup>; Y-J Xue<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, New Brunswick, NJ
- WP 213 **Determination of Fenofibrate and Metabolites in Acidified Human EDTA Plasma by Liquid-Liquid Extraction and LC-MS/MS**; Wei Sun<sup>1</sup>; Lee Winchester<sup>1</sup>; Curtis Sheldon<sup>1</sup>; Alan Dzerk<sup>1</sup>; Chad Briscoe<sup>1</sup>; <sup>1</sup>MDS Pharma Services, Lincoln, NE
- WP 214 **Development of a Highly Sensitive and Selective Quantitative LC-MS/MS Method that Differentiates Pravastatin from Its Major Isomeric Metabolites**; Ernest Y.K. Wong<sup>1</sup>; Dezhong Liu<sup>1</sup>; Anita Towers<sup>1</sup>; Iffat Balkhi<sup>1</sup>; Chrysantha Xavier<sup>1</sup>; Nicola Hughes<sup>1</sup>; <sup>1</sup>Biovail Contract Research, Toronto, Ontario, Canada
- WP 215 **Rapid and Highly Sensitive LC-ESI/MS/MS Method for the Quantitation of Buspirone in Human Plasma: Application to a Pharmacokinetic Study**; Sung-Hee Cho<sup>1</sup>; Ji-Hyung Seo<sup>1</sup>; Sung-Su Kim<sup>1</sup>; Yong-Won Kim<sup>1</sup>; Kyung-Tae Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Kyung Hee University, Seoul, South Korea
- WP 216 **High Throughput and Robust LC/MS/MS Method for Quantitation of Proprietary AT-562890 in Human Plasma and Urine**; Hairui Liang<sup>1</sup>; Justin Toombs<sup>1</sup>; Muna

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- Shrestha<sup>1</sup>; Tauch Socheata<sup>1</sup>; Mark Netsch<sup>1</sup>; <sup>1</sup>Charles River Laboratories, Worcester, MA
- WP 217 **Quantitation of Naltrexone in Human Plasma at the Low pg/mL Level by LC-MS/MS**; Jing Ke<sup>1</sup>; Xin Li<sup>1</sup>; Allan Xu<sup>1</sup>; <sup>1</sup>SFBC Analytical Laboratories, Inc., North Wales, PA
- WP 218 **Simultaneous Determination of Levodopa and Carbidopa in Human Plasma Using a 2D LC-LC/MS-MS Method**; Nancy Zheng<sup>1</sup>; Zong-Ping Zhang<sup>1</sup>; <sup>1</sup>PPD, Madison, Wisconsin
- WP 219 **Quantitative Analysis of Memantine in Human Plasma by LC/MS/MS**; Nancy Zheng<sup>1</sup>; Daniel Dreyer<sup>1</sup>; Zong-Ping Zhang<sup>1</sup>; <sup>1</sup>PPD, Madison, Wisconsin
- PHARMACO KINETICS: METHODS AND APPLICATIONS**
- WP 220 **Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for the Determination of CRx-119, a Novel Syncretic Drug Candidate, in EDTA Human Plasma**; Maresh V Padval<sup>1</sup>; Camille P Granvil<sup>1</sup>; Jennifer Chen<sup>1</sup>; Peter J Elliott<sup>1</sup>; <sup>1</sup>CombinatoRx Inc, Boston, MA
- WP 221 **An LC/MS/MS Assay for Docetaxel in Mouse and Dog Plasma and Mouse Tissues Containing Liposomal Docetaxel: Application to Pharmacokinetics Studies**; Xuejun Zang<sup>1</sup>; Sumsullah Khan<sup>1</sup>; Ateeq Ahmad<sup>1</sup>; Paul Chen<sup>1</sup>; Jenny Ayoub<sup>1</sup>; Yousheng Hua<sup>1</sup>; Imran Ahmad<sup>1</sup>; <sup>1</sup>NeoPharm Inc., Waukegan, IL
- WP 222 **Rapid Determination of Azasetron in Rat Plasma for Pharmacokinetic Studies**; Chang Hun Park<sup>1</sup>; Seungwoo Kang<sup>1</sup>; Hae Jong Jang<sup>1</sup>; Sang Beom Han<sup>3</sup>; Kyung Ryul Lee<sup>2</sup>; Hee Joo Lee<sup>1</sup>; <sup>1</sup>Biocore, Seoul, South Korea; <sup>2</sup>Seoul Medical Science Institute, Seoul, South Korea; <sup>3</sup>Chung-Ang University, Seoul, South Korea
- WP 223 **Evaluation of Accelerator Mass Spectrometry and Triple Quadrupole Mass Spectrometry for use in Microdosing Studies**; Jimmy Flarakos<sup>1</sup>; Rosa G. Liberman<sup>1</sup>; Paul L. Skipper<sup>1</sup>; Steven R. Tannenbaum<sup>1</sup>; Themis Flarakos<sup>2</sup>; Ari Gritsas<sup>2</sup>; Jean Pierre Moreau<sup>2</sup>; Mark L. J. Reimer<sup>2</sup>; <sup>1</sup>Massachusetts Institute of Technology, Cambridge, MA; <sup>2</sup>MDS Pharma Services, Montreal, Canada
- WP 224 **Studying MEK Compound Partitioning into Red Blood Cells**; Wendy W.Y. Zhang<sup>1</sup>; <sup>1</sup>Serono, Rockland, MA
- WP 225 **Quantitative Determination of CRx-026, a Novel Syncretic Anti-cancer Drug Candidate, in EDTA Human Plasma by Liquid Chromatography-Tandem Mass Spectrometry**; Camille P Granvil<sup>1</sup>; Jennifer Chen<sup>1</sup>; Maresh V Padval<sup>1</sup>; Peter J Elliott<sup>1</sup>; <sup>1</sup>CombinatoRx Inc, Boston, MA
- WP 226 **Pharmacokinetic Interactions between Equol and Genistein in Balb/c Mice**; Yu-Ping Wang<sup>1</sup>; Huaxin Song<sup>2</sup>; Nathan C. Twaddle<sup>1</sup>; William G. Helferich<sup>2</sup>; Daniel R. Doerge<sup>1</sup>; <sup>1</sup>National Center for Toxicological Research, Jefferson, AR; <sup>2</sup>University Of Illinois, Urbana-Champaign, IL
- WP 227 **Simple Liquid Chromatography Mass Spectrometric Method for Quantitation of Ondansetron with Granisetron as Internal Standard for Beagle Dog Plasma**; Roger A. Rajewski<sup>1</sup>; Michelle P. McIntosh<sup>1</sup>; Karl S. Schorno<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS
- WP 228 **Practical Solution for Matrix Effect from Dosing Excipients in Pharmacokinetic Analysis using Off-line and On-line Sample Dilution Method**; Fangbiao Li<sup>1</sup>; Zhang Cai<sup>1</sup>; Hamza Kandoussi<sup>1</sup>; Ray Bakhtiar<sup>1</sup>; Rasmy Talaat<sup>1</sup>; <sup>1</sup>Wyeth Pharmaceuticals, Collegeville, PA



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- WP 229 **Bioanalysis of Deferitritin and Its Polyether Analog, a Novel, Orally Active Iron Chelator by Liquid Chromatography-Tandem Mass Spectrometry;** Sujin Ahn<sup>1</sup>; Sirimas Sudsakorn<sup>1</sup>; Cara Conway<sup>1</sup>; Mark Bree<sup>2</sup>; Kerry Culm<sup>3</sup>; Jeffrey Skell<sup>1</sup>; Thomas O'shea<sup>1</sup>; Hanlan Liu<sup>1</sup>; <sup>1</sup>DMPK & Pharmaceuticals, Genzyme, Cambridge, MA; <sup>2</sup>Pharmacology & Preclinical Development, Genzyme, Waltham, MA; <sup>3</sup>Pharmacology & Preclinical Development, Genzyme, Framingham, MA
- WP 230 **Determining Metabolic Kinetic Trends Using LC/MS/MS and PCA Analysis;** Sasaki Tania<sup>1</sup>; Ji Ma<sup>2</sup>; Robert Cho<sup>2</sup>; Elliott Jones<sup>1</sup>; <sup>1</sup>Appliedbiosystems, Foster City, CA; <sup>2</sup>Amgen, South San Francisco, CA
- WP 231 **Characterization of Antibody-Drug Conjugate Ratios for in vivo Sample Analysis Using Affinity Purification Followed by MALDI-TOF Mass Spectrometry;** Qing Zhu<sup>1</sup>; Edward Takach<sup>1</sup>; Mei Zhu<sup>1</sup>; Frank Hsieh<sup>1</sup>; <sup>1</sup>Millennium Pharmaceuticals, Inc, Cambridge, MA
- WP 232 **High Throughput Protein Binding by Rapid Equilibrium Dialysis;** Kevin L. Cook<sup>1</sup>; Dennis M. Kalamaridis<sup>1</sup>; Jose Silva<sup>1</sup>; Jie Chen<sup>1</sup>; Carlo Sensenhauser<sup>1</sup>; Vangala Subrahmanyam<sup>1</sup>; H. K. Lim<sup>1</sup>; <sup>1</sup>Johnson & Johnson PRD, LLC, Raritan, NJ
- WP 233 **Mass Spectrometry, A Tool to Reveal the Mechanisms of Cytochrome b5 on Different Cytochrome P450 Isoforms;** Qiuxia (Elva) Gao<sup>1</sup>; Scott Shaffer<sup>1</sup>; Catalin Doneanu<sup>1</sup>; Arthur Roberts<sup>1</sup>; Elinor Adman<sup>1</sup>; David Goodlett<sup>1</sup>; Sidney Nelson<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- WP 234 **An LC/MS/MS Quantitation Method for Nevirapine (NVP) and Its Two Oxidative Metabolites 4-CANVP and 2-OHNVP and Its Pharmacokinetics in Baboons;** Zhongfa Liu<sup>1</sup>; Patty Havard<sup>1</sup>; Zhiliang Xie<sup>1</sup>; Kenneth K. Chan<sup>1</sup>; <sup>1</sup>the college of Pharmacy, the Ohio State University, Columbus, OH
- WP 235 **HPLC/ESI/MS Method for Quantitative Analysis of a Novel Neuroprotective in Plasma from Various Species Used for Allometric Scaling;** Andrea A. Romeo<sup>1</sup>; Danielle Boulais<sup>1</sup>; Kim Hewitt<sup>1</sup>; Peter Winocour<sup>1</sup>; Alain Boudreault<sup>1</sup>; <sup>1</sup>Aegera Therapeutics Inc., Nun's Island, Quebec
- WP 236 **Mechanism-based CYP450 inactivation and Glutathione-Adduct Trapping as a Strategy for Identifying Potential Reactive Intermediates;** Carlo Sensenhauser<sup>1</sup>; Jie Chen<sup>1</sup>; Kevin L. Cook<sup>1</sup>; Vangala Subrahmanyam<sup>1</sup>; H.K. Lim<sup>1</sup>; <sup>1</sup>J&J Pharmaceutical Research & Development, Raritan, NJ
- WP 237 **An Example of the Utility of Generic Mixed Mode SPE as a Means of Overcoming Ion Suppression in Drug Discovery;** Stuart A Best<sup>1</sup>; <sup>1</sup>Organon Laboratories Ltd, Newhouse, Motherwell, Scotland, UK
- WP 238 **LC/H-ESI MS/MS and Higher Mass Resolution for Quantitative Assay and Pharmacokinetic Study Using Automated Blood Sampling Systems;** Yongxin Zhu<sup>1</sup>; Candice Kissinger<sup>1</sup>; Peter Kissinger<sup>1</sup>; Dipankar Ghosh<sup>2</sup>; Rohan Thakur<sup>2</sup>; <sup>1</sup>Bioanalytical Systems, Inc, West Lafayette, IN; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- WP 239 **Simultaneous Determination of ABT-510 and ABT-388 in Rabbit Plasma using LC MS/MS;** Katty X Wan<sup>1</sup>; Daniel J. Daszkowski<sup>1</sup>; Matthew J. Rieser<sup>1</sup>; <sup>1</sup>Abbott, Abbott Park, IL
- WP 240 **Ultra-Sensitive Quantification of Corticosteroids using Selective Solid Phase Extraction and Reversed-Phase Capillary High Performance Liquid Chromatography**

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- Tandem Mass Spectrometry;** Jun Qu<sup>1</sup>; Robert Straubinger<sup>1</sup>; Yang Qu<sup>1</sup>; <sup>1</sup>SUNY-Buffalo, Amherst, NY
- WP 241 **Automated Method Development to Minimize Sample Carry-over for on-line SPE-LC/MS/MS Quantitation of Compound A and B in Human Plasma;** Dong Wei<sup>1</sup>; Martin Sibum<sup>2</sup>; Qin Yue<sup>1</sup>; Christopher TenHoor<sup>1</sup>; Liyu Yang<sup>1</sup>; <sup>1</sup>Biogen Idec, Inc, Cambridge, MA; <sup>2</sup>Spark Holland BV, AJ Emmen, The Netherlands

### MALDI SAMPLE PREPARATION I

- WP 242 **Applications of a SAM-IMAC Biochip for the Purification and Concentration of Bioengineered or Phosphorylated Proteins with Detection by MALDI-MS;** Christopher M. Belisle<sup>1</sup>; Irene Y. Chen<sup>1</sup>; Julie K. Mirshad<sup>1</sup>; Udo Roth<sup>2</sup>; Kerstin Steinert<sup>2</sup>; John A. Walker, II<sup>1</sup>; <sup>1</sup>Qiagen Sciences, Fremont, CA; <sup>2</sup>Qiagen GmbH, Hilden, Germany
- WP 243 **Effects of Nanoporous Silica Thin Film Parameters on LDI-MS Performance;** Srinivas Iyer<sup>1</sup>; Raea Hicks<sup>1</sup>; Steven Madrid<sup>1</sup>; Andrew Dattelbaum<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM
- WP 244 **Functionalized Monolithic Surfaces for Single Droplet Sample Handling;** Mohammed Kajjout<sup>1</sup>; Xiayang Wang<sup>1</sup>; Christian Rolando<sup>1</sup>; Séverine Le Gac<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- WP 245 **The Use of Reactive Surfaces for On-Chip Immobilization of Biomolecules and Subsequent Purification / Concentration of Analytes for MALDI-MS;** Julie K Mirshad<sup>1</sup>; Christopher M Belisle<sup>1</sup>; Irene Y Chen<sup>1</sup>; Udo Roth<sup>2</sup>; Kerstin Steinert<sup>2</sup>; John A Walker II<sup>1</sup>; <sup>1</sup>Qiagen Sciences, Fremont, CA; <sup>2</sup>Qiagen GmbH, Hilden, DE
- WP 246 **Optimization of the Electrospray Deposition Technique to Produce Better Quantitative MALDI Samples;** Kevin G. Owens<sup>1</sup>; William J. Erb<sup>1</sup>; Rocco Delconte<sup>1</sup>; <sup>1</sup>Drexel University, Philadelphia, PA
- WP 247 **Investigating the Analyte Distribution in MALDI Matrices using MALDI Imaging;** Hui Qiao<sup>1</sup>; Gamini Piyadasa<sup>1</sup>; Oleg V. Krokhnin<sup>1</sup>; Vic Spicer<sup>1</sup>; Kenneth G Standing<sup>1</sup>; Werner Ens<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada
- WP 248 **Enhanced MALDI Ionization Efficiency at the Metal-Matrix Interface: Practical and Mechanistic Consequences of Sample Thickness and Preparation Method;** Gregor McCombie<sup>1</sup>; Richard Knochenmuss<sup>2</sup>; <sup>1</sup>Swiss Federal Institute of Technology (ETH), Zürich, Switzerland; <sup>2</sup>Novartis Institutes for Biomedical Research, Basel, Switzerland
- WP 249 **MALDI on Silicon;** Jae-Kuk Kim<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- WP 250 **Matrix-free Laser Desorption Ionization Mass Spectrometry using Porous Alumina Thin Film Structures;** Ranu Nayak<sup>1</sup>; Daniel R Knapp<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- WP 251 **MALDI-TOFMS High-density Polymer Micro Array for Direct Protein Analysis from Complex Biological Samples;** Alexander Muck<sup>1</sup>; Alfredo Ibanez<sup>1</sup>; Ales Svatos<sup>1</sup>; <sup>1</sup>Max Planck Institute for Chemical Ecology, Jena, Germany
- WP 252 **Improving Monoclonal Antibody and scFv Protein Characterization by Obtaining Complementary MALDI-TOF-MS Spectra from a Single Tryptic Digest;** Adam W. Lucka<sup>1</sup>; Rekha Patel<sup>1</sup>; Bruce A. Andrien<sup>1</sup>; <sup>1</sup>Alexion Pharmaceuticals, Cheshire, CT



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- WP 253 **An Statistical Analysis of Factors Related to ion Suppression in MALDI-TOF mass spectrometry;** Dongmei Yang<sup>1</sup>; Michael S. Wisz<sup>1</sup>; Kevin Ramkissoon<sup>1</sup>; Morgan C. Giddings<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 254 **Advances in MALDI of Small Molecules using Surfactants as Matrix Co-Additives;** David C. Grant<sup>1</sup>; Robert J. Helleur<sup>1</sup>; <sup>1</sup>Memorial University of Newfoundland, St. John's, Canada
- WP 255 **Sublayer Assisted MALDI (SA-MALDI): Practical Applications and Fundamental Studies;** Zaneer M. Segu<sup>1</sup>; Gary R. Kinsel<sup>1</sup>; <sup>1</sup>Southern Illinois University, Carbondale, IL
- WP 256 **Investigation of the First Shot Phenomenon in MALDI Mass Spectrometry of Protein Complexes;** Arno Wortmann<sup>1</sup>; Tatiana Pimenova<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland
- WP 257 **Electrochemically Cleavable Linker Enables High Performance Immunoaffinity Mass Spectrometry by MALDI-TOF-MS;** Mark L. Stolzowicz<sup>1</sup>; Paul Lampe<sup>2</sup>; Heather A. Brauer<sup>2</sup>; <sup>1</sup>Stratos Biosystems, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- WP 258 **Sensitive and Reproducible Detection of Peptides by Maldi-TOF MS using Self-Assembled Monolayer (SAM)-Based Chips – Specifications and Applications;** Udo Roth<sup>1</sup>; Holger Röhl<sup>1</sup>; Matthias Glückmann<sup>2</sup>; Thorsten Jaskolla<sup>3</sup>; Michael Karas<sup>3</sup>; Kerstin Steinert<sup>1</sup>; Karsten Reihls<sup>4</sup>; <sup>1</sup>Qiagen GmbH, Hilden, Germany; <sup>2</sup>Applied Biosystems, Germany; <sup>3</sup>Johann- Wolfgang-Goethe-University of Frankfurt, Germany; <sup>4</sup>Sunyx GmbH, Germany
- WP 259 **Combining Guanidination with Detergent Micelle Treatment Improves Peptide Mapping by MALDI-TOFMS;** David Evason<sup>1</sup>; Vic Parr<sup>1</sup>; <sup>1</sup>SAI, Manchester, UK
- WP 260 **Predicting matrix conditions for drug analysis in tissue by MALDI MS/MS;** Sara L. Frappier<sup>1</sup>; Sheerin K. Shahidi<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN

## INSTRUMENTATION: NEW CONCEPTS I

- WP 261 **Aerodynamic Focusing of Heavy Ions and Nanoparticles;** Xiaoliang Wang<sup>1</sup>; Peter H. McMurry<sup>1</sup>; <sup>1</sup>Mechanical Engineering, University of Minnesota, Minneapolis, MN
- WP 262 **Mass Spectrometry into the Gigadalton Range;** Kenneth C. Wright<sup>1</sup>; Peter T. A. Reilly<sup>1</sup>; William B. Whitten<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- WP 263 **Micro-Cylindrical Ion Trap Mass Spectrometers;** Ashish Chaudhary<sup>1</sup>; Friso H.W. van Amerom<sup>1</sup>; Robert T. Short<sup>1</sup>; <sup>1</sup>University of South Florida, St. Petersburg, Florida
- WP 264 **Studies on Yttria Cated Filaments for Mass Spectrometers;** John J. Manura<sup>1</sup>; <sup>1</sup>Scientific Instrument Services, Ringoes, NJ
- WP 265 **Ultra-High Field Strength Nanoelectrospray via Multiple Embedded Chip-based Electrodes;** Jie Li<sup>1</sup>; Christopher G. Alpha<sup>1</sup>; Barry L. Smith<sup>1</sup>; Thomas N. Corso<sup>1</sup>; <sup>1</sup>Advion BioSystems, Inc., Ithaca, NY
- WP 266 **Micro Ion-Optical Systems Technology [MIST] for Atmospheric Pressure Sources;** David P. Fries<sup>1</sup>; Ross C. Willoughby<sup>2</sup>; Edward W. Sheehan<sup>2</sup>; George Steimle<sup>1</sup>; Stan Ivanov<sup>1</sup>; <sup>1</sup>University of South Florida, St. Petersburg, FL; <sup>2</sup>Chem-Space Associates, Pittsburgh, PA

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- WP 267 **Computer Simulation of a New, AC three rods (tripole), Ion Optic with High Focusing and Mass Filtering Capabilities;** Gary Abdiel Salazar<sup>1</sup>; Tsutomu Masujima<sup>1</sup>; <sup>1</sup>Hiroshima University, Hiroshima, Japan
- WP 268 **Array Ion Detection: Application and Performance of a Second-Generation Focal-Plane Array Camera for MS;** Charles J. Barinaga<sup>1</sup>; David W. Koppelaar<sup>1</sup>; Roger P. Sperline<sup>2</sup>; M. Bonner Denton<sup>2</sup>; Gregory D. Schilling<sup>3</sup>; Francisco J. Andrade<sup>3</sup>; Gary M. Hieftje<sup>3</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Arizona, Tucson, AZ; <sup>3</sup>Indiana University, Bloomington, IN
- WP 269 **Ultra-Compact Orthogonal Acceleration Time-Of-Flight Mass Spectrometer Equipped with Novel Photo Ionisation Source;** Fabian Mühlberger<sup>1</sup>; Marc Gonin<sup>2</sup>; Katrin Fuhrer<sup>2</sup>; Thorsten Streibel<sup>3</sup>; Ralf Zimmermann<sup>1</sup>; <sup>1</sup>GSF Research Centre, Oberschleissheim, Germany; <sup>2</sup>TOFWERK, Thun, Switzerland; <sup>3</sup>University of Augsburg - Analytical Chemistry, Augsburg, Germany
- WP 270 **Integration of a Novel Atmospheric Pressure Interface with AP MALDI FTICR Mass Spectrometer;** Si Wu<sup>1</sup>; Kai Zhang<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Gunnar Skulason<sup>1</sup>; Li Zhou<sup>2</sup>; Milton L. Lee<sup>2</sup>; James E. Bruce<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Brigham Young University, Provo, UT
- WP 271 **Combined Atmospheric and Low Pressure Focusing of Ions;** Kai Zhang<sup>1</sup>; Si Wu<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Gunnar Skulason<sup>1</sup>; David C. Prior<sup>2</sup>; Gordon A. Anderson<sup>2</sup>; James E. Bruce<sup>1</sup>; <sup>1</sup>Depart. of Chemistry, Washington State University, Pullman, WA; <sup>2</sup>Environmental Molecular Sciences Laboratory, PNNL, Richland, WA
- WP 272 **Withdrawn**
- WP 273 **Chemical Characterization of Individual Nanoparticles and Molecules Detected with a New MS System;** Shenji Wang<sup>1</sup>; Murray Johnston<sup>1</sup>; <sup>1</sup>Chem & Biochem Dept, The University of Delaware, Newark, DE
- WP 274 **Evaluation of a Carbon Nanotube-Based Ionization Source;** Charles Parker<sup>1</sup>; Srividya Natarajan<sup>1</sup>; Scott Wolter<sup>1</sup>; Jeffrey Glass<sup>1</sup>; Christopher Bower<sup>2</sup>; Kristin Gilchrist<sup>2</sup>; Brian Stoner<sup>2</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>Research Triangle Institute, International, Research Triangle Park, NC
- WP 275 **Ion Motion Control Experiments and Simulations in the Orbitrap Mass Analyzer;** Qizhi Hu<sup>1</sup>; Richard H. Perry<sup>1</sup>; Guangxiang Wu<sup>1</sup>; Wolfgang R. Plass<sup>2</sup>; Robert J. Noll<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Justus-Liebig Universitaet, Giessen, Germany
- WP 276 **Modeling of a Laminar Flow Interface with Multiple Bends for LC/MS/MS;** Serguei Savtchenko<sup>1</sup>; Gholamreza Jahavery<sup>1</sup>; Chuck Jolliffe<sup>1</sup>; <sup>1</sup>IONICS Mass Spectrometry Group, Concord, ON
- WP 277 **An Ion-Imaging ESI Hadamard Time-of-Flight (HT-TOF) Mass Spectrometer for Studies on Modulation of Charged Particle Beams and Other Fundamental processes;** Ignacio A. Zuleta<sup>1</sup>; Oh-Kyu Yoon<sup>1</sup>; Matt D. Robbins<sup>1</sup>; Griffin K. Barbula<sup>1</sup>; Richard N. Zare<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA
- WP 278 **Development of a High-Pressure Electrodynamical Ion Funnel-Mass Spectrometer Interface;** Yehia M. Ibrahim<sup>1</sup>; Keqi Tang<sup>1</sup>; Aleksey V. Tolmachev<sup>1</sup>; Alexandre A. Shvartsburg<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- WP 279 **Performance Assessment of the New Radiocarbon Accelerator Mass Spectrometry (AMS) Facility in**

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- Seattle; Ugo Zoppi<sup>1</sup>; Ali Arjomand<sup>1</sup>; James Crye<sup>1</sup>;  
<sup>1</sup>Accium Biosciences, Seattle, WA
- WP 280 **A Qit-q-ToF Mass Spectrometer for Multi-Dimensional MS/MS in High Throughput Proteomics**; Houle Wang<sup>1</sup>; David S. Kennedy<sup>1</sup>; Yixin Zhu<sup>1</sup>; Kerry D. Nugent<sup>1</sup>; Gregory K. Taylor<sup>2</sup>; David R. Goodlett<sup>2</sup>; <sup>1</sup>Michrom BioResources, Inc., Auburn, CA; <sup>2</sup>University of Washington, Seattle, WA
- WP 281 **Orthogonal Extraction Ion Mobility Spectrometry**; Victor V. Laiko<sup>1</sup>; <sup>1</sup>MassTech, Inc., Columbia, MD
- INSTRUMENTATION: MASS ANALYZERS (QUADRAPOLES AND TRAPS)**
- WP 291 **Optimization of Parameters for Performing Electron Transfer Dissociation on 2D Linear Ion Traps**; Jae C. Schwartz<sup>1</sup>; Zhiqi Hao<sup>1</sup>; Andreas Huhmer<sup>1</sup>; John E.P. Syka<sup>1</sup>; Joshua J. Coon<sup>2</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA; <sup>2</sup>University of Wisconsin, Madison, WI
- WP 292 **Improving Signal-to-Noise Ratios and Identifying Sources of Noise in Quadrupole MS Systems**; Kevin J. Kuchta<sup>1</sup>; Jian Wei<sup>1</sup>; <sup>1</sup>Extrel CMS, Pittsburgh, PA
- WP 293 **Multiplexed Rectilinear Ion Trap Mass Spectrometer for High-Throughput Analysis**; Amy M. Tabert<sup>1</sup>; Michael P. Goodwin<sup>1</sup>; Jason S. Duncan<sup>1</sup>; Charles D. Fico<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 294 **Extending MS<sup>3</sup> Capabilities on a Quadrupole Hybrid Linear Ion Trap**; Mircea Michael Guna<sup>1</sup>; Bruce Collings<sup>1</sup>; J.C. Yves Le Blanc<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- WP 295 **Polymer Ion Trap — Fabrication, Simulation and Analysis**; Meng Yu<sup>1</sup>; Miriam Fico<sup>1</sup>; R. Graham Cooks<sup>1</sup>; William Chappell<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 296 **A Simple Method to Overcome the Poor Low-Mass Ion Trapping in Enhanced Product Ion Experiment on 4000 Qtrap**; Austin C. Li<sup>1</sup>; Yinghe Li<sup>1</sup>; Tim Mai<sup>1</sup>; Xiangyu Jiang<sup>1</sup>; <sup>1</sup>Covance Laboratories, Inc., Madison, WI
- WP 297 **Real Time Measurement of Isobaric Volatile Organic Compounds Using Proton Transfer Reaction - Linear Ion Trap (PTR-LIT) Mass Spectrometry**; Levi H. Mielke<sup>1</sup>; David E. Erickson<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; Paul B. Shepson<sup>1</sup>; <sup>1</sup>Department of Chemistry, Purdue University, West Lafayette, IN
- WP 298 **High Scan Speed and Mass Resolution with Axial Ejection of Ions from Linear Quadrupole Ion Traps with Added Octopole Fields**; Annie Moradian<sup>1</sup>; Donald J. Douglas<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC
- WP 299 **Free Jet Sampling and Ion Extraction in LC/MS/MS: Modeling and Experimentation**; Ilia Tomski<sup>1</sup>; Graeme Mitchell<sup>2</sup>; Serguei Savtchenko<sup>1</sup>; <sup>1</sup>IONICS Mass Spectrometry Group, Concord, Canada; <sup>2</sup>IONICS MSV, Almere, Netherlands
- WP 300 **Practical Quadrupole Theory: Miniaturization of Rod Diameter, Length, and RF Frequency**; Randall E. Pedder<sup>1</sup>; Theodore Novak<sup>1</sup>; Kenneth A. Pedder<sup>2</sup>; <sup>1</sup>Ardara Technologies L.P., Ardara, PA; <sup>2</sup>Eastern Westmoreland Career & Technology Center, Latrobe, PA
- WP 301 **A Comparison of Charge Capacity Between Two Different Geometries of Three-Dimensional Ion Traps**; John (Ed) George<sup>1</sup>; August Specht<sup>1</sup>; Greg Wells<sup>1</sup>; <sup>1</sup>Varian, Inc., Walnut Creek, CA
- WP 302 **Design and Validation of a Collision Cell for High Speed Triple Quad and QqTOF Instrumentation**; Bill

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- Russ<sup>1</sup>; Harvey Loucks<sup>1</sup>; Bob Crawford<sup>1</sup>; John Fjeldsted<sup>1</sup>;  
<sup>1</sup>Agilent Technologies, Santa Clara, CA
- WP 303 **Novel Ion Trap Focusing Techniques for Use with Distance of Flight (DOF) Time of flight (TOF) Mass Spectrometry (MS)**; Gareth S. Dobson<sup>1</sup>; Christie G. Enke<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM
- WP 304 **A Research-Grade ESI-Linear Ion Trap Mass Spectrometer for Ion-Ion Reactions using Commercial Components**; Matthew W. Soyk<sup>1</sup>; Qin Zhao<sup>1</sup>; Gregg M. Scheiffer<sup>1</sup>; Ethan R. Badman<sup>1</sup>; <sup>1</sup>Iowa State University, Ames, IA
- WP 305 **Realistic Supercomputer Modeling of Ion Cloud Dynamics in RF Accumulation Quadrupoles**; Konstantin S. Chingin<sup>1</sup>; Alexander V. Pozdnev<sup>2</sup>; Alexander M. Popov<sup>2</sup>; Ron M.A. Heeren<sup>3</sup>; Eugene N. Nikolaev<sup>1</sup>; <sup>1</sup>The Institute for Energy Problems of Chem. Physics, Moscow, Russia; <sup>2</sup>Moscow State University, Moscow, Russia; <sup>3</sup>FOM Institute of Atomic and Molecular Physics, Amsterdam, Netherlands
- WP 306 **Mass Analysis with Linear Quadrupole with Added Multipoles Using Stability Islands: Simulations, Theory, and Experiments**; XianZhen Zhao<sup>1</sup>; Zilan Xiao<sup>1</sup>; Annie Moradian<sup>1</sup>; D. J. Douglas<sup>1</sup>; Nikolai Konenkov<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC, Canada
- WP 307 **Dynamic Collision Induced Dissociation of Metal Oxide Ions in a Quadrupole Ion Trap**; Sofie P. Pasilis<sup>1</sup>; Lei Li<sup>2</sup>; Glen P. Jackson<sup>3</sup>; Douglas C. Duckworth<sup>1</sup>; Douglas E. Goeringer<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>GE Advanced Materials, Mt. Vernon, IN; <sup>3</sup>Ohio University, Athens, OH
- WP 308 **Systematic Evaluation of Automatic Gain Control Settings for Shotgun Proteomics: A Case Where Less is More**; Jennifer E. Merrihew<sup>1</sup>; Greg Finney<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- WP 309 **Linear Quadrupole Mass Filters with Added Hexapole Fields**; Don Douglas<sup>1</sup>; Xianzhen Zhao<sup>1</sup>; Nikolai Konenkov<sup>2</sup>; Frank Londry<sup>3</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada; <sup>2</sup>University of Ryazan, Ryazan, Russia; <sup>3</sup>Pangalactic Scientific, Omenee, Canada
- WP 310 **A Low Temperature Quadrupole Ion Trap for IRMPD and Laser Spectroscopy Experiments**; Philip M. Remes<sup>1</sup>; Gary L. Glish<sup>1</sup>; Alessandra L. Ferzoco<sup>1</sup>; <sup>1</sup>University of North Carolina-Chapel Hill, Chapel Hill, NC
- WP 311 **CID in Quadrupole Ion Traps using Resonance Excitation of Higher-Order Secular Frequencies**; Glen P. Jackson<sup>1</sup>; Unige A. Laskay<sup>1</sup>; Bradley J. Nichol<sup>1</sup>; Jennifer J. Hyland<sup>1</sup>; <sup>1</sup>Ohio University, Athens, OH
- WP 312 **Electron Capture Dissociation of Peptide Ions in a Digital Ion Trap**; Francesco L. Brancia<sup>1</sup>; Li Ding<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory, Manchester, UK
- WP 313 **A New Implementation of Non-Destructive Differential Mode Electric Ion Resonance Mass Spectrometry for High Precision Wideband Fourier Transform Analysis**; Michel Aliman<sup>1</sup>; Albrecht Glasmachers<sup>1</sup>; Sevki Gencol<sup>2</sup>; Darko Rozic<sup>3</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany; <sup>2</sup>Scienlab Electronic systems GmbH, Bochum, Germany; <sup>3</sup>Robert Bosch GmbH, Reutlingen, Germany
- WP 314 **Performance Evaluation of a Quadrupole Mass Filter Made of Four Quartz Tubes**; Chang Joon Park<sup>1</sup>; Chang-min Kim<sup>2</sup>; <sup>1</sup>Korea Research Institute of Standards and Science, Daejeon, South Korea; <sup>2</sup>Younglin Instrument, Anyang, South Korea
- WP 315 **On-line MALDI of High Mass Biomolecules with an Ion Trap Mass Spectrometer**; William A. Harris<sup>1</sup>; Peter

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T.A. Reilly<sup>1</sup>; William B. Whitten<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*

### IMAGING MS

- WP 316 **Sequence Identification of a Native Neuropeptide Directly from MS and MS/MS Based Mass Spectrometric Imaging Experiments;** Andrew James<sup>1</sup>; Matthew Willetts<sup>2</sup>; Bill Loyd<sup>3</sup>; Patrick Pribil<sup>1</sup>; <sup>1</sup>*Applied Biosystems/MDS Sciex, Concord, On, Canada*; <sup>2</sup>*Applied Biosystems, Framingham, MA*; <sup>3</sup>*MDS Sciex, Concord, On, Canada*
- WP 317 **Spatial Profiling of Peptides in Rat Brain using MALDI/FT-ICR Mass Spectrometry;** Ioana M. Taban<sup>1</sup>; Jens Fuchser<sup>2</sup>; Yuri van der Burg<sup>1</sup>; Maarten A.F. Altelaa<sup>1</sup>; Liam A. McDonnell<sup>1</sup>; Ron M.A. Heeren<sup>1</sup>; Goekhan Baykut<sup>2</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, The Netherlands*; <sup>2</sup>*Bruker Daltonik, Bremen, Germany*
- WP 318 **Practical Considerations when Choosing Matrix Solutions for MALDI-MS/MS Small Molecule Imaging;** Hema Challa<sup>1</sup>; Charles R. Bredl<sup>1</sup>; Katrina J. Rogers<sup>1</sup>; Douglas S. Mautz<sup>1</sup>; <sup>1</sup>*MDS Pharma Services, Bothell, WA*
- WP 319 **Validation of Organ Specific Protein Markers for Whole-Body MALDI Imaging;** Sheerin K. Shahidi<sup>1</sup>; Kristin E. Burnum<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- WP 320 **Automated Matrix Deposition for MALDI MSI;** Markus Stoeckli<sup>1</sup>; Dieter Staab<sup>1</sup>; Stefan Capretta<sup>1</sup>; <sup>1</sup>*Novartis Institutes for BioMedical Research, Basel, Switzerland*
- WP 321 **Assessment of Bacterial Infection by MALDI Imaging Mass Spectrometry;** Michelle L. Reyzer<sup>1</sup>; Erin H. Seeley<sup>1</sup>; Lisa Zimmerman<sup>1</sup>; Eric P. Skaar<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- WP 322 **The KLT in Imaging Mass Spectrometry and a Technique to Evaluate Image Quality;** Alexis J Polley<sup>1</sup>; Victor C Parr<sup>1</sup>; <sup>1</sup>*Scientific Analysis Instruments, Manchester, UK*
- WP 323 **Development of Mass Microscope with QIT-TOF;** Takahiro Harada<sup>1</sup>; Hideaki Izumi<sup>1</sup>; Sadao Takeuchi<sup>1</sup>; Kiyoshi Ogawa<sup>1</sup>; Yoshikazu Yoshida<sup>1</sup>; Shuichi Shimma<sup>2</sup>; Mitsutoshi Setou<sup>2</sup>; Yuki Sugiura<sup>3</sup>; Machiko Sugiyama<sup>4</sup>; Yutaka Hoshikawa<sup>4</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*The Graduate University for Advanced Studies, Okazaki, Japan*; <sup>3</sup>*Tokyo Institute of Technology, Yokohama, Japan*; <sup>4</sup>*Japanese Foundation for Cancer Research, Tokyo, Japan*
- WP 324 **MALDI-MS Imaging of Biomolecules in Intact Embryos of Drosophila Melanogaster;** Teresita M. Cruz Sanchez<sup>1</sup>; George Agnes<sup>1</sup>; <sup>1</sup>*Simon Fraser University, Burnaby, BC, Canada*
- WP 325 **Imaging MS Analysis of the Effects of Subthalamic Lesions on Protein Expression in the Substantia Nigra;** Malin Andersson<sup>1</sup>; Dale S. Cornett<sup>1</sup>; Ariel Y. Deutch<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Biochemistry, MSRC, Vanderbilt University, Nashville, TN*; <sup>2</sup>*Psychiatry, Pharmacology, Vanderbilt University, Nashville, TN*
- WP 326 **Molecular Depth Profiles of liposomes in a Sugar Matrix;** Juan Cheng<sup>1</sup>; Caiyan Lu<sup>1</sup>; Shawn Parry<sup>1</sup>; Nicholas Winograd<sup>1</sup>; <sup>1</sup>*Pennsylvania State University, University Park, Pennsylvania*
- WP 327 **Recent Instrumental Development in Imaging Mass Spectrometry with 50 Nanometer Lateral Resolution: the NanoSIMS 50L;** Francois Horreard<sup>1</sup>; Francois Hillion<sup>1</sup>; <sup>1</sup>*Cameca, Courbevoie, France*

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- WP 328 **MALDI Imaging of Small Molecular Entity in Brain Tissue using Quadruple Time-of-Flight Mass Spectrometer;** Jun Shen<sup>1</sup>; Xue Ge<sup>1</sup>; Marek Piechowiak<sup>1</sup>; Mitra Mahmoudi<sup>1</sup>; Babu Subramanyam<sup>1</sup>; Jih-Lie Tseng<sup>1</sup>; <sup>1</sup>*Berlex Biosciences, Richmond, CA*
- WP 329 **Toward 3D Mapping of Mouse Brain Proteome by Combining High Throughput Quantitative Proteomics with Voxelation Approach;** Vladislav A Petyuk<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; Mark H Chin<sup>2</sup>; Haixing Wang<sup>1</sup>; Eric A Livesay<sup>1</sup>; Mathew E Monroe<sup>1</sup>; Joshua A Adkins<sup>1</sup>; Navdeep Jaitly<sup>1</sup>; David J Anderson<sup>1</sup>; David G Camp II<sup>1</sup>; Desmond J Smith<sup>2</sup>; Richard D Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*University of California at Los Angeles, Los Angeles, CA*
- WP 330 **Examining the Distribution of the Bioreductive Drug AQ4N and its Metabolites in Treated Tumours by Imaging MALDI-MS;** Sally J. Atkinson<sup>1</sup>; Malcolm R. Clench<sup>1</sup>; Laurence H. Patterson<sup>2</sup>; Paul M. Loadman<sup>2</sup>; <sup>1</sup>*Sheffield Hallam University, Sheffield, UK*; <sup>2</sup>*Institute of Cancer Therapeutics, Bradford, UK*
- WP 331 **Lipid Profiling in Aplysia californica using Intermediate-Pressure MALDI with a Linear Ion Trap;** Michael P. Napolitano<sup>1</sup>; Timothy J. Garrett<sup>1</sup>; Leonid L. Moroz<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*; <sup>2</sup>*The Whitney Laboratory for Marine Bioscience, St. Augustine, FL*
- WP 332 **MALDI-Based Imaging Mass Spectrometry Applied to Rat Nerve Tissue using the ABI 4800 MALDI TOF/TOF Analyzer;** Raf Van de Plas<sup>1</sup>; Bart De Moor<sup>1</sup>; Etienne Waelkens<sup>2</sup>; <sup>1</sup>*K.U.Leuven ESAT-SCD, Leuven, Belgium*; <sup>2</sup>*K.U.Leuven Dept. of Molecular Cell Biology, Leuven, Belgium*; <sup>3</sup>*K.U.Leuven ProMeta, Leuven, Belgium*
- WP 333 **Surface Modification of an RF Polymer with Aptamers for MALDI Sample Preparation;** Hong Yu<sup>1</sup>; James Chaoyong Yang<sup>1</sup>; Weihong Tan<sup>1</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*
- WP 334 **MALDI-MS and SIMS Imaging of Human Fabry Disease Biomarkers;** David Touboul<sup>1</sup>; Sandrine Roy<sup>2</sup>; Dominique P. Germain<sup>3</sup>; Pierre Chaminade<sup>2</sup>; Alain Brunelle<sup>1</sup>; Olivier Laprévote<sup>1</sup>; <sup>1</sup>*Laboratoire de Spectrométrie de Masse ICSN CNRS, Gif sur Yvette, FRANCE*; <sup>2</sup>*E3343 Faculte de Pharmacie Paris XI, Chatenay-Malabry, France*; <sup>3</sup>*Service de Génétique Clinique HEGP AP-HP, Paris, France*
- WP 335 **Computer-Controlled Multi-Channel Inkjet Printing of MALDI Matrices for Imaging Mass Spectrometry;** Dodge L Baluya<sup>1</sup>; Timothy J Garrett<sup>1</sup>; Richard A Yost<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL*
- WP 336 **Applications of Conductive Film as a Sample Support Material for Direct Tissue Mass Spectrometry;** Shuichi Shimma<sup>1</sup>; Masaru Furuta<sup>2</sup>; Yuki Sugiura<sup>3</sup>; Yoshikazu Yoshida<sup>2</sup>; Mitsutoshi Setou<sup>4</sup>; <sup>1</sup>*The Graduate University for Advanced Studies, Okazaki, Aichi, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*Tokyo institute of technology, Yokohama, Kanagawa, Japan*; <sup>4</sup>*National Institute for Physiological Sciences, Okazaki, Aichi, Japan*
- WP 337 **Optimization of the Performance of Automated Matrix Spraying for MALDI Tissue Imaging;** Gordon J. Nye<sup>1</sup>; Jeremy L. Norris<sup>2</sup>; <sup>1</sup>*LEAP Technologies, Carrboro, NC*; <sup>2</sup>*Protein Discovery, Inc., Knoxville, TN*

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### SURFACE ANALYSIS

- WP 338 **Comparison of Molecular Weight Measurements from MALDI-TOF MS and AFM;** Zhenning Hong<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University, Boston, MA*
- WP 339 **Use of Room-Temperature Ionic Liquids (RTILs) for TOF-SIMS Analysis of Biomolecules;** Christine L. Gatlin-Bunai<sup>1</sup>; Peter R. Harris<sup>1</sup>; Christine D. Hopkins<sup>1</sup>; Christopher Brittin<sup>1</sup>; Eugene R. Tracy<sup>1</sup>; William E. Cooke<sup>1</sup>; <sup>1</sup>*College of William and Mary, Williamsburg, VA*
- WP 340 **Lipid Cartography Of Atherosclerotic Plaque. Use Of Cluster TOF-SIMS Mass Spectrometry As A Molecular Imaging Tool In Vascular Pathology;** Sebastián Mas<sup>1</sup>; David Touboul<sup>2</sup>; Alain Brunelle<sup>2</sup>; Paloma Aragoncillo<sup>3</sup>; Jesús Egido<sup>1</sup>; Olivier Laprévote<sup>2</sup>; Fernando Vivanco<sup>1</sup>; <sup>1</sup>*Fundación Jiménez Díaz, Madrid, Spain;* <sup>2</sup>*Institut de Chimie des Substances Naturelles, Gif-sur-Yvette, France;* <sup>3</sup>*Hospital Clínico San Carlos, Madrid, Spain*
- WP 341 **Direct MALDI Analysis of Latex Glove Surfaces – From Sample Preparation to the Identification of Protein Allergens;** Martina Marchetti<sup>1</sup>; Kerstin Strupat<sup>2</sup>; Franz Hillenkamp<sup>2</sup>; Emmanuel Raptakis<sup>3</sup>; Günter Allmaier<sup>1</sup>; <sup>1</sup>*Vienna University of Technology, Vienna, Austria;* <sup>2</sup>*University of Münster, Münster, Germany;* <sup>3</sup>*Shimadzu Biotech-Kratos Analytical, Manchester, UK*
- WP 342 **Crystalline Structures by MALDI Soft Landing Mass Spectrometry;** Hans Joachim Räder<sup>1</sup>; Ali Rouhanipour<sup>1</sup>; Anna Maria Talarico<sup>2</sup>; Vincenzo Palermo<sup>2</sup>; Paolo Samori<sup>2</sup>; Klaus Müllen<sup>1</sup>; <sup>1</sup>*Max Planck Institute for Polymer Research, Mainz, Germany;* <sup>2</sup>*Instituto per la Sintesi Organica e Fotoreattiva, Bologna, Italy*
- WP 343 **Protein-DNA Microarrays for Protein Capture and Direct Readout by MALDI-MS;** Christian F. W. Becker<sup>1</sup>; Ron Wacker<sup>2</sup>; Werner S. Bouschen<sup>3</sup>; Ralf Seidel<sup>1</sup>; Branko Kolaric<sup>1</sup>; Pascal Lang<sup>1</sup>; Hendrick Schroeder<sup>2</sup>; Christof M. Niemeyer<sup>4</sup>; Bernhard Spengler<sup>3</sup>; Roger S. Goody<sup>1</sup>; Martin Engelhard<sup>1</sup>; <sup>1</sup>*Max-Planck-Institut of Molecular Physiology, Dortmund, Germany;* <sup>2</sup>*Chimera Biotec GmbH, Dortmund, Germany;* <sup>3</sup>*Justus-Liebig University Giessen, Giessen, Germany;* <sup>4</sup>*University Dortmund, Dortmund, Germany*
- WP 344 **Surface Vibrational Analysis using Time of Flight Electron Spectroscopy;** Zhongyu Yang<sup>1</sup>; Robert H. Jackson<sup>1</sup>; Brian G. Frederick<sup>1</sup>; <sup>1</sup>*Sillwater Scientific Instruments, Orono, ME*
- WP 345 **High Sensitivity Quantitative Surface Analysis;** Igor V. Veryovkin<sup>1</sup>; Wallis F. Calaway<sup>1</sup>; C. Emil Tripa<sup>1</sup>; Michael R. Savina<sup>1</sup>; Michael J. Pellin<sup>1</sup>; <sup>1</sup>*Argonne National Laboratory, Argonne, IL*

### NON-COVALENT COMPLEXES

- WP 346 **Electrospray Ionization Mass Spectrometry Studies on Interactions between Lithium and other Group 1 Cations with Biologically Active Amines and Neurotransmitters;** Xiao Feng<sup>1</sup>; Cherif Matta<sup>1</sup>; Fuqiang Ban<sup>1</sup>; J. Stuart Grossert<sup>1</sup>; Donald F. Weaver<sup>1</sup>; <sup>1</sup>*Dalhousie University, Halifax, NS, Canada*
- WP 347 **Speciation and Fragmentation of Complexes Containing Poly-Propylene Imine (PPI) Dendrimers and Divalent Metals;** Jason D. Batchelor<sup>1</sup>; Gwendolyn A. Harbour<sup>1</sup>; William D. Price<sup>1</sup>; <sup>1</sup>*Marshall University, Huntington, WV*
- WP 348 **Mass Spectrometric Detection of Metal-Directed Self-Assembly of Conjugated Schiff-Base Macrocyces;** Yun

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- Ling<sup>1</sup>; Cindy Lee<sup>1</sup>; Mark MacLachlan<sup>1</sup>; <sup>1</sup>*University of British Columbia, Vancouver, Canada*
- WP 349 **Characterization of Cu(II)-Substituted, Dimeric Polyoxotungstates by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Gregory A. Khitrov<sup>1</sup>; Firasat Hussain<sup>2</sup>; Ulrich Kortz<sup>2</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL;* <sup>2</sup>*International University Bremen, Bremen, Germany*
- WP 350 **Collision-Induced Dissociation of Cobalt(II)-Amino-Acids Complexes;** Guewen Tournois<sup>1</sup>; William Buchmann<sup>1</sup>; Riccardo Spezia<sup>1</sup>; Jeanine Tortajada<sup>1</sup>; Thierry Cartailier<sup>1</sup>; <sup>1</sup>*Universite d'Evry, Evry, France*
- WP 351 **Spectral Analysis of Dinuclear Rhenium(III) Complexes with Purine Dinucleotides;** Tiffany A. Payne<sup>1</sup>; Elizabeth F. Day<sup>1</sup>; <sup>1</sup>*University of the Pacific, Stockton, CA*
- WP 352 **Screening of  $\beta$ -Amyloid Peptide Inhibitors by Electrospray Ionization Mass Spectrometry;** Fotini Bazoti<sup>2</sup>; Jonas Bergquist<sup>3</sup>; Karin Markides<sup>3</sup>; Anthony Tsaropoulos<sup>1</sup>; <sup>1</sup>*University of Patras, Pharmacy Department, Patras, Greece;* <sup>2</sup>*GATA Research Center, Kifissia, Greece;* <sup>3</sup>*Uppsala University, Chemistry Department, Uppsala, Sweden*
- WP 353 **Mass Spectrometric Characterization of Macrocyclic Complexes Based on S-alkylisothiosemicarbazides and Ortho-Aminobenzaldehyde Capable of Binding Exogenous Cations;** Sergiu P. Paliu<sup>1</sup>; Cesar Contreras<sup>1</sup>; Vadim Druta<sup>2</sup>; Nicolae V. Gerbeleu<sup>2</sup>; John R. Eyler<sup>1</sup>; <sup>1</sup>*University of Florida, Gainesville, FL;* <sup>2</sup>*Academy of Sciences of the Republic of Moldova, Chisinau, Moldova*

### CARBOHYDRATES AND OLIGOSACCHARIDES II

- WP 354 **Ab initio MO Study on the Fragmentation Mechanisms of Carbohydrate in Mass Spectrometry. II. 3'-Sialyllactose and 6'-Sialyllactose;** Takae Takeuchi<sup>1</sup>; Michiko Tajiri<sup>2</sup>; Yoshinao Wada<sup>3</sup>; <sup>1</sup>*Nara Women's Univ., Nara, Japan;* <sup>2</sup>*JST, Izumi, Osaka, Japan;* <sup>3</sup>*Osaka MCHRI, Izumi, Osaka, Japan*
- WP 355 **Electron Capture Dissociation of Oligosaccharides Ionized with Alkali, Divalent, and Transition Metal Adducts;** Julie T. Adamson<sup>1</sup>; Kristina Håkansson<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Michigan, Ann Arbor, MI*
- WP 356 **Solving the Mysteries of a FLAG-Tagged Protein Expressed in CHO Cells;** Pamela K. Cochran<sup>1</sup>; Louise J. Basa<sup>1</sup>; Viswanatham Katta<sup>1</sup>; <sup>1</sup>*Genentech, Inc., South San Francisco, CA*
- WP 357 **Study on Biosynthesis Pathways of Complex-Type N-Glycan in vitro.: Analysis of Branch Specificity of Glycosyltransferases using Tandem Mass Spectrometry;** Hiromi Ito<sup>1</sup>; Akihiko Kameyama<sup>1</sup>; Takashi Sato<sup>1</sup>; Masako Sukegawa<sup>1</sup>; Katsue Kiyohara<sup>1</sup>; Hide-ki Ishida<sup>2</sup>; Hisashi Narimatsu<sup>1</sup>; <sup>1</sup>*AIST, Tsukuba, Japan;* <sup>2</sup>*The Noguchi Institute, Tokyo, Japan*
- WP 358 **Mechanistic Elucidation of the Formation of Reduced 2-Aminopyridine-Derivatized Oligosaccharides in MALDI-MS;** Sadanori Sekiya<sup>1</sup>; Yoshiki Yamaguchi<sup>2</sup>; Koichi Kato<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan;* <sup>2</sup>*Nagoya City University, Nagoya, Japan*
- WP 359 **Structural Characterization of the Brain Gangliosides GM1 and GD1 by High Resolution FT-ICR Tandem Mass Spectrometry;** Carol L. Nilsson<sup>1</sup>; Alan G. Marshall<sup>1</sup>; Jan-Eric Mansson<sup>2</sup>; Mark R. Emmett<sup>1</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL;* <sup>2</sup>*Goteborg University, Goteborg, Sweden*

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- WP 360 **Structural Characterization of N-linked Oligosaccharides on Cetuximab by Quadrupole TOF Mass Spectrometry;** Jun Qian<sup>1</sup>; <sup>1</sup>ImClone Systems Incorporated, NJ
- WP 361 **A Glycomics Application for the Detection of Tissue-Specific Changes in N- and O-glycosylation in the Nematode *Caenorhabditis elegans*;** E. Palaima<sup>1</sup>; J. Zaia<sup>1</sup>; M.J. Gravato-Nobre<sup>2</sup>; J. Hodgkin<sup>2</sup>; C.E. Costello<sup>1</sup>; J. F. Cipollo<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>University of Oxford, UK
- WP 362 **Collision Induced Dissociation of Oligosaccharides Using Quadrupole Ion Trap and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry;** Janne Jänis<sup>1</sup>; Salla Pasanen<sup>1</sup>; Pirjo Vainiotalo<sup>1</sup>; <sup>1</sup>University of Joensuu, Department of Chemistry, Joensuu, Finland
- WP 363 **Off-Line Separation and Deposition of Derivatized Site-Specific N-glycan Pools using Capillary Electrophoresis for Subsequent Analysis by MALDI Mass Spectrometry;** Sergei I. Snovidá<sup>1</sup>; Héléne Perreault<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada
- WP 364 **Improved MS Methods to Analyze Fluorescent ATPS-Labeled Glycans;** Xiaorong (Sharon) Wei<sup>1</sup>; Steven L. Cohen<sup>1</sup>; Melissa Hamm<sup>1</sup>; Charlotte Ip<sup>1</sup>; Richard Rustandi<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- WP 365 **Stabilization and Linkage Determination of Sialic Acids by Selective Derivatization for Analysis by MALDI and Electrospray Ionization Mass Spectrometry;** David J. Harvey<sup>1</sup>; Susan F. Wheeler<sup>1</sup>; Louise Royle<sup>1</sup>; Catherine M. Radcliffe<sup>1</sup>; Umi Abd Hamid<sup>1</sup>; Radka Saldova<sup>1</sup>; Pauline M. Rudd<sup>1</sup>; Raymond A. Dwek<sup>1</sup>; <sup>1</sup>University of Oxford, Oxford, UK
- WP 366 **High Energy CID MALDI-MS/MS as an Enabling Glycan Sequencing Technique for Glycomic Applications and Determination of Novel Glycan Structures;** Sz-Wei Wu<sup>1</sup>; Jin-Mei Chen<sup>1</sup>; Kay-Hooi Khoo<sup>1</sup>; <sup>1</sup>Inst Biol Chem, Academia Sinica, Taipei, Taiwan
- WP 367 **Characterization of Monoclonal Antibody-derived N-linked Glycans using Normal Phase-HPLC/ESI-QTOF MS and MALDI-QTOF MS/MS;** Kelly N. Toler<sup>1</sup>; Tanya Q. Shang<sup>1</sup>; Bruce S. Tangarone<sup>1</sup>; Thomas J. Porter<sup>1</sup>; Jason C. Rouse<sup>1</sup>; <sup>1</sup>Wyeth BioPharma, Andover, MA
- WP 368 **Oligosaccharide Profiling of Recombinant Proteins by MS and Database Searching;** Thomas Nylandsted Krogh<sup>1</sup>; Henrik Rahbek-Nielsen<sup>1</sup>; <sup>1</sup>Protein Science, Novo Nordisk A/S, Måløv, Denmark
- WP 369 **Empirical Rules for Fragmentations of Oligosaccharides during Low-Energy CID in MALDI QIT-TOF Mass Spectrometer;** Akihiko Kameyama<sup>1</sup>; Kazuhiko Fukui<sup>1</sup>; Shuuichi Nakaya<sup>2</sup>; Hiromi Ito<sup>1</sup>; Masako Sukegawa<sup>1</sup>; Hisashi Narimatsu<sup>1</sup>; <sup>1</sup>AIST, Tsukuba, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- WP 370 **A Novel N-glycan from the Extrapallial Fluid Glycoprotein of the Mollusc: *Mytilus edulis*;** Hui Zhou<sup>1</sup>; Andrew J. Hanneman<sup>2</sup>; N. Dennis Chasteen<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>Center for Structural Biology, UNH, Durham, NH; <sup>2</sup>Wyeth Biotech, Andover, MA
- WP 371 **Characterization of the Decorin N-Glycans using Tandem Mass Spectrometry;** May Joy C. Miller<sup>1</sup>; John F. Cipollo<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- WP 372 **A Quantitative Glycomics Technique for Eukaryotic and Prokaryotic N-Linked Protein Glycosylation;** Jianjun Li<sup>1</sup>; Xin Liu<sup>1</sup>; David McNally<sup>1</sup>; Harald Nothaft<sup>1</sup>; Christine M. Szymanski<sup>1</sup>; Jean-Robert Brisson<sup>1</sup>; <sup>1</sup>NRC-Institute for Biological Sciences, Ottawa, Canada

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- WP 373 **Isotopic Labeling of N-linked Glycans for Quantitative Analysis;** Justin M. Prien<sup>1</sup>; David J. Ashline<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>University of New Hampshire, Durham, NH

## GLYCOPROTEINS II

- WP 374 **Screening for Glyco-Proteins in Human Serum Applying Glyco-Specific Magnetic Beads in Combination with LCMALDI;** Katrin Sparbier<sup>1</sup>; Arndt Asperger<sup>1</sup>; Irina Kessler<sup>1</sup>; Thomas Wenzel<sup>1</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Leipzig, Germany
- WP 375 **Mass Spectrometric Detection of Tissue-Derived Proteins in the Blood;** Hui Zhang<sup>1</sup>; Alvin Liu<sup>1</sup>; Paul Loriaux<sup>1</sup>; Bernd Wollscheid<sup>1</sup>; Yong Zhou<sup>1</sup>; Julian Watts<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA
- WP 376 **Characterization of Glycosylation Changes in Human Serum Proteins Using a Combination of Immunoaffinity Depletion, Lectin Affinity Chromatography, RP-HPLC, and LC-MS/MS;** Milan Madera<sup>1</sup>; Yehia Mechref<sup>2</sup>; Iveta Klouckova<sup>1</sup>; Milos V. Novotny<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>National Center for Glycomics and Glycoproteomics, Bloomington, IN
- WP 377 **MSn Analysis of a Glycoprotein Derived from Rat Leptomeningeal Cells with Matrix-Assisted Laser Desorption/Ionization Quadrupole Ion Trap Time-Of-Flight Mass Spectrometry;** Masaki Yamada<sup>1</sup>; Masatomo Watanabe<sup>2</sup>; Kouichi Itoh<sup>2</sup>; Koichi Ishikawa<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Tokushima Bunri University, Kagawa, Japan; <sup>3</sup>Gunma University, Gunma, Japan
- WP 378 **ASC\_GLY\_FLUO: A New Reagent for the Selective Characterization of Glycoproteins on 2D Gel;** Mohammed Kajjout<sup>1</sup>; Christian Rolando<sup>1</sup>; Caroline Tokarski<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- WP 379 **Site-Determination of Mucin-Type O-Glycosylation for Glycoproteomics;** Michiko Tajiri<sup>1</sup>; Yoshinao Wada<sup>2</sup>; <sup>1</sup>CREST, Japan Science & Technology Agency, Kawaguchi, Saitama, Japan; <sup>2</sup>Research Institute, Osaka Medical Center for MCH, Izumi, Osaka, Japan
- WP 380 **Determining Glycoprotein O-Linked Oligosaccharide Structure, Distribution and Monosaccharide Composition by ESI-MS;** John B. Briggs<sup>1</sup>; Bao-Jen Shyong<sup>1</sup>; Rodney Keck<sup>1</sup>; Kathleen Champion<sup>1</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA
- WP 381 **UniPep: A Database of Human N-linked Glycosylation Sites and a Resource for Biomarker Discovery;** Hui Zhang<sup>1</sup>; Paul Loriaux<sup>1</sup>; Jimmy Eng<sup>1</sup>; Andy Keller<sup>1</sup>; Pat Moss<sup>1</sup>; David Campbell<sup>1</sup>; Richard Bonneau<sup>1</sup>; Ning Zhang<sup>1</sup>; Kelly Cooke<sup>1</sup>; Eugene C. Yi<sup>1</sup>; Hookeun Lee<sup>1</sup>; Julian Watts<sup>1</sup>; Richard D. Smith<sup>3</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>IMSB ETH Zurich, University of Zurich, Zurich, CH; <sup>3</sup>Biological Sciences Division, PNNL, Richland, WA
- WP 382 **Direct nanoESI MS Analysis of Glycopeptides Derived from In-Capillary or In-Solution Proteolytic Digests of Glycoproteins;** Gottfried Pohlentz<sup>1</sup>; Stefanie Henning<sup>1</sup>; Michael Mormann<sup>1</sup>; Jasna Peter-Katalinic<sup>1</sup>; <sup>1</sup>Institute for Medical Physics and Biophysics, Münster, Germany
- WP 383 **Direct Comparison of Subsequent LC-MS Runs to Quantify Glycoprotein Enriched Fractions from a Cancer Cell Line During Epidermal-To-Mesenchymal Transition;** Jennifer J. Hill<sup>1</sup>; Arsalan S. Haqqani<sup>1</sup>; Wen Ding<sup>1</sup>; Anne E.G. Lenferink<sup>2</sup>; Maureen D. O'Conner-McCourt<sup>2</sup>; John F. Kelly<sup>1</sup>; <sup>1</sup>National Research Council

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- Canada, Ottawa, Canada; <sup>2</sup>National Research Council Canada, Montreal, Canada
- WP 384 **Quality Control of Intact Proteins and Antibodies by ESI-TOF MS**; Christian Neuss<sup>1</sup>; Matthias Pelzing<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany
- WP 385 **Improved Glycopeptide Fingerprinting and Mass Spectra for Characterization of Recombinant and Isolated Glycoproteins**; Beth L. Gillece-Castro<sup>1</sup>; Thomas E. Wheat<sup>1</sup>; Ziling Lu<sup>1</sup>; Jeffrey R. Mazzeo<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 386 **Characterization of Glycosylation of Human Immunodeficiency Virus Vaccine Protein Antigen gp140**; Mark Schafer<sup>1</sup>; Cathy Chu<sup>1</sup>; Viktorya Levi<sup>1</sup>; Chulani Karunatilake<sup>1</sup>; Paul Jedrzejewski<sup>1</sup>; <sup>1</sup>Chiron Corp., Emeryville, CA
- WP 387 **A Novel Labeling Approach for the Sensitive Detection of Glycoprotein Subclasses by 1-D and 2-D Gel Analysis and Mass Spectrometry**; Brian J Agnew<sup>1</sup>; Nancy Ahnert<sup>1</sup>; Suzanne Buck<sup>1</sup>; Courtenay Hart<sup>1</sup>; Tamara Nyberg<sup>1</sup>; <sup>1</sup>Molecular Probes-Invitrogen, Eugene, Oregon
- WP 388 **Analysis of N-Glycans in Human Blood Serum: Implications for Early Breast Cancer Detection**; Zuzana Kyselova<sup>1</sup>; Yehia Mechref<sup>2</sup>; John A. Goetz<sup>1</sup>; Pilsoo Kang<sup>3</sup>; Milan Madera<sup>3</sup>; Robert Hickey<sup>4</sup>; Milos V. Novotny<sup>3</sup>; <sup>1</sup>METACyt Biochemical Analysis Center, Bloomington, IN; <sup>2</sup>National Center for Glycomics and Glycoproteomics, Bloomington, IN; <sup>3</sup>Indiana University - Chemistry Dept., Bloomington, IN; <sup>4</sup>Indiana University - Faculty of Medicine, Indianapolis, IN
- WP 389 **Characterization of E-cadherin Glycoprotein**; Krystyn E 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>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston University School of Dental Medicine, Boston, MA
- WP 390 **Automated Detection of Unusual Isotope Distributions in Complex Mixtures: Application to the Identification of N-linked Glycosylation Sites of Proteins**; Michael R. Hoopmann<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- WP 391 **Protein Glycosylation Site Mapping in Complex Mixtures by Glycopeptide Enrichment, Partial Deglycosylation and FT ECD-/IRMPD-/CAD Tandem Mass Spectrometry**; Jakob Bunkenborg<sup>1</sup>; Peter Mortensen<sup>1</sup>; Per Hägglund<sup>2</sup>; Irina Kratchmarova<sup>1</sup>; Jens S. Andersen<sup>1</sup>; <sup>1</sup>CEBI, \*University of Southern Denmark, Odense, Denmark; <sup>2</sup>DTU, Biochemistry & Nutrition Group, Copenhagen, Denmark
- WP 392 **Identification of a Novel Wide-Spread Motive for O-Linked Glycosylation in Archaea**; Sander Piersma<sup>1</sup>; Yana Tatur<sup>2</sup>; Marc Stampraad<sup>2</sup>; Ivo Klinkert<sup>1</sup>; Imke Schroeder<sup>3</sup>; Simon de Vries<sup>2</sup>; <sup>1</sup>FOM-AMOLF, Amsterdam, The Netherlands; <sup>2</sup>TU-Delft, Delft, The Netherlands; <sup>3</sup>UCLA, Los Angeles, CA
- WP 393 **The Comprehensive Characterization of an Unusual Bacterial Adhesin by nanoLC-FTICR with Special Focus on N-glycosylation**; Julia Gross<sup>1</sup>; Susan Grass<sup>2</sup>; Alan E. Davis<sup>1</sup>; Joseph W. St. Geme III<sup>2</sup>; <sup>1</sup>Washington University School of Med., St. Louis, MO; <sup>2</sup>Duke University, Durham, NC
- WP 394 **Characterization of N-linked Glycosylation Sites and Glycans of Glycodelins by Means of Tandem Mass Spectrometry**; S. O. Siu<sup>1</sup>; Dave Cox<sup>2</sup>; Calvin K. F. Lee<sup>1</sup>; W. S. B. Yeung<sup>1</sup>; Ivan K. Chu<sup>1</sup>; <sup>1</sup>The University of Hong Kong, Hong Kong SAR, China; <sup>2</sup>MDS Sciex, Concord, Ontario, Canada

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- WP 395 **Identification of Nucleases Associated with Brush Border Membranes and the Nucleic Acid Conducting Channel Complex**; Avelino Teixeira<sup>1</sup>; Edgar Leal-Pinto<sup>1</sup>; Basil Hanss<sup>1</sup>; Paul E. Klotman<sup>1</sup>; John Roboz<sup>1</sup>; <sup>1</sup>Mount Sinai Medical Center, New York, NY
- WP 396 **Effects of Glycosylation on DNA-Anthracycline Binding Probed by Electrospray Ionization Mass Spectrometry (ESI-MS)**; Margaret M. Sheil<sup>1</sup>; Vanessa Tillott<sup>1</sup>; Stephen J. Watt<sup>1</sup>; Renata L.A. Furlan<sup>2</sup>; Gabriel Padilla<sup>2</sup>; Jennifer L. Beck<sup>1</sup>; <sup>1</sup>University of Wollongong, Wollongong, Australia; <sup>2</sup>University of San Paulo, San Paulo, Brazil
- WP 397 **PNA Oligomers Behavior in the Gas Phase Under CID Conditions in High Resolution. For a Better Comprehension of Fragmentation Mechanisms**; Alice Delvolve<sup>1</sup>; Peter Egholm Nielsen<sup>2</sup>; Carlos Afonso<sup>1</sup>; Françoise Fournier<sup>1</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>Lab. Chimie Org et Bio Univ. Pierre et Marie Curie, Paris, France; <sup>2</sup>Dept. Med. Biochem. Genetics Univ. of Copenhagen, Copenhagen, Denmark
- WP 398 **Characterization of Isomeric Benzo[a]pyrene Diol Epoxide Oligonucleotide Adducts using Ion-Pair Reversed Phase Nano LC-MS/MS**; Wennan Xiong<sup>1</sup>; James Glick<sup>1</sup>; Yiqing Lin<sup>1</sup>; Paul Vouras<sup>1</sup>; <sup>1</sup>Barnett Institute, Boston, MA
- WP 399 **DNA Sequencing by MALDI-TOF Mass Spectrometry using Alkali Cleavage of RNA/DNA Chimeras**; Ivo G. Gut<sup>1</sup>; Florence Mauger<sup>1</sup>; Sakina Mezzache<sup>2</sup>; David Gelfand<sup>3</sup>; Rod Fuerst<sup>2</sup>; Keith Bauer<sup>3</sup>; Fred Reichert<sup>3</sup>; Cassandra Calloway<sup>3</sup>; Thomas Koch<sup>2</sup>; <sup>1</sup>Centre National de Genotypage, Evry Cedex, France; <sup>2</sup>Roche Diagnostics GmbH, Penzberg, Germany; <sup>3</sup>Roche Molecular Systems, Alameda, CA
- WP 400 **TIGER MLST Genotyping of Campylobacter jejuni Obtained from Contaminated Chicken Samples Using High Throughput ESI-Mass Spectrometry**; James C. Hannis<sup>1</sup>; Sheri M. Manalili<sup>1</sup>; Thomas A. Hall<sup>1</sup>; Raymond Ranken<sup>1</sup>; Robert E. Mandrell<sup>2</sup>; Clifton K. Fagerquist<sup>2</sup>; William G. Miller<sup>2</sup>; Steven A. Hofstadler<sup>1</sup>; <sup>1</sup>Ibis Therapeutics-A Div. of ISIS Pharmaceuticals, Carlsbad, CA; <sup>2</sup>USDA Produce Safety and Microbiology Research Unit, Albany, CA
- WP 401 **Determination of a Novel Sulphur-Modified Guanine in DNA by LC-MS/MS**; Chunang Gu<sup>1</sup>; Hongxia Wang<sup>1</sup>; Qingchun Zhang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 402 **Collisionally induced Dissociations of Single-Base and Intrastrand Crosslink lesions Induced by Reactive Oxygen Species**; Huachuan Cao<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA
- WP 403 **Mass Spectrometry of the Products of Oligomerisation from Activated Nucleotides of Guanosine with Montmorillonite; Evidence for Cyclic and Cage Structures**; Michael F Aldersley<sup>1</sup>; James P Ferris<sup>2</sup>; Dmitri V Zagorevskii<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute, Troy, NY; <sup>2</sup>New York Center for Studies on the Origin of Life, Troy, NY
- WP 404 **Identification and Quantification of a Guanine-thymine Intrastrand Crosslink Lesion Induced by Cu(II)/H<sub>2</sub>O<sub>2</sub>/Ascorbate**; Haizheng Hong<sup>1</sup>; Huachuan Cao<sup>1</sup>; Yuesong Wang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA
- WP 405 **Identifying RNA by Enzyme Digestion and Mass Spectrometry**; Rune Matthiesen<sup>1</sup>; Gary Schoenhals<sup>2</sup>; Finn

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- Kirpekar<sup>2</sup>; <sup>1</sup>Bioinformatics unit - CIC bioGUNE, Derio, Spain; <sup>2</sup>Biochem. and Mol. Biol., Uni. of Southern Denmark, Odense, Denmark
- WP 406 **Investigation of the Enzymatic Behavior of Benzonase/Alkaline Phosphatase in the Digestion of DNA and DNA Adducts by ESI-LC/MS;** Qing Liao<sup>1</sup>; Norman H. L. Chiu<sup>2</sup>; Chang Shen<sup>3</sup>; Paul Vouros<sup>4</sup>; <sup>1</sup>Harvard University Mass Spec Facility, Cambridge, MA; <sup>2</sup>University of North Carolina, Greensboro, NC; <sup>3</sup>Shenitech, Acton, MA; <sup>4</sup>Northeastern University, Boston, MA
- WP 407 **Evaluation of Broad-Range PCR Followed by Mass Spectrometry to Identify a Blinded Panel of Bacterial Pathogens;** Carson D. Baldwin<sup>1</sup>; Chris A. Whitehouse<sup>1</sup>; Gerald B. Howe<sup>1</sup>; Larry B. Blyn<sup>2</sup>; Dave Ecker<sup>2</sup>; Ranga Sampath<sup>2</sup>; Mark W. Eshoo<sup>2</sup>; Karl Rudnick<sup>3</sup>; Jared J. Drader<sup>2</sup>; Steve A. Hofstadler<sup>2</sup>; Dave Robbins<sup>3</sup>; <sup>1</sup>USAMRIID, Frederick, MD; <sup>2</sup>Ibis Therapeutics, Division of Isis Pharmaceuticals, Carlsbad, CA; <sup>3</sup>SAIC, San Diego, CA
- WP 408 **Optimizing a Mass Spectrometry-Based Approach for the Detection of CMC-derivatized Pseudouridine in RNA;** Anita Durairaj<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 409 **Using Mass Spectrometry to Study Heterogeneous Mixtures of MicroRNAs;** C. Callie Coombs<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 410 **Use of MALDI-TOF, ESI-TOF and GC-MS to Discover how Ethnadenine Damage within DNA is Repaired by AlkB;** James C. Delaney<sup>1</sup>; Lisa Smeester<sup>1</sup>; Cintyu Wong<sup>1</sup>; Lauren E. Frick<sup>1</sup>; Koli Taghizadeh<sup>1</sup>; John S. Wishnok<sup>1</sup>; Catherine L. Drennan<sup>1</sup>; Leona D. Samson<sup>1</sup>; John M. Essigmann<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology, Cambridge, MA
- WP 411 **DNA Binding of New Anthrapyrazoles by ESI-MS-MS;** Suncerae Smith<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; Frank Guziec<sup>2</sup>; Brian Hasinoff<sup>3</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX; <sup>2</sup>Southwestern University, Georgetown, TX; <sup>3</sup>University of Manitoba, Winnipeg, Canada
- WP 412 **Detection and Characterization of Label Retention in Immortal DNA Strands of Mouse Cell Models for Adult Stem Cell Asymmetric Self-Renewal;** Dayana Argoti<sup>1</sup>; Art Lafleur<sup>2</sup>; James Sherley<sup>2</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Barnett Institute-Northeastern University, Boston, MA; <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA
- WP 413 **Investigation of Metal Mediated Binding by Benzoxazoles to DNA by Electrospray Ionization Mass Spectrometry;** Carolyn L. Mazzitelli<sup>1</sup>; Mireya Rodriguez<sup>1</sup>; Sean M. Kerwin<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- WP 414 **Signature Digestion Products of Transfer RNAs: Advantages of Multiple Ribonucleases;** Mahmud Hossain<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 415 **Photochemistry of 5-phenylthiol-2'-deoxyuridine-bearing DNA;** Yu Zeng<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California Riverside, Riverside, CA
- WP 416 **Quantitation of 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine Deoxyguanosine (PhIP-dG) Adducts in Metabolically Competent Human Lymphoblastoid Cells Using Nano-LC-MS/MS;** James Glick<sup>1</sup>; Garrett Ainslie<sup>1</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- WP 417 **LC-ESI-MS/MS Analysis of Peptide-Oligonucleotide Cross-Links: Precursor-Ion Scan Detection and CID-**

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- Induced Fragmentation;** Henning Urlaub<sup>1</sup>; Christof Lenz<sup>2</sup>; Detlev Schleuder<sup>2</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany
- WP 418 **Determination of Deoxynucleosides and Nucleosides Acidity Values using the Kinetic Method;** Clotilde Le Vot<sup>1</sup>; Ying Xu<sup>1</sup>; Carlos Afonso<sup>1</sup>; Françoise Fournier<sup>1</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris 6, Paris, France
- WP 419 **Oligonucleotide Gas-phase H/D Exchange with D<sub>2</sub>S in the Collision Cell of a Q-FT-ICR Mass Spectrometer;** Jingjie Mo<sup>1</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>The University of Michigan, Ann Arbor, MI
- WP 420 **Characterization of a Lipid Hydroperoxide-Derived RNA-Adduct in Rat Intestinal Epithelial Cells by LC/MS/MS;** Peijuan Zhu<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- WP 421 **siRNA Degradation in Human Plasma by LC-ESI-MS;** Sharin E. Roth<sup>1</sup>; <sup>1</sup>Nastech Pharmaceuticals, Inc., Bothell, WA
- WP 422 **ESI-MS Study of Metal Mediated Binding of Quinolone Antibiotics to DNA;** Sarah E. Pierce<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>The University of Texas at Austin, Austin, TX
- WP 423 **HPLC-ESI-MS Identification and Quantification of the Highly Mutagenic DNA Lesions Spiroiminodihydantoin and Guanidinohydantoin;** Peter G. Slade<sup>1</sup>; <sup>1</sup>The University of Montana, Missoula, MT
- WP 424 **Characterization of Oligonucleotide Gas-Phase Fragmentation Pathways by Fourier Transform Ion Cyclotron Double Resonance;** Jiong Yang<sup>1</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- PEPTIDES: FRAGMENTATION AND SEQUENCING III**
- WP 425 **Fragmentation Pathways of Protonated  $\beta$ -Alanine and  $\beta$ -Dipeptides: An Energy-Resolved Tandem Mass Spectrometric and Theoretical Study;** Jackie M. K. Cheng<sup>1</sup>; Onyx O. Y. Chan<sup>1</sup>; Pui K. So<sup>1</sup>; Chun W. Tsang<sup>1</sup>; <sup>1</sup>Hong Kong Polytechnic University, Hong Kong, China
- WP 426 **Tandem Mass Spectrometry of Non-Tryptic Peptides;** Sara P. Gaucher<sup>1</sup>; Anup K. Singh<sup>1</sup>; Jean-Loup M. Faulon<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Livermore, CA
- WP 427 **Dehydration vs. Deamination of N-Terminal Glutamine in Collision-Induced Dissociation of Protonated Peptide Ions;** Lisa Kilpatrick<sup>2</sup>; Pedatsur Neta<sup>1</sup>; Quan-Long Pu<sup>1</sup>; Stephen E. Stein<sup>1</sup>; Sara Yang<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>2</sup>NIST - HML, Charleston, SC
- WP 428 **Fragmentation Mechanisms of Protonated Peptides;** Christian Bleiholder<sup>1</sup>; Sandor Suhai<sup>1</sup>; Bela Paizs<sup>1</sup>; <sup>1</sup>German Cancer Research Center, Heidelberg, Germany
- WP 429 **Quantum Mechanical Studies of Neutral Losses from Peptides with Glutamine in the N-terminal Position;** Christopher R. Kinsinger<sup>1</sup>; Karl K. Irikura<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD
- WP 430 **MS Study of Peptide Profile of Russian Frog Rana Ridibunda;** Albert T. Lebedev<sup>1</sup>; Tatiana Yu Samgina<sup>1</sup>; Konstantin A. Artemenko<sup>1</sup>; Sergey V. Ogurtsov<sup>1</sup>; John H. Bowie<sup>2</sup>; <sup>1</sup>Organic Chemistry Dept., Moscow State University, Moscow, Russia; <sup>2</sup>Adelaide University, Adelaide, Australia
- WP 431 **Reversed Fragmentation Behavior of [M+H]<sup>+</sup> Ions of Alpha-helical Peptides;** Dieter R. Mueller<sup>1</sup>; Bruno Inverardi<sup>1</sup>; Patrick Schindler<sup>1</sup>; Hans Voshol<sup>1</sup>; Jan van Oostrum<sup>1</sup>; <sup>1</sup>Novartis Pharma AG, Basel, Switzerland
- WP 432 **Fragmentation Pathways of Metallated Cyclic Peptides with and without a Crown-Type Auxilliary Ligand in**



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- Ion-Trap and Triple-Quadrupole Mass Spectrometers;** Sheldon M. Williams<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>*Ctr for Research in Mass Spectrometry, York Univ, Toronto, Ontario, Canada*
- WP 433 **Development of a Systematic Process to Identify Process Impurities and Degradation Products of a Synthetic Peptide by MS/MS;** Shawn D Fitzgibbons<sup>1</sup>; Vincy Abraham<sup>1</sup>; <sup>1</sup>*Aptuit, Kansas City, MO*
- WP 434 **Automated De Novo Sequencing of Dual Labeled Peptides;** Laura A. Sharon<sup>1</sup>; James P. Reilly<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*
- WP 435 **Dissociation of Lantibiotics in Negative Ion Mode Tandem Mass Spectrometry;** Anastasia Kalli<sup>1</sup>; Kristina Håkansson<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*
- WP 436 **Kinetic and Mechanistic Studies of Peptide Fragmentation;** John K. Merle<sup>1</sup>; Karl K. Irikura<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 437 **Proton Transfer in Small Peptides;** Juergen Grotemeyer<sup>1</sup>; Osama Abdelrahman<sup>1</sup>; <sup>1</sup>*University Kiel, Kiel, Germany*
- WP 438 **Modeling the Fragmentation of Protonated AGG in a MALDI TOF/TOF Mass Spectrometer;** Benjamin J Bythell<sup>1</sup>; Bela Paizs<sup>2</sup>; Douglas F Barofsky<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*German Cancer Research Center, Heidelberg, Germany*
- WP 439 **Analysis of the Stochastic Variation in LTQ Single Scan Peptide Mass Spectra;** Qunhua Li<sup>1</sup>; Qiangwei Xia<sup>1</sup>; Tiansong Wang<sup>1</sup>; Marina Meila<sup>1</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- WP 440 **Aspartic Acid Side Chain Effect - Experimental and Theoretical Insight;** Marko Rožman<sup>1</sup>; <sup>1</sup>*Institute Ruder Boškovic, Zagreb, Croatia*
- WP 441 **What is the Structure of the b<sub>2</sub> Ions Derived from Protonated Peptides Containing the Proline Residue?;** P. Y. Iris Shek<sup>1</sup>; Houssain El Aribi<sup>1</sup>; Alan C. Hopkinson<sup>1</sup>; K. W. Michael Siu<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*

## PEPTIDES: GENERAL

- WP 450 **Mass Spectrometry Characterization of Disulfide Bonds in MD-1100 an Orally Administered Peptide Designed for the Treatment of IBS-C;** Marco M. Kessler<sup>1</sup>; James D. Wakefield<sup>1</sup>; Li Jing Sun<sup>1</sup>; Angelika Fretzen<sup>1</sup>; Robert W. Busby<sup>1</sup>; <sup>1</sup>*Microbia, Inc., Cambridge, MA*
- WP 451 **Fragmentation of Tertiary Complexes Containing Cu(II), an Amino Acid or Peptide, and Solvents: Generation of Distonic Radical Cations;** Yuyong Ke<sup>1</sup>; P. Y. Iris Shek<sup>1</sup>; Udo H. Verkerk<sup>1</sup>; Alan C. Hopkinson<sup>1</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>*Department of Chemistry and CRMS, York University, Toronto, Canada*
- WP 452 **Identification of Spin-Trapped Free Radicals from Leucine Enkephalin Oxidation under Fenton's Conditions by Tandem Mass Spectrometry;** Conceição Fonseca<sup>1</sup>; Pedro Domingues<sup>1</sup>; Ana Reis<sup>1</sup>; António Ferrer Correia<sup>1</sup>; M Rosario M Domingues<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Aveiro, Aveiro, Portugal*
- WP 453 **Identification of Unknown Pheromone-Like Peptides of the Marine Cephalopod Nautilus Pompilius L. by Mass Spectrometry;** Oliver Schulz<sup>1</sup>; Andreas Roempp<sup>1</sup>; Bettina Westermann<sup>2</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>*Institut fuer Anorganische und Analytische Chemie, Giessen, Germany*; <sup>2</sup>*Institut fuer Allgemeine Zoologie, Giessen, Germany*
- WP 454 **Hydrogen/Deuterium Exchange of Alanine Oligomeric Peptides;** Brittany R. Perkins<sup>1</sup>; Kristin A. Herrmann<sup>1</sup>;

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- Linda Breci<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*University Of Arizona Department of Chemistry, Tucson, AZ*
- WP 455 **A Statistical Model for Peptide Mass Defects and Its Applications;** Xunming Chen<sup>1</sup>; Philip Savickas<sup>3</sup>; Darryl Pappin<sup>1</sup>; Marvin Vestal<sup>2</sup>; <sup>1</sup>*Applied Biosystems, Framingham, MA*; <sup>2</sup>*Virgin Instrument, Sudbury, MA*; <sup>3</sup>*Shire Pharm, Cambridge, MA*
- WP 456 **Mechanism and Energetics & Beta;-Alanine Methylamide Ion and Radical Dissociations in the Gas Phase;** Chunxiang Yao<sup>1</sup>; Erik A. Syrtstad<sup>1</sup>; Frantisek Turecek<sup>1</sup>; <sup>1</sup>*Department of Chemistry/University of Washington, Seattle, WA*
- WP 457 **Accurate Mass Measurements of Biomolecules with Newly Developed MALDI-TOF Mass Spectrometer with a Spiral Optical System and its Applications;** Junichi Osuga<sup>1</sup>; Takaya Satoh<sup>1</sup>; Takafumi Sato<sup>1</sup>; Akihiko Kusai<sup>1</sup>; Jun Tamura<sup>1</sup>; David Vargas<sup>2</sup>; <sup>1</sup>*JEOL Ltd., Akishima, Tokyo, Japan*; <sup>2</sup>*JEOL USA, Inc., Peabody, MA*
- WP 458 **MS Intensities of Peptides in Matrix-Assisted Laser Desorption/Ionization (MALDI) Mass Spectrometry;** Yasushi Shigeri<sup>1</sup>; Rie Tanaka<sup>1</sup>; Ryuichi Arakawa<sup>2</sup>; Tomoya Kinumi<sup>1</sup>; <sup>1</sup>*Natl Inst of Advanced Industrial Sci & Tech, Ikeda, Osaka, Japan*; <sup>2</sup>*Kansai University, Suita, Osaka, Japan*
- WP 459 **Role of UV-absorbing and Basic Groups in Enhancing Signal Intensity of Peptides in MALDI-TOF Mass Spectrometry;** Jong-Seo Kim<sup>1</sup>; Hie-Joon Kim<sup>1</sup>; <sup>1</sup>*Seoul National University, Seoul, Korea*
- WP 460 **In vitro Stability and Degradation Identification of Therapeutic Peptide by LC-MS/MS;** Hongyan Li<sup>1</sup>; Chun Li<sup>1</sup>; Keyang Xu<sup>1</sup>; Gary L. Skiles<sup>1</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*
- WP 461 **Characterization of Dimeric Linkage of rhPTH(1-34) Induced by Heat, Humidity and Light Stress;** Lihua Huang<sup>1</sup>; Stanley Szweczyk<sup>1</sup>; Alice Riggan<sup>1</sup>; <sup>1</sup>*Eli Lilly and Company, Indianapolis, IN*

## PEPTIDES: POST-TRANSLATIONAL MODIFICATIONS II

- WP 462 **Kinetics Measurement of Human Tyrosylprotein Sulfotransferase using Reverse-Phase Liquid Chromatography coupled to Electrospray Ionization Mass Spectrometry;** Lieza Marie A Danan<sup>1</sup>; Julie A Leary<sup>1</sup>; <sup>1</sup>*Genome Center, University of California, Davis, CA*
- WP 463 **Isolation and Identification of a Novel Impurity Observed in Development Samples of a Therapeutic Peptide;** Andrew W. Carr<sup>1</sup>; Gregory M. Beck<sup>1</sup>; Bryan J. Harmon<sup>1</sup>; Karen J. Hywood<sup>1</sup>; Andreas Kaerner<sup>1</sup>; Amareth Lim<sup>1</sup>; Tim A. Smitka<sup>1</sup>; <sup>1</sup>*Eli Lilly and Company, Indianapolis, IN*
- WP 464 **A Study of Snake Venoms and Comparison of Members from the Genera *Crotalus* and *Calloselasma* using nanoHPLC MS/MS;** Clare L. Smith<sup>1</sup>; Edward Dudley<sup>2</sup>; Gareth Brenton<sup>1</sup>; Russell P Newton<sup>3</sup>; <sup>1</sup>*Mass Spectrometry Research Unit, Chemistry, Swansea, Wales*; <sup>2</sup>*Biomolecular Analysis through Mass Spectrometry, Swansea, Wales*; <sup>3</sup>*Biochemistry Group, Swansea, Wales*
- WP 465 **Site-Specific Protein S-glutathiolation Modulates the Electron Transfer and Superoxide Generation Activities of Mitochondrial NADH Ubiquinone Reductase (NQR);** Liwen Zhang<sup>1</sup>; Kari B. Green-Church<sup>1</sup>; Nan Kleinholz<sup>1</sup>; Rhonda Pitsch<sup>3</sup>; Chwen-Lin Chen<sup>2</sup>; Jay L. Zweier<sup>2</sup>; Yeong-Renn Chen<sup>2</sup>; <sup>1</sup>*MS&P Facility, The Ohio State University, Columbus, OH*; <sup>2</sup>*Davis HLRI, The Ohio State University, Coulmbus, OH*;



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- <sup>3</sup>Henry M. Jackson Found. for the Adv. of Mil. Med, Dayton, OH
- WP 466 **Mass Spectrometry to Dissect the Mechanism whereby Destabilizing Mutations in the Tumour Suppressor Protein p53 Exhibit Enhanced Ubiquitination;** David G Saliba<sup>1</sup>; Harumi Shimizu<sup>2</sup>; Pat R. R. Langridge-Smith<sup>3</sup>; Ted R. Hupp<sup>1</sup>; <sup>1</sup>University of Edinburgh, Cancer Research UK, Edinburgh, UK; <sup>2</sup>Genentech, San Francisco, Ca; <sup>3</sup>University of Edinburgh, Edinburgh, UK
- WP 467 **Characterization Of Peptide O-linked Glycoforms Using a Combination of  $\beta$ -Elimination, Tryptic Digestion, and MALDI-TOF TOF MS;** Patricia Molina<sup>1</sup>; John B. Briggs<sup>1</sup>; Kathleen Champion<sup>1</sup>; <sup>1</sup>Genentech, Inc, South San Francisco, CA
- WP 468 **Mass Spectrometric Characterization of Human Aromatase;** Mike Aguiar<sup>1</sup>; Robert Masse<sup>2</sup>; Bernard F. Gibbs<sup>1</sup>; <sup>1</sup>McGill University, Montreal, Canada; <sup>2</sup>MDS Pharma Services, Saint Laurent (Montreal), Canada
- WP 469 **Post-Translational Modification Analyses using 1,5-Diaminonaphthalene as a Matrix;** Yuko Fukuyama<sup>1</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan
- WP 470 **FT-ICR MS-Based Structural Characterization of a Novel Conotoxin from *Conus monile*: Determination of Bromotryptophan by use of Electron Capture Dissociation;** Sudarslal Sadasivan Nair<sup>1</sup>; Mark R Emmett<sup>1</sup>; Carol L Nilsson<sup>1</sup>; Krishnan K.S<sup>2</sup>; Balaram Padmanabhan<sup>3</sup>; Alan G Marshall<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Tata Institute of Fundamental Research, Mumbai, India; <sup>3</sup>Indian Institute of Science, Bangalore, India
- WP 471 **Ribosomal Protein Isoform Determination;** Michael B. Strader<sup>1</sup>; Cai Chen<sup>1</sup>; Anthony J. Makusky<sup>1</sup>; Jeffrey A. Kowalak<sup>1</sup>; Sanford P. Markey<sup>1</sup>; <sup>1</sup>National Institute of Mental Health, Bethesda, MD
- WP 472 **Complexity of the Peptide Complement in *Conus* Venom Duct Partially Unraveled by Chromatography and Mass Spectrometry;** Timothy A. Richmond<sup>1</sup>; Zora Lebaric<sup>2</sup>; Suresh P. Annangudi<sup>1</sup>; Carl Elliger<sup>2</sup>; William F. Gilly<sup>2</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL; <sup>2</sup>Hopkins Marine Station Stanford University, Pacific Grove, CA
- WP 473 **Anion-Electron Reactions as a Tool for Establishing the Presence and Location of Acidic Post-Translational Modifications in Singly Charged Peptides;** Gabriela Grigorean<sup>1</sup>; Kristina Håkansson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- WP 474 **Combined CID/ETD Ion Trap MS for Improved Characterization of Glycopeptides;** Markus Lubeck<sup>1</sup>; Ralf Hartmer<sup>1</sup>; Victor G. Fursey<sup>2</sup>; Andreas Brekenfeld<sup>1</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA
- WP 475 **Exploring the Sialome using Titanium Dioxide and Mass Spectrometry - Identification of Sialic Acid Containing Peptides From Glycosylated Proteins;** Søren S. Jensen<sup>1</sup>; Niels H. H. Heegaard<sup>2</sup>; Lene Jacobsen<sup>1</sup>; Martin R. Larsen<sup>1</sup>; <sup>1</sup>Biochemistry and Molecular Biology, Odense, Denmark; <sup>2</sup>State Serum Institute, Copenhagen, Denmark
- WP 476 **Novel Mass Spectrometry Strategies for Facile Mapping of Protein S-Nitrosylation Sites in Relation to Identification of Controlled Cysteine Oxidation;** Kuan-Ting Pan<sup>1</sup>; Yi-Yun Chen<sup>1</sup>; Shu-Yu Lin<sup>1</sup>; Tzu-Ching Meng<sup>2</sup>; Kay-Hooi Khoo<sup>2</sup>; <sup>1</sup>Core Facilities for Proteomics Research, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan

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- WP 477 **Use of Internal Standard Peptides to Enhance the Specificity and Sensitivity of Multiplexed Precursor-Ion-Like Scanning Technique for Quadrupole Time-Of-Flight Instruments;** Marc Gentzel<sup>1</sup>; Matthias Wilm<sup>1</sup>; <sup>1</sup>EMBL, Heidelberg, Germany

### PHOSPHORYLATED PROTEINS

- WP 478 **Analysis of Histidine Phosphorylation of Histone H4;** Paul V. Attwood<sup>1</sup>; Xin L. Zu<sup>1</sup>; Paul G. Besant<sup>1</sup>; Axel Imhof<sup>2</sup>; <sup>1</sup>The University of Western Australia, Crawley, Australia; <sup>2</sup>Ludwig-Maximilians University of Munich, Munich, Germany
- WP 479 **Identification of Novel Phosphorylation Sites in Huntingtin Protein Using Combined Vacuum-MALDI LTQ Linear Ion Trap and Q-TOF Platforms;** Bradford W Gibson<sup>1</sup>; Birgit Schilling<sup>1</sup>; Xin Cong<sup>1</sup>; Cameron Torcassi<sup>1</sup>; Michael P Cusack<sup>1</sup>; Christopher A Ross<sup>2</sup>; Lisa M Ellerby<sup>1</sup>; <sup>1</sup>Buck Institute for Age Research, Novato, CA; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- WP 480 **Determination of Absolute Phosphorylation Stoichiometry by MALDI-MS using Proteolytic O18-Labeling;** Wenzhu Zhang<sup>1</sup>; Wenhui Zhao<sup>1</sup>; Wei Gu<sup>1</sup>; <sup>1</sup>Columbia University, New York, NY
- WP 481 **Specific Fractionation and Identification of Multiply Phosphorylated Peptides by Immobilized pH Gradient Isoelectric Focusing Electrophoresis and LC-ESI-MS/MS;** Jinglan Wang<sup>1</sup>; Shaohui Sui<sup>2</sup>; Jingfeng Liu<sup>2</sup>; Yangjun Zhang<sup>1</sup>; Yun Cai<sup>1</sup>; Xiaohong Qian<sup>1</sup>; <sup>1</sup>Beijing Institute of Radiation Medicine, Beijing, P.R. China; <sup>2</sup>Beijing Proteomics Research Center, Beijing, P.R. China
- WP 482 **Automatic Off-Line Enrichment of Phosphorylated Peptides by Titanium Dioxide;** Manfred R. Raida<sup>1</sup>; Bantscheff Marcus<sup>1</sup>; Duempelfeld Birgit<sup>1</sup>; Kuster Bernhard<sup>1</sup>; <sup>1</sup>Cellzome AG, Heidelberg, Germany
- WP 483 **Identification of Phosphorylation Sites and Their Biological Relevance on the Nap1 Protein Using Fe(III) IMAC Enrichment and Reversed-Phase C18 LC-MS/MS-ETD;** Ken G. Victor<sup>1</sup>; Meredith Calvert<sup>1</sup>; A. Celeste Ptak<sup>1</sup>; Jeffrey Shabanowitz<sup>1</sup>; Lucy Pemberton<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA
- WP 484 **Development of a Robust Strategy for the Enrichment of Phosphorylated Proteins and Peptides from Complex Mixtures;** Christian Collin-Hansen<sup>1</sup>; Erol E. Gulcicek<sup>1</sup>; Terence Wu<sup>1</sup>; Kenneth R. Williams<sup>1</sup>; Angus C. Nairn<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT
- WP 485 **Proteomic Analysis of PP2A/B56 $\gamma$ 1-Associated Cardiac Proteins Reveals Phosphorylation-Regulated Players that Participate in Excitation-Contraction Coupling and Heart-Failure Development;** Xing W. Zhou<sup>1</sup>; Malkanthi Mudannayake<sup>1</sup>; Terry B. Rogers<sup>1</sup>; <sup>1</sup>University of Maryland School of Medicine, Baltimore, MD
- WP 486 **Strategies for Investigating Protein Phosphorylation in the Mouse Hippocampus;** Emma L. Schofield<sup>1</sup>; Andrew J Thompson<sup>1</sup>; Helen L Byers<sup>2</sup>; John Stephenson<sup>1</sup>; Brian Anderton<sup>1</sup>; Malcolm A Ward<sup>2</sup>; <sup>1</sup>Institute of Psychiatry, London, UK; <sup>2</sup>Proteome Sciences plc, London, UK
- WP 487 **Phosphoproteomic Analysis of Linker Histone H1 from Growing and Starved Tetrahymena Cells;** Benjamin A. Garcia<sup>3</sup>; Swati Joshi<sup>2</sup>; C. Eric Thomas<sup>3</sup>; Raghu Chitta<sup>4</sup>; Jeffrey Shabanowitz<sup>4</sup>; Neil L. Kelleher<sup>3</sup>; Craig A. Mizzen<sup>3</sup>; C. David Allis<sup>2</sup>; Donald F. Hunt<sup>4</sup>; <sup>1</sup>Institute of Genomic Biology, Urbana, IL; <sup>2</sup>Rockefeller University, New York, NY; <sup>3</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>4</sup>University of Virginia, Charlottesville, VA

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- WP 488 **Detection of Phosphopeptide-Metal Ion Complexes by MALDI-MS;** Wolfgang H. Fischer<sup>1</sup>; Jessica D. Read<sup>1</sup>; <sup>1</sup>The Salk Institute, La Jolla, CA
- WP 489 **Combined Enzymatic and Data Mining Approaches for Comprehensive Phosphoproteome Analyses in sub-Cellular Protein Extracts of Macrophages;** Maria Marcantonio<sup>1</sup>; Matthias Trost<sup>3</sup>; Michel Desjardins<sup>3</sup>; Pierre Thibault<sup>2</sup>; <sup>1</sup>Department of Biochemistry, Université de Montréal, Montreal, Canada; <sup>2</sup>Institute for Research in Immunology and Cancer, Montreal, Canada; <sup>3</sup>Dept. of Pathol. and Cell Biol., Univ. of Montreal, Montreal, Canada
- WP 490 **Identification of Direct Binding Partners and Phosphorylation of Serum Response Factor during Myoblast Cell Differentiation using nano-LC-MS/MS and MALDI-TOF-TOF;** Zhe Zhang<sup>1</sup>; Xueyin Huang<sup>2</sup>; Emanuel Schreiber<sup>3</sup>; Balasubramani Manimalha<sup>3</sup>; Wen Yan<sup>2</sup>; Billy W Day<sup>1</sup>; Jorge L Sepulveda<sup>2</sup>; <sup>1</sup>Dep. of Pharmaceutical Science, U of Pittsburgh, Pittsburgh, PA; <sup>2</sup>Department of Pathology, U of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Genomics and Proteomics Core Laboratory, Pittsburgh, PA
- WP 491 **Phosphorylation of the Cardiac Contractile Apparatus by PKC- $\beta$ 2 Evaluated by Stable Isotope Labeling;** Jennifer E. Grant<sup>1</sup>; Martha M. Vestling<sup>2</sup>; Jeffery W. Walker<sup>1</sup>; <sup>1</sup>University of Wisconsin Medical School, Madison, WI; <sup>2</sup>University of Wisconsin Department of Chemistry, Madison, WI
- WP 492 **Structural Characterization and Identification of Post-Translational Modifications of Human eIF3 Protein Complex by Nano-LC-LTQ-FTMS;** Eugen Damoc<sup>1</sup>; Christopher S. Fraser<sup>2</sup>; Elena Catalina Damoc<sup>1</sup>; Jennifer A. Doudna<sup>2</sup>; Julie A. Leary<sup>1</sup>; <sup>1</sup>Genome Center, University of California, Davis, CA; <sup>2</sup>University of California, Berkeley, CA
- WP 493 **Identification of Post-Translational Modifications on Heterochromatin Protein 1 by LC-MS/MS;** Hillary A. 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
- WP 494 **Metal Nanoparticle based Polymer Monolithic Columns Dedicated to the Specific Trapping of Phosphopeptides;** Séverine Le Gac<sup>1</sup>; François Dupire<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- WP 495 **Chemical Approaches for the Identification and Quantitative Analysis of Protein Phosphorylation by Mass Spectrometry;** Eileen M. Woo<sup>1</sup>; Hironori Funabiki<sup>1</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>Rockefeller University, New York, NY
- WP 496 **Optimizing Isolation and Mass Spectrometric Analysis of Phosphopeptides by Microfractionation on Bruker PAC-MALDI Target Plates;** Roland D. Türk<sup>1</sup>; Dietbert Neumann<sup>1</sup>; Helene Rechsteiner<sup>2</sup>; Theo Wallimann<sup>1</sup>; René A. Brunisholz<sup>2</sup>; <sup>1</sup>Institute Cell Biology, ETH-Hönggerberg, Zürich, Switzerland; <sup>2</sup>FGCZ, ETHZ, Switzerland
- WP 497 **Identification of Phosphorylation Sites on Murine  $\beta$ 2PIX-a Protein using Fe(III) IMAC Enrichment and RP-HPLC-MS/MS Analysis;** Erin D. Jeffery<sup>1</sup>; Mark W. Mayhew<sup>1</sup>; Joy M. Polefrone<sup>1</sup>; Alan F. Horwitz<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA

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- WP 498 **Determination of the Phosphorylation Sites in Non-Structural Protein 5A of Hepatitis C Virus by FTICR Mass Spectrometry;** Oleg N. Kharybin<sup>1</sup>; Alexander V. Ivanov<sup>3</sup>; Eugene N. Nikolaev<sup>2</sup>; <sup>1</sup>The Institute for Biomedical Chemistry, Moscow, Russia; <sup>2</sup>The Institute for Energy Probl. Chem.Physics, Moscow, Russia; <sup>3</sup>Engelhardt Institute of Molecular Biology, Moscow, Russia
- WP 499 **A Sensitive Method For Detecting Phosphorylated Tyrosines On a Linear Ion Trap Using Pseudo-MS3;** Mark Szewc<sup>1</sup>; Scott Peterman<sup>1</sup>; Kevin McHale<sup>1</sup>; Tonya Pekar<sup>1</sup>; <sup>1</sup>Thermo Electron, Somerset, NJ

## PROTEIN CONFORMATION II

- WP 500 **Exploring the Domain Structure and DNA Binding Regions of b Protein from Bacteriophage I by Mass Spectrometry;** Zengru Wu<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- WP 501 **Disulfide Bond Confirmation of a Humanized anti-C5 Complement Monoclonal Antibody and its Single Chain Homolog by Peptide Mapping;** Bruce A. Andrien Jr.<sup>1</sup>; Rekha Patel<sup>1</sup>; Adam W. Lucka<sup>1</sup>; <sup>1</sup>Alexion Pharmaceuticals Inc., Cheshire, CT
- WP 502 **Ion Mobility as a Tool for Determining Prion Conformations and Diagnosing Mad Cow Disease;** Megan Grabenauer<sup>1</sup>; Thomas Wytenbach<sup>1</sup>; Susan Slade<sup>2</sup>; Teresa Pinheiro<sup>2</sup>; James Scrivens<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
- WP 503 **Assessing Conformational Heterogeneity of Natively Unstructured Proteins with ESI MS;** Agva K. Frimpong<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, Massachusetts
- WP 504 **Nitration of Tyrosine Residues in Different Isoforms of the Prion Protein;** Holly D. Cox<sup>1</sup>; Chris W. Lennon<sup>1</sup>; Scott P. Hennelly<sup>1</sup>; Michele A. McGuirl<sup>1</sup>; <sup>1</sup>University of Montana, Missoula, MT
- WP 505 **Using Electrospray Ionization Mass Spectrometry to Study the Stoichiometry and Surface Areas of Amyloid Aggregates of Beta-2-Microglobulin;** Kwasi Antwi<sup>1</sup>; Kevin R. Anderson<sup>1</sup>; R. Srikanth<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA
- WP 506 **Conformation of (Bio)Molecules in the Gas Phase Studied by Fluorescence Resonance Energy Transfer;** Maxim Dashtiev<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>Swiss Federal Institute of Technology, ETH, Zurich, Switzerland
- WP 507 **Probing Conformations of Large Proteins by FAIMS: A New Characterization Method Based on Direction-Specific Ion Mobilities?;** Alexandre A. Shvartsburg<sup>1</sup>; Tadeusz Bryskiewicz<sup>2</sup>; Randy Purves<sup>2</sup>; Luyi Ding<sup>2</sup>; David A. Barnett<sup>2</sup>; Barbara Ells<sup>2</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; Roger Guevremont<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Ionalytics/Thermo Electron Corporation, Ottawa, Canada
- WP 508 **Limited Proteolysis and Matrix-Assisted Desorption/Ionization Mass Spectrometry for the Interpretation of Ribosomal Protein Topography;** Daisy M. Hamburg<sup>1</sup>; Moo-Jin Suh<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 509 **Dose-Dependent Protein Oxidative Surface Mapping: A Novel Method for Monitoring Protein Conformational Change Due to Oxidative Damage;** Joshua S. Sharp<sup>1</sup>; Daniel M. Sullivan<sup>2</sup>; John Cavanagh<sup>2</sup>; Kenneth B. Tomer<sup>1</sup>; <sup>1</sup>NIEHS, Research Triangle Park, NC; <sup>2</sup>North Carolina State University, Raleigh, NC

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- WP 510 **Quantitative Investigation of the Stability and Conformational Change of Protein by Laser Spray Mass Spectrometry;** Xiangguo Shi<sup>1</sup>; Atsushi Takamizawa<sup>2</sup>; Yoshifumi Nishimura<sup>1</sup>; Kenzo Hiraoka<sup>2</sup>; Satoko Akashi<sup>1</sup>; <sup>1</sup>*Yokohama City University, Yokohama, Japan*; <sup>2</sup>*University of Yamanashi, Kofu, Japan*
- WP 511 **Segmental Charge Distributions of Cytochrome c on Transfer into the Gas Phase;** Kathrin Breuker<sup>1</sup>; <sup>1</sup>*University of Innsbruck, Innsbruck, Austria*
- WP 512 **Disulfide Linked Portal Region of CRABP I, Study of the Protein and its Interaction with RAR by Mass Spectrometry;** Virginie Sjoelund<sup>1</sup>; Igor Kaltashov<sup>1</sup>; <sup>1</sup>*University of Massachusetts Amherst, Amherst, MA*
- WP 513 **Protein Surface Mapping Using Peroxynitrite and Mass Spectrometry;** Mark R. Olbris<sup>1</sup>; Angela M. Fahey<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*
- WP 514 **Topologically Informative Residues of Large Proteins Can Be Marked by Photochemical Oxidation and Mapped by Mass Spectrometry;** Carlee McClintock<sup>1</sup>; Robert L. Hettich<sup>2</sup>; <sup>1</sup>*University of Tennessee, Knoxville, TN*; <sup>2</sup>*Oak Ridge National Lab, Oak Ridge, TN*
- WP 515 **Photoaffinity Labeling of P450Cam by an Imidazole-tethered Benzophenone Probe;** Michael J Trnka<sup>1</sup>; Catalin E Doneanu<sup>2</sup>; William F Tragger<sup>2</sup>; <sup>1</sup>*University of California, San Francisco, CA*; <sup>2</sup>*University of Washington, Seattle, WA*
- WP 516 **Human Amelogenin Degradation by MMP-20 in Tooth Enamel Development Studied by SDS PAGE, MALDI TOF MS and LC MS/MS;** Wu Li<sup>1</sup>; Sarah Robinson<sup>1</sup>; Stefan Habelitz<sup>1</sup>; Thuan Le<sup>1</sup>; Li Zhu<sup>1</sup>; Shengwu Wang<sup>1</sup>; Kotaro Tanimoto<sup>1</sup>; Venu Varanasi<sup>1</sup>; Markus Hardt<sup>1</sup>; Steven Hall<sup>1</sup>; Pamela DenBesten<sup>1</sup>; H. Ewa Witkowska<sup>1</sup>; <sup>1</sup>*UCSF, San Francisco, CA*

## BIOINFORMATICS III

- WP 517 **RAAMS: An Algorithm for Automatically Interpreting Mass Spectra of <sup>18</sup>O Labeled Isotopic Clusters;** Christopher J Mason<sup>1</sup>; Jeanette E Eckel-Passow<sup>1</sup>; Kenneth L Johnson<sup>1</sup>; Terry M Therneau<sup>1</sup>; Ann L Oberg<sup>1</sup>; David C Muddiman<sup>2</sup>; H Robert Bergen, III<sup>1</sup>; <sup>1</sup>*Mayo Clinic College of Medicine, Rochester, MN*; <sup>2</sup>*North Carolina State University, Raleigh, NC*
- WP 518 Moved to poster 578
- WP 519 **A Fisher Ratio Algorithm for Third Order Separation Instrumentation Data to Identify Significant Chemical Components when Differentiating Complex Samples;** Karisa M. Pierce<sup>1</sup>; Jamin C. Hoggard<sup>1</sup>; Janiece L. Hope<sup>1</sup>; Petrie M. Rainey<sup>1</sup>; Andrew N. Hoofnagle<sup>1</sup>; Rhona M. Jack<sup>2</sup>; Bob W. Wright<sup>3</sup>; Robert E. Synovec<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Children's Hospital Regional Medical Center, Seattle, WA*; <sup>3</sup>*Pacific Northwest National Laboratory, Richland, WA*
- WP 520 **Accidental Data Independent Collision Induced Dissociation on the LTQFT;** Shawna M. Hengel<sup>1</sup>; Scott Shaffer<sup>1</sup>; Gregory Taylor<sup>1</sup>; Alex Scherl<sup>1</sup>; Alexandre Masselot<sup>2</sup>; Pierre-Alain Binz<sup>2</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*GeneBio, Geneva, Switzerland*
- WP 521 **Sub-ppm Mass Accuracy and Improved Peptide Identification from FTMS;** Rob Grothe<sup>1</sup>; Darren Kessner<sup>1</sup>; Jon Katz<sup>1</sup>; David Agus<sup>1</sup>; Parag Mallick<sup>1</sup>; <sup>1</sup>*Cedars-Sinai Medical Center, Los Angeles, CA*
- WP 522 **Annotation of the Yeast Proteome with PeptideAtlas;** Nichole L. King<sup>1</sup>; Eric W. Deutsch<sup>1</sup>; Jimmy Eng<sup>1</sup>; Jeff Ranish<sup>1</sup>; Brian Raught<sup>4</sup>; James Edde<sup>1</sup>; Alexey I.

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- Nesvizhskii<sup>5</sup>; Parag Mallick<sup>6</sup>; Daniel B. Martin<sup>1</sup>; Mark Flory<sup>7</sup>; Hookeun Lee<sup>3</sup>; Henry Lam<sup>1</sup>; Ruedi Aebersold<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>*Swiss Federal Institute of Technology, ETH, Zurich, Switzerland*; <sup>4</sup>*University of Toronto, Toronto, Canada*; <sup>5</sup>*University of Michigan Medical School, Ann Arbor, MI*; <sup>6</sup>*Cedars-Sinai Medical Center, Los Angeles, CA*; <sup>7</sup>*Wesleyan University, Middletown, CT*
- WP 523 **A Cyber Infrastructure for Biomarker Discovery in Mass Spectrometry-Based Proteomics;** Xiang Zhang<sup>1</sup>; Seza Orcun<sup>1</sup>; Shrinivas Jandhyala<sup>1</sup>; Mourad Ouzzani<sup>1</sup>; Ivan Baxter<sup>1</sup>; David E Salt<sup>1</sup>; Ahmed Elmagarmid<sup>1</sup>; Fred E Regnier<sup>1</sup>; V Jo Davison<sup>1</sup>; Joseph Pekny<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- WP 524 **Quantified Peptide Signal in MALDI-TOF Data;** Timothy Randolph<sup>1</sup>; Bree Mitchell<sup>1</sup>; Dale McLerran<sup>2</sup>; Paul Lampe<sup>2</sup>; Ziding Feng<sup>2</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*
- WP 525 **Using Data Self-Calibration and Accurate Mass Fingerprint Searching To Enhance Proteomics Identifications within Complex Mixtures;** Ryan M. Danell<sup>1</sup>; Cameron O. Scarlett<sup>2</sup>; Severine A. Patat<sup>2</sup>; J. Paul Speir<sup>3</sup>; Christoph H. Borchers<sup>2</sup>; <sup>1</sup>*Danell Consulting, Greenville, NC*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*; <sup>3</sup>*Bruker Daltonics, Billerica, MA*
- WP 526 **BioLCCC-MS/MS Tools: a Comprehensive Approach to Sequence Dependent Retention Time Prediction;** Irina A. Tarasova<sup>1</sup>; Alexander V. Gorshkov<sup>2</sup>; Victor V. Evreinov<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, Russia*; <sup>2</sup>*Institute of Chemical Physics, Moscow, Russia*; <sup>3</sup>*Biological and Medical Center, Uppsala University, Uppsala, Sweden*
- WP 527 **Robust, Quantitative Comparison of Features from Multiple Mass Spectra;** Daniel Fasulo<sup>1</sup>; Anne-Katrin Emde<sup>1</sup>; <sup>1</sup>*Siemens Corporate Research, Princeton, NJ*
- WP 528 **Rapid Microorganism Identification Database (RMIDB);** Nathan J. Edwards<sup>1</sup>; Fernando Pineda<sup>2</sup>; <sup>1</sup>*University of Maryland, College Park, MD*; <sup>2</sup>*Johns Hopkins Bloomberg School of Public Health, Baltimore, MD*
- WP 529 **NeuroPred: A Tool for Predicting Neuropeptides from Prohormones;** Andinet Amare<sup>1</sup>; Bruce R. Southey<sup>1</sup>; Amanda B. Hummon<sup>1</sup>; Tyler A. Zimmerman<sup>1</sup>; Sandra L. Rodriguez-Zas<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois at Urbana-Champaign, Urbana, IL*
- WP 530 **SpectraST: An Open-Source MS/MS Spectra-Matching Library Search Tool for Targeted Proteomics;** Henry Lam<sup>1</sup>; Eric Deutsch<sup>1</sup>; James Edde<sup>1</sup>; Jimmy Eng<sup>1</sup>; Nichole King<sup>1</sup>; Sara Yang<sup>2</sup>; Jeri Roth<sup>2</sup>; Lisa Kilpatrick<sup>2</sup>; Pedatsur Neta<sup>2</sup>; Steve Stein<sup>2</sup>; Ruedi Aebersold<sup>1</sup>; <sup>1</sup>*Institute for Systems Biology, Seattle, WA*; <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 531 **Combined LC-MS and LC-MS/MS Inferential Framework for Reliable and Reproducible Discovery of Candidate Biomarkers;** O. Vitek<sup>1</sup>; A. S. Garbutt<sup>1</sup>; J. S. Edde<sup>1</sup>; Daniel B. Martin<sup>1</sup>; R. Aebersold<sup>1</sup>; <sup>1</sup>*Institute for Systems Biology, Seattle, WA*
- WP 532 **The Hidden Dimension of Peptide Mass Spectra - Identification of Characteristic Mass Shifts by Correlation Analysis;** Michael D. Hoffman<sup>1</sup>; Matthew J.

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- Sniatynski<sup>1</sup>; Jason C. Rogalski<sup>1</sup>; Juergen Kast<sup>1</sup>;  
<sup>1</sup>University of British Columbia, Vancouver, BC
- WP 533 **SMART (Search by MAss and Retention Time) - A New Tool for HPLC-MALDI MS Peptide Mass Fingerprinting**; Oleg V. Krokhin<sup>1</sup>; Vic Spicer<sup>1</sup>; Kenneth G. Standing<sup>1</sup>; John A. Wilkins<sup>1</sup>; Werner Ens<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada
- WP 534 **MassSense, a New Software for Peptide Detection and Segmentation of Unlabeled Peptide Ions in Comparative Proteome Analyses**; Gagandeep Jaitly<sup>1</sup>; Navdeep Jaitly<sup>2</sup>; Eric Bonneau<sup>1</sup>; Mihaela Ghitun<sup>1</sup>; Christelle Pomies<sup>1</sup>; Marie-Helene Fortier<sup>1</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>IRIC-Universite de Montreal, Montreal, QC; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- WP 535 **A Novel Method for Model-Based Feature Extraction in Mass Spectra**; Karin Noy<sup>2</sup>; Daniel Fasulo<sup>1</sup>; <sup>1</sup>Siemens Corporate Research, Princeton, NJ; <sup>2</sup>Ben Gurion University of the Negev, Beer-Sheva, Israel
- WP 536 **Novel Method for Detection of Low Abundant Peaks**; Grzegorz M Boratyn<sup>1</sup>; Michael Merchant<sup>1</sup>; Jon B Klein<sup>2</sup>; <sup>1</sup>University of Louisville, Louisville, KY; <sup>2</sup>Veterans Administration Medical Center, Louisville, KY
- WP 537 **An Analysis of Search Strategies with the Paragon<sup>TM</sup> Algorithm**; Ignat Shilov<sup>1</sup>; Sean Seymour<sup>1</sup>; Alpesh Patel<sup>1</sup>; Sean Keating<sup>1</sup>; Alex Loboda<sup>1</sup>; Christie Hunter<sup>1</sup>; Daniel Schaeffer<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA
- WP 538 **Reanalysis of Unassigned High Quality Spectra from Published Datasets Can Provide Biologically Interesting New Insights**; Alexey I. Nesvizhskii<sup>1</sup>; James S. Eddes<sup>2</sup>; Ruedi Aebersold<sup>3</sup>; <sup>1</sup>University of Michigan Medical School, Ann Arbor, MI; <sup>2</sup>Institute for Systems Biology, Seattle, WA; <sup>3</sup>Swiss Federal Institute of Technology, Zurich, Switzerland
- WP 539 **PEAKS-Q: Software for MS-based Quantitative Proteomics**; Weijie Yang<sup>2</sup>; Weiwu Chen<sup>1</sup>; Iain Rogers<sup>1</sup>; Sean Bendall<sup>2</sup>; Derek Smith<sup>3</sup>; Bin Ma<sup>2</sup>; Gilles Lajoie<sup>2</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, ON; <sup>2</sup>University of Western Ontario, London, ON; <sup>3</sup>University of Victoria Proteomics Centre, Victoria, BC
- WP 540 **Combining MALDI-FTMS and Biostatistics to Identify Biomarkers of Prion Diseases**; Joshua J. Schmidt<sup>1</sup>; Allen Herbst<sup>2</sup>; Sean McIlwain<sup>3</sup>; David Page<sup>3</sup>; Judd Aiken<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin, Madison, WI; <sup>2</sup>Animal Health and Biomedical Sciences, U. of WI, Madison, WI; <sup>3</sup>Department of Statistics, U. of Wisconsin, Madison, WI
- WP 541 **A Reference Library of Peptide Ion Fragmentation Spectra: Yeast**; Steve Stein<sup>1</sup>; Lisa Kilpatrick<sup>2</sup>; Pedatsur Neta<sup>1</sup>; Jeri Roth<sup>1</sup>; Xiaoyu (Sara) Yang<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>NIST-HML, Charleston, SC
- WP 542 **The Use of TOF-MS and Chemometrics to Discriminate Organically and Conventionally Grown Grapefruit**; Pei Chen<sup>1</sup>; Gene E Lester<sup>2</sup>; McAuley Brandon<sup>1</sup>; Meyer Robert<sup>2</sup>; Harnly James<sup>1</sup>; <sup>1</sup>USDA, Beltsville Human Nutrition Research Center, Beltsville, MD; <sup>2</sup>USDA, Agricultural Research Service, Weslaco, TX
- WP 543 **ProRata: a Software Package with Improved Point and Interval Estimation of Protein Abundance Ratio for Quantitative Shotgun Proteomics**; Nagiza F Samatova<sup>1</sup>; Chongle Pan<sup>1</sup>; Guruprasad Kora<sup>1</sup>; David Tabb<sup>1</sup>; W. Hayes McDonald<sup>1</sup>; Dale Pelletier<sup>1</sup>; Greg Hurst<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- WP 544 **Evaluation of Mass Spectrometry-Based Identification of Plant Proteins with Different Existing Sequence Databases and a New Non-Redundant Compiled**

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- Database**; Kris Laukens<sup>1</sup>; Filip Lemièr<sup>1</sup>; Eric Bonnet<sup>2</sup>; Eddy L. Esmans<sup>1</sup>; Harry A. Van Onckelen<sup>1</sup>; Geert De Jaeger<sup>2</sup>; Erwin J. Witters<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium; <sup>2</sup>Ghent University, Ghent, Belgium
- WP 545 **How Much Data is Lost and How Do We Check?: Pushing the Limits of Data Preprocessing by Weighting Different Converters**; Ali Alkaabi<sup>1</sup>; Christian Panse<sup>1</sup>; Bernd Roschitzki<sup>1</sup>; Frank Potthast<sup>1</sup>; Ralph Schlapbach<sup>1</sup>; Bertran Gerrits<sup>1</sup>; <sup>1</sup>Functional Genomics Center Zurich, Uni/ETH Zurich, Zurich, Switzerland
- WP 546 **Selection of Protein Database for DB Searches as a Crucial Factor in Large Scale Proteomics Comparison Studies**; Michael Andersen<sup>1</sup>; Soeren Schandorff<sup>1</sup>; Hans Jespersen<sup>1</sup>; Ole Vorm<sup>1</sup>; Alexandre Podtelebnikov<sup>1</sup>; <sup>1</sup>Proxeon, Odense, Denmark
- WP 547 **An Innovative Approach to Quality Assessment of Tandem Mass Spectra**; Seungjin Na<sup>1</sup>; Eunok Paek<sup>1</sup>; <sup>1</sup>University of Seoul, Seoul, Korea
- WP 548 **The Plastid Proteomics Data Base; an Integrative Proteomics Data Base for Plastid Proteomes of Arabidopsis Thaliana and Maize**; Qi Sun<sup>1</sup>; Andrea Rudella<sup>1</sup>; Giulia Friso<sup>1</sup>; Wojciech Majeran<sup>1</sup>; Jimmy Ytterberg<sup>1</sup>; Lisa Giacomelli<sup>1</sup>; Jie An<sup>1</sup>; Heidi Rutschow<sup>1</sup>; klaas van Wijk<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY

## PROTEOMICS: BIOMARKERS

- WP 549 **Protein Marker and Antibody Characterization by Top-down Quadrupole-Fourier Transform Mass Spectrometry Analysis**; Shaun M. McLoughlin<sup>1</sup>; Scott E. Warder<sup>1</sup>; Richard D. Burton<sup>1</sup>; Laura J. Miesbauer<sup>1</sup>; Joseph L. Meuth<sup>1</sup>; Tamara J. Streltzer<sup>1</sup>; Robert W. Johnson<sup>1</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
- WP 550 **Dietary Biomarkers can be Detected by MALDI-TOF in a Dose-Dependent Manner and Across Different Study Populations**; Heather Ann Brauer<sup>1</sup>; Yutaka Yasui<sup>2</sup>; Johanna W. Lampe<sup>1</sup>; Paul D. Lampe<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>University of Alberta, Edmonton, Edmonton, Canada
- WP 551 **Differential Proteomic Analysis of Protein Expression and Localization During Osteoclastogenesis**; Cornelia Czupalla<sup>1</sup>; Eberhard Krause<sup>2</sup>; Theresia Pursche<sup>1</sup>; Bernard Hoflack<sup>1</sup>; <sup>1</sup>Biotechnological Center, University of Technology, Dresden, Germany; <sup>2</sup>Institute of Molecular Pharmacology, Berlin, Germany
- WP 552 **Direct Maldi (Dt-Maldi) Identification of Histone 2a2, Tubulin β-2 Chain, Myelin Basic Protein in Human and Murine Cells And Tissues**; P H Pevsner<sup>1</sup>; F Naftolin<sup>1</sup>; D Hillman<sup>1</sup>; Joseph P Fox<sup>1</sup>; BK Stall<sup>1</sup>; DC Miller<sup>1</sup>; D Keegan<sup>1</sup>; E Newcomb<sup>1</sup>; A Fadiel<sup>2</sup>; S Wishnie<sup>3</sup>; F Licciardi<sup>1</sup>; J Grifo<sup>1</sup>; A Stern<sup>1</sup>; H Samuels<sup>1</sup>; <sup>1</sup>NYU, New York, NY; <sup>2</sup>Yale, New Haven, CT; <sup>3</sup>Shimadzu, Columbia, MD
- WP 553 **Proteomic Biomarker Discovery Associated with the JNK Pathway and Fibrosis**; Lilly Wong<sup>1</sup>; Dunrui Wang<sup>1</sup>; Quang Pham<sup>1</sup>; Christian R. Lombardo<sup>1</sup>; <sup>1</sup>Celgene, San Diego, CA
- WP 554 **Analysis of Extracellular Matrix Proteins Expressed during Osteoblast Differentiation by Differential Expression Profiling**; Takako Miyamoto<sup>1</sup>; Hisaaki Taniguchi<sup>1</sup>; <sup>1</sup>University of Tokushima, Tokushima, Japan
- WP 555 **Temporal Analysis of the Rat Urinary Proteome as a Window Into Kidney Maturation**; Richard Lee<sup>1</sup>; Mohini Lutchman<sup>1</sup>; Flavio Monigatti<sup>1</sup>; Bogdan Budnik<sup>1</sup>; Thomas Patterson<sup>1</sup>; Andrew Briscoe<sup>1</sup>; Zach Waldon<sup>1</sup>; Brian Hekking<sup>1</sup>; Judith Steen<sup>1</sup>; Michael Freeman<sup>1</sup>; Hanno

# WEDNESDAY POSTERS

## POSTER SPACE

- Steen<sup>1</sup>; <sup>1</sup>Children's Hospital Boston/Harvard Medical School, Boston, MA
- WP 556 **Identification of Chlamydia pneumoniae Antigens Via Immuno&Minus;Proteomics Using High Resolution FTICR Mass Spectrometry;** Iuliana Susnea<sup>1</sup>; Sebastian Bunk<sup>1</sup>; Corinna Hermann<sup>1</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>University of Konstanz, Konstanz, Germany
- WP 557 **Construction of the Proteomic Profiles on Human Kidney Cancer Tissues using the NBS Method;** Taro Masuda<sup>1</sup>; Noboru Okamura<sup>2</sup>; Kazuki Suganuma<sup>1</sup>; Hisato Tanaka<sup>2</sup>; Makoto Watanabe<sup>1</sup>; Ei-ichi Matsuo<sup>1</sup>; Susumu Tsunasawa<sup>1</sup>; Akinobu Gotoh<sup>2</sup>; Toshiro Shirakawa<sup>2</sup>; Shuji Terao<sup>2</sup>; Katsuhiko Okumura<sup>2</sup>; Osamu Nishimura<sup>1</sup>; <sup>1</sup>Life Science Laboratory, Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kobe University Graduate School of Medicine, Kobe, Japan
- WP 558 **Differential Expression of Vitreous Proteins in Proliferative Diabetic Retinopathy (PDR);** Jungeun Park<sup>1</sup>; Sang Jin Kim<sup>1</sup>; Sangmi Kim<sup>1</sup>; Hong Kyu Lee<sup>1</sup>; Kyong Soo Park<sup>1</sup>; Hyeong Gon Yu<sup>1</sup>; Youngsoo Kim<sup>1</sup>; <sup>1</sup>Seoul National University, College of Medicine, Seoul, South Korea
- WP 559 **Top Down Sequencing of Apolipoprotein A-I for the Identification of Mutations and Post-translational Modifications;** Michael J. Roth<sup>1</sup>; Baohai Shao<sup>2</sup>; Jay W. Heinecke<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois Urbana-Champaign, Urbana, IL; <sup>2</sup>University of Washington, Seattle, WA
- WP 560 **Endogenous Peptide Biomarker Quantitation in Biological Fluids using On-line Immunoaffinity LC/MS/MS on a Triple Quadrupole, AQUA+: What Happens after Discovery?;** Dawn R Dufield<sup>1</sup>; Michael Schlittler<sup>1</sup>; Mollisa Elrick<sup>1</sup>; Olga Nemirovskiy<sup>1</sup>; Kevin Duffin<sup>2</sup>; Micky Tortorella<sup>1</sup>; Anne-Marie Malfait<sup>1</sup>; Elizabeth Arner<sup>1</sup>; <sup>1</sup>Pfizer, St. Louis, MO; <sup>2</sup>Eli Lilly, Indianapolis, IN
- WP 561 **Proteomic Profile of Keratinocytes and Skin in Response to the Induction of UV-Irradiation and Chemical-Toxicant;** Shuqing Liu<sup>1</sup>; Ming-Zhong Sun<sup>1</sup>; Liming Liu<sup>1</sup>; Thomas S McComick<sup>1</sup>; Kevin D Cooper<sup>1</sup>; Mark R Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH
- WP 562 **Imaging via LA-ICP-MS: Measurement of Cancer Biomarkers;** Cameron McLeod<sup>1</sup>; J. Seuma<sup>1</sup>; J. Bunch<sup>1</sup>; A. Cox<sup>1</sup>; C. Murray<sup>2</sup>; <sup>1</sup>University of Sheffield, Sheffield, UK; <sup>2</sup>Medical Solutions, Nottingham, UK
- WP 563 **Technical Versus Biological Variations in LC-MS Analysis of Complex Biological Samples;** Sudha Rajagopalan<sup>1</sup>; Nicole Kawachi<sup>1</sup>; Peicheng Du<sup>1</sup>; Abadi Negassa<sup>1</sup>; Edward Nieves<sup>1</sup>; Ruth Angeletti<sup>1</sup>; Michael Prystowsky<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, New York, NY
- WP 564 **Early Detection of Ragwort Toxicosis: Analysis of Dehydromonocrotaline (DHM) Adducts of Proteins and Peptides;** Rowan E. Moore<sup>1</sup>; Sallyann V. Wales<sup>1</sup>; Phillip D. Whitfield<sup>1</sup>; Derek C. Knottenbelt<sup>1</sup>; Robert J. Beynon<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, UK
- WP 565 **Covalent Adducts Arising from Reaction of Cytochrome C with a Series of Lipid Hydroperoxides;** Michelle V. Williams<sup>1</sup>; John S. Wishnok<sup>1</sup>; Steven R. Tannenbaum<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology, Cambridge, MA
- WP 566 **2D/MS Proteomic Study for the Discovery of New Biomarkers Candidates of Colorectal Cancer;** Richard Joubert<sup>1</sup>; Petra Prefot<sup>1</sup>; Gitte Boehm<sup>1</sup>; Juergen Schaefer<sup>1</sup>;

## POSTER SPACE

- Josef Schwarz<sup>1</sup>; <sup>1</sup>Proteome Sciences R&D GmbH & Co KG, Frankfurt, Germany
- WP 567 **Tandem Mass Spectrometry for the Identification and Detection of Fungal Plant Pathogens;** Neerav D. Padliya<sup>1</sup>; Wesley M. Garrett<sup>1</sup>; Kimberly B. Campbell<sup>1</sup>; Jian Feng<sup>2</sup>; Daniel Q. Naiman<sup>2</sup>; Bret Cooper<sup>1</sup>; <sup>1</sup>U.S. Department of Agriculture, Beltsville, MD; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- WP 568 **Differential Proteomics Analysis of Osteoarthritis and Control Synovial Fluids;** Linhong Jing<sup>1</sup>; Mary C. Charlesworth<sup>1</sup>; James T. Bronk<sup>1</sup>; Benjamin Madden<sup>1</sup>; Melinda Miller<sup>1</sup>; Linda Benson<sup>1</sup>; H. Robert Bergen, III<sup>1</sup>; Mark E. Bolander<sup>1</sup>; <sup>1</sup>Mayo Clinic College of Medicine, Rochester, MN
- WP 569 **Ambient Temperature Effects on the Drosophila Proteome: An Age-dependent Profile;** Renâ A. Sowell<sup>1</sup>; John F. Kellie<sup>1</sup>; Thomas C. Kaufman<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- WP 570 **Human Tumor Metastasis: Identification of Posttranslational Modifications Using On-line Intact Protein Molecular Mass Characterization and Tandem Mass Spectrometry;** Paweena Kreunin<sup>1</sup>; Chul Yoo<sup>1</sup>; Virginia Urquidí<sup>2</sup>; David M Lubman<sup>1</sup>; Steve Goodison<sup>2</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>University of Florida, Jacksonville, FL
- WP 571 **Reproducible Protein Markers of Osmoregulation in Mouse Kidney Cell Cultures;** Lewis M. Brown<sup>1</sup>; Christopher J. Rivard<sup>2</sup>; Juan M. Capasso<sup>2</sup>; Tomas Berl<sup>2</sup>; <sup>1</sup>U. of Colorado at Denver and Health Sciences Ctr., Aurora, CO; <sup>2</sup>U. of Colorado at Denver and Health Sciences Ctr., Denver, CO
- WP 572 **Sequential Solubilization of Proteins from Biopsies from Inclusion Body Myositis compared to Polymyositis or Normal Muscle: A Proteomic Analysis;** Ronan Walsh<sup>1</sup>; David Sarracino<sup>2</sup>; Anthony Amato<sup>1</sup>; Bryan Krastins<sup>2</sup>; Steven Greenberg<sup>1</sup>; Kenneth Parker<sup>1</sup>; <sup>1</sup>Brightman and Women's Hospital, Boston, MA; <sup>2</sup>Harvard Partners Center for Genetics & Genomics, Cambridge, MA
- WP 573 **Proteomics of a Drosophila Model of Parkinson's Disease;** Zhiyin Xun<sup>1</sup>; Renâ Sowell<sup>1</sup>; Thomas C. Kaufman<sup>1</sup>; David E. Clemmer<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN
- WP 574 **Marker Peptide Screening in Macrophages and Neutrophils by Whole Cell MALDI: Thymosin beta-4 in Macrophages;** Lakshmi Kannan<sup>1</sup>; Narayan Rath<sup>2</sup>; Rohana Liyanage<sup>3</sup>; Jackson Lay, Jr.<sup>3</sup>; <sup>1</sup>Cell & Molecular Biology/University of Arkansas, Fayetteville, AR; <sup>2</sup>United States Department of Agriculture/ARS, Fayetteville, AR; <sup>3</sup>Chemistry and Biochemistry/University Arkansas, Fayetteville, AR
- WP 575 **Differential Proteomic Analysis of Articular Cartilage Tissue from Normal and Osteoarthritic Patients;** Amanda L Bemis<sup>1</sup>; Zhiyong Yang<sup>1</sup>; Wei Liu<sup>1</sup>; Eunice Wang<sup>1</sup>; Carl Flannery<sup>1</sup>; Elisabeth Morris<sup>1</sup>; Yong C Qiu<sup>1</sup>; Jiang X Wu<sup>1</sup>; <sup>1</sup>Wyeth Research, Cambridge, MA
- WP 576 **Biomarker Studies Using the Phosphoproteome;** Thomas De Vijlder<sup>1</sup>; Kris Laukens<sup>1</sup>; Filip Lemièr<sup>1</sup>; Walter Van Dongen<sup>1</sup>; Robin Tuytten<sup>1</sup>; Eddy L. Esman<sup>1</sup>; Harry A. Van Onckelen<sup>1</sup>; Marleen Maras<sup>1</sup>; Wim De Coen<sup>1</sup>; Erwin J. Witters<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium
- WP 577 **Proteomic Analysis of High-Grade Dysplastic Cells Obtained From ThinPrep® Cervical Slides Using Laser Capture Microdissection and Mass**

**Spectrometry;** Ye Gu<sup>1</sup>; Shiaw-Lin Wu<sup>1</sup>; William Hancock<sup>1</sup>; Barry Karger<sup>1</sup>; Jane Meyer<sup>2</sup>; David Hanlon<sup>2</sup>; James Linder<sup>2</sup>; Larry Burg<sup>2</sup>; <sup>1</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>2</sup>Cytac Corporation, Marlborough, MA

# PROTEOMICS: TECHNIQUE COMPARISONS

- WP 578 **Accurate Mass Triggered MS/MS Enhances Sensitivity and Specificity for Verification of Novel Computationally Predicted Proteins;** Betty Chang<sup>1</sup>; Sarah Calvo<sup>1</sup>; David Pagliarini<sup>2</sup>; Vamsi K. Mootha<sup>3</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Center For Human Genetic Research, MGH, Boston, MA; <sup>3</sup>Department of Systems Biology, Harvard Medical Sch, Boston, MA
- WP 579 **Proteomic Comparison of Muscle Biopsies from Inclusion Body Myositis, Non-specific Myositis, and Normal Muscle;** Kenneth Parker<sup>1</sup>; Ronan Walsh<sup>1</sup>; Bryan Krastins<sup>2</sup>; Anthony Amato<sup>1</sup>; Stephen Greenberg<sup>1</sup>; David Sarracino<sup>2</sup>; <sup>1</sup>Brighman and Women's Hospital, Boston, MA; <sup>2</sup>Harvard Partners Center for Genetics & Genomics, Cambridge, MA
- WP 580 **Comparison of Bottom-Up Protein Identification Methods;** Magnus Palmblad<sup>1</sup>; Laurence V Bindschedler<sup>1</sup>; Trevor M Gibson<sup>1</sup>; Rainer K Cramer<sup>1</sup>; <sup>1</sup>The University of Reading, Reading, UK
- WP 581 **Comprehensive Analysis Luminal Plasma Membrane Proteins in Endothelium of Rat Lung in vivo;** Yan Li<sup>1</sup>; Hui-luen Huang<sup>1</sup>; Jing-yi Yu<sup>1</sup>; Eberhard Durr<sup>2</sup>; Phil Oh<sup>1</sup>; Jan Schnitzer<sup>1</sup>; <sup>1</sup>Sidney Kimmel Cancer Centre, San Diego, CA; <sup>2</sup>Merck & Co., Inc, Philadelphia, PA
- WP 582 **Analysis of Protein Mixtures by Mass Spectrometry: An Information Theory Study based on Computer Simulation;** Jian Liu<sup>1</sup>; Paul Chrisman<sup>1</sup>; David Erickson<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 583 **Increasing the Number of Identified Peptides with High Measured Mass Accuracy on CID Fragments;** Alexander Scherl<sup>1</sup>; Manhong Wu<sup>2</sup>; Scott Shaffer<sup>1</sup>; Gregory K. Taylor<sup>1</sup>; Alexandre Masselot<sup>3</sup>; Pierre-Alain Binz<sup>3</sup>; Samuel I. Miller<sup>2</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>Dpt. of Med. Chemistry, University of Washington, Seattle, WA; <sup>2</sup>Dpt. of Microbiology, University of Washington, Seattle, WA; <sup>3</sup>GeneBio SA, Geneva, Switzerland
- WP 584 **Optimizing Chemical Cleavage for LC-MS Profiling;** Joerg Karolat<sup>1</sup>; Rebecca Sutphen<sup>1</sup>; Ted Gauthier<sup>2</sup>; Richard Yip<sup>1</sup>; John Koomen<sup>1</sup>; <sup>1</sup>H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL; <sup>2</sup>University of South Florida Chemistry Department, Tampa, FL
- WP 585 **Comparison of LC-ESI MS/MS and LC-MALDI TOF/TOF Analysis of iTRAQ Labeled Complex Samples;** Leanne B Ohlund<sup>1</sup>; Darryl B Hardie<sup>1</sup>; Phil Jakubowski<sup>1</sup>; Derek S Smith<sup>1</sup>; Monica Elliott<sup>1</sup>; Axel Bergman<sup>2</sup>; Domanik Domanski<sup>1</sup>; <sup>1</sup>University of Victoria, Victoria, Canada; <sup>2</sup>iCapture Centre, Vancouver, Canada
- WP 586 **Data-Directed Versus Targeted MS/MS For Protein Identification Of Complex Proteomics Samples;** Tom A. van de Goor<sup>1</sup>; Mihaela Ghitun<sup>2</sup>; Eric Bonneil<sup>2</sup>; Pierre Thibault<sup>2</sup>; Christine Miller<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Universite de Montreal, Montreal, Canada
- WP 587 **Comparison of Protein/Peptide Analysis using Two Techniques: Nanolc MALDI MS/MS and NanoLC ESI MS/MS;** Sandra Hofmann<sup>1</sup>; Matthias Glückmann<sup>2</sup>; Jacqueline Burré<sup>1</sup>; Tobias Beckhaus<sup>1</sup>; Malte Schürken<sup>1</sup>; Herbert Zimmermann<sup>1</sup>; Walter Volknandt<sup>1</sup>; Michael

Karas<sup>1</sup>; <sup>1</sup>J.W. Goethe University, Frankfurt am Main, Germany; <sup>2</sup>Applied Biosystems, Darmstadt, Germany

- WP 588 **Benchmarking the Performance of a New Search Algorithm;** Lauren K. Mansfield<sup>1</sup>; Alpesh A. Patel<sup>1</sup>; Sean L. Seymour<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA
- WP 589 **Proteome vs. Transcriptome: Comparisons between Microarray Data and Proteomics Data for the Organism *Yersinia pestis*;** Kim K. Hixson<sup>1</sup>; Mary S. Lipton<sup>2</sup>; Harold R. Udseth<sup>1</sup>; Sandra McCutchen-Maloney<sup>3</sup>; <sup>1</sup>Environmental Molecular Sciences Laboratory/PNNL, Richland, WA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Lawrence Livermore National Laboratory, Livermore, CA
- WP 590 **Investigation of LC-MALDI Matrix Spotting for Improved TOF/TOF Analysis by Combined Spotting and Acquisition Strategies;** Darryl Hardie<sup>1</sup>; Philip Jakubowski<sup>1</sup>; Angela Jackson<sup>1</sup>; Leanne Ohlund<sup>1</sup>; <sup>1</sup>UVic Genome B.C. Proteomics Centre, Victoria, Canada
- WP 591 **Complimentary Techniques for Protein Separation and Identification by MS in Animal Models of Heart Failure;** Irina Neverova<sup>1</sup>; Jennifer E. Van Eyk<sup>2</sup>; <sup>1</sup>Queen's University, Kingston, Ontario, Canada; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- WP 592 **Enhanced Nano electrospray Ionization Efficiencies and Increased Peptide Coverage through Optimal Solvent Selection;** Thomas N. Corso; Colleen K. Van Pelt; Jie Li; A. Celeste Ptak; Jack Henion; Advion BioSystems, Inc., Ithaca, NY
- WP 593 **Quantitative Evaluation of Product Ion Abundances from the Top-down and Bottom-up Dissociation of *S. aureus* and *E. coli* Dihydroneopterin Aldolase;** Gwynyth Scherperel<sup>1</sup>; Katherine Rank<sup>1</sup>; Gavin E. Reid<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- WP 594 **Combined Power of High-Throughput MALDI-TOF/TOF and Sensitive Nano-LC-MS/MS Analyses in Protein Identification For 2D Gel Separated Samples;** Sabine Baumgart<sup>1</sup>; Robert W. Sherwood<sup>1</sup>; Sheng Zhang<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY
- WP 595 **Flagellar Protein Identification: Nano-LC MALDI-FTMS Versus Automated Nano-LC On-Chip ESI-FTMS;** Sarah R. Hart<sup>1</sup>; Stephen C.C. Wong<sup>1</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>The University of Manchester, Manchester, UK
- WP 596 **Comparative Methods for Native Serum Peptides Analysis by an oMALDI QqTOF Mass Spectrometer;** Chris Lock<sup>1</sup>; Suzanne Ackloo<sup>1</sup>; Ken Evans<sup>2</sup>; John Marshall<sup>3</sup>; <sup>1</sup>MDS Sciex, Concord, Canada; <sup>2</sup>Ontario Cancer Research Network, MaRS, Toronto, Canada; <sup>3</sup>Ryerson University, Toronto, Canada
- WP 597 **Forbidden Zones in Proteomics and its Ramifications and Possibilities for Analysis of Complex Protein Mixtures;** Jennifer L. Frahm<sup>1</sup>; Brian E. Howard<sup>1</sup>; Steffen Heber<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC
- WP 598 **Investigation of Multi-Dimensional Chromatography Coupled with Mass Spectrometry for the 2D Prefractionation of Intact Proteins from Complex Matrices;** Andy D. Mahan<sup>1</sup>; John A. Masucci<sup>1</sup>; Bill J. Jones<sup>1</sup>; Gary W. Caldwell<sup>1</sup>; <sup>1</sup>Johnson and Johnson Pharmaceutical R&D LLC, Spring House, PA
- WP 599 **Comparison of Protein Identification by Two-Dimensional Liquid Chromatography Mass Spectrometry Using pH or Salt Elution;** Hu Zhou<sup>1</sup>; Qing-Run Li<sup>1</sup>; Jie Dai<sup>1</sup>; Rong Zeng<sup>1</sup>; <sup>1</sup>Shanghai Institutes for Biological Sciences, Shanghai, China

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- WP 600 **Shotgun Proteomic Analysis of *Streptomyces scabies* by Quadrupole Linear Ion Trap Mass Spectrometry Using Three Prefractionation Methods;** Sheng Zhang<sup>1</sup>; David Schneider<sup>2</sup>; Madhumita Joshi<sup>3</sup>; Robert Sherwood<sup>1</sup>; Rosemary Loria<sup>3</sup>; <sup>1</sup>Proteomics Core Facility, Cornell University, Ithaca, NY; <sup>2</sup>US Plant Soil and Nutrition Laboratory, Ithaca, NY; <sup>3</sup>Plant Pathology, Cornell University, Ithaca, NY
- WP 601 **Multi-Platform Proteomic Study of Human Follicular Fluid;** Georgia Dolios<sup>1</sup>; Martha Luna<sup>2</sup>; Alan Copperman<sup>2</sup>; Rong Wang<sup>1</sup>; <sup>1</sup>Mount Sinai School of Medicine, New York, NY; <sup>2</sup>Reproductive Medicine Associate of New York, New York, NY
- WP 602 **Gel- and Gas-Phase Enhanced Tandem MS Analyses Applied to Organellar Proteomics;** Sebastian Wiese<sup>1</sup>; Thomas Gronemeyer<sup>1</sup>; Rob Ofman<sup>2</sup>; Ronald Wanders<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Bettina Warscheid<sup>1</sup>; <sup>1</sup>Medical Proteom-Center, Ruhr-University Bochum, Bochum, Germany; <sup>2</sup>University of Amsterdam, Amsterdam, Netherlands
- WP 603 **Comparison of Proteomic Methods for Tear Profiling;** Kari B. Green-Church<sup>1</sup>; Kelly K. Nichols<sup>1</sup>; Ronelito J. Perez<sup>1</sup>; Bryan M. Ham<sup>1</sup>; Nan M. Kleinholz<sup>1</sup>; Rhonda L. Pitsch<sup>2</sup>; Jason J. Nichols<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Henry M. Jackson Found. for the Adv. of Mil. Med., Dayton, OH
- WP 604 **Data-Dependent Electron Capture Dissociation (ECD) for the Characterisation of Signalling Proteins;** Helen J. Cooper<sup>1</sup>; Andrew J. Creese<sup>1</sup>; John K. Heath<sup>1</sup>; Robert H. Insall<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK
- WP 605 **Comparative Analysis of Protein Identification Data from Direct LC-MS/MS and 1D-SDS-PAGE-LC-MS/MS on ING1 Co-Immunoprecipitate;** Morgan F. Hughes<sup>1</sup>; Michael W. Russell<sup>1</sup>; Karl T. Riabowol<sup>1</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, Canada
- WP 606 **Label-free Quantitative Proteomics: Understanding the Role of Chromatographic Separation to Overall Information Content by High Resolving Power FTMS;** Matthew T. Mazur<sup>1</sup>; Fanyu Meng<sup>1</sup>; Yi Du<sup>1</sup>; Ekaterina G. Deyanova<sup>1</sup>; Weixun Wang<sup>1</sup>; Nathan A. Yates<sup>1</sup>; Ronald C. Hendrickson<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, Rahway, NJ

## PROTEOMICS: SAMPLE PREPARATION III

- WP 607 **A rapid MALDI/TOF Procedure for the Analysis of Intact Hydrophobic Proteins;** Mahbod Hajivandi<sup>1</sup>; Mike Blanton<sup>2</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>Invitrogen, Carlsbad, California; <sup>2</sup>TTHSC, Lubock, Texas
- WP 608 **Efficient Trypsin, ArgC- and LysC-Like Digestion Procedures, Exploiting One Enzyme and Chemical Modifications to Facilitate Protein Characterization and Identification;** Tsetska Takova<sup>2</sup>; Sven Andrecht<sup>1</sup>; Anja Seiler<sup>1</sup>; Robertus Hendriks<sup>1</sup>; <sup>1</sup>Merck KGaA, Darmstadt, Germany; <sup>2</sup>EMD Biosciences, Inc., Madison, WI
- WP 609 **A Comparison of Three Sample Preparation Methods for a Mass Spectrometry Based Assay for Cardiac Troponin T in Rat Plasma;** Van M. Hoang<sup>1</sup>; Caroline K. Ferraro<sup>1</sup>; Frank D. Sistare<sup>1</sup>; William H. Schaefer<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA
- WP 610 **C-Terminal Charge-Tagging of Proteins for the Sequencing with MALDI-MS;** Takashi Nakazawa<sup>1</sup>; Minoru Yamaguchi<sup>2</sup>; Kimiko Nishida<sup>1</sup>; Mutsumi Oka<sup>1</sup>; Ayako Hamazaki<sup>1</sup>; Hiroki Kuyama<sup>2</sup>; Eiji Ando<sup>2</sup>; Taka-aki Okamura<sup>3</sup>; Norikazu Ueyama<sup>3</sup>; Shigemi Norioka<sup>3</sup>; Susumu Tsunasawa<sup>2</sup>; <sup>1</sup>Nara Women's University, Nara,

## POSTER SPACE

- Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Osaka University, Osaka, Japan
- WP 611 **A Combined Solid Phase Extraction LCMS Approach for Identification of Peptides in Meat;** Meelis Tikk<sup>1</sup>; Caroline Nebel<sup>1</sup>; Henrik J. Andersen<sup>1</sup>; <sup>1</sup>Danish Institute of Agricultural Sciences, Tjele, Denmark
- WP 612 **Direct Desorption of in-situ Digested Immobilised Proteins Following Separation using 1D-HPLC and Automated Robotic Sample Deposition;** Helen V. Montgomery<sup>1</sup>; Cornelia Koy<sup>2</sup>; Thomas Deierling<sup>2</sup>; Michael O. Glocker<sup>2</sup>; Koichi Tanaka<sup>3</sup>; <sup>1</sup>Koichi Tanaka Mass Spec Research Laboratory, Manchester, UK; <sup>2</sup>Proteome Center, Univ. of Rostock, Rostock, Germany; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- WP 613 **De novo Sequencing of Peptide on MALDI-TOF MS Target Plate by Chemical Reaction;** Kenji Miyazaki<sup>1</sup>; Hiroaki Torii<sup>1</sup>; Reiji Teramoto<sup>1</sup>; Ken'ichi Kamijo<sup>1</sup>; Akira Tsugita<sup>1</sup>; <sup>1</sup>Proteomics Research Center, NEC corp., Tsukuba, Japan
- WP 614 **Antigen Retrieval Facilitates Proteomic Analysis of Formalin-Fixed Brain Tissues;** Mark J. Raftery<sup>1</sup>; Farid Rahimi<sup>2</sup>; Glenda M. Halliday<sup>2</sup>; Carolyn L. Geczy<sup>1</sup>; Claire E. Shepherd<sup>2</sup>; <sup>1</sup>University of New South Wales, Sydney, Australia; <sup>2</sup>Prince of Wales Medical Research Institute, Sydney, Australia
- WP 615 **Evaluation of LC-ESI/LC-MALDI MS in the Analysis of Photosystem I and II-Complex of Barley;** Marten F. Snel<sup>1</sup>; Diana Uria<sup>1</sup>; Therese McKenna<sup>1</sup>; James Langridge<sup>1</sup>; Alistair Wallace<sup>1</sup>; Bernhard Granvogel<sup>2</sup>; V. Reisinger<sup>2</sup>; Lutz A. Eichacker<sup>2</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>Ludwig-Maximilians-Universitaet, Munich, Germany
- WP 616 **Rapid and Time-controlled Protein Digest by Trypsin-coated Magnetic Particles prior to Mass Spectrometric Analysis;** Sylvia Tigrett<sup>1</sup>; Michel Canton<sup>1</sup>; Thomas Elssner<sup>2</sup>; Markus Kostrzewa<sup>2</sup>; Karine Pacaud-Mercier<sup>1</sup>; <sup>1</sup>Agro-Bio, La Ferte St Aubin, France; <sup>2</sup>Bruker, Leipzig, Germany
- WP 617 **A Method for Controlling the Post Sampling Stability of Proteomics Samples;** Karl Sköld<sup>1</sup>; Marcus Svensson<sup>1</sup>; Per Svenningsson<sup>2</sup>; Göran Palmers<sup>3</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Lab for Biological and Medical Mass Spectrometry, Uppsala, Sweden; <sup>2</sup>Karolinska Institute, Stockholm, Sweden; <sup>3</sup>Denator Biotechnology, Göteborg, Sweden
- WP 618 **Proteomic Analysis of the Arabidopsis thaliana Endomembrane Compartment using Alternative Extraction Techniques;** Srijeet K. Mitra<sup>1</sup>; John A. Gantt<sup>1</sup>; James F. Ruby<sup>1</sup>; Steven D. Clouse<sup>1</sup>; Michael B. Goshe<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC
- WP 619 **Evaluation of In-Gel Protein Digestion Extraction Protocols: How Important are the Steps Involved?;** Stephen Macha<sup>1</sup>; Susan Russell<sup>1</sup>; Larry Sallans<sup>1</sup>; Patrick Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 620 **Improved Sample Preparation Method for Characterization of Postranslational Modifications at the Low-Nanogram Protein Levels using Nano-LC LTQ-FT MS;** Lingyun Li<sup>1</sup>; Tomas Rejtár<sup>1</sup>; Shujia Dai<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- WP 621 **Identification and Quantification of Secreted Proteins and Cell Surface Proteins from Solid Tissues;** Yuan Tian<sup>1</sup>; Yong Zhou<sup>1</sup>; Ruedi Aebersold<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Institute for Systemsbiology, Seattle, WA
- WP 622 **Experimental Approach For Large-Scale Proteome Measurements From Small Amounts (low mg) Of Microbial Cultures;** Melissa R. Thompson<sup>1</sup>; Jennifer M. Froelich<sup>3</sup>; Brian Erickson<sup>2</sup>; Nathan C. VerBerkmoes<sup>1</sup>;



# WEDNESDAY POSTERS

## POSTER SPACE

- Robert L. Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee, Knoxville, TN; <sup>3</sup>Michigan State University, East Lansing, MI
- WP 623 **Target Protein Identification - Cross-linking Radiolabeled & Photoreactive Probes with Proteins, Followed by Mass Spectrometry;** Hideji Fujiwara<sup>1</sup>; Antony Yem<sup>1</sup>; Jerry Colca<sup>1</sup>; Olga Nemirovskiy<sup>1</sup>; Melissa Radabaugh<sup>1</sup>; Connie Evans<sup>1</sup>; Heidi Hope<sup>1</sup>; Richard Head<sup>1</sup>; W. Rodney Mathews<sup>1</sup>; <sup>1</sup>Pfizer Inc., Chesterfield, MO
- WP 624 **Profile of Secreted Proteins from Primary Human Chondrocytes Using a Reversible Gel Cell Encapsulation Culture System;** Michael D. Knierman<sup>1</sup>; Dennis A. Laska<sup>1</sup>; Richard E. Higgs<sup>1</sup>; Kevin L. Duffin<sup>1</sup>; John E. Hale<sup>1</sup>; <sup>1</sup>Eli Lilly and Co., Greenfield, IN
- WP 625 **Levitated Droplet and Dried Droplet Sample Preparation Strategies with Alternative Ionic Compounds and Common Matrices Applied to Hydrophobic Protein Sequencing;** Diem Ly Van<sup>1</sup>; Teresita M. Cruz Sanchez<sup>1</sup>; George Agnes<sup>1</sup>; <sup>1</sup>Simon Fraser University, Burnaby, BC, Canada
- WP 626 **On-line HPLC/UV/MS Detection and Characterization of Leachables from Protein Drugs using a Reverse Phase Phenyl Column;** Lin Zhu<sup>1</sup>; Anneli Depaolis<sup>1</sup>; Ghobrial Ibrahim<sup>1</sup>; Basant Sharma<sup>1</sup>; <sup>1</sup>GBSC/Centocor, Raritan, , NJ
- WP 627 **Prespotted AnchorChip Targets as Archiving Platform for Proteomics Samples;** Christine Luebbert<sup>1</sup>; Christian Ziegmann<sup>2</sup>; Detlev Suckau<sup>1</sup>; Oksana Gvozdyak<sup>3</sup>; Martin Schuerenberg<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Eppendorf Polymere GmbH, Oldenburg, Germany; <sup>3</sup>Bruker Daltonics, Billerica, MA
- WP 628 **Transcriptional and Post-Transcriptional Mechanisms of Human COX-2 Gene Regulation by DNA/RNA-Affinity Capture-mLC/MS/MS;** Thomas K. Bane<sup>1</sup>; <sup>1</sup>City of Hope National Medical Center, Duarte, CA
- WP 629 **Mechanistic Studies of a Two-Step Formaldehyde Cross-linking Reaction by Mass Spectrometry;** Judy Toews<sup>1</sup>; Peter Schubert<sup>1</sup>; Juergen Kast<sup>1</sup>; <sup>1</sup>The Biomedical Research Centre, UBC, Vancouver, Canada
- WP 630 **Identification of Protein-Protein Interaction Sites Using Molecular Pendants, Affinity Chromatography and Mass Spectrometry;** Jason G Williams<sup>1</sup>; Katina Johnson<sup>1</sup>; Kenneth B Tomer<sup>1</sup>; <sup>1</sup>National Institute of Environmental Health Science, RTP, NC

## PROTEOMICS: 2D ELECTROPHORESIS

- WP 636 **Proteomic Analysis of Differential Expressed Protein by Proteasome Inhibitor MG132 and Heat Shock Stress;** Jaeho Jeong<sup>1</sup>; Yung Hee Kim<sup>1</sup>; Ah-Ran Kim<sup>1</sup>; Kong-Joo Lee<sup>1</sup>; <sup>1</sup>Center for Cell Signaling Research, Seoul, Korea
- WP 637 **Proteomic Analysis of Intestinal Epithelial Cells Along Crypt - Villus Axis;** Jinsook Chang<sup>1</sup>; John M. Mariadason<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Albert Einstein College of Medicine, Bronx, NY
- WP 638 **Changes in Ribosomes Associated with Drug Resistance;** Faith A Hays<sup>1</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD
- WP 639 **Alterations in Protein Expression Associated with Neuroprotection: Investigation of the Mechanism Using Novel Multicolor Fluorescent Zdyes and 2DE;** Britt Alsaker<sup>1</sup>; David Fouchard<sup>1</sup>; Kevin Spicka<sup>1</sup>; Rajani Gurram<sup>1</sup>; Paul Grieco<sup>1</sup>; Duane Mooney<sup>1</sup>; Don Thorne<sup>3</sup>; Melodie Weller<sup>2</sup>; David Poulsen<sup>2</sup>; Edward Dratz<sup>1</sup>;

## POSTER SPACE

- <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>University of Montana, Missoula, Montana; <sup>3</sup>Zdye, LLC, Bozeman, MT
- WP 640 **Development and Use of Image Merging Software to Increase the Dynamic Range of Protein Detection in Fluorescently Labeled 2D Gels;** Mark K Clements<sup>1</sup>; Brian Bothner<sup>1</sup>; Don Thorne<sup>2</sup>; Edward Dratz<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Zdye, LLC, Gallatin Gateway, MT
- WP 641 **Zdyes: A New Differential Fluorescent 2D Gel Approach and Agilent ChipLC analysis of the Yeast Alpha Mating Factor Response;** Matt Shipman<sup>1</sup>; David Fouchard<sup>1</sup>; Rajaiah Gurram<sup>1</sup>; Kevin Spicka<sup>1</sup>; Duane Mooney<sup>1</sup>; Walid Maaty<sup>1</sup>; Linda Hyman<sup>1</sup>; Kathy Sheehan<sup>1</sup>; Mark Clements<sup>1</sup>; Jonathan Hilmer<sup>1</sup>; Don Thorne<sup>2</sup>; Paul Grieco<sup>1</sup>; Edward Dratz<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Zdye LLC, Gallatin Gateway, MT
- WP 642 **Differential Proteomic Analysis of Hyperthermophilic Virus-Infected Sulfolobus Sulfataricus Archaea using 2DE DIGE and Novel Multicolor Fluorescent Zdyes;** Walid Maaty<sup>1</sup>; Britt Alsaker<sup>1</sup>; David Fouchard<sup>1</sup>; Kevin Spicka<sup>1</sup>; Rajaiah Gurram<sup>1</sup>; Mark Clements<sup>1</sup>; Jonathan Hilmer<sup>1</sup>; Paul Grieco<sup>1</sup>; Don Thorne<sup>2</sup>; Brian Bothner<sup>1</sup>; Edward Dratz<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Zdye, LLC, Gallatin Gateway, MT
- WP 643 **Improved MS-Compatibility of Silver Nitrate-Stained Proteins from 2-DE Gels by Use of ZipPlates for the In-Gel Digest;** Grit Nebrich<sup>1</sup>; Marion Herrmann<sup>1</sup>; Dijana Sagi<sup>1</sup>; Joachim Klose<sup>1</sup>; Patrick Giavalisco<sup>1</sup>; <sup>1</sup>Charité - Institute for Human Genetics, Berlin, Germany
- WP 644 **Alternations in Mouse Liver Endosomal Protein Profiles Induced by Apolipoprotein E and B100 Deficiency;** Anshu Chen<sup>1</sup>; Hong Yang<sup>1</sup>; DongFang Wu<sup>1</sup>; ZhongMao Guo<sup>1</sup>; <sup>1</sup>Meharry Medical College, Nashville, TN

## PROTEOMICS: QUANTITATION TECHNIQUES III

- WP 645 **Quantitative Mass Spectrometric Immunoassay permutations in the MALDI endeavor toward Clinical Proteomics;** Kemmons A. Tubbs<sup>1</sup>; Urban A. Kiernan<sup>1</sup>; Eric E. Niederkofler<sup>1</sup>; Dobrin Nedelkov<sup>1</sup>; Allan L. Bieber<sup>1</sup>; Randall W. Nelson<sup>1</sup>; <sup>1</sup>Intrinsic Bioprobes, Inc, Tempe, AZ
- WP 646 **A Proteomic Study of Archaeal Viral and Host Proteins;** Lars Liepold<sup>1</sup>; Walid Maaty<sup>1</sup>; Brian Bothner<sup>1</sup>; Trevor Douglas<sup>1</sup>; Mark Young<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT
- WP 647 **Protein Expression Ratios from Porphyromonas gingivalis Using Different Approaches to non-Label Based Quantitation;** Tiansong "Tony" Wang<sup>1</sup>; Qiangwei Xia<sup>1</sup>; Fred Taub<sup>1</sup>; Yoonsuk Park<sup>2</sup>; Richard J. Lamont<sup>2</sup>; Murray Hackett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Florida, Gainesville, FL
- WP 648 **Proteomic Analysis of Rat Liver after Chronic Treatment with Tamoxifen and Phenobarbital;** Jason T. Taylor<sup>1</sup>; Richard C. Jones<sup>1</sup>; Sheeno Thyparambil<sup>1</sup>; Yvonne P. Dragan<sup>1</sup>; Ricky D. Edmondson<sup>1</sup>; <sup>1</sup>National Center for Toxicological Research, Jefferson, AR
- WP 649 **Evaluation of Biological Variability in the Proteomic Characterization of a Hydrogen-Producing Mutant of Rhodospseudomonas Palustris;** Brian Erickson<sup>2</sup>; Melissa Thompson<sup>2</sup>; Nathan C. VerBerkmoes<sup>1</sup>; Dale Pelletier<sup>3</sup>; Simona Romagnoli<sup>4</sup>; Bing Zhang<sup>5</sup>; Richard Laguna<sup>4</sup>; Nagiza F. Samatova<sup>5</sup>; Robert L. Hettich<sup>1</sup>; Frank W. Larimer<sup>3</sup>; Robert F Tabita<sup>4</sup>; <sup>1</sup>Chemical Sciences Division, Oak Ridge National Lab, Oak Ridge, TN; <sup>2</sup>Genome Science and Technology UT/ORNL, Oak Ridge, TN; <sup>3</sup>Life



# WEDNESDAY POSTERS

## POSTER SPACE

- Sciences Division, Oak Ridge National Lab, Oak Ridge, TN; <sup>4</sup>Department of Microbiology, The Ohio State Univ, Columbus, OH; <sup>5</sup>Computer Science Division, Oak Ridge National Lab, Oak Ridge, TN
- WP 650 **Non-invasive Clinical Detection of Potential Drug Induced Toxicity in Urine;** Annette R. Erskine<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- WP 651 **An LCMS Method to Understand Differences Between Natural Isolates;** Esteban Martinez Garcia<sup>1</sup>; Jeffrey C. Silva<sup>2</sup>; Craig A. Dorschel<sup>2</sup>; Scott J. Geromanos<sup>2</sup>; Roberto G. Kolter<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Waters Corporation, Milford, MA
- WP 652 **Comparison of Alternate Scanning LC-MS Data across Multiple Instruments for Large-Scale Proteomic Studies;** Craig A Dorschel<sup>1</sup>; Scott J Geromanos<sup>1</sup>; Marc V Gorenstein<sup>1</sup>; Guo-Zhong Li<sup>1</sup>; Jeffrey C Silva<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 653 **Identification and Relative Quantification of Membrane Proteins by Surface Biotinylation and Two-Dimensional Peptide Mapping;** Christoph Rösli<sup>1</sup>; Giuliano Elia<sup>1</sup>; Dario Neri<sup>1</sup>; <sup>1</sup>Institute of Pharmaceutical Sciences, ETH Zurich, Zurich, Switzerland
- WP 654 **Incorporation of an Internal Trypsin Cleavage Site into Protein-AQUATM Standards for Absolute Quantification;** Jeffrey J Porter<sup>1</sup>; Justin Wildsmith<sup>1</sup>; David K Stone<sup>1</sup>; Dian Er Chen<sup>1</sup>; Kevin M Ray<sup>1</sup>; Graham B I Scott<sup>1</sup>; <sup>1</sup>Sigma-Aldrich Biotechnology, Saint Louis, MO
- WP 655 **Nano-LC, Dual Channel (Cy-3, Cy-5) Laser Induced Fluorescence (LIF) Detector, Nano-ESI-MS Hyphenation for Quantitative Proteomics;** Florence Guerad<sup>1</sup>; Jocelyne Tahar<sup>2</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France; <sup>2</sup>Picometrics, Toulouse, France
- WP 656 **Three Label Free Quantification Methods Investigated and Applied to Study Murine Purkinje Cell Degeneration: Sequence Coverage, Peptide Count and ROOMS;** Soyoung Ryu<sup>1</sup>; Byron Gallis<sup>1</sup>; Lisa Chakrabarti<sup>1</sup>; Scott A. Shaffer<sup>1</sup>; Dragan Radulovic<sup>2</sup>; Al LaSpada<sup>1</sup>; David R. Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Florida Atlantic University, Boca Raton, FL
- WP 657 **An Isotope-Free Method for Quantitative Proteomics;** Zhenyu Huang<sup>1</sup>; Xiaoning Lu<sup>1</sup>; Jianjun Zhai<sup>1</sup>; Haining Zhu<sup>1</sup>; <sup>1</sup>University of Kentucky, Lexington, KY
- WP 658 **Quantitative Analysis of Nuclear Proteins from the Human Pathogen *Trypanosoma cruzi*;** James A. Atwood III<sup>1</sup>; Fernanda Ludolf<sup>2</sup>; Arthur Nuccio<sup>1</sup>; Todd A. Minning<sup>3</sup>; Brent Weatherly<sup>3</sup>; Rick L. Tarleton<sup>3</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center, Athens, GA; <sup>2</sup>Santa Casa de Belo Horizonte, Belo Horizonte, Brazil; <sup>3</sup>Center for Tropical and Emerging Global Disease, Athens, GA
- WP 659 **Beyond Protein Profiling: Measurement of Changes in Isoforms and Phosphorylation Due to Stroke;** Martha D. Stapels<sup>1</sup>; Grace M. Credo<sup>1</sup>; Jennifer Fournier<sup>1</sup>; Martin Gilar<sup>1</sup>; John C. Gebler<sup>1</sup>; Aaron White<sup>2</sup>; Giuseppe Pignataro<sup>2</sup>; Roger P. Simon<sup>2</sup>; An Zhou<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Legacy Research, Portland, OR
- WP 660 **Quantitative Multi-Variable Proteome Analysis Using Difference Gel Electrophoresis and Mass Spectrometry to Study Iron Regulation Pathways in *Staphylococcus aureus*;** David B. Friedman<sup>1</sup>; Corbin A. Whitwell<sup>1</sup>; Devin Stauff<sup>1</sup>; Eric P. Skaar<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN

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- WP 661 **Proteomic Study of BDNF Induced Changes in the Membrane-Associated Proteome of Hippocampal Neurons;** Bruno Manadas<sup>1</sup>; Spiros D. Garbis<sup>2</sup>; Michael Fountoulakis<sup>2</sup>; Carlos B. Duarte<sup>1</sup>; <sup>1</sup>Center for Neuroscience and Cell Biology, Coimbra, Portugal; <sup>2</sup>Biomedical Research of the Academy of Athens, Athens, Greece
- WP 662 **Analysis and Quantification of Diagnostic Markers and Protein Signatures for Gaucher Disease by Means of LC-MS;** Johannes P.C. Vissers<sup>1</sup>; Mark Ritchie<sup>1</sup>; Jim L. Langridge<sup>1</sup>; Johannes M.F.G. Aerts<sup>2</sup>; <sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>Academic Medical Center, University of Amsterdam, Amsterdam, NL
- WP 663 **Label-Free Differential Quantitation of Relative Peptide Intensities Without Peak Detection in an Orbitrap LC/MS System;** Greg L. Finney<sup>1</sup>; Adele R. Blackler<sup>2</sup>; Michael Hoopmann<sup>1</sup>; Christine C. Wu<sup>2</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Colorado Health Sciences Center, Denver, CO
- WP 664 **Quantitative Proteomics: LC- Laser Induced Fluorescence Detector coupled to ESI Mass Spectrometry;** Junichi Masuda<sup>1</sup>; Nicole Y. Morgan<sup>2</sup>; Anthony J. Makusky<sup>3</sup>; Masayuki Nishimura<sup>1</sup>; Shuzo Maruyama<sup>4</sup>; Paul D. Smith<sup>2</sup>; Terry M. Phillips<sup>2</sup>; Jeffrey A. Kowalak<sup>3</sup>; Sanford P. Markey<sup>3</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Inc., Columbia, MD; <sup>2</sup>DBEPS/ORS/NIH, Bethesda, MD; <sup>3</sup>NIMH/NIH, Bethesda, MD; <sup>4</sup>Shimadzu Corporation, Kyoto, Japan
- WP 665 **Rapid Quantitation of Proteins and Peptides Using a LC/MS/MS Based Multiplexed Amino Acid Analysis Method;** Wendy L. White<sup>1</sup>; Jon D. Williams<sup>1</sup>; <sup>1</sup>GlaxoSmithKline, Research Triangle Park, NC
- WP 666 **Proteomic analysis of drug treated *Mycobacterium smegmatis*;** Rong Wang<sup>1</sup>; Edward M. Marcotte<sup>1</sup>; <sup>1</sup>ICMB, UT Austin, Austin, TX
- WP 667 **pH-Reversible Fluorescent Tags for Quantifying Protein Post-Translational Modifications;** Alan A. Doucette<sup>1</sup>; Harman Clair<sup>1</sup>; <sup>1</sup>Dalhousie University, Halifax, Canada
- WP 668 **Standard Protein Mixtures for Accurate Protein Identification and Expression Measurements;** Jason M. Hogan<sup>1</sup>; Roger Higdon<sup>1</sup>; Elizabeth V. Landorf<sup>2</sup>; Frank R. Collart<sup>2</sup>; Eugene Kolker<sup>1</sup>; <sup>1</sup>The Biotech Institute, Bothell, WA; <sup>2</sup>Argonne National Lab, Argonne, IL

## THURSDAY POSTERS

### POSTER SPACE

### THURSDAY POSTERS

These posters should be set up at 7:30 am on Thursday and removed at 2:30 pm. Be sure to use the poster space number next to the title.

#### ATMOSPHERIC CHEMISTRY

- ThP 9 **TOF-SIMS Study of Individual Marine Particles;** Yuri Desyaterik<sup>1</sup>; Daniel Gaspar<sup>1</sup>; Alexander Laskin<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*
- ThP 10 **Ozone Reaction Kinetics of the Oxidation of Tyrosine and Histidine Residues;** Julie A. Lloyd<sup>1</sup>; Murray V. Johnston<sup>1</sup>; <sup>1</sup>*University of Delaware, Newark, DE*
- ThP 11 **On-Line Real-Time Detection of Oligomers in Secondary Organic Aerosol with the ATOFMS;** Deborah S. Gross<sup>1</sup>; Markus Gaelli<sup>2</sup>; Markus Kalberer<sup>3</sup>; Andre Prevot<sup>4</sup>; Josef Dommen<sup>4</sup>; Urs Baltensperger<sup>4</sup>; <sup>1</sup>*Carleton College, Northfield, MN*; <sup>2</sup>*TSI Incorporated, Shoreview, MN*; <sup>3</sup>*ETH Zürich, Zürich, Switzerland*; <sup>4</sup>*Paul Scherrer Institut, Villigen PSI, Switzerland*
- ThP 12 **Extraction of Taxonomic Chemical Information from Bacterial Cells Using Differential Mobility Spectrometry and Multi-Way Principal Component Analysis;** Satendra Prasad<sup>1</sup>; Hartwig Schmidt<sup>1</sup>; Robert Gueth<sup>1</sup>; Jaya V. Rao<sup>1</sup>; Whitney Fort<sup>1</sup>; Geoffrey B. Smith<sup>1</sup>; Gary A Eiceman<sup>1</sup>; <sup>1</sup>*New Mexico State University, Las Cruces, NM*
- ThP 13 **The Effect of Needle Voltage on the Negative Ion Formation Using Atmospheric Pressure Corona Discharge Ionization (APCDI) in Air;** Kanako Sekimoto<sup>1</sup>; Mitsuo Takayama<sup>1</sup>; <sup>1</sup>*Yokohama City University, Yokohama, Japan*

#### ATMOSPHERIC PRESSURE PHOTO IONIZATION

- ThP 14 **Atmospheric Pressure Photoionization: Investigation of Proton Transfer in Complex Mixtures;** Jeremiah M. Purcell<sup>1</sup>; Ryan P. Rodgers<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Donald F. Smith<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*
- ThP 15 **Electrospray-Atmospheric Pressure Laser Ionization (ES-APLI): A New Interface for LC-MS Coupling;** Oliver J. Schmitz<sup>1</sup>; Stefan Droste<sup>1</sup>; Marc Schellenträger<sup>1</sup>; Marc Constapel<sup>1</sup>; Ralf Schiewek<sup>1</sup>; Siegm. Gäßl<sup>1</sup>; Matthias Lorenz<sup>2</sup>; Klaus J. Brockmann<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*University of Wuppertal, Analytical Chemistry, Wuppertal, Germany*; <sup>2</sup>*University of Wuppertal, Physical Chemistry, Wuppertal, Germany*
- ThP 16 **Atmospheric-Pressure Laser Ionization (APLI): A New Interface for GC-MS Coupling;** Ralf Schiewek<sup>1</sup>; Stefan Droste<sup>1</sup>; Marc Constapel<sup>1</sup>; Oliver J. Schmitz<sup>1</sup>; Siegm. Gäßl<sup>1</sup>; Matthias Lorenz<sup>2</sup>; Klaus J. Brockmann<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*University of Wuppertal, Analytical Chemistry, Wuppertal, Germany*; <sup>2</sup>*University of Wuppertal, Physical Chemistry, Wuppertal, Germany*
- ThP 17 **Mechanism of [M+H]<sup>+</sup> Formation in APPI Mass Spectrometry: Identification of an Acetonitrile Impurity and Possible Involvement in the Protonation Phenomenon;** Amin. M. Kamel<sup>1</sup>; Patrick Jeanville<sup>2</sup>; Kevin Colizza<sup>1</sup>; <sup>1</sup>*Pfizer Global Research and Development, Groton, CT*; <sup>2</sup>*Thermo Electron Corporation, West Palm Beach, FL*
- ThP 18 **Determination of the Ion Acceptance Volume of Atmospheric Pressure Ionization Sources using APLI;** Klaus J. Brockmann<sup>1</sup>; Matthias Lorenz<sup>1</sup>; Ralf Schiewek<sup>2</sup>; Marc Constapel<sup>2</sup>; Oliver J. Schmitz<sup>2</sup>; Siegm. Gäßl<sup>2</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>*University of Wuppertal, Physical*

### POSTER SPACE

- Chemistry, Wuppertal, Germany*; <sup>2</sup>*University of Wuppertal, Analytical Chemistry, Wuppertal, Germany*
- ThP 19 **Determination of Lipophilicity and Solubility Using LC-MS with APPI;** Angelo Filosa<sup>1</sup>; Pascal Turcotte<sup>1</sup>; <sup>1</sup>*AstraZeneca R&D Montreal, St Laurent, Canada*
- ThP 20 **Application of Atmospheric Pressure Photoionization Mass Spectrometry in the Aquatic Environment;** Sean M. Backus<sup>1</sup>; Suzanne Batchelor<sup>1</sup>; John Struger<sup>1</sup>; L. Mark Hewitt<sup>1</sup>; <sup>1</sup>*Environment Canada, Burlington, Canada*
- ThP 21 **On the Ionization Mechanisms in APPI vs. APLI;** Matthias Lorenz<sup>1</sup>; Klaus J. Brockmann<sup>1</sup>; Ralf Schiewek<sup>2</sup>; Marc Constapel<sup>2</sup>; Oliver J. Schmitz<sup>2</sup>; Siegm. Gäßl<sup>2</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>*University of Wuppertal, Physical Chemistry, Wuppertal, Germany*; <sup>2</sup>*University of Wuppertal, Analytical Chemistry, Wuppertal, Germany*
- ThP 22 **The Hydrolysis Reaction Mechanism of Alkanox P24: An HPLC-APPI-MS Investigation;** Malvina M. Papanastasiou<sup>1</sup>; Adam McMahon<sup>2</sup>; Norman S. Allen<sup>1</sup>; Brian J. Johnson<sup>3</sup>; Klaus Keck-Antoine<sup>3</sup>; <sup>1</sup>*Manchester Metropolitan University, Manchester, UK*; <sup>2</sup>*University of Manchester, Molecular Imaging Centre, Manchester, UK*; <sup>3</sup>*Chemtura, Herentals, Belgium*
- ThP 23 **Investigation of THF as a Dopant in Different Introducing Ways in LC-APPI/MS Analysis;** Yanxuan Cai<sup>1</sup>; Oliver McConnell<sup>1</sup>; Alvin C. Bach<sup>1</sup>; <sup>1</sup>*Wyeth Research, Princeton, NJ*
- ThP 24 **Investigation into the Suitability of Various Compounds for Promoting Charge Exchange Ionization in Dopant-Assisted Atmospheric Pressure Photoionization for Reverse-Phase LC/MS;** Derek Smith<sup>1</sup>; Damon Robb<sup>1</sup>; Michael Blades<sup>1</sup>; <sup>1</sup>*University of British Columbia, Vancouver, Canada*
- ThP 25 **Detection of Polycyclic Aromatic Hydrocarbon by Liquid Chromatography-Atmospheric Pressure Photoionization-Mass Spectrometry;** Xia Zhang<sup>1</sup>; Michelle Somers<sup>1</sup>; Jerome Robles<sup>1</sup>; Mary J. Wornat<sup>1</sup>; <sup>1</sup>*Louisiana State University, Baton Rouge, LA*
- ThP 26 **Validation of an Assay to Quantitate Vitamin K and Vitamin K Epoxide in Rat Serum Utilizing HPLC/MS/MS with Photo-Ionization;** Kimberly A. Navetta<sup>1</sup>; Jennifer L. Colangelo<sup>1</sup>; <sup>1</sup>*Safety Sciences Groton, Pfizer Global R&D, Groton, CT*
- ThP 27 **Structural Elucidation of Liquid Crystal Display (LCD) Materials by Means of LC-APPI-FT-ICR-MS/MS;** Shigeru Sakamoto<sup>1</sup>; Julie Horner<sup>2</sup>; Rohan Thakur<sup>2</sup>; Masayuki Kubota<sup>1</sup>; <sup>1</sup>*Thermo Electron, Yokohama, Japan*; <sup>2</sup>*Thermo Electron, San Jose, CA*
- ThP 28 **APPI-LC/MS Analysis of Triacylglycerols – Strategies for Selections of Mobile Phase Solvent Systems and VUV Lamps for Optimum Performance;** Sheng-Suan Cai<sup>1</sup>; Luke C. Short<sup>1</sup>; Jack A. Syage<sup>1</sup>; <sup>1</sup>*Syagen Technology, Inc, Tustin, CA*
- ThP 29 **Atmospheric Pressure Photo Ionisation Normal Phase Chiral LCMS;** Mark William Harrison<sup>1</sup>; <sup>1</sup>*AstraZeneca, macclesfield, United Kingdom*
- ThP 30 **Evaluation of APPI for the Analysis of Pharmaceutical Compounds in Support of Bioanalytical Research in Drug Discovery;** Asoka Ranasinghe<sup>1</sup>; Hongwei Zhang<sup>1</sup>; Cecilia L. Chi<sup>1</sup>; Georgia Cornelius<sup>1</sup>; Steven Wu<sup>1</sup>; Timothy V. Olah<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*
- ThP 31 **Use of MALDI matrixes as dopant in Atmospheric Pressure Photoionization;** Alexandre Giuliani<sup>1</sup>; Aicha Sabir - Bagag<sup>1</sup>; Vincent Guerinéau<sup>1</sup>; Olivier Laprêve<sup>1</sup>; <sup>1</sup>*CNRS-ICSN, Gif-sur-Yvette, France*

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- ThP 32 **Investigation of Surface-Assisted (SA) LDI-TOFMS for the Characterization of Organometallic and Coordination Compounds;** David Thomas<sup>1</sup>; Mark F. Wyatt<sup>1</sup>; Bridget K. Stein<sup>1</sup>; A. Gareth Brenton<sup>1</sup>; <sup>1</sup>EPSRC National Mass Spec. Service Centre, Swansea, U.K.
- ThP 33 **Jet Desorption Ionization - A New Ionization Method for Tissue Analysis;** Zoltan Takats<sup>1</sup>; Maria Katona<sup>3</sup>; Noemi Czuczy<sup>1</sup>; Reka Skoumal<sup>2</sup>; <sup>1</sup>Chemical Research Center of HAS, Budapest, Hungary; <sup>2</sup>National Institute of Cardiology, Budapest, Hungary; <sup>3</sup>Rational Drug Design CRC, Budapest, Hungary
- ThP 34 **Controlled Fragmentation in Laser Desorption Ionization from Laser-Induced Silicon Microcolumn Arrays;** Yong Chen<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>The George Washington University, Washington, DC
- ThP 35 **Forensic Applications of Electrospray-assisted Laser Desorption Ionization (ELDI) Mass Spectrometry for Direct Chemical Analysis on Solids;** Sy-Chyi Tseng<sup>1</sup>; Min-Zong Huang<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan
- ThP 36 **Desorption Electrospray Ionization and Electrosonic Spray Ionization for Solid- and Solution-Phase Analysis of Industrial Polymers;** Marcela Nefliu<sup>1</sup>; Andre Venter<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- ThP 37 **Electrospray-Assisted Laser Desorption Ionization (ELDI) Mass Spectrometry for Direct Characterization of The Chemical Compounds on The Thin-Layer Chromatography (TLC) Plate;** Min-Zong Huang<sup>1</sup>; Shu-Yao Lin<sup>1</sup>; Ya-Lin Ma<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan
- ThP 38 **A New Matrix-Free SIMS: Electrospray Droplet Impact;** Kenzo Hiraoka<sup>1</sup>; Daiki Asakawa<sup>1</sup>; Kunihiro Mori<sup>1</sup>; <sup>1</sup>University of Yamanashi, Kofu 400-8511, Yamanashi
- ThP 39 **Electrospray-Assisted Laser Desorption Ionization Mass Spectrometry for Characterizing Proteins in Biological Media under Ambient Conditions;** Min-Zong Huang<sup>1</sup>; Jen-Yih Lee<sup>3</sup>; Hsiu-Jung Hsu<sup>1</sup>; Jing-Yueh Jeng<sup>2</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan; <sup>2</sup>Chia-Nan University of Pharmacy and Science, Tainan, Taiwan; <sup>3</sup>Center for Disease Control - Kaohsiung Branch, Kaohsiung, Taiwan

### INSTRUMENTATION: ION SOURCES

- ThP 40 **Newly Developed CryoSpray Ionization Device and its Combination with Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy;** Kazunori Saito<sup>1</sup>; Yoshihisa Sei<sup>2</sup>; Daisuke Higo<sup>1</sup>; Mitsuo Nakamura<sup>3</sup>; Ryoji Saho<sup>3</sup>; Shinichi Miki<sup>1</sup>; Kentaro Yamaguchi<sup>2</sup>; <sup>1</sup>Bruker Daltonics KK, Yokohama, Kanagawa, Japan; <sup>2</sup>Tokushima Bunri University, Sanuki, Kagawa, Japan; <sup>3</sup>Japan Thermal Engineering Co Ltd, Sagami-hara, Kanagawa, Japan
- ThP 41 **Investigations into ESI Emitter Electrode Potential Control to Optimize Low-end Linear Dynamic Range and Attainable Limits of Detection;** Michael C. Granger<sup>1</sup>; David Meyer<sup>1</sup>; Qi Zhang<sup>1</sup>; Milind P. Nagale<sup>1</sup>; Paul Gamache<sup>1</sup>; Ian N. Acworth<sup>1</sup>; Vilmos Kertesz<sup>2</sup>; Gary J. Van Berkel<sup>2</sup>; <sup>1</sup>ESA Biosciences, Inc., Chelmsford, MA; <sup>2</sup>Oak Ridge National Laboratory, OBMS, Oak Ridge, TN
- ThP 42 **Transmission Geometry MALDI Mass Microscopy;** Jae-Kuk Kim<sup>1</sup>; Fan Huang<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA

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- ThP 43 **Characterization of the Effect of an Atmospheric Pressure Ion Lens on an Electrospray Ion Source;** Alison E. Holliday<sup>1</sup>; Rong Yi<sup>1</sup>; David D.Y. Chen<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada
- ThP 44 **Alternately Pulsed Nano-electrospray Ionization/Atmospheric Pressure Chemical Ionization for Ion/Ion Reactions in an Electrodynamical Ion Trap;** Xiaorong Liang<sup>1</sup>; Yu Xia<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- ThP 45 **Investigating the Fundamental Mechanisms of Electrospray Ionization Using a New Electrospray Membrane Probe;** Craig M. Whitehouse<sup>1</sup>; Thomas P. White<sup>1</sup>; <sup>1</sup>Analytica of Branford, Inc., Branford, CT
- ThP 46 **Very High Sensitivity Cantilever Polysilicium ESI Tips Compatible with Standard Analytical Chromatography Fittings;** S  verine Le Gac<sup>1</sup>; Steve Arscott<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universit   des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- ThP 47 **A Temperature Programmable Atmospheric Pressure Interface for LC/MS Analysis;** John (Ed) George<sup>1</sup>; August Specht<sup>1</sup>; Thierry Faye<sup>1</sup>; <sup>1</sup>Varian, Inc., Walnut Creek, CA
- ThP 48 **Aperture Arrays for Atmospheric Pressure Sources;** Edward W Sheehan<sup>1</sup>; Ross C Willoughby<sup>1</sup>; <sup>1</sup>Chem-Space Associates, Inc., Pittsburgh, PA
- ThP 49 **Silanized Inner-surfaces for Reduced Peptide Adsorption in Nanoelectrospray;** Yongseok Choi<sup>1</sup>; Troy D. Wood<sup>1</sup>; <sup>1</sup>The State University of New York at Buffalo, Buffalo, NY
- ThP 50 **The Effect of the Laser Beam Profile on MALDI;** Jens Hoehndorf<sup>1</sup>; Andreas Haase<sup>1</sup>; Markus Kayser<sup>1</sup>; Armin Holle<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany
- ThP 51 **Development of a Pulsed, Multiplexed, nano-Electrospray Ionization Source;** Jared M. Bushey<sup>1</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- ThP 52 **Chaotic Transitions Between Electrospray Regimes;** Ioan Marginean<sup>1</sup>; Peter Nemes<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, DC
- ThP 53 **Low Attomole Sensitivity with Optimised MALDI Zoom Optics;** Mark D Mills<sup>1</sup>; Stephen P Thompson<sup>1</sup>; Victor C Parr<sup>1</sup>; <sup>1</sup>Scientific Analysis Instruments, Manchester, U.K.
- ThP 54 **Variable Temperature Target for Infrared and Ultraviolet MALDI MS;** James A. Hill<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>JAHIS, Arlington, MA
- ThP 55 **Development of IR-MALDI TOFMS Using a Mid-infrared DFG Laser;** Sachiko Yoshihashi-Suzuki<sup>1</sup>; Izuru Sato<sup>1</sup>; Hisanao Hazama<sup>2</sup>; Yoshiaki Takatani<sup>2</sup>; Kunio Awazu<sup>1</sup>; <sup>1</sup>Osaka University, Suita Osaka, Japan; <sup>2</sup>Kawasaki Heavy Industries, Akashi Hyogo, Japan
- ThP 56 **Fused-Droplet Electrospray Ionization (FD-ESI) Mass Spectrometry for Samples Temperature Ranging from -100 to +1,000   C;** Jing-Yueh Jeng<sup>2</sup>; Jia-Jiun Liu<sup>1</sup>; Chia-Cheng Lee<sup>1</sup>; Chia-Chi Tsao<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan; <sup>2</sup>Chia-Nan University of Pharmacy and Science, Tainan, Taiwan
- ThP 57 **Automated Atmospheric Pressure Photoionization GC/MS on an LC/MS Instrument;** Barbara S. Larsen<sup>1</sup>; Richard G. McKay<sup>1</sup>; Charles N. McEwen<sup>1</sup>; <sup>1</sup>DuPont Corporate Center for Analytical Sciences, Wilmington, DE
- ThP 58 **Fabrication of Plastic Microfluidic Devices Containing Monolithic Column Arrays for ESI MS Proteomic Analysis by Hot Embossing with Nickel Masters;** Jian

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- ThP 59 **Evaluation of the Simplified Ion Funnel;** Tanner M. Schaub<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, Florida
- ThP 60 **Fabrication of High Aspect Ratio, Open Tubular and Monolithic Silica Electrospray Emitters by Chemical Etching;** Ryan T. Kelly<sup>1</sup>; Jason S. Page<sup>1</sup>; Keqi Tang<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 61 **Accurate Mass Measurement of C-6 Heteroaryl Purine Nucleosides Using AP-MALDI TOF Mass Spectrometry;** Larry M. Russon<sup>1</sup>; Pallavi Lagisetty<sup>2</sup>; Mahesh K Lakshman<sup>2</sup>; Craig M Whitehouse<sup>1</sup>; <sup>1</sup>Analytica of Branford, Inc, Branford, CT; <sup>2</sup>The City University of New York, New York, NY

## ION MOBILITY II

- ThP 62 **ESI Ion mobility Spectrometry of Carbohydrate Isomers;** Joseph Zaia<sup>1</sup>; Iain Campuzano<sup>2</sup>; Kevin Giles<sup>2</sup>; Keith Compson<sup>2</sup>; Robert Bateman<sup>2</sup>; Catherine Costello<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Waters Corporation, Manchester, UK
- ThP 63 **Revealing the Mode of Action of Beta-defensins with Ion Mobility Mass Spectrometry;** Perdita E Barran<sup>1</sup>; Bryan J McCullough<sup>1</sup>; Hayden Eastwood<sup>1</sup>; Jason Kalapothakis<sup>1</sup>; Karen Taylor<sup>2</sup>; Julia Dorin<sup>2</sup>; Robert H Bateman<sup>3</sup>; Derek MacMillan<sup>4</sup>; Paul Kemper<sup>5</sup>; <sup>1</sup>The University of Edinburgh, Edinburgh, UK; <sup>2</sup>MRC-Human Genetics Unit, Edinburgh, UK; <sup>3</sup>Waters, Manchester, UK; <sup>4</sup>UCL, London, UK; <sup>5</sup>UCSB, Santa Barbara, CA
- ThP 64 **A Comparison of Travelling Wave and Drift Tube Ion Mobility Separations;** Jason L Wildgoose<sup>1</sup>; Kevin Giles<sup>1</sup>; Steve D Pringle<sup>1</sup>; Stormy L Koeniger<sup>2</sup>; Stephen J Valentine<sup>3</sup>; Robert H Bateman<sup>1</sup>; David E Clemmer<sup>2</sup>; <sup>1</sup>Waters MS Technologies Centre, Manchester, UK; <sup>2</sup>Indiana University, Bloomington, IN; <sup>3</sup>Predictive Physiology and Medicine, Bloomington, IN
- ThP 65 **Metabolomics by MALDI-IMMS;** Kimberly A. Kaplan<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Denise Langlais<sup>2</sup>; Thomas F. Egan<sup>2</sup>; Agnes Tempez<sup>2</sup>; Albert J. Schultz<sup>2</sup>; Amina Woods<sup>3</sup>; William F. Siems<sup>1</sup>; Herbert H. Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Ionwerks, Houston, TX; <sup>3</sup>NIDA, Baltimore, MD
- ThP 66 **The Effects of Temperature Control in FAIMS Separation;** Christopher K. Hilton<sup>1</sup>; Richard A. Yost<sup>1</sup>; Michael W. Belford<sup>2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- ThP 67 **Influence of Methylation on Protein Structures as Revealed by a Combined Ion-Mobility and Mass-Spectrometry Examination;** Yuzhu Guo<sup>1</sup>; P. Y. Iris Shek<sup>1</sup>; Bruce A. Thomson<sup>2</sup>; K.W. Michael Siu<sup>1</sup>; <sup>1</sup>York University, Toronto, Ontario, Canada; <sup>2</sup>MDS SCIEX, Concord, Ontario, Canada
- ThP 68 **Liquid Chromatography Coupled with a Mass Spectrometer Incorporating a Travelling Wave Ion Mobility Spectrometer for Analysing Complex Tryptic Peptide Mixtures;** Christopher Hughes<sup>1</sup>; Steven Pringle<sup>1</sup>; James Langridge<sup>1</sup>; Kevin Giles<sup>1</sup>; Jason Wildgoose<sup>1</sup>; Robert H Bateman<sup>1</sup>; <sup>1</sup>Waters Corporation MS Technologies Centre, Manchester, UK
- ThP 69 **Studying Non-covalent Metalloprotein Complexes by Travelling Wave-based Ion Mobility Mass Spectrometry;** Vibhuti J. Patel<sup>1</sup>; Jonathan P. Williams<sup>1</sup>; Kevin Giles<sup>2</sup>; Robert H. Bateman<sup>2</sup>; Michael T. Bowers<sup>3</sup>;

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- James H. Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Waters MS Technologies, Manchester, UK; <sup>3</sup>University of California, Santa Barbara, CA
- ThP 70 **Evaluation of the Effects of Temperature and Pressure on the Transmission of Ions Through a FAIMS Device;** David A. Barnett<sup>1</sup>; Michael Belford<sup>1</sup>; Jean-Jacques Dunyach<sup>1</sup>; Paul Atherton<sup>1</sup>; Randy W. Purves<sup>1</sup>; <sup>1</sup>Thermo Electron, San Jose, CA
- ThP 71 **Evaluation of a Parallel Plate Differential Mobility Analyzer for Protein Mobility Measurements;** John P. van Nostrand<sup>1</sup>; Bruce A. Thomson<sup>2</sup>; K. W. Michael Siu<sup>1</sup>; <sup>1</sup>Centre for Research in Mass Spec, York University, Toronto, Ontario, Canada; <sup>2</sup>MDS SCIEX, Concord, Ontario, Canada
- ThP 72 **Gas Phase Chiral Separations by Ion Mobility Mass Spectrometry (IMMS);** Herbert H. Hill Jr<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Ching Wu<sup>2</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Excellims Inc., Boston, MA
- ThP 73 **Effect of FAIMS Electrode Dimensions on Peak Shape, Separation and Transmission Efficiency;** Michael W. Belford<sup>1</sup>; Jean-Jacques Dunyach<sup>1</sup>; Randy Purves<sup>1</sup>; David Barnett<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA
- ThP 74 **Ion Mobility –TOFMS of Phospholipids;** J. Albert Schultz<sup>1</sup>; Shelley N. Jackson<sup>2</sup>; Michael Ugarov<sup>1</sup>; Thomas Egan<sup>1</sup>; Amina S. Woods<sup>2</sup>; <sup>1</sup>Ionwerks Inc., Houston, TX; <sup>2</sup>NIDA IRP, NIH, Baltimore, MD
- ThP 75 **Miniature Differential Mobility Spectrometer Interface for Enhanced Performance of an AP MALDI/MS System;** Sergei A. Ilchenko<sup>1</sup>; Robert J. Cotter<sup>2</sup>; Eugeny Krylov<sup>3</sup>; Raanan Miller<sup>3</sup>; Erkinjon Nazarov<sup>3</sup>; <sup>1</sup>Center for Proteomics, Case Western Reserve Univ., Cleveland, OH; <sup>2</sup>Middle Atlantic MS Lab., Johns Hopkins Univ., Baltimore, MD; <sup>3</sup>Sionex Corporation, Bedford, MA
- ThP 76 **Metabolomics with Ion Mobility Mass Spectrometry (IMMS);** Prabha Dwivedi<sup>1</sup>; Kimberly A. Kaplan<sup>1</sup>; Thomas F. Egan<sup>2</sup>; Agnes Tempez<sup>2</sup>; Albert J. Schultz<sup>2</sup>; Herbert H. Hill Jr<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Ionwerks Inc., Houston, TX
- ThP 77 **Characterisation of Isomeric Oligosaccharides and N-linked Glycans by Travelling Wave Based Ion Mobility Mass Spectrometry;** Richard J Holland<sup>1</sup>; Jonathan P Williams<sup>1</sup>; David J Harvey<sup>2</sup>; Robert H Bateman<sup>3</sup>; Kevin Giles<sup>3</sup>; Michael T Bowers<sup>4</sup>; James H Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Oxford Glycobiology Institute, Oxford, UK; <sup>3</sup>Waters MS Technologies, Manchester, UK; <sup>4</sup>University of California, Santa Barbara, CA

## ESI/NANOSPRAY SAMPLE PREPARATION

- ThP 78 **Fully Automated Sample Pre-Concentration and Chip Based Nanoelectrospray;** Reinaldo Almeida<sup>12</sup>; Mark Baumart<sup>12</sup>; Mark Allen<sup>12</sup>; Tom Corso<sup>12</sup>; Colleen van Pelt<sup>12</sup>; <sup>1</sup>Advion BioSciences, Norwich, UK; <sup>2</sup>Advion BioSciences, Ithaca, NY
- ThP 79 **Nanospray Emitters of Entrapped ODS Particles For Efficient Electrospray and Online Preconcentration of Analytes;** Terry B. Koerner<sup>1</sup>; Feng Sheng<sup>1</sup>; Richard D. Oleschuk<sup>1</sup>; <sup>1</sup>Queen's University, Kingston, Ontario
- ThP 80 **Multilayer Microfabricated Electrospray Emitter for On-Line Sample Manipulation and ESI-MS Analysis;** Jamie M. Iannacone<sup>1</sup>; Jennifer A. Jakubowski<sup>1</sup>; Paul W. Bohn<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL
- ThP 81 **Use of nano-Liquid Chromatography–Electro Spray Mass Spectrometry in Drug Discovery;** Gunnar

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- Stenhagen<sup>1</sup>; Hasse Karlsson<sup>2</sup>; <sup>1</sup>AstraZeneca R&D, Mölndal, Sweden; <sup>2</sup>Medical Biochemistry, Göteborg, Sweden
- ThP 82 **High Sensitivity Nanospray Chip Nozzles for Direct Infusion and Online NanoLC**; Sau Lan T. Staats<sup>1</sup>; Ike Ajagba<sup>1</sup>; <sup>1</sup>Phoenix S&T, Inc., Elkton, Maryland
- ThP 83 **A Comparative Study of ESI, nano ESI and Polymer Chip Nano ESI Ion Sources for Optimum Sensitivity and Sample Throughput**; Craig Love<sup>1</sup>; Uwe Effelsberg<sup>1</sup>; Alex Mordehai<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 84 **Optimizing the Use of Chip-based Infusion Nanoelectrospray Tandem Mass Spectrometry for the Rapid Analysis of Complex Proteomes**; Ana G. Pereira-Medrano<sup>1</sup>; Alistair Sterling<sup>2</sup>; Ambrosius PL. Snijders<sup>1</sup>; Kenneth F. Reardon<sup>3</sup>; Phillip C. Wright<sup>1</sup>; <sup>1</sup>University of Sheffield, Sheffield, UK; <sup>2</sup>Advion BioSciences Ltd, Norwich, UK; <sup>3</sup>Colorado State University, Fort Collins, CO
- ThP 85 **Reduction of Phospholipid Matrix Effects in Electrospray Ionization by Adding Colloidal Silica and Manganese Chloride**; Dale Schoener<sup>1</sup>; Marzena Noren<sup>1</sup>; Jim Lehman<sup>1</sup>; Patrick Lin<sup>1</sup>; <sup>1</sup>Alta Analytical Laboratory, El Dorado Hills, CA
- ThP 86 **A Direct Observation on the Formation of Ordered Clusters in Solution by Cold-spray Ionization Mass Spectrometry**; Masatoshi Kawahata<sup>1</sup>; Yoshihisa Sei<sup>1</sup>; Kentaro Yamaguchi<sup>1</sup>; Hiroko Seki<sup>2</sup>; <sup>1</sup>Tokushima Bunri University, Sanuki-city, Kagawa; <sup>2</sup>Chiba University, Chiba-city, Chiba
- ThP 87 **Unique Decomposition Pathways of Brevetoxins Enabled by Fluoride Anion Attachment in Negative Ion Electrospray**; Weiqun Wang<sup>1</sup>; Richard B. Cole<sup>1</sup>; <sup>1</sup>University of New Orleans, New Orleans, LA
- ThP 88 **Porous Polymer Monolith Emitters Produce Cold Nanospray**; David V. Dearden<sup>1</sup>; Nannan Fang<sup>1</sup>; Binghe Gu<sup>1</sup>; Milton L. Lee<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- ThP 89 **Cold-spray Ionization: A Mass Spectrometric Reaction Tracking**; Yoshihisa Sei<sup>1</sup>; Hiroshi Danjo<sup>1</sup>; Masatoshi Kawahata<sup>1</sup>; Tomoko Hatakeyama<sup>1</sup>; Jun Tamura<sup>2</sup>; Kentaro Yamaguchi<sup>1</sup>; <sup>1</sup>TokushimaBunri University, Sanuki-city, Japan; <sup>2</sup>JEOL Ltd., Akishima-city, Japan

## MICRO AND NANO SCALE SEPARATIONS

- ThP 90 **Indication of Peptide Charge State in CE-MALDI-MS Data for Proteolytic Digests of Escherichia Coli Heparin-binding Proteins**; Brad J. Williams<sup>1</sup>; William K. Russell<sup>1</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- ThP 91 **Interrogation of Post Translational Modifications on Transcription Factors by nano-LC-LTQ-FTMS/MS**; Lihua Jiang<sup>1</sup>; Michael T. Boyne II<sup>1</sup>; Paul M. Thomas<sup>1</sup>; Andrew J. Forbes<sup>1</sup>; Ling Wang<sup>2</sup>; Varsha Likehite<sup>1</sup>; John Ervin<sup>3</sup>; Gary A. Valaskovic<sup>4</sup>; Philip A. Cole<sup>2</sup>; John A. Katzenellenbogen<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>the Johns Hopkins University, Baltimore, MD; <sup>3</sup>Eksigent Technologies, LLC, Dublin, CA; <sup>4</sup>New Objective, Inc, Woburn, MA
- ThP 92 **Developing Polymer Microchips for CE-ESI-MS**; April L. Dupre<sup>1</sup>; Justin S. Mecomber<sup>1</sup>; Collin Wetzel<sup>1</sup>; H. Brian Halsall<sup>1</sup>; William R. Heineman<sup>1</sup>; Carl J. Seliskar<sup>1</sup>; Kenneth R. Wehmeyer<sup>2</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>Procter and Gamble Pharmaceuticals, Mason, OH

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- ThP 93 **Comparison of Gradient Slope, Column Length, and Particle Sizes for Analysis of Peptides on a 10,000 psi nanoLC/MS/MS Platform**; Jeffrey W. Finch<sup>1</sup>; Hongji Liu<sup>1</sup>; Keith Fadgen<sup>1</sup>; Geoff Gerhardt<sup>1</sup>; James P. Murphy<sup>1</sup>; John C. Gebler<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- ThP 94 **Integration of Microfluidics to Electrospray Ionization Mass Spectrometry Using a Chip-embedded SU-8 Electrospray Tip**; Seung-min Park<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY
- ThP 95 **High Pressure, Transparent Microfluidic Coupling Method for Nanobore LC-MS**; Jeffrey Wynn<sup>1</sup>; Adam W. Perala<sup>1</sup>; Christopher J. Toher<sup>1</sup>; Gary A. Valaskovic<sup>1</sup>; <sup>1</sup>New Objective Inc., Woburn, MA
- ThP 96 **Fast and High Quality Peptide Mapping Using Silica Nano-Monoliths in On- and Off-line Capillary LC-ESI- and LC-MALDI-MS/MS**; Sven Andrecht<sup>1</sup>; Dieter Lubda<sup>1</sup>; Almut Rapp<sup>1</sup>; Robertus Hendriks<sup>1</sup>; Karin Cabrera<sup>1</sup>; <sup>1</sup>Merck KGaA, Darmstadt, Germany
- ThP 97 **Drastic Increase in Resolution and Sensitivity in Complex Proteomic Analysis by a Novel Ultra-High-Pressure Split-less Nano-HPLC System**; Frank Yang<sup>1</sup>; Diane Cripps<sup>2</sup>; Stefani Thomas<sup>2</sup>; Austin Yang<sup>2</sup>; Richard Xu<sup>1</sup>; Gordon Hsu<sup>1</sup>; <sup>1</sup>Micro-Tech Scientific, Vista, CA; <sup>2</sup>University of Southern California, Los Angeles, CA
- ThP 98 **Fully Integrated Chip-based LC-ESI Systems with Flow Sensor and Feedback Control**; Yunan Miao<sup>1</sup>; Jason Shih<sup>2</sup>; Yu-Chong Tai<sup>2</sup>; Terry D. Lee<sup>1</sup>; <sup>1</sup>Beckman Research Institute of the City of Hope, Duarte, CA; <sup>2</sup>California Institute of Technology, Pasadena, CA
- ThP 99 **High Performance Reverse Phase Monolithic Capillary Columns for Direct Injection of Crude Proteomics Sample**; Séverine Le Gac<sup>1</sup>; Kamal Tobal<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- ThP 100 **Analyses of Intact Proteins from Complex Cell Extracts Using an Integrated Microfluidic Devices Coupled to a Time-of-Flight Instrument**; Mihaela Ghitun<sup>1</sup>; Eric Bonneil<sup>1</sup>; Christelle Pomies<sup>1</sup>; Reid Brennen<sup>2</sup>; Hongfeng Yin<sup>2</sup>; Kevin Killeen<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>IRIC, Université de Montréal, Montréal, Canada; <sup>2</sup>Agilent Technologies, Palo Alto, CA
- ThP 101 **Using Chromatographic Resolution to Increase Sensitivity and Spectral Information in LC/MS Peptide Mapping**; Ziling Lu<sup>1</sup>; Beth L. Gillece-Castro<sup>1</sup>; Thomas E. Wheat<sup>1</sup>; Jeffrey R. Mazzeo<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- ThP 102 **Microfluidic Chip for Biomarker Screening in Cancer Cell Extracts**; Hetal Sarvaia<sup>1</sup>; Iulia M. Lazar<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute & State University, Blacksburg, VA
- ThP 103 **Performance of Polystyrene-Divinylbenzene Monolithic ESI Needles for nanoLC-MS/MS Peptide Sequencing**; Mark van Gils<sup>1</sup>; Robert van Ling<sup>2</sup>; Bjorn de Haan<sup>2</sup>; Bas Dolman<sup>2</sup>; Remco Swart<sup>2</sup>; <sup>1</sup>Dionex Corp., Sunnyvale, CA; <sup>2</sup>LC Packings - Dionex, Amsterdam, Netherlands
- ThP 104 **Withdrawn**
- ThP 105 **A Comparison of Matrix Effects, Speed and Sensitivity in UPLC™ and HPLC**; Erin E. Chambers<sup>1</sup>; Claude Mallet<sup>1</sup>; Diane Diehl<sup>1</sup>; Jeffrey Mazzeo<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- ThP 106 **Integration of Microfluidic Devices and FTICR Mass Spectrometry**; Mariam S ElNaggar<sup>1</sup>; Richard A Mathies<sup>1</sup>; Evan R Williams<sup>1</sup>; <sup>1</sup>University of California, Berkeley, CA
- ThP 107 **Using the Inherent Electrochemistry in a Microfabricated Nanospray Emitter System for**

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- Analytical Advantage;** Vilmos Kertesz<sup>1</sup>; Gary J. Van Berkel<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 108 **Electrocapture-based Separation for Mass Spectrometry of Biomolecules;** Juan Astorga-Wells<sup>1</sup>; Susanne Vollmer<sup>1</sup>; Tomas Bergman<sup>1</sup>; Hans Jörnvall<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Stockholm, Sweden
- ThP 109 **Open-Channel Silicon-Based Electrospray Emitter Tips for Coupling with PDMS Microfluidic Systems;** Matthew D. Robbins<sup>1</sup>; Yiqi Luo<sup>1</sup>; Griffin K. Barbula<sup>1</sup>; Oh Kyu Yoon<sup>1</sup>; Ignacio A. Zuleta<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA
- ThP 110 **Confident Identification of Proteins Analyzed by One Sequenced Peptide from Tryptic Digests of pH Fractions Using Monolithic HPLC/MS/MS;** Chul S. Yoo<sup>1</sup>; Tasneem Patwa<sup>1</sup>; Paweena Kreunin<sup>1</sup>; Fred R. Miller<sup>2</sup>; Christian G. Huber<sup>3</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Babara Ann Karmanos Cancer Institute, Detroit, MI; <sup>3</sup>Saarland University, Saarbrücken, Germany
- ThP 111 **Microchip LC-MALDI-MS Using Multiple Monolithic Column Arrays;** Kyung Won Ro<sup>1</sup>; Jian Liu<sup>1</sup>; Daniel R. Knapp<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- ThP 112 **A Sheathless PMMA chip-CE/ESI/MS Interface Utilizing a Wire-assisted Epoxy-gluing Method;** Fu-An Li<sup>1</sup>; Guor-Rong Her<sup>1</sup>; <sup>1</sup>Dept. of Chemistry, National Taiwan University, Taipei, Taiwan
- ThP 113 **Nano-LC-FTMS Analysis of Native and Chemically Modified Nucleic Acids;** Alexei Gapeev<sup>1</sup>; Zhi Shi Guo<sup>1</sup>; Daniel Fabris<sup>1</sup>; <sup>1</sup>University of Maryland Baltimore County, Baltimore, MD
- ThP 114 **Optimization of Nanobore Capillary Trapping Column Geometries for the Analysis of Peptide Mixtures;** John M Neveu<sup>1</sup>; William S Lane<sup>1</sup>; Gary A Valaskovic<sup>2</sup>; <sup>1</sup>Harvard Univ. Microchem. and Proteomics Analysis, Cambridge, MA; <sup>2</sup>New Objective Inc., Woburn, MA

## MALDI SAMPLE PREPARATION II

- ThP 115 **MALDI TOF Mass Spectrometry of Cucurbiturils;** Zbynek Spalt<sup>1</sup>; Shaban Elost<sup>1</sup>; Josef Havel<sup>1</sup>; <sup>1</sup>Masaryk University, Brno, Czech Republic
- ThP 116 **Sub-microliter Volume Online Concentration/Fractionation of Phosphopeptides Prior to MALDI MS Analysis;** Haixia Zhang<sup>1</sup>; Kashmira Rustomji<sup>1</sup>; Ken K.-C. Yeung<sup>1</sup>; <sup>1</sup>The University of Western Ontario, London, ON, Canada
- ThP 117 **Derivatized Carbon Nanotubes as Matrix for MALDI-TOF MS Analysis;** Graham A. McGibbon<sup>1</sup>; Ming Xue<sup>1</sup>; Huaming Li<sup>1</sup>; Alex Adronov<sup>1</sup>; <sup>1</sup>McMaster University, Hamilton, ON, Canada
- ThP 118 **Direct lipids Analyses in Brain Tissue and E. Coli Extract Using Graphite-Assisted Laser Desorption/Ionization Mass Spectrometry;** Sangwon Cha<sup>1</sup>; Edward S. Yeung<sup>1</sup>; <sup>1</sup>Ames Laboratory-US DOE, Iowa State University, Ames, IA
- ThP 119 **PiezoLC Microdispenser for LC Separation and MALDI-TOF Analysis;** Patrick W. Cooley<sup>1</sup>; Ting Chen<sup>1</sup>; David B. Wallace<sup>1</sup>; Femia Hopwood<sup>2</sup>; Andrew Gooley<sup>2</sup>; Frantisek Svec<sup>3</sup>; <sup>1</sup>MicroFab Technologies, Inc., Plano, TX; <sup>2</sup>Proteome Systems, Ltd., North Ryde, Australia; <sup>3</sup>The Molecular Foundry, LBNL, Berkeley, CA
- ThP 120 **Microfluidic Polymeric Integrated Selective Enrichment Target for Sample Preparation and MALDI MS Sample Presentation;** Simon Ekström<sup>1</sup>; Lars Wallman<sup>1</sup>; Gyorgy Marko-Varga<sup>2</sup>; Göran Heldin<sup>3</sup>; Thomas Laurell<sup>1</sup>; <sup>1</sup>Lund University, Lund Institute of

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- Technology, Lund, Sweden; <sup>2</sup>Lund University, Lund, Sweden; <sup>3</sup>Microplast AB, Skara, Sweden
- ThP 121 **Application of Solvent-free Sample Preparation Methods for MALDI-TOFMS to Organometallic and Coordination Compounds;** Laura Hughes<sup>1</sup>; Mark F. Wyatt<sup>1</sup>; Bridget K. Stein<sup>1</sup>; A. Gareth Brenton<sup>1</sup>; <sup>1</sup>EPSRC National Mass Spec. Service Centre, Swansea, U.K.
- ThP 122 **Rapid and Efficient Sample Clean up on Hydrophobic Probe Surface for MALDI Analysis;** Appavu K. Sundaram<sup>1</sup>; Gavin E. Black<sup>1</sup>; Nelli I. Taranenko<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; <sup>1</sup>MassTech, Inc., Columbia, MD
- ThP 123 **Use of Nitrocellulose Membranes for Protein Characterization by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry;** Jose L. Luque-Garcia<sup>1</sup>; Ge Zhou<sup>2</sup>; Tung-Tien Sun<sup>2</sup>; Thomas A. Neubert<sup>1</sup>; <sup>1</sup>Skirball Institute. New York University, New York, NY; <sup>2</sup>Epithelial Biology Unit. New York University, New York, NY
- ThP 124 **Using Fe<sub>3</sub>O<sub>4</sub> Particles as the Matrix and Concentrating Probe for SALDI-MS Analysis of Peptides and Proteins;** Wei-Yu Chen<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>National Chiao Tung University, Hsinchu, Taiwan
- ThP 125 **Comparative Study of Separation Methods for Human Whole Saliva by MALDI-TOF-MS;** Linda Nagore<sup>1</sup>; Conor Mullens<sup>1</sup>; Robert Christy<sup>2</sup>; John Kalns<sup>2</sup>; Lexi Mitchell<sup>2</sup>; Stephan Bach<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, Texas; <sup>2</sup>Hyperion Biotechnology Inc., San Antonio, Texas
- ThP 126 **Using magnetic Particles Coated with Alumina as the Concentrating Probes to Rapidly Enrich Phosphopeptides from Complex Samples;** Cheng-Tai Chen<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>National Chiao Tung University, Hsinchu, Taiwan
- ThP 127 **Affinity Capture Using Fluorescent Dye-Embedded Magnetic Nanoparticles for the Analysis of Pathogens;** Ya-Shiuan Lin<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>National Chiao Tung University, Hsinchu, Taiwan
- ThP 128 **Novel Nanoparticle Preparations as Adaptable and Selective Probes for Biological MALDI Mass Spectrometry;** Katherine A Stumpo<sup>1</sup>; Edward T. Castellana<sup>1</sup>; David H Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- ThP 129 **Further Investigations Into the Use of Pencil Lead as a MALDI-TOFMS Matrix;** G John Langley<sup>1</sup>; Julie M Herniman<sup>1</sup>; Marc S Townell<sup>1</sup>; Claudie Black<sup>2</sup>; Chris Poile<sup>2</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>AWE Aldermaston, Reading, UK
- ThP 130 **Investigation of a Fast, Reproducible LC and Spotting System for Protein Id and Biomarker Discovery;** Dominic Gostick<sup>1</sup>; Matthew Willetts<sup>1</sup>; Brian Williamson<sup>1</sup>; Peter Kovarik<sup>2</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>MDS Sciex, Concord, ON
- ThP 131 **Trypsin Digestion of Proteins Immobilized on the Hydrophobic Surface of an Elastomeric Device;** Xiaoxi (Kevin) Chen<sup>1</sup>; Anthony Murawski<sup>1</sup>; Guannan Kuang<sup>2</sup>; Dan Sexton<sup>2</sup>; William Galbraith<sup>1</sup>; <sup>1</sup>BD Biosciences, Bedford, MA; <sup>2</sup>Dyax Corp., Cambridge, MA
- ThP 132 **Dirty Cheap High Precision Automated LC MALDI Plate Spotting;** Steven H. Seeholzer<sup>1</sup>; <sup>1</sup>Fox Chase Cancer Center, Philadelphia, PA
- ThP 133 **Novel Solventless Sample Preparation Method for MALDI-TOF MS Analysis of Synthetic Polymers;** Patricia M. Peacock<sup>1</sup>; <sup>1</sup>Dupont, Wilmington, DE

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- ThP 134 **Sample Concentrator for AP-MALDI Plate;** Mukta M. Shukla<sup>1</sup>; Ashok K. Shukla<sup>1</sup>; Nelli I. Taranenko<sup>2</sup>; Vladimir M. Doroshenko<sup>2</sup>; <sup>1</sup>Glygen Corp., Columbia, MD; <sup>2</sup>Mass Tech Inc., Columbia, MD
- ThP 135 **Development and Application of Affinity MALDI Plates;** Andre P. Seale<sup>1</sup>; Hyoung Soon Park<sup>2</sup>; Jeong Heon Lee<sup>1</sup>; Lucia A. de Jesus<sup>1</sup>; Yangsun Kim<sup>1</sup>; <sup>1</sup>Proteonik Inc., Ansan, South Korea; <sup>2</sup>Probiom Co. Ltd., Seoul, South Korea
- ThP 136 **Isotopic Analysis of Actinides Using MALDI TOF MS and Pencil Lead as a Matrix;** Claudia K Black<sup>1</sup>; Chris Poile<sup>1</sup>; G John Langley<sup>2</sup>; Julie Herniman<sup>2</sup>; <sup>1</sup>AWE Aldermaston, Reading, Berkshire, UK; <sup>2</sup>University of Southampton, Southampton, UK

### INSTRUMENTATION: NEW CONCEPTS II

- ThP 137 **Detection of Intact Proteins with DESI-MS: Application to Microorganism Biomarker Detection;** Yong-Seung Shin<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY
- ThP 138 **Reduction of Chemical Background Interferences in API LC-MS using Exclusive Chemical Reactions with a Reagent;** Xinghua Guo<sup>1</sup>; Andries P. Bruins<sup>1</sup>; Tom Covey<sup>2</sup>; <sup>1</sup>University of Groningen, Groningen, The Netherlands; <sup>2</sup>MDS Sciex, Concord, Canada
- ThP 139 **Laser-driven Acoustic Desorption of Organic Molecules from Back-Irradiated Solid Foils;** Alexander V. Zinovev<sup>1</sup>; Wallis F. Calaway<sup>1</sup>; Michael J. Pellin<sup>1</sup>; Igor V. Veryovkin<sup>1</sup>; <sup>1</sup>Argonne National Laboratory, Argonne, IL
- ThP 140 **Eliminating Post-Purification Liquid Handling Through Immediate Fraction Analysis Using a MUX Purification Factory;** Michael M. Kwok<sup>1</sup>; John Isbell<sup>1</sup>; Ding Yuan<sup>1</sup>; <sup>1</sup>Genomics Institute of the Novartis Research Foundation, San Diego, CA
- ThP 141 **Surface Induced Dissociation (SID) in a Quadrupole Time of Flight Mass Spectrometer - Towards the Study of Larger Biomolecules;** Asiri S. Galhena<sup>1</sup>; Shai Dagan<sup>1</sup>; Christopher M. Jones<sup>1</sup>; Richard L. Beardsly<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, Arizona
- ThP 142 **Using Collision Activation Dissociation (CAD) and Electron Transfer Dissociation (ETD) to Identify Peptides and Proteins;** Paul C. Goodley; Ning Tang; David Horn; <sup>1</sup>Agilent Technologies, Santa Clara, California
- ThP 143 **Acoustic Desorption/Ionization with Room Temperature Ionic Liquids (RTIL) as a Source for MS;** Peter R. Harris<sup>1</sup>; Christine L. Gatlin-Bunai<sup>1</sup>; K. Aurelia Ball<sup>2</sup>; Eugene R. Tracy<sup>1</sup>; William E. Cooke<sup>1</sup>; <sup>1</sup>College of William & Mary, Williamsburg, VA; <sup>2</sup>Middlebury College, Middlebury, VT
- ThP 144 **On-line Atmospheric Pressure Sampling Laser Desorption Ionization;** Damien A. Narcisse<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, Louisiana
- ThP 145 **Reactive Landing of Peptide Ions on Surfaces: A Novel Approach for Preparation of Peptide Arrays Using Soft Landing;** Peng Wang<sup>1</sup>; Omar Hadjar<sup>1</sup>; Jean H. Futrell<sup>1</sup>; Paul L. Gassman<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 146 **Applying Superfluid Helium Nanodroplets to the Study of Ions: New Possibilities;** Travis M. Falconer<sup>1</sup>; William K. Lewis III<sup>1</sup>; Aaron M. Johnson<sup>1</sup>; Raymond J. Bemish<sup>2</sup>; Gary L. Glish<sup>1</sup>; Roger E. Miller<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Pfizer Inc., Groton, CT

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- ThP 147 **Design and Performance of a Novel Instrument for Soft-Landing of Bio-Molecular Ions on Surfaces;** Omar Hadjar<sup>1</sup>; Peng Wang<sup>1</sup>; Yury Dessiatierik<sup>1</sup>; Jean H. Futrell<sup>1</sup>; A. Scott Lea<sup>1</sup>; Jason Green<sup>2</sup>; R. Graham Cooks<sup>2</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratories, Richland, WA; <sup>2</sup>Purdue University, West Lafayette, IN
- ThP 148 **Toward Soft-Landing of Protein Complexes as Sample Preparation for Imaging by Electron Microscopy;** Douglas A. Simmons<sup>1</sup>; Brandon T. Ruotolo<sup>1</sup>; Justin L. P. Benesch<sup>1</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, United Kingdom
- ThP 149 **The Identification and Characterization of Heavily Posttranslationally Modified Proteins on Chips Through Chemical Modification;** Bernard F. Gibbs<sup>1</sup>; Robert Masse<sup>2</sup>; Mike Aguiar<sup>1</sup>; <sup>1</sup>McGill University, Montreal, Canada; <sup>2</sup>MDS Pharma Services, Saint Laurent (Montreal), Canada
- ThP 150 **Surface-Surface (Ping-Pong) Neutralization-Reionization Mass Spectrometry;** Luke E. Adams<sup>1</sup>; Xinli Yang<sup>1</sup>; František Tureček<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA

### PORTABLE INSTRUMENTATION

- ThP 151 **Calibration of a Field-Portable GC/MS for Chemical Warfare Agents and Toxic Industrial Chemicals;** Jon Onstot<sup>1</sup>; Corrie Carnes<sup>1</sup>; Robert Walton<sup>2</sup>; Charles Sadowski<sup>3</sup>; Jacqueline Piotrowski<sup>2</sup>; Jonathan Chambers<sup>1</sup>; Richard Ludwick<sup>1</sup>; David Hodgson<sup>1</sup>; <sup>1</sup>Midwest Research Institute, Kansas City, MO; <sup>2</sup>Navy Environmental Health Center, Portsmouth, VA; <sup>3</sup>Inficon Corporation, Syracuse, NY
- ThP 152 **Hand-portable Gas Chromatograph-Mass Spectrometer System Based on a Miniature Toroidal RF Ion Trap for Detection and Identification of Threat Agents;** Edgar D. Lee<sup>1</sup>; Jeffrey L. Jones<sup>1</sup>; Randall W. Waite<sup>1</sup>; Samuel E. Tolley<sup>1</sup>; Steven R. Lo Forte<sup>1</sup>; Kenneth D. Nemelka<sup>1</sup>; Harold D. Tolley<sup>1</sup>; Gary B. Collins<sup>1</sup>; Jesse A. Contreras<sup>2</sup>; James R. Oliphant<sup>1</sup>; Jacolin A. Murray<sup>2</sup>; Gregory E. Henry<sup>1</sup>; H. Dennis Tolley<sup>2</sup>; Alan L. Rockwood<sup>3</sup>; Stephen A. Lammert<sup>2</sup>; Milton L. Lee<sup>2</sup>; <sup>1</sup>Palmar Technologies, Highland, UT; <sup>2</sup>Brigham Young University, Provo, UT; <sup>3</sup>ARUP Inst. for Clinical and Experimental Pathology, Salt Lake City, UT
- ThP 153 **Handheld Rectilinear Ion Trap Mass Spectrometer;** Liang Gao<sup>1</sup>; Qingyu Song<sup>1</sup>; Charles D. Fico<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Garth E. Patterson<sup>2</sup>; Brent Knecht<sup>2</sup>; Jason L. Springston<sup>2</sup>; Adam D. Keil<sup>1</sup>; Robert J. Noll<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Aston Lab/Purdue University, West Lafayette, IN; <sup>2</sup>Griffin Analytical Technologies Inc., West Lafayette, IN
- ThP 154 **Detection of Novel Biomarkers with the TinyTOF: Potential for Point-of-Care Mass Spectrometry;** Christine A. Jelinek<sup>1</sup>; Sara C. McGrath<sup>1</sup>; Theresa G. Evans-Nguyen<sup>1</sup>; Robert J. Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 155 **Withdrawn**
- ThP 156 **Axial Time of Flight Mass Spectrometry (Axial-TOF-MS);** Brian G. Frederick<sup>1</sup>; Jay LeGore<sup>1</sup>; Robert Jackson<sup>1</sup>; Bronson Crothers<sup>1</sup>; Daniel Martin<sup>1</sup>; <sup>1</sup>Stillwater Scientific Instruments, Orono, ME
- ThP 157 **Characterization of the Biological Agent Detection and Identification Capabilities of a Field Portable Mass Spectrometer;** Kevin J. Hart<sup>1</sup>; Cyril V. Thompson<sup>1</sup>; Arpad A. Vass<sup>1</sup>; Marcus B. Wise<sup>1</sup>; Wayne H. Griest<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN

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- ThP 158 **Performance Characterization of High Pressure Electron Multipliers Under Poor (30 Milli-Torr) Vacuum Conditions**; Raymond Cochran<sup>1</sup>; Bruce N Laprade<sup>1</sup>; <sup>1</sup>BURLE Electro-Optics, Sturbridge, MA
- ThP 159 **Investigations of Membrane Introduction Transport Phenomena in an Underwater Mass Spectrometer**; Ryan J. Bell<sup>1</sup>; Friso H.W. van Amerom<sup>2</sup>; Peter G. Wenner<sup>1</sup>; Strawn K. Toler<sup>2</sup>; R. Timothy Short<sup>2</sup>; Robert H. Byrne<sup>1</sup>; <sup>1</sup>University of South Florida, St Petersburg, FL; <sup>2</sup>Center for Ocean Technology, St Petersburg, FL
- ThP 160 **Desorption Electrospray Ionization with a Portable Mass Spectrometer: In-situ Analysis of Ambient Surfaces**; Christopher C. Mulligan<sup>1</sup>; Nari N. Talaty<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN

### FLAVORS AND FRAGRANCES

- ThP 161 **Characterization of Reaction Products and Kinetics of Maillard Reactions of Dark Malts with Amino Acids by Chromatography and Mass Spectrometry**; Katrina E. Vaitkunas<sup>1</sup>; Victor Ryzhov<sup>1</sup>; Andrea Weinecke<sup>2</sup>; Robert Sobel<sup>2</sup>; <sup>1</sup>Northern Illinois University, De Kalb, IL; <sup>2</sup>Flavors of North America, Inc., Geneva, IL
- ThP 162 **A 3-Stage Preconcentrating Inlet for Trace Analysis of Volatile Headspace Organics by Gas Chromatography / Electron-Impact Ionization Mass Spectrometry**; Daniel B. Cardin<sup>1</sup>; Chris Casteel<sup>1</sup>; <sup>1</sup>Entech Instruments, Inc, Simi Valley, CA
- ThP 163 **Rapid Testing of Olive Oil Quality Using SIFT-MS**; Murray McEwan<sup>1</sup>; Brett M Davis<sup>1</sup>; <sup>1</sup>University of Canterbury, Christchurch, New Zealand
- ThP 164 **Early Detection of Fire by Smoldering Odor**; Takashi Nohmi<sup>1</sup>; <sup>1</sup>Nohmi Bosai Co Ltd, Shinjuku, Tokyo Japan
- ThP 165 **Using Chemometrics to Show a Direct Relationship between Analytical and Sensory Data**; Wayne E. Wargo<sup>1</sup>; Susan M. Fawcett<sup>1</sup>; Michael E. Larson<sup>1</sup>; Janis E. Dugle<sup>1</sup>; <sup>1</sup>Abbott Laboratories - RPD, Columbus, OH

### DRUG METABOLISM: REACTIVE INTERMEDIATES AND ADDUCTS

- ThP 166 **The Development of a Strategy for Unambiguous Identification of Reactive Intermediate/Metabolite**; Xue Snow Ge<sup>1</sup>; Jun Shen<sup>1</sup>; Babu Subramanyam<sup>1</sup>; Jih-Lie Tseng<sup>1</sup>; <sup>1</sup>Berlex Biosciences, Richmond, CA
- ThP 167 **Covalent Binding of a p38 MAP Kinase Inhibitor AMG 476 to Rat Hemoglobin**; Chun Li<sup>1</sup>; Sekhar Surapaneni<sup>1</sup>; Jeana Warren<sup>1</sup>; Gondi Kumar<sup>1</sup>; Dawei Zhang<sup>1</sup>; Celia Dominguez<sup>1</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA
- ThP 168 **Comparison of Mass Spectrometry Methods for the Detection of Glutathione Conjugates**; Yuan Chen<sup>1</sup>; Gargi Choudhary<sup>2</sup>; Quynh Ho<sup>1</sup>; Diane Cho<sup>2</sup>; Fitch William<sup>1</sup>; <sup>1</sup>Roche Palo Alto LLC, Palo Alto, CA; <sup>2</sup>Thermo Electron Corporation, San Jose, CA
- ThP 169 **Identification the Reactive Site of Wortmannin with Respect to Covalent Protein Binding**; Jianyao Wang<sup>1</sup>; Lin Deng<sup>1</sup>; William DeMaio<sup>1</sup>; Fangbiao Li<sup>1</sup>; Rasmy Talaat<sup>1</sup>; <sup>1</sup>Wyeth, Collegeville, PA
- ThP 170 **Studies of the Protein Adducts of Carbamazepine and Phenytoin Reactive Metabolites**; Ling Xu<sup>1</sup>; Wei Lu<sup>2</sup>; Ying Yang<sup>1</sup>; Jack Uetrecht<sup>2</sup>; <sup>1</sup>PMSC, Faculty of Medicine, U of Toronto, Toronto, Canada; <sup>2</sup>Faculty of Pharmacy & Faculty of Medicine, Toronto, Canada
- ThP 171 **Ultrafiltration LC-MS-MS Identification of Alkyl Phenols in Prempro that Form Electrophilic Metabolites**; Aarti D. Sawant<sup>1</sup>; Hong Liu<sup>1</sup>; Benjamin M.

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- Johnson<sup>1</sup>; Judy L. Bolton<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL
- ThP 172 **Alkylation of DNA by Electrophilic Metabolites of p-Cresol from Prempro**; Long Yuan<sup>1</sup>; Judy L. Bolton<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL
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- ThP 174 **Reactive Intermediate Screening Using Negative Ion Tandem Mass Spectrometry**; Yau Yi Lau<sup>1</sup>; Robert Steffek<sup>1</sup>; Peter Dandliker<sup>1</sup>; <sup>1</sup>Abbott Laboratories, Abbott Park, IL
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- ThP 177 **LC/MS Method for the Simultaneous Determination of Buprenorphine, Norbuprenorphine and the Enantiomers of Methadone and EDDP in Human Plasma**; Maria E. Rodriguez-Rosas<sup>1</sup>; Michelle R. Lofwall<sup>2</sup>; Eric C. Strain<sup>2</sup>; Irving W. Wainer<sup>1</sup>; <sup>1</sup>National Institute on Aging, NIH, Baltimore, MD; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
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- ThP 179 **Microsomal Metabolism, Plasma Protein Binding, Plasma and Urine Concentrations of Methadone and EDDP by a Validated Enantiomeric LC/ESI-MS-MS**; Shen-Nan Lin<sup>1</sup>; Lollita Lamm<sup>1</sup>; Yan Chang<sup>1</sup>; Ryan Nielsen<sup>1</sup>; Mark K. Greenwald<sup>3</sup>; Todd Hieronymus<sup>2</sup>; Mahmoud S. Ahmed<sup>2</sup>; David E. Moody<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>The University of Texas Medical Branch, Galveston, TX; <sup>3</sup>Wayne State University, School of Medicine, Detroit, MI
- ThP 180 **Evaluation of Chiral Differentiation Using Chemical Ionization in a Hybrid Quadrupole Ion Trap Mass Spectrometer**; Teresa M. Vail<sup>1</sup>; O. David Sparkman<sup>1</sup>; Patrick R. Jones<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA
- ThP 181 **LC/MS Chiral Methods and its Application in Bioanalysis**; Dawei Zhou<sup>1</sup>; Yong-Xi Li<sup>1</sup>; Zhe-ming Gu<sup>1</sup>; <sup>1</sup>XenoBiotic Laboratories, Inc., Plainsboro, NJ
- ThP 182 **Improving Chromatographic Performance and Throughput in Bioanalysis with Supercritical Fluid Chromatography-MS/MS (SFC-MS/MS)**; Luca C. Matassa<sup>1</sup>; Chris R. Bowerbank<sup>1</sup>; Ti Zhang<sup>1</sup>; <sup>1</sup>Tandem Labs, Salt Lake City, Utah, 84124
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Derek B. Laskar<sup>1</sup>; Daniel B. Kassel<sup>1</sup>; <sup>1</sup>Takeda SD, Inc., San Diego, CA

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- ThP 185 **Elemental Composition Elucidation Method and Software for Identifying Low Molecular Weight Chemicals by Exact Mass MS/MS;** Shigeru Suzuki<sup>1</sup>; Yukio Oonishi<sup>2</sup>; <sup>1</sup>Chubu University, Kasugai, JAPAN; <sup>2</sup>Environmental Research Institute Inc., Osaka, JAPAN
- ThP 186 **Application of Speciation Analysis Using HPLC-ICP-MS and HPLC-ESI-MS for the Investigation of Metal-Containing Species in Pharmaceutical Process Research;** Qiang Tu<sup>1</sup>; Tiebang Wang<sup>1</sup>; Christopher Welch<sup>1</sup>; Peng Wang<sup>1</sup>; Xiujuan Jia<sup>1</sup>; Michael Doyle<sup>2</sup>; <sup>1</sup>Merck & Co., Inc., Rahway, NJ; <sup>2</sup>University of Maryland, College Park, MD
- ThP 187 **Lipidomics in Leech Brain Regeneration by Cluster TOF-SIMS Imaging;** Karim Arafah<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Delphine Debois<sup>2</sup>; Remi Lemaire<sup>1</sup>; Alain Brunelle<sup>2</sup>; Olivier Laprevote<sup>2</sup>; Isabelle Fournier<sup>1</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>MALDI Imaging Team, FRE CNRS 2933, Univ. of Lille, Villeneuve d'Ascq, France; <sup>2</sup>Laboratoire de Spectrométrie de Masse, ICNS-CNRS, Gif-sur-Yvette, France
- ThP 188 **Distinguishing Stereo- and Structural Isomers with Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and Principle Component Analysis;** Elena SF Berman<sup>1</sup>; Kristen S. Kulp<sup>1</sup>; Mark G. Knize<sup>1</sup>; Kuang Jen Wu<sup>1</sup>; <sup>1</sup>Lawrence Livermore Nat Lab, Livermore, CA
- ThP 189 **Enhanced Metabolite Profiling Through Affinity Capture and Isotope Labeling;** Grace O'Maille<sup>1</sup>; Linh Hoang<sup>1</sup>; Anders Nordström<sup>1</sup>; Eden Go<sup>1</sup>; Paul O'Maille<sup>2</sup>; Chuan Qin<sup>1</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>The Salk Institute for Biological Studies, La Jolla, CA
- ThP 190 **Advanced Software for Multi Analyte Screening of ToF-MS Data Using Library Searching and Accurate Mass Confirmation;** Jeff Goshawk<sup>1</sup>; Peter Hancock<sup>1</sup>; Daniel McMillan<sup>1</sup>; <sup>1</sup>Waters Corp., MS Technologies Centre, Manchester, UK
- ThP 191 **High-Throughput Small Molecule Determination: A Comparison of MUX-LC and UPLC with LC/UV/ELSD/TOFMS Systems;** Jim Conboy<sup>1</sup>; Navin Varshney<sup>1</sup>; Michele Kelly<sup>1</sup>; <sup>1</sup>Pfizer Inc, Groton, CT
- ThP 192 **A Generic Quantitative Analysis of Nucleoside Analogs by LC/MS/MS;** Tuyen Nguyen<sup>1</sup>; Xin Zhang<sup>1</sup>; Jakal Amin<sup>1</sup>; Christopher Marlor<sup>2</sup>; Gohar Mushtaq<sup>2</sup>; Doug Buechter<sup>2</sup>; <sup>1</sup>Charles River Labs, Bioanalytical Chemistry, Worcester, MA; <sup>2</sup>Achillion Pharmaceuticals, New Haven, CT
- ThP 193 **An Approach for the Analytical Evaluation of a Large, Small-molecule, Chemical Database;** Christopher C. Lai<sup>1</sup>; Holly L. Haley<sup>1</sup>; Lawrence R. Phillips<sup>2</sup>; John H. Cardellina<sup>2</sup>; Marc C. Nicklaus<sup>3</sup>; Johannes H. Voight<sup>1</sup>; Joseph J. Barchi<sup>1</sup>; Nouri Neamati<sup>3</sup>; James A. Kelley<sup>1</sup>; <sup>1</sup>Center for Cancer Research, NCI, NIH, Frederick, MD; <sup>2</sup>Developmental Therapeutics Program, NCI, NIH, Frederick, MD; <sup>3</sup>School of Pharmacy, USC, Los Angeles, CA

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- ThP 196 **Characterization of Bis(diaryl)Aminoxylys, Tetramethylpyrrolidineaminoxyl Substituted Peptides and Tetramethylpiperidineaminoxyl Based Biradicals by EI MS;** Boris V. Rozynov<sup>1</sup>; <sup>1</sup>Aspen Research Corporation, St Paul, MN
- ThP 197 **Use of LC-MS/MS for the Evaluation of the Presence of Impurities in Two Novel PET Tracers;** Kerry A. Riffel<sup>1</sup>; Terence Hamill<sup>1</sup>; Eric Hostetler<sup>1</sup>; H. Donald Burns<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- ThP 198 **The Use of ESI-LCMS and MALDI Mass Spectrometry in the Analysis and Characterisation of Synthetic Phospholipids and Betaines;** Stephen J Rumbelow<sup>1</sup>; Kevin W Penfield<sup>1</sup>; <sup>1</sup>Uniqema Technical Center, New Castle, Delaware
- ThP 199 **Diversity of Photo-Labeling/Crosslinking on Small Molecules: A Liquid Chromatography/Tandem Mass Spectrometric Investigation;** Takemichi Nakamura<sup>1</sup>; Naoki Kanoh<sup>2</sup>; Kaori Honda<sup>2</sup>; Hiroyuki Osada<sup>2</sup>; <sup>1</sup>RIKEN, Biomolecular Characterization, Wako, Saitama, Japan; <sup>2</sup>RIKEN, Antibiotics Lab, Wako, Saitama, Japan
- ThP 200 **Does Resolution Actually Impact on Accurate Mass Determinations?;** Federico Riccardi Sirtori<sup>1</sup>; Maristella Colombo<sup>1</sup>; <sup>1</sup>Nerviano Medical Sciences, Nerviano (Milan), Italy
- ThP 201 **Investigation and Characterization of Bis-Retinoid Pyridinium Compound Photooxidation Products by HPLC-MS;** Aleksey S. Kononikhin<sup>2</sup>; Marina A. Jakovleva<sup>2</sup>; Mikhail A. Ostrovskiy<sup>2</sup>; Eugene N. Nikolaev<sup>1</sup>; <sup>1</sup>The Institute for Energy Probl. Chem. Physics, Moscow, Russia; <sup>2</sup>The Institute for Biochemical Physics, Moscow, Russia
- ThP 202 **Automated LC-MS/MS Impurity Analysis;** Alina Dindyal-Popescu<sup>1</sup>; J.C. Yves Le Blanc<sup>1</sup>; Julie Wingate<sup>1</sup>; Jean-Claude Wolff<sup>2</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Concord, Canada; <sup>2</sup>GlaxoSmithKline, Stevenage, United Kingdom
- ThP 203 **Multiresidue Pesticide Screening by LC-ESI-TOF MS;** Petra Decker<sup>1</sup>; Christian Neusuess<sup>1</sup>; Matthias Pelzing<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany
- ThP 204 **True Automated Exact Mass of Pharmaceutically Relevant Synthetic Compounds – Is it Ready for Prime Time?;** Justin G. Stroh<sup>1</sup>; Christopher Petucci<sup>1</sup>; Scott Brecker<sup>1</sup>; Yanxun Cai<sup>1</sup>; <sup>1</sup>Wyeth Research, Collegeville, PA
- ThP 205 **Automated Chemical Logic to Improve Prediction of Chemical Formula;** Eva Duchoslav<sup>1</sup>; J.C. Yves Le Blanc<sup>1</sup>; Julie Wingate<sup>1</sup>; Alina Dindyal-Popescu<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- ThP 206 **Qualitative Analysis of the Fragmentation Reactions of Negative Organic Ions in Drug Discovery;** Christopher Petucci<sup>1</sup>; Scott Brecker<sup>1</sup>; Justin Stroh<sup>1</sup>; <sup>1</sup>Wyeth Research, Collegeville, PA
- ThP 207 **Use of LC-MS and Hydrogen/Deuterium Exchange to Distinguish N-Oxides and Hydroxylated Forms of**

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- ThP 208 **Structural Elucidation by Composition Formula Predictor Software Using MS<sup>n</sup> Data;** Holly M. Shackman<sup>1</sup>; Joy M. Ginter<sup>1</sup>; Joseph P. Fox<sup>1</sup>; Masayuki Nishimura<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 209 **Alkylloxycarbonylation as an Alternative Method for Liquid Chromatographic-Mass Spectrometric Analysis of Urinary Diuretics;** Junghyun Son<sup>1</sup>; Jong-Dae Kim<sup>1</sup>; Ju-Yeon Moon<sup>1</sup>; Dong-Hyun Kim<sup>1</sup>; Man Ho Choi<sup>1</sup>; <sup>1</sup>Korea Institute of Science and Technology, Seoul, Korea
- ThP 210 **Barbiturate Analysis by USP 28 -NF23 General Chapter <361>, Isn't It Time for an Upgrade?;** Mark Jacyno<sup>1</sup>; Reno Nguyen<sup>1</sup>; Mark Waksmonski<sup>1</sup>; <sup>1</sup>Grace Davison, Deerfield, IL
- ThP 211 **Evaluation of Using MALDI -TOF/MS and Electrospray TOF/MS for Biomarker Discovery;** Yulin Huang<sup>1</sup>; David Ho<sup>1</sup>; Keith Ohm<sup>1</sup>; Lily Li<sup>1</sup>; <sup>1</sup>PharmaKD Inc., Woburn, MA
- ThP 212 **Analysis of Fullerene Derivatives by Ion Trap and Time-of-Flight Mass Spectrometry;** K. Janota<sup>1</sup>; Christopher Smart<sup>2</sup>; <sup>1</sup>Agilent Technology, Paramus, NJ; <sup>2</sup>Vassar College, Poughkeepsie, NY
- ThP 213 **Energy-resolved Fragmentation of Acyl Homoserine Lactones;** Nathan D. Leigh<sup>1</sup>; <sup>1</sup>University of Missouri - Columbia, Columbia, MO
- ThP 214 **The Characterization of Phenolic Content in Almond industry "Waste" by Negative Ion ESI Capillary LC/MS;** Bruce Wilcox<sup>1</sup>; Christine Hughey<sup>2</sup>; Lilian Were<sup>2</sup>; <sup>1</sup>Eksigent Technologies, Dublin, CA; <sup>2</sup>Chapman University, Orange, CA
- ThP 215 **Automated Elemental Composition Determination and Correlation of Precursor with Product Ions Based on Orthogonal Acceleration, Time-of-Flight Mass Spectra;** G. Wayne Sovocool<sup>1</sup>; Michael C. Zumwalt<sup>2</sup>; Andrew H. Grange<sup>1</sup>; <sup>1</sup>U.S. EPA, ORD, NERL, ESD, Las Vegas, NV; <sup>2</sup>Agilent Technologies, Englewood, CO
- ThP 216 **Speciation of Selenium-Enriched Samples by Parallel Elemental and Molecular Mass Spectrometry (PEMMS) and Peak Parameterization;** J. Thomas Brenna<sup>1</sup>; Gavin L. Sacks<sup>1</sup>; Louis A. Derry<sup>1</sup>; Gerald F. Combs<sup>2</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>USDA- Human Nutrition Research Center, Grand Forks, ND
- ThP 217 **Characterization of Di- and Tri-substituted Sulfonated Azo Dyes by LC/ESI/MS/MS, LC/ESI/MS and LC/CI/MS;** James M. Chapman<sup>1</sup>; Cagney Bennett<sup>1</sup>; Andrea Dolezal<sup>1</sup>; Scott Niemann<sup>2</sup>; <sup>1</sup>Rockhurst University, Kansas City, MO; <sup>2</sup>CSS Analytical Company, Shawnee, KS

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- ThP 218 **Detection and Identification of Ricin and Abrin Using SELDI-TOF Mass Spectrometry;** Rajaseger Ganapathy<sup>1</sup>; Vidhya Novem<sup>1</sup>; Jessica Huizhen Woo<sup>1</sup>; <sup>1</sup>Defence Medical & Environmental Research Institute, Singapore
- ThP 219 **Synthesis and Characterization of Oligodeoxynucleotides Containing Tandem Lesions of Thymidine Glycol and 8-oxo-2'-Deoxyguanosine;** Yuesong Wang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of California, Riverside, CA
- ThP 220 **Plasma Source Differential Ion Suppression During Routine Sample Analysis By A Validated LC-MS/MS**

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- ThP 221 **Effects of the Environmental Contaminant Bisphenol A on the Rat Pituitary Proteome;** Francesco Giorgianni<sup>1</sup>; Amira Wohabrebbi<sup>1</sup>; Laura Canesi<sup>2</sup>; Yingxin Zhao<sup>1</sup>; Dominic M. Desiderio<sup>1</sup>; Achille Cappiello<sup>3</sup>; Pierangela Palma<sup>3</sup>; Sarka Beranova-Giorgianni<sup>1</sup>; <sup>1</sup>University of Tennessee Health Science Center, Memphis, TN; <sup>2</sup>University of Genoa, Genoa, Italy; <sup>3</sup>University of Urbino, Urbino, Italy
- ThP 222 **Determination of Heterocyclic Aromatic Amines in Cooked Muscle Tissue by Electrospray Ionization HPLC/MS/MS;** Michael Erickson<sup>1</sup>; Thomas Fillmore<sup>1</sup>; <sup>1</sup>Columbia Analytical Services, Kelso, WA
- ThP 223 **A Novel Approach to the Quantitation of 1,3-Butadiene Gas in Human Exhalate;** Kirk Newland<sup>1</sup>; Toby Julian<sup>1</sup>; Ridha Nachi<sup>1</sup>; Lee Zhu<sup>1</sup>; <sup>1</sup>MDS Pharma Services, Lincoln, NE
- ThP 224 **Toxicological Studies on Mimics of EHC-93 Particle Types on a Human Lung Epithelial Cell-line (A549) in vitro;** Ndukauba M. Elegbasim<sup>2</sup>; Goerge R. Agnes<sup>2</sup>; Stephen F. Van Eeden<sup>3</sup>; <sup>1</sup>Simon Fraser University, Burnaby, BC, Canada; <sup>2</sup>Simon Fraser University, Burnaby, BC, Canada; <sup>3</sup>University of British Columbia, Vancouver, BC, Canada
- ThP 225 **ReLiquid Chromatography-Tandem Mass Spectrometry Method using Heated Electro-spray Ionization for the Determination of Specific Metabolites of Contemporary Pesticides in Urine;** Roberto Bravo<sup>1</sup>; Jessica Norrgran<sup>1</sup>; Paula A Restrepo<sup>1</sup>; Amanda M. Bishop<sup>2</sup>; Ralph D. Jr. Whitehead<sup>1</sup>; Larry L. Needham<sup>1</sup>; Dana B. Barr<sup>1</sup>; <sup>1</sup>Centers For Disease Control and Prevention, Atlanta, Georgia; <sup>2</sup>Battelle, Atlanta, Georgia
- ThP 226 **Determination of Extractable Formaldehyde in Metered-Dose Packaging Components by HPLC-MS;** Anulfo Valdez<sup>1</sup>; F. Sedinam Amegavibor<sup>1</sup>; Stephen A. Ampofo<sup>1</sup>; Yaping Zhu<sup>1</sup>; Lex A. Adjei<sup>1</sup>; <sup>1</sup>Kos Pharmaceuticals, Inc., Cranbury, NJ
- ThP 227 **Simultaneous Quantification of 3-Nitrotyrosine and 3-Bromotyrosine in Human Urine by Isotope Dilution Liquid Chromatography/Electrospray Ionization-Tandem Mass Spectrometry;** Wei-Loong Chiu<sup>1</sup>; Hauh-Jyun Candy Chen<sup>1</sup>; <sup>1</sup>National Chung Cheng University, Ming-Hsiung, Chia-Yi, Taiwan
- ThP 228 **Reactivity of Acrolein with Peptidyl Amino Acid Residues;** Jian Cai<sup>1</sup>; Aruni Bhatnagar<sup>1</sup>; William M. Pierce, Jr.<sup>1</sup>; <sup>1</sup>University of Louisville, Louisville, KY
- ThP 229 **Examination of Isocyanate Adducts of Human Serum Albumin by Matrix Assisted Laser Desorption Ionisation - Mass Spectrometry;** Tasneem Muharib<sup>1</sup>; Malcolm R Clench<sup>1</sup>; John White<sup>2</sup>; Duncan A Rimmer<sup>2</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>Health and Safety Laboratory, Buxton, UK
- ThP 230 **Recognizing the Proteomic Patterns of Induced Toxicity with 1D-ZOOMER Approach;** Andrey Lisitsa<sup>1</sup>; Igor Nikitin<sup>1</sup>; Alexey Podoplelov<sup>1</sup>; Alexander Archakov<sup>1</sup>; Herbert Thiele<sup>2</sup>; <sup>1</sup>Institute of Biomedical Chemistry, Moscow, Russia; <sup>2</sup>Bruker Daltonics GmbH, Bremen, Germany
- ThP 231 **Mass Spectrometric Analysis of Synaptosomal Protein Modification Upon Exposure to Selected &alpha;,&beta;-Unsaturated Carbonyl Compounds;**

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- ThP 233 **Liquid Chromatography/Tandem Mass Spectrometric Method for the Simultaneous Determination of Six Tobacco-Specific Nitrosamine Metabolites;** Huiling Lee<sup>1</sup>; Giing Chiying Wang<sup>1</sup>; Dennis Paul Hsientang Hsieh<sup>1</sup>; <sup>1</sup>Division of Environmental Health and Occupational, Miaoli, Taiwan R.O.C
- ThP 234 **General Unknown Screening of Drugs and Toxic Compounds in Human Samples Using on Hybrid Triple Quadrupole - Linear Ion-Trap Instruments;** Pierre Marquet<sup>1</sup>; Joaquim Soares Granja<sup>2</sup>; <sup>1</sup>University hospital, Limoges, France; <sup>2</sup>Applied Biosystems, Courtaboeuf, France
- ThP 235 **Measurement of Protein Cross-Links o,o'-Dityrosine in Human Urine by Isotope Dilution Liquid Chromatography/Electrospray Ionization-Tandem Mass Spectrometry;** Chia-Ming Chang<sup>1</sup>; Hauh-Jyun Candy Chen<sup>1</sup>; <sup>1</sup>National Chung Cheng University, Ming-Hsiung, Chia-Yi, Taiwan
- ThP 236 **Quantitative Analysis of Alkyldiphenoxide Disulfonates in Anodic Seal Baths by LC-ESI-(Ion Trap)MS and HPLC-UV;** Edward Elizondo<sup>1</sup>; Chris Hanthorn<sup>1</sup>; <sup>1</sup>Henkel Technologies, Madison Heights, MI
- ThP 237 **Identification of Novel Proteins and their Covalent Adducts by Reactive Metabolites of Molinate using Mass Spectrometry;** William T. Jewell<sup>1</sup>; Andrew Campbell<sup>1</sup>; Marion G. Miller-Sears<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA
- ThP 238 **The Inflammation Potential of Particulate Matter as a Function of Its Chemical Composition;** Allen Haddrell<sup>1</sup>; George Agnes<sup>1</sup>; Simone Gross<sup>2</sup>; Stephan van Eeden<sup>2</sup>; Allan Bertram<sup>2</sup>; <sup>1</sup>Simon Fraser University, Vancouver, BC; <sup>2</sup>University of British Columbia, Vancouver, BC
- ThP 239 **Quantitation of Methyl Phosphotriester DNA Adduct of Thymidyl (3'-5') thymidine by LC-APCI-MS/MS;** Fagen Zhang<sup>1</sup>; Michael J. Bartels<sup>1</sup>; Lynn H. Pottenger<sup>1</sup>; B. Bhaskar Gollapudi<sup>1</sup>; Melissa R. Schisler<sup>1</sup>; <sup>1</sup>The Dow Chemical Company, Midland, Michigan
- ThP 240 **Determination of Chlorpyrifos and its Metabolites in Rat Blood Using Liquid Chromatography-Tandem Mass Spectrometry;** Leah N. Williamson<sup>1</sup>; Alvin V. Terry<sup>1</sup>; Michael G. Bartlett<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- ThP 241 **Simultaneous Determination of Four Trace Elements in Human Urine by Dynamic Reaction Cell ICP-MS;** Dongmei Zhou<sup>1</sup>; Sum Chan<sup>1</sup>; Richard E. Reitz<sup>1</sup>; <sup>1</sup>Quest Diagnostics Nichols Institute, San Juan Capistrano, CA
- ThP 242 **Determination of Oxidative DNA Damage in Human Bronchoalveolar Cells by Immunoaffinity Purification and LC/MS/MS;** Dipti Mangal<sup>1</sup>; <sup>1</sup>Center for Pharmacology, Philadelphia, PA
- ThP 243 **Quantification of N-(deoxyguanosin-8-yl)-4-Aminobiphenyl Adducts in N-hydroxy-4-Aminobiphenyl Dosed Human Lymphoblastoid Cells and Their Relationship to Mutation, Toxicity, and Gene Expression Profiling;** Elaine M. Ricicki<sup>1</sup>; Wen Luo<sup>2</sup>; Helmut Zarbl<sup>2</sup>; Paul Vourros<sup>1</sup>; <sup>1</sup>Northeastern

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- University, Boston, MA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- ThP 244 **The Analysis of Alprazolam in Synthetic Urine Via Dual Column Switching;** Charles Yang<sup>1</sup>; Jonathan Beck<sup>1</sup>; Rohan Thakur<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA
- ThP 245 **Improved Dose Metric for Monitoring VX-G Analog in Rats Using GC Tandem Mass Spectrometry (GC-MS/MS);** Jeffrey M. McGuire<sup>1</sup>; Ronald A. Evans<sup>1</sup>; Edward M. Jakubowski<sup>1</sup>; Sandra A. Thomson<sup>1</sup>; <sup>1</sup>US Army Edgewood CB Center, Aberdeen Proving Ground, MD
- ThP 246 **Detection of Ethylene and Propylene Oxide Metabolites in Urine by GC/MS;** Jeffrey S. Snow<sup>1</sup>; Michael F. Martin<sup>1</sup>; Timothy R. Croley<sup>1</sup>; <sup>1</sup>Commonwealth of Virginia, Richmond, VA
- ThP 247 **Development and Validation of a LC/MS TOF Method for Determining Isopropyl Methylphosphonic Acid in Minipig Plasma following Sarin Vapor Exposures;** Ronald A. Evans<sup>1</sup>; Julie A. Renner<sup>2</sup>; Edward M. Jakubowski<sup>1</sup>; Sandra A. Thomson<sup>1</sup>; <sup>1</sup>U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD; <sup>2</sup>SAIC, Gunpowder Branch, MD
- ThP 248 **LC-ES/MS/MS Quantification of O<sup>6</sup>-Alkyldeoxyguanosines in DNA from Mice Exposed to Alkylating Agents;** Mona I. Churchwell<sup>1</sup>; Frederick A. Beland<sup>1</sup>; Daniel R. Doerge<sup>1</sup>; <sup>1</sup>FDA/NCTR, Jefferson, AR
- ThP 249 **Methodology for Creating and Depositing Particulate Matter Onto Cells with MALDI-ToF-MS Monitoring of Differential Expression of Secreted Cytokines;** Edward Lau<sup>1</sup>; Alice Kardjaputri<sup>1</sup>; George Agnes<sup>1</sup>; Stephan van Eeden<sup>2</sup>; <sup>1</sup>Simon Fraser University, Vancouver, Canada; <sup>2</sup>University of British Columbia, Vancouver, Canada
- ThP 250 **A Quantitative Screen for Multiple Classes of Illicit Drugs and Their Primary Metabolites in Human Biological Fluids by LC/MS/MS;** Kevin J. McHale<sup>1</sup>; Angela C. Springfield<sup>2</sup>; <sup>1</sup>Thermo Electron, Somerset, NJ; <sup>2</sup>Tarrant County Medical Examiner, Fort Worth, TX
- ION ACTIVATION AND DISSOCIATION**
- ThP 251 **Charge-Remote Fragmentation of Free Fatty Acids under FAB Conditions;** Valery G. Voinov<sup>1</sup>; Hong Ji<sup>1</sup>; Jeff Morré<sup>1</sup>; Douglas F. Barofsky<sup>1</sup>; Max L. Deinzer<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 252 **Effect of the Surface Morphology on the Energy Transfer in Ion-Surface Collisions;** Zhibo Yang<sup>1</sup>; Omar Hadjar<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 253 **Surface-Induced Dissociation of Molecular Ions in a Digital Ion Trap Mass Spectrometer;** Osamu Furuhashi<sup>1</sup>; Kengo Takeshita<sup>1</sup>; Hideaki Izumi<sup>1</sup>; Kiyoshi Ogawa<sup>1</sup>; Yoshikazu Yoshida<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Li Ding<sup>2</sup>; Michael Sudakov<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Research Laboratory (Europe) Ltd, Manchester, UK
- ThP 254 **A Variational Treatment of the Unimolecular Dissociations of Ionized Methyl Substituted Hydrazine Compounds;** Anne-Marie Boulanger<sup>1</sup>; Emma E. Rennie<sup>1</sup>; Paul M. Mayer<sup>1</sup>; David M. P. Holland<sup>2</sup>; David A. Shaw<sup>2</sup>; <sup>1</sup>University of Ottawa, Ottawa, Canada; <sup>2</sup>Daresbury Laboratory, Daresbury, UK
- ThP 255 **Exploiting Electron Transfer Dissociation Reactions Using High Temperature Bath Gas;** Brittany D.M. Hodges<sup>1</sup>; Hongling Han<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN

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- ThP 256 **Enhancement of Infrared Multiphoton Dissociation Efficiency in a Quadrupole Ion Trap using Metal Complexes with Chromophoric Ligands;** Michael Pikulski<sup>1</sup>; Jeffrey J. Wilson<sup>1</sup>; Apolonio Aguilar<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>The University of Texas at Austin, Austin, TX
- ThP 257 **Ion-Surface Collisions on Cl, Br, and F Terminated Self-Assembled Monolayers (SAMs);** Karen E. Joyce<sup>1</sup>; Zhuhua Qi<sup>1</sup>; Amy Graham<sup>1</sup>; Neal R. Armstrong<sup>1</sup>; Ronald Wysocki<sup>1</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- ThP 258 **CID Fragmentation Pathways of THG and Trenbolone;** Fuyu Guan<sup>1</sup>; Cornelius E. Uboh<sup>2</sup>; Lawrence R. Soma<sup>1</sup>; Scott Peterman<sup>3</sup>; Youwen You<sup>1</sup>; Jeffrey Rudy<sup>2</sup>; <sup>1</sup>University of Pennsylvania, Kennett Square, PA; <sup>2</sup>PA Equine Toxicol. & Research Center, West Chester, PA; <sup>3</sup>Thermo Electron, Finnigan LC-MS, Somerset, NJ
- ThP 259 **Electron Photodetachment and Subsequent Fragmentation of Multiply Charged DNA Ions Under UV-Visible Laser Irradiation;** Valerie Gabelica<sup>1</sup>; Thibault Tabarin<sup>2</sup>; Frederic Rosu<sup>1</sup>; Rodolphe Antoine<sup>2</sup>; Isabelle Compagnon<sup>2</sup>; Michel Broyer<sup>2</sup>; Edwin De Pauw<sup>1</sup>; Philippe Dugourd<sup>2</sup>; <sup>1</sup>University of Liège, Liège, Belgium; <sup>2</sup>University of Lyon I, Lyon, France
- ThP 260 **Effective Temperatures and the Mobile Proton in Activated Ions, Evaluated by Thermal Extrapolation and by ab initio Calculations;** Michael Mautner<sup>1</sup>; Arpad Somogyi<sup>2</sup>; Christian Bleiholder<sup>3</sup>; Bela Paizs<sup>3</sup>; <sup>1</sup>Virginia Commonwealth U., Richmond, Virginia; <sup>2</sup>University of Arizona, Tucson, AZ; <sup>3</sup>German Cancer Research Center, Heidelberg, Germany
- ThP 261 **Improved Isolation Efficiency Using Higher Resolution Isolation in an Ion Trap Mass Spectrometer;** Karen Salomon<sup>1</sup>; Min He<sup>1</sup>; Jae Schwartz<sup>1</sup>; Gargi Choudhary<sup>1</sup>; Diane Cho<sup>1</sup>; <sup>1</sup>Thermo Electron Corp., San Jose, CA
- ThP 262 **Kinetics of Surface Induced Dissociation Using Laser Desorption of C<sub>60</sub> and Silicon Nano Powder Assisted Ionization of N(CH<sub>3</sub>)<sub>4</sub><sup>+</sup>;** Sung Hwan Yoon<sup>1</sup>; Dylan Boday<sup>1</sup>; Chaminda Gamage<sup>1</sup>; Wujuan Wen<sup>1</sup>; Kent Gillig<sup>1</sup>; Shai Dagan<sup>1</sup>; Vicki Wysocki<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- ThP 263 **Addition of Radical Traps Quenches Backbone Electron Capture Dissociation and Redirects it to the Aromatic Sidechains;** Marina A. Belyayev<sup>1</sup>; Jason J. Cournoyer<sup>1</sup>; Cheng Lin<sup>1</sup>; Bogdan A. Budnik<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; <sup>1</sup>Boston University, Boston, MA
- ThP 264 **Probing Collisional Excitation in Ion-Molecule Collisions by Fluorescence Detection;** Clement Poon<sup>1</sup>; Paul M. Mayer<sup>1</sup>; <sup>1</sup>University of Ottawa, Ottawa, Canada
- ThP 265 **ECD of Heptameric gp31 Non-Covalent Complexes Causes Disassembly with Remarkable Charge Separation;** Rimco B.J. Geels<sup>1</sup>; Albert J.R. Heck<sup>2</sup>; Saskia M. van der Vies<sup>3</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM-AMOLF, Amsterdam, Netherlands; <sup>2</sup>Utrecht University, Utrecht, Netherlands; <sup>3</sup>Vrije Universiteit, Amsterdam, Netherlands
- ThP 266 **Metal Ion Binding Affinities and Activation of Phosphate Esters Studied by Threshold Collision-Induced Dissociation and Theory Calculations;** Chunhai Ruan<sup>1</sup>; Hai Huang<sup>1</sup>; Mary T. Rodgers<sup>1</sup>; <sup>1</sup>Wayne state university, Detroit, MI
- ThP 267 **CID Achieved During Mass Acquisition in a QIT-MS Using a Two-frequency Excitation Waveform;** Unige

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A. Laskay<sup>1</sup>; Jennifer J. Hyland<sup>1</sup>; Glen P. Jackson<sup>1</sup>; <sup>1</sup>Ohio University, CICI, Athens, OH

### CARBOHYDRATES AND OLIGOSACCHARIDES III

- ThP 291 **Monoclonal Antibody Carbohydrate Structure Sequencing using Mass Spectrometry and OSCAR: an Algorithm for Assigning Oligosaccharide Topology from MSn Data;** Yan-Hui Liu<sup>1</sup>; Mei Lin<sup>2</sup>; David J. Ashline<sup>3</sup>; Vernon Reinhold<sup>3</sup>; Michael Grace<sup>2</sup>; Birendra N. Pramanik<sup>1</sup>; <sup>1</sup>Schering-Plough Research Institute, Kenilworth, New Jersey; <sup>2</sup>Bristol-Myers Squibb, Hopewell, New Jersey; <sup>3</sup>Department of Chemistry, University of New Hampshire, Durham, New Hampshire
- ThP 292 **Sugar Stereochemistry on Mass Spectrometry;** Yoko Ohashi<sup>1</sup>; Hiroshi Hatase<sup>1</sup>; Takashi Hirano<sup>1</sup>; Shojiro Maki<sup>1</sup>; Haruki Niwa<sup>1</sup>; <sup>1</sup>University of Electro-Communications, Chofu, Tokyo, Japan
- ThP 293 **High-throughput Glycomic Profiling through On-line Permethylolation and LC/MS;** Pilsoo Kang<sup>1</sup>; Yehia Mechref<sup>1</sup>; Milos V. Novotny<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>National Center of Glycomics and Glycoproteomic, Bloomington, IN; <sup>3</sup>METACyt Biochemical Analysis Center, Bloomington, IN
- ThP 294 **Investigation of Glycan Release Methods for Screening Oligosaccharide Biomarkers in Human Serum;** Hyun Joo An<sup>1</sup>; Bensheng Li<sup>1</sup>; Crystal Kirmiz<sup>1</sup>; Suzanne Miyamoto<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- ThP 295 **Automated Detection of Glycan Isobars with the Bioinformatics Tool GlySpy;** Anthony J. Lapadula<sup>1</sup>; David J. Ashline<sup>1</sup>; Hailong Zhang<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>Center for Structural Biology, UNH, Durham, NH
- ThP 296 **LC-MS Detection of Monosaccharides from Yeast Selected for Xylose Consumption;** Lindsay M. Comeaux<sup>1</sup>; R. Paul Levine<sup>2</sup>; Allis S. Chien<sup>1</sup>; Gavin J. Sherlock<sup>3</sup>; <sup>1</sup>Vincent Coates Foundation Mass Spectrometry Lab, Stanford, CA; <sup>2</sup>Department of Biological Sciences, Stanford, CA; <sup>3</sup>Department of Genetics, Stanford, CA
- ThP 297 **Towards the Automated Profiling of Glycans Using nano-PGC FT-ICR MS and IRMPD;** Brian H. Clowers<sup>1</sup>; Katherine Schubothe<sup>1</sup>; Richard Seipert<sup>1</sup>; Crystal Kirmiz<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- ThP 298 **Highly sensitive MALDI MS<sup>n</sup> for Identification of Polysulfated Oligosaccharides by a Simple Pyrene-Derivatization Method;** Junko Amano<sup>1</sup>; Fumio Tougasaki<sup>1</sup>; Koichi Tanaka<sup>2</sup>; <sup>1</sup>The Noguchi Institute, Tokyo, JAPAN; <sup>2</sup>Shimadzu Corporation, Kyoto, JAPAN
- ThP 299 **"Glyco-Peakfinder" – Automated Annotation for MS Peaks of Carbohydrates and Data Base Search in EUROCarbDB;** Kai Maass<sup>1</sup>; René Ranzinger<sup>2</sup>; Hildegard Geyer<sup>1</sup>; Rudolf Geyer<sup>1</sup>; Claus W. von der Lieth<sup>2</sup>; <sup>1</sup>University of Giessen, Giessen, Germany; <sup>2</sup>German Cancer Research Center, Heidelberg, Germany
- ThP 300 **GlycoScreen: A Screening Tool for Comparative Analyses and Assurance of Glycan Profiles;** Hailong Zhang<sup>1</sup>; David J. Ashline<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>Center for Structural Biology, UNH, Durham, NH
- ThP 301 **LC/MS Study of Iodine Attachment for Quantitative Analysis of Carbohydrates by Isotope Dilution Assay;** Eduard Rogatsky<sup>1</sup>; Daniel. T Stein<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine of Yeshiva Uni, Bronx, NY
- ThP 302 **Analysis of Isobaric Oligosaccharide Mixtures by Sequential Mass Spectrometry;** David J. Ashline<sup>1</sup>;

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- Anthony J. Lapadula<sup>1</sup>; Vernon N. Reinhold<sup>1</sup>; <sup>1</sup>*Center for Structural Biology, UNH, Durham, NH*
- ThP 303 **Prefractionation of the Human Serum Glycome Using Lectin Affinity**; Caroline S. Chu<sup>1</sup>; Crystal Kirmiz<sup>1</sup>; Bensheng Li<sup>1</sup>; Brian Clowers<sup>1</sup>; Hyun Joo An<sup>1</sup>; Suzanne Miyamoto<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, Davis, CA*
- ThP 304 **Quantitation of Oligosaccharides in Human Milk Using Deuterium Labeled Standards**; Milady Ninonuevo<sup>1</sup>; Riccardo LoCascio<sup>2</sup>; Robert Ward<sup>3</sup>; David Mills<sup>2</sup>; J. Bruce German<sup>3</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of California, Davis, CA*; <sup>2</sup>*Viticulture & Enology, University of California, Davis, CA*; <sup>3</sup>*Food Science & Technology, University of California, Davis, CA*
- ThP 305 **Capillary Electrophoresis-Mass Spectrometry of Carbohydrates**; J. Tim Smith<sup>1</sup>; Brad J. Williams<sup>1</sup>; Ann Privett<sup>2</sup>; Carson J. Cameron<sup>1</sup>; <sup>1</sup>*Southeastern Oklahoma State Univ, Durant, OK*; <sup>2</sup>*Xavier University, New Orleans, LA*
- ThP 306 **Automated Mass Spectrometric Determination of N-Linked Glycan Structures Using a Custom Built Glycan Structure Database**; Jian M. Ren<sup>1</sup>; Lingyun Li<sup>1</sup>; Tomas Rejtar<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*
- ThP 307 **LC/MS Approach for the Analysis of Reduced and Permethylated Oligosaccharides**; John F. Cipollo<sup>1</sup>; Joy Contado-Miller<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Boston University School of Medicine MSRR, Boston, MA 02118*
- ThP 308 **Profiling of Oligosaccharides in non-Human Mammalian Milk**; Nannan Tao<sup>1</sup>; Milady R. Ninonuevo<sup>1</sup>; Katherine J. Hinde<sup>2</sup>; Brian clowers<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, Davis, CA*; <sup>2</sup>*University of California, Los Angeles, Los Angeles, CA*
- ThP 309 **Glycoprotein Identification and Glycosylation Analysis of Human Serum by Fourier Transform Mass Spectrometry (FTMS)**; Bensheng Li<sup>1</sup>; Crystal Kirmiz<sup>1</sup>; Hyun-Joo An<sup>1</sup>; Caroline Chu<sup>1</sup>; Brian Clowers<sup>1</sup>; Suzanne Miyamoto<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>*University of California-Davis, Davis, CA*
- ThP 310 **Characterization of Plant Polysaccharides Using Online Normal-Phase LC-MALDI-TOF/TOF Tandem Mass Spectrometry**; Sarah L Maslen<sup>1</sup>; Alex Adam<sup>2</sup>; Paul Dupree<sup>3</sup>; Elaine Stephens<sup>1</sup>; <sup>1</sup>*Chemistry Department, Cambridge University, Cambridge, UK*; <sup>2</sup>*Dionex UK Ltd, Camberley, UK*; <sup>3</sup>*Biochemistry Department, University of Cambridge, Cambridge, UK*
- ThP 311 **Annotating the Milk Glycome**; Latasha Lamotte<sup>1</sup>; Milady Ninonuevo<sup>1</sup>; Youmie Park<sup>1</sup>; Jinhua Zhang<sup>1</sup>; Robert Ward<sup>1</sup>; J. Bruce German<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*University of California, Davis, California*

### IMAGING MS II

- ThP 312 **Direct and Indirect Imaging-MS for Identification of Biomarkers in Tissue Sections**; Erika R. Amstalden<sup>1</sup>; Stefan Luxembourg<sup>1</sup>; Sander Piersma<sup>1</sup>; Iwona Sobczak-Elbourne<sup>2</sup>; Rainer Bischoff<sup>2</sup>; Ate G.J. van der Zee<sup>2</sup>; Ali R. Vaezzadeh<sup>3</sup>; Catherine G. Zimmermann-Ivol<sup>3</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands*; <sup>2</sup>*University of Groningen, Groningen, The Netherlands*; <sup>3</sup>*Biomedical Proteomics Research Group, Geneva Univ., Geneva, Switzerland*

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- ThP 313 **Imaging of Target Proteins in Histological Sections by MALDI Mass Spectrometry**; Gwendoline Thiery<sup>1</sup>; Mikhail S. Shchepinov<sup>2</sup>; Edwin M. Southern<sup>2</sup>; Ivo G. Gut<sup>2</sup>; <sup>1</sup>*Centre National de Genotypage, Evry Cedex, France*; <sup>2</sup>*Oxford Gene Technology, Yarnton, United Kingdom*
- ThP 314 **Direct Profiling of Lipids in Rat Brain Tissue Using Desorption Electrospray Ionization Mass Spectrometry**; Justin M. Wiseman<sup>1</sup>; Thomas A. Blake<sup>1</sup>; Qingyu Song<sup>1</sup>; Demian Ifa<sup>1</sup>; James E. Woods<sup>2</sup>; Candice Kissinger<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Bioanalytical Systems Inc., West Lafayette, IN*
- ThP 315 **The Ethanol Triton X-100 Sandwich Method Yields High Resolution and M/z MALDI Mass Spectral Images on Tissue**; Barbara D. Leinweber<sup>1</sup>; Terrence J. Monks<sup>1</sup>; Serrine S Lau<sup>1</sup>; <sup>1</sup>*College of Pharmacy, U of Arizona, Tucson, AZ*
- ThP 316 **Peptide Imaging in Neural Tissue**; M. Reid Groseclose<sup>1</sup>; Malin Andersson<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- ThP 317 **Coregistered Analysis of Proteomic Imaging and Magnetic Resonance Imaging**; Tuhin K. Sinha<sup>1</sup>; Jeffrey J. Luci<sup>1</sup>; Sheerin K. Shahidi<sup>2</sup>; Benoit M. Dawant<sup>3</sup>; John C. Gore<sup>1</sup>; Dale S. Cornett<sup>2</sup>; <sup>1</sup>*Institute Of Imaging Science, Nashville, Tennessee*; <sup>2</sup>*Mass Spectrometry Research Center, Nashville, Tennessee*; <sup>3</sup>*Electrical Engineering and Computer Science, Nashville, Tennessee*
- ThP 318 **Imaging at Atmospheric Pressure by MALDI Mass Spectrometry**; Yue Li<sup>1</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, DC*
- ThP 319 **Determination of Loperamide in Mouse Brain Tissue Using MALDI MS Imaging and Comparison with Quantitative ESI LC-MS/MS Analysis**; Young G. Shin<sup>1</sup>; Teresa Dong<sup>1</sup>; Bilin Chou<sup>1</sup>; Kapil Menghrajani<sup>1</sup>; Achintya K. Sinhababu<sup>1</sup>; Patrick J. Rudewicz<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*
- ThP 320 **Tissue Section Profiling of Phospholipids and Dosed Drug Levels to Characterize Drug Induced Phospholipidosis Using MALDI-TOF/TOF Mass Spectrometry**; Edward J. Takach<sup>1</sup>; Qing Zhu<sup>1</sup>; Frank Hsieh<sup>1</sup>; <sup>1</sup>*Millennium Pharmaceuticals, Cambridge, MA*
- ThP 321 **Enhanced TOF-SIMS Imaging Using Automated Peak Picking**; William E. Cooke<sup>1</sup>; Eugene R. Tracy<sup>1</sup>; Haijian Chen<sup>1</sup>; Christine Hopkins<sup>1</sup>; Dariya I. Malyarenko<sup>1</sup>; Maciek Sasinowski<sup>2</sup>; Dennis M. Manos<sup>1</sup>; <sup>1</sup>*College of William and Mary, Williamsburg, VA*; <sup>2</sup>*INCOGEN, Inc., Williamsburg, VA*
- ThP 322 **Determination of the Distribution of Loperamide in FVB and mdr1a/1b (-/-) Mouse Brain Tissue Sections using MALDI MS Imaging**; Teresa Dong<sup>1</sup>; Young G. Shin<sup>1</sup>; Achintya K. Sinhababu<sup>1</sup>; Patrick J. Rudewicz<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*
- ThP 323 **Combining MALDI MS and Novel Microscale Protein Isolation Techniques for the Characterization of Disease Progression in Thin Tissue Sections**; Hans-Rudolf Aerni<sup>1</sup>; Dale S. Cornett<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*
- ThP 324 **MALDI Imaging MS and cDNA Analysis Reveal Changes in Protein Profiles and Gene Expression in Chemical-Induced Renal Tumors**; Serrine S Lau<sup>1</sup>; Barbara D. Leinweber<sup>1</sup>; Pierre Chaurand<sup>2</sup>; Richard M. Caprioli<sup>2</sup>; Terrence J. Monks<sup>1</sup>; <sup>1</sup>*College of Pharmacy, U of Arizona, Tucson, AZ*; <sup>2</sup>*Vanderbilt University Medical Center, Nashville, TN*

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- ThP 325 **Two-step Matrix Crystallization Technique Improves Resolution and Signal-to-Noise Ratio in Direct Tissue MALDI Analysis on Tissue Surface;** Yuki Sugiura<sup>1</sup>; Shuichi Shimma<sup>2</sup>; Takahiro Harada<sup>3</sup>; Mitsutoshi Setou<sup>2</sup>; <sup>1</sup>Tokyo Institute of Technology, Yokohama, Japan; <sup>2</sup>The Graduate University for Advanced Studies, Aichi, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 326 **Atmospheric Pressure MALDI Imaging Mass Spectrometry;** Berk Oktem<sup>1</sup>; Victor V. Laiko<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; Shelley N. Jackson<sup>2</sup>; Hay-Yan J. Wang<sup>2</sup>; Amina S. Woods<sup>2</sup>; <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>National Institute on Drug Abuse, NIH, Baltimore, MD
- ThP 327 **Characterising Oral Cancer Tissue Using MALDI MS with Chemical Printing;** Soyab Patel<sup>1</sup>; Royston Goodacre<sup>1</sup>; Phil Sloan<sup>2</sup>; Nalin Thakker<sup>2</sup>; Alan Barnes<sup>3</sup>; Neil Loftus<sup>3</sup>; <sup>1</sup>School of Chemistry, The University of Manchester, Manchester, United Kingdom; <sup>2</sup>School of Dentistry, The University of Manchester, Manchester, United Kingdom; <sup>3</sup>Shimadzu Biotech, Manchester, United Kingdom
- ThP 328 **Effects of Metal Coating for UV-MALDI-a-TOF Mass Spectrometry Imaging (MALDI MSI) and Direct Tissue Analysis in UV/IR-MALDI-o-TOF Mass Spectrometry;** Maxence Wisztorski<sup>1</sup>; Klaus Dreisewerd<sup>2</sup>; Franz Hillenkamp<sup>2</sup>; Stefan Berkenkamp<sup>3</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>MALDI Imaging Team, FRE CNRS 2933, Univ. of Lille, Villeneuve d'Ascq, France; <sup>2</sup>Institute of Medical Physics and Biophysics, Muenster, Germany; <sup>3</sup>Sequenom GmbH, Hamburg, Germany
- ThP 329 **Enhanced Processing of Tissue Imaging Data;** Min Yang<sup>1</sup>; Andrew James<sup>1</sup>; Gordana Ivosev<sup>1</sup>; Ron Bonner<sup>1</sup>; <sup>1</sup>MDS Sciex, Concord, ON, Canada
- ThP 330 **MALDI Imaging: Pitfalls and Solutions for Sample Preparation and Data Evaluation;** Soeren-Oliver Deininger<sup>1</sup>; Martin Schuerenberg<sup>1</sup>; Christine Luebbert<sup>1</sup>; Arne Fuetterer<sup>1</sup>; Sergej Dikler<sup>2</sup>; Matthias Ebert<sup>3</sup>; Christoph Roeken<sup>4</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Billerica, MA; <sup>3</sup>Klinikum rechts der Isar, TU Muenchen, Munich, Germany; <sup>4</sup>Pathology, Charite University Hospital, Berlin, Germany
- ThP 331 **Histology Directed MALDI-TOF Tissue Profiling of Metastatic Breast Cancer;** Erin H. Seeley<sup>1</sup>; Rachel E. Ellsworth<sup>2</sup>; Darrell L. Ellsworth<sup>2</sup>; Jeffrey A. Hooke<sup>3</sup>; Dale S. Cornett<sup>1</sup>; Craig D. Shriver<sup>3</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Windber Research Institute, Windber, PA; <sup>3</sup>Walter Reed Army Medical Center, Washington, DC
- ThP 332 **New Insights in Sample Preparation for MALDI Imaging and New Developments to Approach Specific MALDI Imaging of the Transcriptome;** Isabelle Fournier<sup>1</sup>; Remi Lemaire<sup>1</sup>; Maxence Wisztorski<sup>1</sup>; Jonathan Stauber<sup>1</sup>; Olivia Jardin-Mathe<sup>1</sup>; Robert Day<sup>2</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>MALDI Imaging Team, FRE CNRS 2933, Univ. of Lille, Villeneuve d'Ascq, France; <sup>2</sup>Pharmacology Dept, Univ of Sherbrooke, SHerbrooke, Canada
- ThP 333 **Direct Analysis and MALDI Imaging on Formalin-Fixed Paraffin-Embedded (FFPE) Tissues : Application to Parkinson Disease;** Remi Lemaire<sup>1</sup>; Annie Desmons<sup>1</sup>; Patrick Ducoroy<sup>3</sup>; Jean Claude Tabet<sup>2</sup>; Michel Salzet<sup>1</sup>; isabelle Fournier<sup>1</sup>; <sup>1</sup>Neuroimmunologie des annelides, imagerie MALDI, Villeneuve d'ascq, France; <sup>2</sup>Synthese structure fonction molecules bioactives, Paris, France; <sup>3</sup>Plateforme proteomique IFR 100, Dijon, France

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- ThP 334 **Identifying Early Proteomic Markers of Kanamycin Induced Nephrotoxicity through Direct Tissue Profiling Using MALDI MS;** Kristen D Herring<sup>1</sup>; Axel Ducret<sup>2</sup>; Deming Mi<sup>1</sup>; Richard M Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>2</sup>F. Hoffman-La Roche Ltd., Basel, Switzerland
- ThP 335 **Profiling of Lipids at the Tumour:Liver Margin in Colorectal Liver Metastasis by Imaging MALDI-MS;** Sally J. Atkinson<sup>1</sup>; Ali Majeed<sup>2</sup>; Nigel Bird<sup>2</sup>; David Mangnall<sup>2</sup>; Michael M. Burrell<sup>3</sup>; Malcolm R. Clench<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, United Kingdom; <sup>2</sup>Royal Hallamshire Hospital, Sheffield, United Kingdom; <sup>3</sup>Sheffield University, Sheffield, UK
- LIPIDS: STRUCTURAL ANALYSIS AND PROFILING**
- ThP 336 **Identification of Resolvins, Protectin-D1, and Other Omega-3 Fatty-Acid Derived Lipid-Mediators Via Liquid Chromatography-Electrospray/Low Collision Energy Tandem Mass Spectrometry: Fragmentation Mechanisms;** Song Hong<sup>1</sup>; Yan Lu<sup>1</sup>; Yong Yang<sup>1</sup>; Katherine Gotlinger<sup>1</sup>; Charles Serhan<sup>1</sup>; <sup>1</sup>Brigham & Women's Hospital/Harvard Medical School, Boston, MA
- ThP 337 **Distinction of cis and Trans Isomers of Monounsaturated Fatty Acid by FAB MS in Negative Ion Mode;** Hong Ji<sup>1</sup>; Valery G. Voinov<sup>1</sup>; Max L. Deinzer<sup>1</sup>; Douglas F. Barofsky<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 338 **Atmospheric Pressure Covalent Adduct Chemical Ionization (APCACI) for Structural Elucidation of Triacylglycerols;** Yichuan Xu<sup>1</sup>; J. Thomas Brenna<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY
- ThP 339 **Analysis of Phospholipids in Protein Microdomains using Isotope Tagged Derivatives;** Kathleen A. Harrison<sup>1</sup>; Bridget S. Wilson<sup>2</sup>; Robert C. Murphy<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Aurora, CO; <sup>2</sup>University of New Mexico Cancer Research Center, Albuquerque, NM
- ThP 340 **Identification of Acylation Patterns and Novel Modifications in Lipid A species from Francisella using a Vacuum-MALDI LTQ Linear Ion Trap;** Birgit Schilling<sup>1</sup>; Molly K. McLendon<sup>2</sup>; Nancy J. Phillips<sup>3</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; <sup>3</sup>University of California, San Francisco, CA
- ThP 341 **Characterization of the Mouse Liver Mitochondrial Polyunsaturated Lipidome by ESI-MS/MS/MS;** Kristal M. Maner<sup>1</sup>; J. Thomas Brenna<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY
- ThP 342 **Withdrawn**
- ThP 343 **Unravelling Lipidomes of Lipid Related Disorders Quantitatively by Comprehensive and Automated Lipid Profiling;** Marcus Stahlman<sup>2</sup>; Gun-Britt Forsberg<sup>1</sup>; Mark Baumert<sup>3</sup>; Eva Duchoslav<sup>4</sup>; Jan Borén<sup>2</sup>; Kim Ekroos<sup>1</sup>; <sup>1</sup>AstraZeneca, Mölndal, Sweden; <sup>2</sup>Wallenberg Laboratory for Cardiovascular Research, Gothenburg, Sweden; <sup>3</sup>Advion BioSciences Inc, Norwich, UK; <sup>4</sup>MDS Sciex, Concord, Canada
- ThP 344 **Electrospray Mass Spectrometry Ocular Lipid Study: Fragmentation of Cis-9-octadecenamide, Negative Mode Reduction of Oleic Acid and Mono-unsaturated Wax Ester Oxidation;** Bryan M. Ham<sup>1</sup>; Kari B. Green-Church<sup>1</sup>; Jason J. Nichols<sup>2</sup>; Kelly K. Nichols<sup>2</sup>; <sup>1</sup>Mass Spec. & Proteo. Facility, Ohio State Univ., Columbus, OH; <sup>2</sup>College of Optometry, Ohio State Univ., Columbus, OH

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- ThP 345 **In situ Analyses of Cardiolipin in Mitochondria-Rich Rat Organ Sections;** Hay-Yan J. Wang<sup>1</sup>; Shelley N. Jackson<sup>1</sup>; Amina S. Woods<sup>1</sup>; <sup>1</sup>NIDA-IRP, NIH, DHHS, Baltimore, MD
- ThP 346 **Ozonolysis of Phospholipid Double Bonds During Electrospray Ionization: OZESI - A New Tool for Structure Determination;** Michael C. Thomas<sup>1</sup>; Todd W. Mitchell<sup>1</sup>; Stephen J. Blanksby<sup>1</sup>; <sup>1</sup>University of Wollongong, Wollongong, Australia
- ThP 347 **Analytical Systems for Neutral-lipids by Mass Spectrometry;** Toshiaki Houjou<sup>1</sup>; Masaki Ishikawa<sup>1</sup>; Yasuhiro Iida<sup>1</sup>; Mayuko Ishida<sup>2</sup>; Takao Shimizu<sup>1</sup>; Ryo Taguchi<sup>1</sup>; <sup>1</sup>The University of Tokyo, Tokyo, Japan; <sup>2</sup>SHIMADZU Corporation, Kyoto, Japan
- ThP 348 **Structural Characterization of Glycosphingolipids and Toxin Receptor Gangliosides by IRMPD with TLC/VC-FTMS;** Vera B. Ivleva<sup>1</sup>; Anne A. Wolf<sup>2</sup>; Wayne I. Lencer<sup>2</sup>; Peter B. O'Connor<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Children's Hospital, Boston, MA
- ThP 349 **Lipids Profiling of Fish Oils from Wild and Farmed Salmon by Matrix Assisted Laser Desorption/Ionization Mass Spectrometry;** Omar Belgacem<sup>1</sup>; Emmanuel Raptakis<sup>1</sup>; Gerald Stuebiger<sup>2</sup>; <sup>1</sup>Shimadzu Biotech, Manchester, United Kingdom; <sup>2</sup>Institut of Chemical technologies and analysis, Vienna, Austria
- ThP 350 **A Mass Spectrometric Approach to Analyze the Lipid Composition of Detergent-Resistant Membranes Isolated from Cells;** Catharina Crone<sup>1</sup>; Göran Hübner<sup>1</sup>; Buko Lindner<sup>1</sup>; <sup>1</sup>Research Center Borstel, Borstel, Germany
- ThP 351 **Quantitative and Qualitative Analysis of Total Brain Gangliosides using LC Interfaced with a Hybrid Triple Quadrupole/Linear Ion Trap Mass Spectrometer;** Doina Caraiman<sup>1</sup>; Tom Biesenthal<sup>1</sup>; Johnnie Brown<sup>2</sup>; <sup>1</sup>Applied Biosystems-MDS Sciex, Concord, Canada; <sup>2</sup>Applied Biosystems, Framingham, MA
- ThP 352 **Characterization of Gangliosides from Mouse Brain by MALDI-TOF/TOF;** Kenneth H.N. Chan<sup>1</sup>; Patrick Pribil<sup>2</sup>; Willard Costain<sup>1</sup>; Warren W. Wakarchuk<sup>1</sup>; Li Jianjun<sup>1</sup>; <sup>1</sup>National Research Council of Canada, IBS, Ottawa, Canada; <sup>2</sup>Applied Biosystem / MDS SCIEX, Concord, Canada
- ThP 353 **Quantitative Analysis of Glycerophospholipids by LC-MS Using Odd-Carbon Internal Standards;** Jeff D. Moore<sup>1</sup>; Stephen B. Milne<sup>2</sup>; Walter A. Shaw<sup>1</sup>; Alex H. Brown<sup>2</sup>; <sup>1</sup>Avanti Polar Lipids, Alabaster, AL; <sup>2</sup>Vanderbilt University Medical Center, Nashville, TN
- ThP 354 **Shotgun Analysis of Intact Phospholipids by Nanoflow LC/MS/MS;** Myeong Hee Moon<sup>1</sup>; Dae Young Bang<sup>1</sup>; <sup>1</sup>Yonsei University, Seoul, Korea
- ThP 355 **Quantitative Analysis of Sphingolipids by Liquid Chromatography-Triple Quadrupole and Hybrid Quadrupole-Ion Trap (QTrap) Tandem Mass Spectrometry;** Jeremy C. Allegood<sup>1</sup>; M. Cameron Sullards<sup>1</sup>; Alfred H. Merrill Jr.<sup>1</sup>; Jeff D. Moore<sup>2</sup>; Walter A. Shaw<sup>2</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Avanti Polar Lipids, Inc., Alabaster, AL
- ThP 356 **Tandem Mass Spectrometry of Francisella novicida (U112) Lipid A Reveals Temperature Dependent Remodeling;** Scott A Shaffer<sup>1</sup>; Thomas F Kalhorn<sup>1</sup>; Megan D Harvey<sup>1</sup>; Robert K Ernst<sup>1</sup>; David R Goodlett<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA

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- ThP 357 **Rapid Characterization of Edible Oils by Direct MALDI MS Analysis of Triacylglycerols;** Jackson Lay, Jr.<sup>1</sup>; Rohana Liyanage<sup>1</sup>; Bill Durham<sup>1</sup>; John Brooks<sup>2</sup>; <sup>1</sup>Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR; <sup>2</sup>Crime Scene Unit, Fayetteville Police Department, Fayetteville, AR

## LIPIDS: BIOCHEMISTRY AND SIGNALING

- ThP 358 **Method Development for Profiling Postprandial Changes in Monocyte Membrane Lipids Using Chip-Based Nanospray-Fourier Transform-Ion Cyclotron Resonance-Mass Spectrometry;** Nabil Saad<sup>1</sup>; Laura Higgins<sup>1</sup>; John Rutledge<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, CA
- ThP 359 **Remodeling of Docosahexaenoic Acid Containing Phospholipids During Stimulation Monitored by Electrospray LC/MS;** Yang Suk Kim<sup>1</sup>; Jong Seong Kang<sup>2</sup>; Hee Yong Kim<sup>1</sup>; <sup>1</sup>NIAAA, NIH, Rockville, MD; <sup>2</sup>Coll. Pharm. CNU, Daejeon, Korea
- ThP 360 **Structural and Functional Analysis of the Lipid Binding Properties of a Sec14-like Domain Using Nanospray Mass Spectrometry;** Sven Fraterman<sup>1</sup>; Steffan Welti<sup>1</sup>; Klaus Scheffzek<sup>1</sup>; Matthias Wilm<sup>1</sup>; <sup>1</sup>European Molecular Biology Laboratory, Heidelberg, Germany
- ThP 361 **A Novel LC/MS Cell-based Assay to Investigate SCD1 Activity;** Michael J. Greig<sup>1</sup>; Roslyn Dillon<sup>1</sup>; B. Ganesh Bhat<sup>1</sup>; <sup>1</sup>Pfizer Global R&D, San Diego, CA
- ThP 362 **Identification of an Endogenous Ligand of the C. Elegans Nuclear Receptor DAF-12 Using GC-MS;** Jason M Held<sup>1</sup>; Matthew S Gill<sup>1</sup>; Mark White<sup>1</sup>; Gordon J Lithgow<sup>1</sup>; Bradford W Gibson<sup>1</sup>; <sup>1</sup>Buck Institute for Age Research, Novato, CA
- ThP 363 **Sphingolipidomics: A New Tool to Study Mitochondrial Dysfunction in the Aging Heart;** Alan W. Taylor<sup>1</sup>; Jeffrey S. Monette<sup>1</sup>; Regis Moreau<sup>1</sup>; Tory M. Hagen<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 364 **Improved Long-Chain Fatty Acyl-Coenzyme A Quantitation by HPLC-ESI MS/MS and Distinction of Alternative Biosynthetic Pathways Using Stable Isotope-Labeling;** Christopher A. Haynes<sup>1</sup>; M. Cameron Sullards<sup>1</sup>; Elaine W. Wang<sup>1</sup>; Alfred H. Merrill, Jr.<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- ThP 365 **Lipidomics: Study of Total Phospholipids in Immortalized Liver Cells Exposed to Different Fatty Acid Substrates;** Michael Pagliassotti<sup>1</sup>; Jessica Prenni<sup>1</sup>; Phil Ryan<sup>1</sup>; Paul Rainville<sup>2</sup>; Andrew Baker<sup>3</sup>; <sup>1</sup>Colorado State University, Ft. Collins, CO; <sup>2</sup>Waters, Milford, MA; <sup>3</sup>Waters, Dublin, CA
- ThP 366 **Lipidomics Approaches to Fatty Acid Amides Using LC-MS/MS;** Bo Tan<sup>1</sup>; David K. O'Dell<sup>1</sup>; Heather B. Bradshaw<sup>1</sup>; M. Francesca Monn<sup>1</sup>; Y. William Yu<sup>1</sup>; Harini Srinivasan<sup>1</sup>; Jocelyn F. Krey<sup>2</sup>; J. Michael Walker<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Stanford University, Palo Alto, CA
- ThP 367 **Feasibility of Breath Condensate Lipids & Eicosanoids as Non-invasively Collected Biomarker Predictors of Pulmonary Pathobiology;** Sung-Chan Jo<sup>1</sup>; James M Cantu<sup>1</sup>; Owen R. Moss<sup>2</sup>; Edilberto Bermudez<sup>2</sup>; David C White<sup>1</sup>; <sup>1</sup>Center for Biomarker Analysis, Univ. Tennessee, Knoxville, TN; <sup>2</sup>CIIT, Center for Health Research, Research Triangle Park, NC
- ThP 368 **Characterization of Protein Adduction by Reactive Lipid Oxidation-Derived Electrophiles;** Simona G. Codreanu<sup>1</sup>; Daniel C. Liebler<sup>1</sup>; <sup>1</sup>Vanderbilt University



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- Medical Center, Nashville, TN; <sup>2</sup>Mass Spectrometry Research Center, Nashville, TN
- ThP 369 **Leukotriene A4 inhibition of Viral Replication;** Kelly M Wynalda<sup>1</sup>; Joseph A Hankin<sup>1</sup>; Jessica L Krank<sup>1</sup>; Carlos E Catalano<sup>1</sup>; Helene A Gaussier<sup>1</sup>; Robert C Murphy<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, Colorado
- ThP 370 **Application of Combined Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) in Screening for X-linked Adrenoleukodystrophy (X-ALD) in Newborns;** Walter C. Hubbard<sup>1</sup>; Ann B. Moser<sup>3</sup>; Anita Liu<sup>3</sup>; Hugo W. Moser<sup>3</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Kennedy-Krieger Institute, Baltimore, MD; <sup>3</sup>Kennedy-Krieger Institute, Baltimore, MD
- ThP 371 **Using ESI-MS to Verify the Presence of Sulfogalactosylglycerolipid (SGG) in Lipid Rafts Isolated from Pig Sperm;** Arman Yaghoubian<sup>1</sup>; Andrew J. Norris<sup>1</sup>; Julian P. Whitelegge<sup>1</sup>; Maroun Bou Khalil<sup>2</sup>; Hongbin Xu<sup>2</sup>; Nongnui Tanphaichitr<sup>2</sup>; Kym F. Faull<sup>1</sup>; <sup>1</sup>UCLA Pasarow Mass Spectrometry Laboratory, Los Angeles, California; <sup>2</sup>Ottawa Health Research Institute, Ottawa, Canada

### LIPIDS: OXIDIZED LIPIDS AND STEROLS

- ThP 372 **Detection of Enantiomers of Epoxyeicosatrienoic Acid Derivatives by Chiral-Phase High Performance Liquid Chromatography/ Tandem Mass Spectrometry;** A. Clementina Mesaros<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- ThP 373 **5-oxo-EETE Synthesis Under Conditions of Cell Death and Oxidative Stress in Human Leukemic Cells;** Aaron E. Ransome<sup>1</sup>; Robert C. Murphy<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, CO
- ThP 374 **Targeted Chiral Lipidomics Analysis of COX-2-Mediated 15(S)-Hydroxy-eicosatetraenoic Acid Metabolism;** Angela Y. Wehr<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- ThP 375 **Development of a Rapid and Sensitive Method for Sterol Analysis by HPLC-ESI-MS;** Erin C McCrum<sup>1</sup>; Jeffrey G McDonald<sup>1</sup>; <sup>1</sup>University of Texas Southwestern Medical Center, Dallas, TX
- ThP 376 **Identification of Covalent (Phospho)Lipid-Peptide Adducts: Separation by Liquid Chromatography Coupled with Tandem Mass Spectrometry;** Ana Reis<sup>1</sup>; M Rosário M Domingues<sup>1</sup>; Pedro Domingues<sup>1</sup>; <sup>1</sup>University of Aveiro, Aveiro, Portugal
- ThP 377 **Chiral Lipidomics Analysis of Cyclooxygenase-2-Mediated Arachidonic Acid Metabolism;** Seon Hwa Lee<sup>1</sup>; Michelle V. Williams<sup>1</sup>; Angela Wehr<sup>1</sup>; Yunxian Liu<sup>1</sup>; Raymond N. DuBois<sup>2</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Vanderbilt University Medical Center, Nashville, TN
- ThP 378 **Determination of Isoprostanes in Urine from Smokers and Nonsmokers by Liquid Chromatography/Tandem Mass Spectrometry;** Gary D. Byrd<sup>2</sup>; Michael W. Ogden<sup>2</sup>; Weiyang Yan<sup>1</sup>; <sup>1</sup>Wake Forest University Medical Center, Winston Salem, NC; <sup>2</sup>R. J. Reynolds Tobacco Company, Winston Salem, NC
- ThP 379 **Analysis of Oxidized Phosphatidylcholines Using Structure Specific Survey or Focused Multiple Reaction Monitoring with Reverse Phase LC/MS/MS;** Ryo Taguchi<sup>1</sup>; Yasuhiro Iida<sup>1</sup>; Hiroki Nakanishi<sup>1</sup>; Takao Shimizu<sup>1</sup>; <sup>1</sup>Grad. Sch. Med., The Univ. Tokyo, Tokyo, Japan; <sup>2</sup>Crest, Jst, Kawaguchi, Saitama, Japan

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- ThP 380 **Ascorbylation and Glutathionylation of Lipid Peroxidation Products as Potential Biomarkers of Oxidative Stress Response;** Heather M. Conway<sup>1</sup>; Ruth Gordillo<sup>1</sup>; Nicholas G. Kesinger<sup>1</sup>; John Sowell<sup>1</sup>; Cristobal L. Miranda<sup>1</sup>; Jan F. Stevens<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 381 **Analysis of Neurosteroid Glucuronides from Mouse Brain by Capillary-Liquid Chromatography-Tandem Mass Spectrometry;** Sirkku E. Jäntti<sup>1</sup>; Petteri Piepponen<sup>2</sup>; Anne Tammimäki<sup>2</sup>; Risto Kostianen<sup>2</sup>; Raimo A. Ketola<sup>1</sup>; <sup>1</sup>Drug Discovery and Development Technology Center, Helsinki, FINLAND; <sup>2</sup>University of Helsinki, Helsinki, FINLAND
- ThP 382 **LC-ESI-MS/MS Analysis of trans-4-hydroxy-2-nonenal Enantiomers and Metabolites;** Ales Honzatkó<sup>1</sup>; Jiri Brichac<sup>1</sup>; Matthew J Picklo<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND
- ThP 383 **High Sensitivity LC/MS Analysis of Lipid Hydroperoxide-Derived Glutathione Adducts;** Xin Tang<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; Ian A Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- ThP 384 **LC-MS Analysis and Identification of Oxidized Lipid Components in Minimally Modified Low Density Lipoprotein;** Richard Harkewicz<sup>1</sup>; Yury I. Miller<sup>1</sup>; Agnes Boullier<sup>1</sup>; Joseph L. Witztum<sup>1</sup>; Edward A. Dennis<sup>1</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA

### BIOINFORMATICS IV

- ThP 385 **The Use of an Open Architecture LIMS Solution to Address the Complexity of Proteomic Workflows, Data Management, and Analysis;** Sau-Mei Leung<sup>1</sup>; Manimalha Balasubramani<sup>2</sup>; <sup>1</sup>GenoLogics Life Sciences Software Inc., Victoria, BC, Canada; <sup>2</sup>Genomics & Proteomics Core Laboratories, UPITT, Pittsburgh, PA
- ThP 386 **Classification of MS-MS Peptide Spectra to Predict Primary Structure Using Pattern Detection and Matching Techniques;** Jennifer Broughton<sup>1</sup>; Sujeewa Alwis<sup>2</sup>; Michael P May<sup>1</sup>; Jim Austin<sup>2</sup>; <sup>1</sup>Shimadzu Research Laboratory (Europe) Ltd, Manchester, UK; <sup>2</sup>Cybula Ltd, York, UK
- ThP 387 **The mzXML Schema Version 3.0;** Patrick G.A. Pedrioli<sup>2</sup>; James S. Eddes<sup>1</sup>; Jimmy K. Eng<sup>3</sup>; Nichole L. King<sup>1</sup>; Brian Pratt<sup>4</sup>; David Shteynberg<sup>1</sup>; Joshua M. Tasman<sup>1</sup>; Ning Zhang<sup>1</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Institute for Molecular Systems Biology (ETH), Zurich, Switzerland; <sup>3</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>4</sup>Insilicos, Seattle, WA
- ThP 388 **Large Scale Identification of SILAC peptides by Delay Series Autocorrelation and Convolution Mapping;** Matthew J Sniatynski<sup>1</sup>; Jason C Rogalski<sup>1</sup>; Michael D Hoffman<sup>1</sup>; Leonard J Foster<sup>2</sup>; Juergen Kast<sup>1</sup>; <sup>1</sup>The Biomedical Research Centre, Vancouver, BC; <sup>2</sup>UBC Centre for Proteomics, Vancouver, BC
- ThP 389 **System for Interactive Analysis and Comparison of Mass Spectrometry Proteomics Experiments;** Mark Igra<sup>1</sup>; Adam Rauch<sup>2</sup>; Peter Hussey<sup>2</sup>; Joshua Eckels<sup>2</sup>; Martin McIntosh<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>LabKey Software, Seattle, WA
- ThP 390 **New MS Peak Picking and Quality Assessment Tools for Proteomics;** Thomas O Patterson<sup>1</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Childrens Hospital, Boston, MA
- ThP 391 **ProteinCenter: A New Bioinformatics Application for Processing of Large-Scale Proteomics Data Sets;** Ole Vorm<sup>1</sup>; Hans Jespersen<sup>1</sup>; Morten Bern<sup>1</sup>; Soeren Schandorff<sup>1</sup>; Alexandre Podtelejnikov<sup>1</sup>; Peter Venø<sup>1</sup>;



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- Martin Damsbo<sup>1</sup>; Soren Larsen<sup>1</sup>; Brian Ramsgaard<sup>1</sup>; Erik Nielsen<sup>1</sup>; Jacob Kristensen<sup>1</sup>; Kenneth Budin<sup>1</sup>; <sup>1</sup>Proxeon, Odense, Denmark
- ThP 392 **2D Mass Spectra Correlation – Semi Automatic Tool for Modified Peptide Discovery**; Ilan Vidavsky<sup>1</sup>; Don L. Rempel<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- ThP 393 **A Novel Visualization Tool for Common Mass Spectrometric File Formats**; Erik J Nilsson<sup>1</sup>; Brian S Pratt<sup>1</sup>; Bryan J Prazen<sup>1</sup>; <sup>1</sup>Insilicos, Seattle, WA
- ThP 394 **Simultaneous Optimization of the Accuracy and Yield of Peptide / Protein Identification with Multiple Search Engines with in-situ Error Estimation**; Wen Yu<sup>1</sup>; J. Alex Taylor<sup>1</sup>; Sharon Wong-Madden<sup>1</sup>; Robert DuBose<sup>1</sup>; Scott Patterson<sup>2</sup>; <sup>1</sup>Bioinformatics, Seattle, WA; <sup>2</sup>Molecular Sciences, Thousand Oaks, CA
- ThP 395 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data**; Luis Mendoza<sup>1</sup>; Eric W. Deutsch<sup>1</sup>; James S. Eddes<sup>1</sup>; Jimmy K. Eng<sup>2</sup>; Robert Hubley<sup>1</sup>; Andrew Keller<sup>3</sup>; Nichole L. King<sup>1</sup>; Xiao-jun Li<sup>4</sup>; Alexey I. Nesvizhskii<sup>5</sup>; Patrick Pedrioli<sup>6</sup>; David Shteynberg<sup>1</sup>; Joshua M. Tasman<sup>1</sup>; Bernd Wollschied<sup>1</sup>; Ning Zhang<sup>1</sup>; Ruedi Aebersold<sup>6</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>3</sup>Rosetta Biosoftware, Seattle, WA; <sup>4</sup>Homestead Clinical Corporation, Seattle, WA; <sup>5</sup>University of Michigan, Ann Arbor, MI; <sup>6</sup>Institute for Molecular Systems Biology, ETH Zurich, Zurich, Switzerland
- ThP 396 **A Software Shell for MS Data Processing and Management**; Yang Su<sup>1</sup>; Sequin Huang<sup>2</sup>; Hua Huang<sup>1</sup>; David H. Perlman<sup>1</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>Present address Waters Corp, Milford, MA
- ThP 397 **A Dynamic-Link Library for Predicting Peptide CID Spectra Through Kinetic Modeling**; Zhongqi Zhang<sup>1</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA
- ThP 398 **Recent Advances in Reliability, Performance and Usability of the Trans-Proteomic Pipeline (TPP) Software Tools**; Brian S Pratt<sup>1</sup>; <sup>1</sup>Insilicos LLC, Seattle, WA
- ThP 399 **PIKE: Protein Information and Knowledge Extractor**; J. Alberto Medina-Aunon<sup>1</sup>; Marcus Macht<sup>2</sup>; Juan Pablo Albar<sup>1</sup>; Herbert Thiele<sup>2</sup>; <sup>1</sup>Centro Nacional de Biotecnología - CSIC, Madrid, Spain; <sup>2</sup>Bruker Daltonik, GmbH, Bremen, Germany
- ThP 400 **Delivering Mass Spectrometry Tools to the Masses**; Carmen M. Pancerella<sup>1</sup>; Dan Fabris<sup>2</sup>; Julian Eaton<sup>2</sup>; Irwin D. Kuntz<sup>3</sup>; Larry A. Rahn<sup>1</sup>; Andrew Rothfuss<sup>1</sup>; Ken Sale<sup>1</sup>; Christine L. Yang<sup>1</sup>; Malin M. Young<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Livermore, CA; <sup>2</sup>University of Maryland, Baltimore County, Baltimore, MD; <sup>3</sup>University of California, San Francisco, San Francisco, CA
- ThP 401 **ASCQ\_ME: A New Engine for Peptide Mass Fingerprinting Directly from Mass Spectrum Without Mass List Extraction**; Jean-Charles Boisson<sup>1</sup>; Pierre Laurence<sup>1</sup>; Laetitia Vermeulen-Jourdan<sup>1</sup>; El-Ghazali Talbi<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Universite des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
- ThP 402 **Schema for the Integration of 2-D Gel Electrophoresis Data with Mass Spectrometry Analysis Results**; Romesh Stanislaus<sup>1</sup>; John Arthur<sup>1</sup>; Balaji Rajagopalan<sup>4</sup>; Rick Moerschell<sup>3</sup>; Brian McGlothlen<sup>3</sup>; Jonas Almeida<sup>2</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Univ. Texas MDAnderson Cancer Center, Houston, TX;

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- <sup>3</sup>BioRad Laboratories, Hercules, CA; <sup>4</sup>Wake Forest University School of Medicine, Winston-Salem, NC
- ThP 403 **Integrated Proteomics Environment for Automated High Throughput Analysis of MS Data**; Bruce D Pascal<sup>1</sup>; Mark R Southern<sup>1</sup>; Mohammad Fallahi<sup>1</sup>; Michael J Chalmers<sup>1</sup>; Scott A Busby<sup>1</sup>; Nicholas Tsinoremas<sup>1</sup>; Christopher Mader<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, Jupiter, FL
- ThP 404 **An Open Access, Peer Reviewed, Peer-to-Peer Based Proteomics Data Dissemination and Archival System**; Jayson A Falkner<sup>1</sup>; Philip C Andrews<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- ThP 405 **InSilicoSpectro - Proteomics Open-Source Library**; Jacques Colinge<sup>1</sup>; Alexandre Masselot<sup>2</sup>; Erik Pitzer<sup>1</sup>; Ron D. Appel<sup>3</sup>; <sup>1</sup>Upper Austria University of Applied Sciences, Hagenberg, Austria; <sup>2</sup>GeneBio S.A., Geneva, Switzerland; <sup>3</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland
- ThP 406 **A New High Speed Method of Preparing Reports from MASCOT Search Results**; Jermaine O. Rouson<sup>1</sup>; Cameron O. Scarlett<sup>1</sup>; Bradley Bone<sup>1</sup>; Timothy J. Kirksey<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- ThP 407 **The Wildcat Toolbox: A Set of Perl Utilities for Data and Database Manipulation**; Paul A. Haynes<sup>2</sup>; Linda Brecl<sup>1</sup>; Susan Miller<sup>1</sup>; James Rohrbaugh<sup>3</sup>; Michael Galligan<sup>1</sup>; Timothy Radabaugh<sup>1</sup>; Fatimah Hickman<sup>1</sup>; Nirav Merchant<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Macquarie University, Sydney, Australia; <sup>3</sup>Air Force Institute of Technology, Wright-Patterson AFB, OH
- ThP 408 **Open Source Tools for the Accurate Mass and Time (AMT) Tag Proteomics Pipeline**; Navdeep Jaitly<sup>1</sup>; Matthew E. Monroe<sup>1</sup>; Kyle Littlefield<sup>1</sup>; Don S. Daly<sup>1</sup>; Gordon A. Anderson<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 409 **Associative Networks for the Exploration of Proteomic Data**; Ioannis K. Moutsatsos<sup>1</sup>; Patrick Cody<sup>1</sup>; John B. Damask<sup>2</sup>; Peter Warren<sup>1</sup>; <sup>1</sup>Wyeth Research, Cambridge, MA; <sup>2</sup>Damask Solutions LLC, Somerville, MA
- ThP 410 **RAPID: Coordinated Visualization of Multiple Charge States from Individual or Isotopically Labeled Peptides in Liquid Chromatography Mass Spectrometry Experiments**; D. Leif Rustvold<sup>1</sup>; Phillip Wilmarth<sup>1</sup>; Surendra Dasari<sup>1</sup>; Larry David<sup>1</sup>; <sup>1</sup>Oregon Health & Science University, Portland, OR
- ThP 411 **Visual Basic .NET Tools for Enhancements in Proteomics, Automation and Data Analysis in a Modern Mass Spectrometry Laboratory**; Adrian R. Woolfitt<sup>1</sup>; Hercules Moura<sup>1</sup>; John R. Barr<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA

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- ThP 412 **Identification of Phospholipids in Lipid Extracts Using 4.7 Tesla Electrospray-Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI-FTICR MS)**; Seonghyun Yu<sup>1</sup>; Kun Cho<sup>1</sup>; Younghwan Kim<sup>2</sup>; Soojin Park<sup>1</sup>; Hanbin Oh<sup>1</sup>; <sup>1</sup>Sogang University, Seoul, Korea; <sup>2</sup>Korea Basic Science Institute, Daejeon, Korea
- ThP 413 **Desorption Electrospray Ionization (DESI): New Applications of Differential Metabolomics for Cancer Detection**; Nari Talaty<sup>1</sup>; Zhengzheng Pan<sup>1</sup>; Huanwen Chen<sup>1</sup>; Daniel Raftery<sup>1</sup>; R Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- ThP 414 **Metabonomics Approaches to Profiling Biological Matrices Using a Hybrid LTQ-Orbitrap Mass Spectrometer**; Petia Shipkova<sup>1</sup>; Robert Langish<sup>1</sup>; Emily

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- Luk<sup>1</sup>; Bethanne Warrack<sup>1</sup>; Serhiy Hnatyshyn<sup>1</sup>; Mark Sanders<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*
- ThP 415 **Quantitative Profiling of Primary and Secondary Amine-Contained Metabolites in Urine Using Differential Reductive Amination Labeling and LC-MS**; Chengjie Ji<sup>1</sup>; Kevin Guo<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Alberta*
- ThP 416 **Development of New Methods for Comprehensive High-Throughput Glycosphingolipidomics**; Steven B. Levery<sup>1</sup>; Yunsen Li<sup>1</sup>; Heather Eichert<sup>1</sup>; Emma Arigi<sup>1</sup>; <sup>1</sup>*University of New Hampshire, Durham, NH*
- ThP 417 **Determination of Arachidonic Acid Metabolites in Rat Brain Striatum Microdialysate by LC-MS/MS Utilizing Electron Capture Atmospheric Pressure Chemical Ionization**; Ge Zu<sup>1</sup>; Li Zhang<sup>1</sup>; Steven Foster<sup>1</sup>; Monika Wrona<sup>1</sup>; Glenn Dryhurst<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*
- ThP 418 **Towards Metabolome Profiling with Single Cell MALDI-TOF MS**; Stanislav S. Rubakhin<sup>1</sup>; Nathan R. Bohn<sup>1</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>*University of Illinois, Urbana, IL*
- ThP 419 **A New Sample Preparation Method for Human Plasma/Serum Metabolomics Study by Liquid-Chromatography Mass Spectrometry (LC/MS)**; Xiang He<sup>1</sup>; Christopher Becker<sup>1</sup>; <sup>1</sup>*Biomarker Discovery Sciences, PPD Inc., Menlo Park, CA*
- ThP 420 **A Lipidomics Approach in *Sinorhizobium Meliloti* as a Tool in Functional Genomics**; Libia Saborido Basconcillo<sup>1</sup>; Brian E. McCarry<sup>1</sup>; <sup>1</sup>*Chemistry Department/McMaster University, Hamilton, ON, Canada*
- ThP 421 **Enhancement of Amino Acid Analysis by Liquid Chromatography/Electrospray Ionization Mass Spectrometry Through Charged and Deuterium-Coded Derivatization**; Wen-Chu Yang<sup>1</sup>; Hamid Mirzaei<sup>1</sup>; Xiuping Liu<sup>1</sup>; Fred E. Regnier<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- ThP 422 **Advanced Tools for LC/MS Metabolomics Studies of Secondary Metabolism Using the Model Legume *Medicago truncatula***; David V. Huhman<sup>1</sup>; Scott M. Peterman<sup>2</sup>; Manor Askenazi<sup>3</sup>; Stacey Allen<sup>1</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>*The Samuel Roberts Noble Foundation, Ardmore, OK*; <sup>2</sup>*Thermo Electron, Somerset, NJ*; <sup>3</sup>*BRIMS Center, Cambridge, MA*
- ThP 423 **Differential Detection of Endogenous Metabolites Using a Dual Mode Ionization Source on an Atmospheric Pressure Ionization Time-of-Flight Mass Spectrometer (API-TOF)**; David Weil<sup>1</sup>; Steve Fischer<sup>1</sup>; Theodore Sana<sup>1</sup>; Laura A. Egnash<sup>2</sup>; Michael D. Reily<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*CA and Discovery Biomarkers, Pfizer Global R and D, Ann Arbor, MI*
- ThP 424 **Data Analysis for High Resolution, High-Throughput Metabolomics**; Norma H. Pawley<sup>1</sup>; Steven P. Brumby<sup>1</sup>; Kwasi G. Mawuenyega<sup>1</sup>; Munehiro Teshima<sup>1</sup>; Clifford J. Unkefer<sup>1</sup>; Pat J. Unkefer<sup>1</sup>; <sup>1</sup>*Los Alamos National Laboratory, Los Alamos, NM*
- ThP 425 **Combined Analysis of NMR and LC/MS Data: Observations in Urine Samples From a Smoker Study**; Markus Godejohann<sup>1</sup>; Hartmut Schäfer<sup>1</sup>; Christian Fischer<sup>1</sup>; Peter Neidig<sup>1</sup>; Manfred Spraul<sup>1</sup>; Duk-Young Han<sup>2</sup>; Eunil Lee<sup>3</sup>; Gabriela Zurek<sup>4</sup>; Carsten Baessmann<sup>4</sup>; <sup>1</sup>*Bruker BioSpin GmbH, Rheinstetten, Germany*; <sup>2</sup>*KBSI Seoul, Seoul, South-Korea*; <sup>3</sup>*Korea University, Seoul, South-Korea*; <sup>4</sup>*Bruker Daltonik GmbH, Bremen, Germany*

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- ThP 426 **Development of a Human Plasma and Serum Metabolomic Feature Database and Application in the Study of Type 1 Diabetes Mellitus**; Thomas O. Metz<sup>1</sup>; Christina M. Sorensen<sup>1</sup>; Stephen J. Callister<sup>1</sup>; Matthew E. Monroe<sup>1</sup>; Jennifer S.D. Zimmer<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Patricia W. Mueller<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*U.S. Centers for Disease Control and Prevention, Atlanta, GA*
- ThP 427 **Metabolic and Proteomic Profiling of Cerebrospinal Fluid and Serum for Schizophrenia**; Hilary Major<sup>1</sup>; Therese McKenna<sup>1</sup>; Christopher Hughes<sup>1</sup>; Jeffrey T.-J Huang<sup>2</sup>; Sabine Bahn<sup>2</sup>; <sup>1</sup>*Waters Corporation, Manchester, United Kingdom*; <sup>2</sup>*University of Cambridge, Cambridge, United Kingdom*
- ThP 428 **A Metabolomics Approach to the Changes in Liver Phospholipids from Rats Treated with Tamoxifen Using Electrospray Ionization Mass Spectrometry Analysis**; Ricky D. Holland<sup>1</sup>; Michelle Wiest<sup>2</sup>; Macdonald Morris<sup>2</sup>; Rebecca Baillie<sup>2</sup>; Yvonne P. Dragan<sup>1</sup>; Laura Schnackenberg<sup>1</sup>; Stacy Dial<sup>1</sup>; Naito Akihiro<sup>1</sup>; Richard D. Beger<sup>1</sup>; <sup>1</sup>*National Center for Toxicological Research, Jefferson, AR*; <sup>2</sup>*Lipomics Technologies Inc., West Sacramento, CA*
- ThP 429 **Benefits of Capillary LC for Metabolomic Analyses**; Tanya N. Gamble<sup>1</sup>; Pauline J. Vollmerhaus<sup>1</sup>; Alina Dindyal-Popescu<sup>1</sup>; Ron Bonner<sup>1</sup>; <sup>1</sup>*Applied Biosystems/MDS SCIEX, Concord, Canada*
- ThP 430 **An Automated LC-MS/MS Platform for Metabolomics Pathway Quantification - Application to a Type II Diabetic Mouse Model**; Steven L. Ramsay<sup>1</sup>; Wolfgang Stöggli<sup>1</sup>; Wolfgang Guggenbichler<sup>1</sup>; Katusservani Bernardo<sup>1</sup>; Klaus Weinberger<sup>1</sup>; Armin Graber<sup>1</sup>; <sup>1</sup>*Biocrates Life Sciences, Innsbruck, Tirol*
- ThP 431 **Structure Elucidation of Important Unknown Endogenous Urinary Metabolites Using UPLC/MS-Directed Fraction Collection**; John P. Shockcor<sup>1</sup>; Paul Lefebvre<sup>1</sup>; Paul Rainville<sup>1</sup>; Rob Plumb<sup>1</sup>; Warren Potts<sup>1</sup>; Jose Castro-Perez<sup>1</sup>; <sup>1</sup>*Waters Corp., Milford, MA*
- ThP 432 **Profiling the Mammalian Metabolome and Its Application to Toxicity Prediction Using High Temperature and Pressure LC/MS-*oa*-TOF with Novel Statistical Analysis**; Robert Plumb<sup>1</sup>; Jeremy Nicholson<sup>1</sup>; Ian Wilson<sup>3</sup>; Kelly Johnson<sup>2</sup>; Paul Rainville<sup>2</sup>; <sup>1</sup>*Imperial College, London, UK*; <sup>2</sup>*Waters Corporation, Milford, MA*; <sup>3</sup>*Astra Zeneca, Macclesfield, UK*
- ThP 433 **Development of Solid Phase Extraction Methods for Metabonomics Screening and Targeted Biomarker Analysis by LC-MS and NMR**; Laura A Egnash<sup>1</sup>; Laura M Sardelli<sup>1</sup>; Lora C Robosky<sup>1</sup>; Michael D Reily<sup>1</sup>; <sup>1</sup>*Pfizer Global Research and Development, Ann Arbor, MI*
- ThP 434 **Precise Identification of Molecular Species of Phosphatidylethanolamine and Phosphatidylserine by Neutral Loss Survey with MS<sup>3</sup> and Accurate Mass Measurement**; Mayuko Ishida<sup>1</sup>; Shinichi Yamaguchi<sup>1</sup>; Junichi Taniguchi<sup>1</sup>; Junko Iida<sup>1</sup>; Kozo Miseki<sup>1</sup>; Osamu Nishimura<sup>1</sup>; Takao Shimizu<sup>2</sup>; Ryo Taguchi<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*The University of Tokyo, Tokyo, Japan*
- ThP 435 **Identification of Coenzyme A Activated Substances by Accurate Mass Determination Using ESI Triple-Quadrupole Mass Spectrometry**; Christoph Magnes<sup>1</sup>; Thomas R. Pieber<sup>1</sup>; Werner Regittinig<sup>2</sup>; Frank M. Sinner<sup>1</sup>; <sup>1</sup>*Joanneum Research, Graz, Austria*; <sup>2</sup>*Medical University, Graz, Austria*

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- ThP 436 **Identification of Metabolic Biomarkers of Disease by FT-ICR MS**; Stephen C.C. Wong<sup>1</sup>; Warwick B. Dunn<sup>1</sup>; David I. Broadhurst<sup>1</sup>; Mark Baumert<sup>2</sup>; Alistair Stirling<sup>2</sup>; Douglas B. Kell<sup>1</sup>; Simon J. Gaskell<sup>1</sup>; <sup>1</sup>*The University of Manchester, Manchester, UK*; <sup>2</sup>*Advion Biosciences Ltd, Hethersett, Norwich, UK*
- ThP 437 **Single-Column Multi-Mode HPLC Separation and its Application for Amino Acid Analysis**; Zhihui Wen<sup>1</sup>; Ying Zhang<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, AB, Canada*
- ThP 438 **Optimization of Experimental Parameters for Reproducible Urine Analysis During Conduct of a Pre-Clinical Metabonomics Study in Rabbits**; Richard Schneider<sup>1</sup>; Andrew Butler<sup>1</sup>; Marielle Delnomdedieu<sup>1</sup>; <sup>1</sup>*Pfizer Global Research & Development, Groton, CT*
- ThP 439 **Metabolic Profiling of Cerebral Spinal fluid Utilizing Gas Chromatography Mass Spectrometry with Negative Chemical Ion Detection**; James A. Eckstein<sup>1</sup>; Gina M. Londino<sup>1</sup>; Kalpana M. Merchant<sup>1</sup>; Bradley L. Ackermann<sup>1</sup>; <sup>1</sup>*Eli Lilly and Company, Greenfield, IN*
- ThP 440 **Unbiased Selection of Aroma Producing Bacteria by Metabolomics**; Heike Schaefer<sup>1</sup>; Stefan Irmeler<sup>1</sup>; <sup>1</sup>*Agroscope Liebefeld-Posieux (ALP), Bern, Switzerland*
- ThP 441 **Identification and Quantification of Human Metabolites from Plasma Using HPLC, MS and NMR**; Lisa N. Nikolai<sup>1</sup>; David S. Wishart<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*
- ThP 442 **Purification and Structural Characterization of Novel Metabolic Substrates in Pathogenic Bacteria by Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry (HILIC-MS) and NMR**; Evelyn C. Soo<sup>1</sup>; Dave J McNally<sup>2</sup>; Joseph PM Hui<sup>1</sup>; Annie J. Aubry<sup>2</sup>; Kenneth KK Mui<sup>3</sup>; Susan M Logan<sup>2</sup>; Patricia Guerry<sup>4</sup>; Jean-Robert Brisson<sup>2</sup>; <sup>1</sup>*NRC-Institute for Marine Biosciences, Halifax, Canada*; <sup>2</sup>*NRC-Institute for Biological Sciences, Ottawa, Canada*; <sup>3</sup>*University of Waterloo, Waterloo, Canada*; <sup>4</sup>*Naval Medical Research Center, Silver Spring, MD*
- ThP 443 **Metabolite Analysis of Fermenting and Respiring Yeast Cells using GCxGC-TOFMS and chemometrics**; Rachel E. Mohler<sup>1</sup>; Kenneth M. Dombek<sup>1</sup>; Jamin C. Hoggard<sup>1</sup>; Elton T. Young<sup>1</sup>; Robert E. Synovec<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*
- ThP 444 **Metabolite Profiling in Human Urine by NMR and MS**; Mulu Gebre<sup>1,2,3,4,5</sup>; Lisa Nikolai<sup>1,2,3,4,5</sup>; Godwin Amegbey<sup>1,2,3,4,5</sup>; David Wishart<sup>1,2,3,4,5</sup>; Liang Li<sup>1,2,3,4,5</sup>; <sup>1</sup>*University of Alberta, Edmonton, AB, Canada*; <sup>2</sup>*University of Alberta, Edmonton, AB, Canada*; <sup>3</sup>*University of Alberta, Edmonton, AB, Canada*; <sup>4</sup>*University of Alberta, Edmonton, AB, Canada*; <sup>5</sup>*University of Alberta, Edmonton, AB, Canada*
- ThP 445 **New Tools in Metabonomics: Application of Sensitive MRM Scans Together with New Scaling Procedures to Detect Reactive Metabolites in Humans**; Silvia Wagner<sup>1</sup>; Karoline Scholz<sup>1</sup>; Lyle Burton<sup>2</sup>; Wolfgang Voelkel<sup>1</sup>; <sup>1</sup>*University of Wuerzburg, Wuerzburg, Germany*; <sup>2</sup>*Applied Biosystems, Concord, Canada*
- ThP 446 **Cell-Based Metabolite Identification for Expanding the Human Metabolome MS/MS Database**; Melisa A. Clements<sup>1</sup>; Sandra L. Marcus<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Alberta*
- ThP 447 **Development and Characterization of a HILIC LC-MS Method for Metabolomic Analysis of Polar Analytes in Urine**; Kara M Pearson<sup>1</sup>; Danny W Choo<sup>1</sup>; William H Schaefer<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*

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- ThP 450 **Identification of Endogenous Glycine Conjugates in Normal Rat Urine Using LTQ-FTMS System**; Yutai Li<sup>1</sup>; Qiuwei Xu<sup>1</sup>; Amy Fitzpatrick Loughlin<sup>1</sup>; William H Schaefer<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*
- ThP 451 **Urinary Polyamines and N-acetylated Polyamines in Four Patients with Alzheimer's Disease as their N-ethoxycarbonyl-N-pentafluoropropionyl Derivatives by GC-SIM-MS Method**; Kyoung R. Kim<sup>1</sup>; Sunmie Lee<sup>1</sup>; Man J. Paik<sup>1</sup>; Kyung H. Cho<sup>2</sup>; <sup>1</sup>*Sungkyunkwan University, Suwon, South Korea*; <sup>2</sup>*Seoul Women's University, Seoul, South Korea*
- ThP 452 **A Stable Isotope Dilution LC-MS/MS Method to Analyze Pathways of Benzo[a]pyrene-Mediated DNA-Adduct Formation**; Stacy L. Gelhaus<sup>1</sup>; Qian Ruan<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; Trevor M. Penning<sup>1</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*
- ThP 453 **Metabolome Analysis of Steady State Bacterial Cultures by High-Resolution Mass Spectrometry**; Munehiro Teshima<sup>1</sup>; Kwasi G. Mawuenyega<sup>1</sup>; Norma H. Pawley<sup>1</sup>; Clifford J. Unkefer<sup>1</sup>; Pat J. Unkefer<sup>1</sup>; <sup>1</sup>*Los Alamos National Laboratory, Los Alamos, NM*
- ThP 454 **Metabolite Profiling by LC/ESI-TOF MS Combined with XCMS Analysis for Biomarker Discovery**; Hiroto Morita<sup>1</sup>; Grace O'Maille<sup>1</sup>; Elizabeth J. Want<sup>1</sup>; Anders Nordström<sup>1</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*
- ThP 455 **A Metabolomics Study of Camellia Sinensis (Tea)**; Chris L. Stumpf<sup>1</sup>; Paul D. Rainville<sup>1</sup>; John Shockcor<sup>1</sup>; Robert S. Plumb<sup>1</sup>; James N. Willis<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*
- ThP 456 **Characterization of Myxobacteria Producing Secondary Metabolites by HPLC-MS Screening and Principal Component Analysis (PCA)**; Daniel Krug<sup>1</sup>; Birgit Schneider<sup>2</sup>; Gabriela Zurek<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Jim Cunningham<sup>3</sup>; Rolf Mueller<sup>1</sup>; <sup>1</sup>*Saarbruecken University, Saarbruecken, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*Bruker Daltonics, Billerica, MA*
- ThP 457 **Investigation of Delta-Aminolevulinic Acid for Use as a Small Molecule Biomarker for Zinc Status in Humans**; Na Pi<sup>1</sup>; Ellen Fung<sup>1</sup>; David Killilea<sup>1</sup>; Bruce Ames<sup>1</sup>; <sup>1</sup>*Children's Hospital Oakland Research Institute, Oakland, CA*
- ThP 458 **Combining Unbiased and Targeted Mass Spectrometry-Based Metabolomics Methods for Profiling Pre- and Post-Liver Transplantation in Hepatitis C Virus Subjects**; Brett R. Wenner<sup>1</sup>; James R. Bain<sup>1</sup>; Amany Zekry<sup>1</sup>; Olga Ilkayeva<sup>1</sup>; Don C. Rockey<sup>1</sup>; Christopher B. Newgard<sup>1</sup>; John G. McHutchison<sup>1</sup>; Robert D. Stevens<sup>1</sup>; <sup>1</sup>*Duke University Medical Center, Durham, NC*
- ThP 459 **Identification of Sugar-Phosphates and Sugar-Nucleotides in a Metabolomics Study of E. coli Cell Lysates**; Joseph P. M. Hui<sup>1</sup>; Jie Yang<sup>2</sup>; Jon S. Thorson<sup>2</sup>; Evelyn C. Soo<sup>1</sup>; <sup>1</sup>*NRC - Institute for Marine Biosciences, Halifax, Canada*; <sup>2</sup>*University of Wisconsin - School of Pharmacy, Madison, WI*
- ThP 460 **Profiling of Catecholamines and their Metabolites in Rat Brain Extract using Liquid Chromatography/Atmospheric Pressure Photoionization Mass Spectrometry**; Jason A. Starkey<sup>1</sup>; Tatiana Rojkovicova<sup>1</sup>; Yehia Mechref<sup>2</sup>; William J. McBride<sup>3</sup>; Milos V. Novotny<sup>1</sup>; <sup>1</sup>*Department of Chemistry, Indiana University, Bloomington, Indiana*; <sup>2</sup>*METACyt*

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- Biochemical Analysis Center, Bloomington, Indiana;  
<sup>3</sup>Department of Psychiatry, Indiana University,  
 Indianapolis, Indiana
- ThP 461 **Identification and Characterization of Metabolites and Markers Indicative of Effectiveness of Schizophrenia Treatment;** Geron Bindseil<sup>1</sup>; J.C. Yves Le Blanc<sup>1</sup>; Lyle Burton<sup>1</sup>; Julie Wingate<sup>1</sup>; <sup>1</sup>Applied Biosystems|MDS Sciex, Concord, Canada
- ThP 462 **Free Amino Acid Levels in brain Cortex Tissues of Three Mouse Models with Alzheimer's Disease as Their N (O,S)-ethoxycarbonyl/tert-butyl dimethylsilyl Derivatives;** Man J. Paik<sup>1</sup>; In S. Cho<sup>1</sup>; Inhee. Mook-Jung<sup>2</sup>; Kyoung R. Kim<sup>1</sup>; <sup>1</sup>Sungkyunkwan University, Suwon, South Korea; <sup>2</sup>Seoul National University College of Medicine, Seoul, South Korea
- ThP 463 **Investigating the Distribution of Metabolites in Wheat by Imaging Matrix-Assisted Laser Desorption Ionisation Mass Spectrometry;** Caroline J Earnshaw<sup>1</sup>; Malcolm R Clench<sup>1</sup>; Mike M Burrell<sup>2</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, UK; <sup>2</sup>University of Sheffield, Sheffield, UK
- ThP 464 **Metabolite Profiling of an Obese Murine Model;** David Mutch<sup>1</sup>; Grace O'Maille<sup>1</sup>; Chuan Qin<sup>1</sup>; Gary Siuzdak<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA
- ThP 465 **Metabolite Profiles in Developing Oranges;** Kwasi G Mawuenyega<sup>1</sup>; Munehiro Teshima<sup>1</sup>; Norma H Pawley<sup>1</sup>; Clifford J Unkefer<sup>1</sup>; Pat J Unkefer<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM
- ThP 466 **Identification and Characterization of SbSTS1-derived Secondary Metabolites in Transgenic Arabidopsis by Means of Tandem Mass Spectrometry;** Corey N. W. Lam<sup>1</sup>; Christine K. Y. Yu<sup>1</sup>; Fiona H. Y. Shiu<sup>1</sup>; J. C. Yves Le Blanc<sup>2</sup>; Clive Lo<sup>1</sup>; Ivan K. Chu<sup>1</sup>; <sup>1</sup>The University of Hong Kong, Hong Kong, China; <sup>2</sup>MDS Sciex, Concord, Ontario, Canada
- ThP 467 **Stable Isotopes and Mass Spectrometry. Flux Analysis of the Fructose-6-P-phosphoketolase Shunt Pathway in Bifidobacterium;** Anthony Adeuya<sup>1</sup>; Terence R. Whitehead<sup>2</sup>; Neil P. Price<sup>1</sup>; <sup>1</sup>USDA-ARS-NCAUR, Bioproducts & Biocatalysis Research, Peoria, IL; <sup>2</sup>USDA-ARS-NCAUR, Fermentation Biotechnology Research, Peoria, IL

### NON-COVALENT INTERACTIONS II

- ThP 468 **Nanoelectrospray Mass Spectrometry to Study the Structure and Dynamics of Homogeneous and Heterogeneous Noncovalent Protein Complexes;** Alexander J Painter<sup>1</sup>; Justin Benesch<sup>1</sup>; Carol V Robinson<sup>1</sup>; <sup>1</sup>Cambridge University, Cambridge, United Kingdom
- ThP 469 **Study of Interactions and Determination of Binding Affinity Constants of Ape1 to E3330 or c-Jun by PLIMSTEX;** Bich T. N. Vu<sup>1</sup>; Millie M. Georgiadis<sup>2</sup>; John-Stephen A. Taylor<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- ThP 470 **ESI-MS of Proteins in Urea;** Lynda J Donald<sup>1</sup>; Vladimir M. Collado<sup>1</sup>; Harry W. Duckworth<sup>1</sup>; Kenneth G. Standing<sup>1</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Manitoba, Canada
- ThP 471 **Laser Spray Mass Spectrometry; A Promising Tool for the Analysis of Stability of Biological Macromolecules in Solution;** Satoko Akashi<sup>1</sup>; Xiangguo Shi<sup>1</sup>; Atsushi Takamizawa<sup>2</sup>; Yoshifumi Nishimura<sup>1</sup>; Kenzo Hiraoka<sup>2</sup>; <sup>1</sup>Yokohama City University, Yokohama, Japan; <sup>2</sup>University of Yamanashi, Kofu, Japan

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- ThP 472 **Characterization of Ribosomes by Chemical Cross-linking and Mass Spectrometry;** Soheil Pourshahian<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Cincinnati, Cincinnati, OH
- ThP 473 **A Novel Fluorescent Isotopically-Coded MALDI-Cleavable Crosslinker, BiPS;** Evgeniy V. Petrotchenko<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- ThP 474 **Behavior of Beta-Carboline Toward Nucleosides, Nucleobases and Oligonucleotides in Electrospray;** Ying Xu<sup>1</sup>; Clotilde Le Vot<sup>1</sup>; Xiao Chun Dong<sup>2</sup>; Carlos Afonso<sup>1</sup>; Françoise Fournier<sup>1</sup>; Ren Wen<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris 6, Paris, France; <sup>2</sup>Fudan University, Shanghai, China
- ThP 475 **Surface-Induced Dissociation of Non-Covalent Protein Complexes: Comparisons to Collision-Induced Dissociation;** Christopher M Jones<sup>1</sup>; Richard L Beardsley<sup>1</sup>; Asiri S Galhena<sup>1</sup>; Shai Dagan<sup>1</sup>; Charles Cheng<sup>1</sup>; Vicki H Wysocki<sup>1</sup>; <sup>1</sup>The University of Arizona, Tucson, AZ
- ThP 476 **Nano-ESI-MS Study of Non-Denatured Nuclear Receptor Complexes Helps to Define a Network of Protein-Protein interactions;** Alan M. Sandercock<sup>1</sup>; Herbert Nar<sup>2</sup>; Thilo A. Fligge<sup>2</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, United Kingdom; <sup>2</sup>Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach/Riss, Germany
- ThP 477 **Biological Aggregates in Solution and the Gas Phase;** Hannah V Florance<sup>1</sup>; Jess Lippens<sup>1</sup>; Bryan McCullough<sup>1</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>University of Edinburgh, Edinburgh, United Kingdom
- ThP 478 **Elucidating the Binding Selectivity of Bivalent Glutathione S-Transferase Inhibitors by H/D Exchange Mass Spectrometry;** Liming Hou<sup>1</sup>; Sumit S. Mahajan<sup>1</sup>; Catalin Doneanu<sup>1</sup>; William M. Atkins<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 479 **Crosslinking and Mass Spectrometry for Identifying Protein-protein Interaction Sites in Activator-Multi-component Protein Complexes;** Kun Lu<sup>1</sup>; Evgeniy V. Petrotchenko<sup>1</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- ThP 480 **Noncovalent Protein-Protein Complexes Studied by ESI-MS: Distinguishing "Real" Signals from Dissociation and Clustering Artifacts;** Belal M. Hossain<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Ontario N6A 5B7, Canada
- ThP 481 **MALDI-MS and MALDI-MS/MS of Oligonucleotide/Polycation Complexes;** Peran Terrier<sup>1</sup>; William Buchmann<sup>1</sup>; Gregoire Zin<sup>1</sup>; Valerie Gabelica<sup>2</sup>; Edwin De Pauw<sup>2</sup>; Jeanine Tortajada<sup>1</sup>; <sup>1</sup>LAMBE UMR 8587 CNRS/CEA/Universite d'Evry, Evry, France; <sup>2</sup>Universite de Liege, Liege, Belgium
- ThP 482 **Emerging Technologies for Mass Spectrometry of Noncovalent Complexes: Structural Determination Via Collision-Induced Dissociation, Spectral Deconvolution, and Ion Mobility;** Justin LP Benesch<sup>1</sup>; Brandon T Ruotolo<sup>1</sup>; Adam RC McKay<sup>1</sup>; Carol V Robinson<sup>1</sup>; <sup>1</sup>University of Cambridge, Cambridge, UK
- ThP 483 **Fully Automated Chip-Based Nanoelectrospray Tandem Mass Spectrometry for the Determination of Noncovalent Protein-Carbohydrate Interaction;** Alina D. Zamfir<sup>1</sup>; Martin G. Peter<sup>2</sup>; Jasna Peter-Katalinic<sup>1</sup>; <sup>1</sup>Institute for Medical Physics and Biophysics, Münster, Germany; <sup>2</sup>Chemistry Institute, Potsdam, Germany

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- ThP 484 **DNA-Drug Complexes Probed by ESI and MALDI and Different Ion Activation Methods;** Todd H. Mize<sup>1</sup>; Arpad Somogyi<sup>2</sup>; <sup>1</sup>Bio5 Institute--University of Arizona, Tucson, AZ; <sup>2</sup>Department of Chemistry--University of Arizona, Tucson, AZ
- ThP 485 **Probing the Structure of Protein Complexes Using Covalent Derivatization and Two-Dimensional Protein Chromatography/Mass Spectrometry;** Richard L. Beardsley<sup>1</sup>; Xiaohui Liu<sup>1</sup>; William E. Running<sup>1</sup>; James P. Reilly<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- ThP 486 **Equilibrium Dialysis LC/ESI-MS/MS for Characterizing Protein-Ligand Interactions;** Terri L. Quenzer<sup>1</sup>; Ben Bolanos<sup>1</sup>; Catherine Pham<sup>1</sup>; Jiangli Yan<sup>1</sup>; Michael J. Greig<sup>1</sup>; <sup>1</sup>Pfizer Global R&D - La Jolla, San Diego, CA

## PROTEINS GENERAL II

- ThP 487 **Proton-Deuteron Amide Exchange Studies by MS and NMR: A New Method for Protein NMR Resonance Assignment;** Lianmei Feng<sup>1</sup>; James Prestegard<sup>1</sup>; Ronald Orlando<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA, USA
- ThP 488 **Automated Intermediate Mass Correction for Protein Open-Access LC/MS;** Jon D. Williams<sup>1</sup>; Craig D. Wagner<sup>1</sup>; John T. Hall<sup>1</sup>; Wendy L. White<sup>1</sup>; <sup>1</sup>GlaxoSmithKline, Research Triangle Park, NC
- ThP 489 **Structural Variations in the Peanut Allergen Ara h 2;** Kevin J. Shefcheck<sup>1</sup>; Carmen D. Westphal<sup>1</sup>; John H. Callahan<sup>1</sup>; <sup>1</sup>US Food and Drug Administration, College Park, MD
- ThP 490 **Profiling of Soluble Proteins in Wine by Nano-High-Performance Liquid Chromatography/Tandem Mass Spectrometry;** Sung Won Kwon<sup>1</sup>; Jae Sung Pyo<sup>1</sup>; Jeong Hill Park<sup>1</sup>; <sup>1</sup>Seoul National University, Seoul, South Korea
- ThP 491 **Mapping the Interaction Between Bacterial Transferrin Binding Protein B and human Transferrin via Hydrogen-Deuterium Exchange Mass Spectrometry;** Michael J. Eggertson<sup>1</sup>; David C. Schriemer<sup>1</sup>; Anthony B. Schryvers<sup>1</sup>; Jessmi Ling<sup>1</sup>; Collin Shima<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB Canada
- ThP 492 **MALDI Imaging of Retina and MALDI Profiling of Isolated Rod Cells;** Joshua L. Johnson<sup>1</sup>; Daniel D. Oprian<sup>1</sup>; Jeffery N. Agar<sup>1</sup>; <sup>1</sup>Brandeis University, Waltham, MA
- ThP 493 **Production and Characterization of ABL1 Wild-Type and Gleevec® Resistant Mutant Kinases using LC-MS/MS, Radioactive and Z-LYTE™ Assays;** Jill K. Wolken<sup>1</sup>; Krishne Gowda<sup>1</sup>; Tina Hallis<sup>1</sup>; Mark Maffitt<sup>1</sup>; Richard Somberg<sup>1</sup>; Chris Armstrong<sup>1</sup>; Mary Ozers<sup>1</sup>; Kurt Vogel<sup>1</sup>; Baigen Mei<sup>1</sup>; <sup>1</sup>Invitrogen, Madison, WI
- ThP 494 **Analysis of Glue Droplets on Spider Egg Case Silk Using MALDI/TOF/TOF Mass Spectrometry;** Xiaoyi Hu<sup>1</sup>; Jing Yuan<sup>1</sup>; Arnold M. Falick<sup>2</sup>; Craig A. Vierra<sup>1</sup>; Anne M. F. Moore<sup>1</sup>; O. David Sparkman<sup>1</sup>; Patrick R. Jones<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA; <sup>2</sup>HHMI MS Lab, University of California, Berkeley, Berkeley, CA
- ThP 495 **Development of H/D Exchange Mass Spectrometry as a Biophysical Assay for the Classification of Nuclear Receptor Modulators;** Michael J. Chalmers<sup>1</sup>; Scott A. Busby<sup>1</sup>; Swati Prasad<sup>1</sup>; Bruce D. Pascal<sup>1</sup>; Mark Southern<sup>1</sup>; Sandra Cervino<sup>1</sup>; Patrick R. Griffin<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, Jupiter, Florida
- ThP 496 **Identification of Copper-Binding Plant Proteins Using Immobilized Metal-Ion Affinity Chromatography, Gel Electrophoresis and LC-MS/MS;** Cory A. Sonntag<sup>1</sup>; Andrew RS Ross<sup>2</sup>; Douglas JH Olson<sup>2</sup>; <sup>1</sup>University of

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- Saskatchewan, Saskatoon, Canada; <sup>2</sup>NRC-Plant Biotechnology Institute, Saskatoon, Canada
- ThP 497 **Characterization of the Murine Myelin Basic Protein: Structural Analysis of an Intrinsically Unstructured Protein;** Christine M. Hager-Braun<sup>1</sup>; Kenneth B. Tomer<sup>2</sup>; Michael B. Goshe<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>National Institute of Environmental Health Science, Research Triangle Park, NC
- ThP 498 **Dynamic Analysis of the Heat Shock Protein 60 and its Gene Expression in Thermoanaerobacter Tengcongensis Induced by Temperature Increase;** Bo Meng<sup>1</sup>; <sup>1</sup>Beijing Genomics Institute, Beijing, China
- ThP 499 **Determination of Proteins in Infant Formula by High-Performance Liquid Chromatography-Electrospray Tandem Mass Spectrometry;** Jae Sung Pyo<sup>1</sup>; Jeong Hill Park<sup>1</sup>; Sung Won Kwon<sup>1</sup>; <sup>1</sup>Seoul National University, Seoul, South Korea
- ThP 500 **High Sequence Coverage by In-Capillary Proteolytic Digest: Identification and/or Sequencing of Hemoglobins Directly from Blood Samples;** Gottfried Pohlentz<sup>1</sup>; Stefanie Henning<sup>1</sup>; Michael Mormann<sup>1</sup>; Jasna Peter-Katalinic<sup>1</sup>; <sup>1</sup>Institute for Medical Physics and Biophysics, Münster, Germany

## MODIFIED PROTEINS: OXIDATION

- ThP 501 **Mass Spectroscopic Characterization of Protein Oxidation by Pyrroloquinoline Quinone;** Takeshi Ishii<sup>1</sup>; Mitsugu Akagawa<sup>2</sup>; Yuji Naito<sup>3</sup>; Toshikazu Yoshikawa<sup>3</sup>; Shigenori Kumazawa<sup>1</sup>; <sup>1</sup>University of Shizuoka, Shizuoka, Japan; <sup>2</sup>Osaka Prefecture University, Sakai, Japan; <sup>3</sup>Kyoto Prefectural University of Medicine, Kyoto, Japan
- ThP 502 **The Oxidation of Yeast Alcohol Dehydrogenase by Hydrogen Peroxide in vitro;** Lijie Men<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California at Riverside, Riverside, CA
- ThP 503 **Post Translational Modifications of Human Transthyretin as Potential Biomarkers for Type 2 Diabetes;** Qinfeng Liu<sup>1</sup>; Erik N. Hansen<sup>2</sup>; Naji N. Abumrad<sup>2</sup>; Daniel C. Liebler<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt University Medical Center, Nashville, TN
- ThP 504 **Identification of Specific Protein Carbonylation Sites in Model Oxidations of Human Serum Albumin;** Ani Temple<sup>1</sup>; Ten-Yang Yen<sup>1</sup>; Scott Gronert<sup>1</sup>; <sup>1</sup>San Francisco State University, San Francisco, CA
- ThP 505 **Methionine Oxidation and Specific Tyrosine Chlorination: Potential Mechanism for Impaired ABCA1-dependent Cholesterol Efflux Activity of Apolipoprotein A-I by Myeloperoxidase;** Baohai Shao<sup>1</sup>; Michael N. Oda<sup>2</sup>; Nathan Brot<sup>3</sup>; John F. Oram<sup>1</sup>; Jay W. Heinecke<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Children's Hospital Oakland Research Institute, Oakland, CA; <sup>3</sup>Weill Medical College of Cornell University, New York, NY
- ThP 506 **LC/MS Methods in Study of Photo-Degradations of Therapeutic Recombinant IgG Molecules;** Himanshu Gadgil<sup>1</sup>; Doug Banks<sup>1</sup>; Gary Pipes<sup>1</sup>; Vipa Hobbs<sup>1</sup>; Timothy Osslund<sup>1</sup>; Pavel Bondarenko<sup>1</sup>; Robert Rush<sup>1</sup>; <sup>1</sup>Amgen Inc, Thousand Oaks, CA
- ThP 507 **Characterization of the Post-Translational Modifications of Two Sources of Recombinant Oligomeric Adiponectin;** Jennifer F. Nemeth<sup>1</sup>; Audrey Baker<sup>1</sup>; Karen Becker<sup>1</sup>; Haiyan Jiang<sup>1</sup>; Bethany Swencki-Underwood<sup>1</sup>; Justin Sprenkle<sup>1</sup>; Mark Cunningham<sup>1</sup>; Todd Schraw<sup>2</sup>; Philipp E. Scherer<sup>2</sup>; Ian James<sup>1</sup>; Ray Sweet<sup>1</sup>; <sup>1</sup>Centocor Research and Development, Radnor,

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- PA; <sup>2</sup>Albert Einstein College of Medicine, New York, New York
- ThP 508 **Bottom-Up vs Top-Down Mass Spectrometric Characterization Of Heme-Protein Free Radicals Induced By Oxidative Damage;** Leesa J Deterding<sup>1</sup>; Suchandra Bhattacharjee<sup>1</sup>; Dario C Rameriz<sup>1</sup>; Ronald P Mason<sup>1</sup>; Kenneth B. Tomer<sup>1</sup>; <sup>1</sup>NIEHS, NIH, DHHS, Research Triangle Park, NC
- ThP 509 **Identification and Quantification of Post-Translational Modifications on Large Intact Proteins by LC/ESI-TOF MS;** Da Ren<sup>1</sup>; Dean Liu<sup>1</sup>; Gang Xiao<sup>1</sup>; Himanshu Gadgil<sup>1</sup>; Bill Callahan<sup>1</sup>; Sabine Paterson<sup>1</sup>; Pavel Bondarenko<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, California
- ThP 510 **ESI- and MALDI-MS Studies of Covalently Modified Peroxiredoxin and Superoxide Dismutase: Targets of Quinone Methide Lung Tumor Promoters;** Oleg V. Kirichenko<sup>1</sup>; Brent W. Meier<sup>1</sup>; Jose D. Gomez<sup>1</sup>; John A. Thompson<sup>1</sup>; <sup>1</sup>University of Colorado Health Sciences Center, Denver, CO
- ThP 511 **Structural and Catalytic Effects of Biological Oxidants on Group VI Group VIA Phospholipase A<sub>2</sub>;** Haowei Song<sup>1</sup>; Shuzhong Bao<sup>1</sup>; Sasanka Ramanadham<sup>1</sup>; John Turk<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- ThP 512 **Modification, Degradation, and Inactivation of Mitochondrial and Cytosolic Proteins in Alcohol-Exposed Animal Livers and Hepatoma Cells;** Byoung J. Song<sup>2</sup>; Brian L. Hood<sup>1</sup>; Bong-Jo Kim<sup>2</sup>; Kwan-Hoon Moon<sup>2</sup>; Soo-Kyung Suh<sup>2</sup>; James P. Hardwick<sup>2</sup>; David A. Lucas<sup>1</sup>; Thomas P. Conrads<sup>1</sup>; Timothy D. Veenstra<sup>1</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>National Institute on Alcohol Abuse and Alcoholism, Bethesda, MS
- ThP 513 **Conclusive Determination of Carbonylated Proteins from Rat Skeletal Muscle Mitochondria Using Affinity Enrichment, iTRAQ Reagent Labeling and MS/MS Analysis;** Hongwei Xie<sup>1</sup>; Danni Li<sup>1</sup>; LaDora V. Thompson<sup>1</sup>; Edgar A. Arriaga<sup>1</sup>; Timothy J. Griffin<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN
- ThP 514 **Rapid Screening of 4HNE Adducts on Creatine Kinase Brain Isoform by Direct Infusion LTQ-FT MS and MS/MS;** Shannon M Eliuk<sup>1</sup>; Erin M Shonsey<sup>1</sup>; Matthew B Renfrow<sup>1</sup>; Marion Kirk<sup>1</sup>; Stephen Barnes<sup>1</sup>; Helen Kim<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL
- ThP 515 **A Detailed Map of Oxidative Post-translational Modifications of Human p21ras using Fourier Transform Mass Spectrometry;** Cheng Zhao<sup>1</sup>; Mahadevan Sethuraman<sup>1</sup>; Nicolas Clavreul<sup>1</sup>; Parminder Kaur<sup>1</sup>; Richard Cohen<sup>1</sup>; Peter O'Connor<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- ThP 516 **De Novo Sequencing and Characterization of Post-translational Modifications of an Amyloidogenic Immunoglobulin Kappa Light Chain;** Yan Jiang<sup>1</sup>; Roger Theberge Theberge<sup>1</sup>; Jeremy Eberhard<sup>1</sup>; Greg Karamitis<sup>1</sup>; Tatiana Prokaeva<sup>1</sup>; Lawreen H. Connors<sup>1</sup>; Martha Skinner<sup>1</sup>; Cheng Lin<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA

### PROTEIN CONFORMATION III

- ThP 517 **Transferrin : Receptor Binding in vivo Using Novel Footprinting Approach;** Ming-Zhong Sun<sup>1</sup>; Olga Zak<sup>2</sup>; Guozhong Xu<sup>1</sup>; Rutao Liu<sup>2</sup>; Phil Aisen<sup>2</sup>; Mark R Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Albert Einstein College of Medicine, Bronx, NY
- ThP 518 **Determining the Conformation of ApoA-I on Phospholipid rHDL Discs Using Chemical Cross-linking and Mass Spectrometry;** Michael J. Thomas<sup>1</sup>;

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- Shaila Bhat<sup>1</sup>; Michael P. Samuel<sup>1</sup>; Mary G. Sorci-Thomas<sup>1</sup>; <sup>1</sup>Wake Forest University Health Science, Winston-Salem, NC
- ThP 519 **Time-resolved Footprinting Approach to Examine the Dynamics of Ca<sup>2+</sup> Dependent Activation of Gelsolin;** Janna G Kiselar<sup>13</sup>; Paul A Janmey<sup>2</sup>; Mark R Chance<sup>13</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Case Western Reserve University, Cleveland, OH
- ThP 520 **Inside of a Molecular Machine: Examination of the ClpAP Protease via Synchrotron Radiolysis and Mass Spectrometry;** Jen Bohon<sup>1</sup>; Sayan Gupta<sup>1</sup>; Laura D. Jennings<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA
- ThP 521 **Three Integrative Computational Tools for a Chemical Protein Crosslinking Workflow using Isotope-Coded Crosslinkers and Mass Spectrometry: iXLINK, doXLINK and XlinkViewer;** Jan Seebacher<sup>1</sup>; Parag Mallick<sup>3</sup>; Ning Zhang<sup>1</sup>; James S. Eddes<sup>1</sup>; Ruedi Aebersold<sup>4</sup>; Michael H. Gelb<sup>2</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Louis Warschaw Prostate Cancer Center, Cedars-Sina, Los Angeles, CA; <sup>4</sup>Federal Institute of Technology, Zürich, Switzerland
- ThP 522 **Probing Laminin Self-Interactions Using Isotope-Labeled Cross-Linkers and ESI-FTICR Mass Spectrometry;** Stefan Kalkhof<sup>1</sup>; Sebastian Haehn<sup>2</sup>; Christian Ihling<sup>1</sup>; Neil Smyth<sup>3</sup>; Andrea Sinz<sup>1</sup>; <sup>1</sup>BBZ, University of Leipzig, Leipzig, Germany; <sup>2</sup>University of Cologne, Cologne, Germany; <sup>3</sup>University of Southampton, Southampton, UK
- ThP 523 **Determining Inter-Residue Distances in Proteins from Sequential Cross-linking Rate Measurements (SCRaM): A Mass Spectrometry-based Alternative to FRET;** Joseph Schoeniger<sup>1</sup>; Richard Jacobsen<sup>1</sup>; Christopher Behrens<sup>1</sup>; Kenneth Sale<sup>1</sup>; <sup>1</sup>Sandia National Labs, Livermore, CA
- ThP 524 **Exploring of Protein-Protein Interaction by Cross-linking Reactions and Mass Spectrometry;** Miroslav Sulc<sup>1</sup>; Katerina Peslova<sup>2</sup>; Jana Michalova<sup>2</sup>; Tomas Obsil<sup>3</sup>; Petr Novak<sup>1</sup>; Petr Hodek<sup>2</sup>; <sup>1</sup>Institute of Microbiology AVCR, Prague, Czech Republic; <sup>2</sup>Dept. of Biochemistry, Charles University, Prague, Czech Republic; <sup>3</sup>Institute of Physiology AVCR, Prague, Czech Republic
- ThP 525 **Structural Analysis of Interdomain Interactions and DNA Binding by the TATA Binding Protein (TBP) by Synchrotron Radiolysis and Mass Spectrometry;** Sayan Gupta<sup>1</sup>; Sergei Khrapunov<sup>2</sup>; Janna Kiselar<sup>1</sup>; Jen Bohon<sup>1</sup>; Mark R. Chance<sup>1</sup>; Michael Brenowitz<sup>2</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Albert Einstein College of Medicine, Bronx, NY
- ThP 526 **Akt-Membrane Interaction Probed by Chemical Cross-Linking and Mass Spectrometry: the Effect of Phosphatidylserine (PS) on Akt Activation;** Bill X. Huang<sup>1</sup>; Hee-Yong Kim<sup>1</sup>; <sup>1</sup>NIH/NIAAA, Rockville, MD
- ThP 527 **Modeling of the Cofilin-Actin Binary Complex Using Protein Footprinting Data;** J. K. Amisha Kamal<sup>1</sup>; Jing-Qu Guan<sup>2</sup>; Steven C. Almo<sup>3</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University School of Medicine, Cleveland, OH; <sup>2</sup>PhytoCeutica, Inc., New Haven, CT; <sup>3</sup>Albert Einstein College of Medicine, Bronx, NY
- ThP 528 **Monitoring Conformational Changes in Protein Complexes Using Chemical Cross-linking and FTMS: The Influence of Calcium to Calmodulin - Melittin**

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- Complex;** Anastassios E. Giannakopoulos<sup>1</sup>; Peter J. Derrick<sup>1</sup>; Vladimir Havlicek<sup>2</sup>; Petr Novak<sup>2</sup>; <sup>1</sup>University of Warwick, Coventry, United Kingdom; <sup>2</sup>Institute of Microbiology, Prague, Czech Republic
- ThP 529 **Chemical Cross-Linking and X-Ray footprinting Coupled to Mass Spectrometry as a Tool for Protein Structure Elucidation;** Amadeu H Iglesias<sup>1</sup>; Nilson T Zanchin<sup>1</sup>; Fabio C Gozzo<sup>1</sup>; <sup>1</sup>Brazilian Synchrotron Light Laboratory, Campinas, Brazil
- ThP 530 **Detection of Conformational Changes in Beta-Arrestin by Cross-Linking and Mass Spectrometry;** Jennifer L. Cable<sup>2</sup>; Evgeniy V. Petrotchenko<sup>1</sup>; Nikolay V. Dokholyan<sup>1</sup>; Kunhong Xiao<sup>2</sup>; J. Michael Dial<sup>1</sup>; Robert J. Lefkowitz<sup>2</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Duke University, Durham, NC
- ThP 531 **Nested Rigid Crosslinkers for the Conformational Probing of Proteins and Protein/Ligand Complexes by ESI-FTMS;** Qingrong Zhang<sup>1,3</sup>; Liz Crosland<sup>2</sup>; Daniele Fabris<sup>1,3</sup>; <sup>1</sup>University of Maryland Baltimore County, Baltimore, MD; <sup>2</sup>Villa Julie College, Stevenson, MD; <sup>3</sup>University of Maryland Baltimore County, Baltimore, MD
- ThP 532 **Cross-linking Proteins with APAX. An Aptly Positioned Azide Group Enables Facile MS Detection of Cross-Linked Peptides;** Piotr T. Kasper<sup>1</sup>; Jaap Willem Back<sup>1</sup>; Géraldine Masson<sup>2</sup>; Aloysius F. Hartog<sup>2</sup>; Leo J. de Koning<sup>1</sup>; Jan H. van Maarseveen<sup>2</sup>; Anton O. Muijsers<sup>1</sup>; Luitzen de Jong<sup>1</sup>; Chris G. de Koster<sup>1</sup>; <sup>1</sup>SILS, University of Amsterdam, Amsterdam, The Netherlands; <sup>2</sup>HIMS, University of Amsterdam, Amsterdam, The Netherlands
- ThP 533 **Mapping Dimerization Interfaces of Mammalian Adenylyl Cyclase by Chemical Cross-linking Combined with MALDI-TOF and Nano-LC-ESI Mass Spectrometry;** Yan Li<sup>1</sup>; Tung-Chung Mou<sup>1</sup>; Haydn L. Ball<sup>1</sup>; Stephen R. Sprang<sup>1</sup>; <sup>1</sup>University of Texas Southwestern Medical Center, Dallas, TX

### PROTEINS: FOLDING

- ThP 534 **Phenomenon of Cryogenic Chemical Oxidation of Proteins;** David M. Hambly<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- ThP 535 **Extension of SUPREX to the Thermodynamic Analysis of Multi-State Folding Proteins and their Ligand Complexes;** Liangjie Tang<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- ThP 536 **Probing Protein Structure as a Function of Side Chain Availability: Selective Noncovalent Attachment of 18-Crown-6 to Lysine Side Chains;** Ryan R Julian<sup>1</sup>; Tony Ly<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- ThP 537 **Unfolding in the SH3 Domain of the Abelson Tyrosine Kinase probed with Hydrogen Exchange Mass Spectrometry;** Shugui Chen<sup>1</sup>; James M. Hochrein<sup>1</sup>; Anthony P. Schiavone<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA
- ThP 538 **Characterization of an Autonomous Folding Unit for LR<sup>3</sup>IGF-I by Hydrogen/Deuterium Exchange-Mass Spectrometry;** Xue Li<sup>1</sup>; Jiong Yu<sup>2</sup>; William J Wedemeyer<sup>1</sup>; Steven P Gygi<sup>2</sup>; J Throck Watson<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>Harvard Medical School, Boston, MA
- ThP 539 **Folding and Assembly Kinetics of Noncovalent Protein Complexes on the Millisecond Time Scale;** Lars Konermann<sup>1</sup>; Anne C. Dempsey-Rintala<sup>1</sup>; Gary S. Shaw<sup>1</sup>;

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- Yu Li<sup>1</sup>; Jingxi Pan<sup>1</sup>; <sup>1</sup>The University of Western Ontario, London, ON, Canada
- ThP 540 **Straightforward Determination of Disulfide Linkages in Proteins: The Case of beta- N-acetyl-Hexosaminidase from *Aspergillus oryzae*;** Petr Novak<sup>1</sup>; Petr Man<sup>1</sup>; Petr Pompach<sup>1</sup>; Katerina Hofbauerova<sup>1</sup>; Karel Bezouska<sup>1</sup>; <sup>1</sup>Institute of Microbiology, Prague, Czech Republic
- ThP 541 **Determination of the Binding Constants of Calbindin D28k to Calcium Ions by Direct Infusion Using the PLIMSTEX Technique;** Sandra A. Kerfoot<sup>1</sup>; Don Rempel<sup>1</sup>; Rajiv Kumar<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Mayo Clinic, Rochester, MN
- ThP 542 **Probing the Solvent-Exposed Surface of a Moving Macromolecular Machine;** Marek Daniel Koter<sup>1</sup>; Paul David Gershon<sup>1</sup>; <sup>1</sup>University of California, Irvine, CA
- ThP 543 **Rapid Mapping of Protein Conformational Landscapes by Automated Data Acquisition and Analysis of Multiplexed HXMS Timecourses;** Allis S. Chien<sup>1</sup>; Judith Frydman<sup>2</sup>; Andrew D. Miranker<sup>3</sup>; Sheila S. Jaswal<sup>2</sup>; <sup>1</sup>SU Mass Spectrometry, Stanford University, Stanford, CA; <sup>2</sup>Dept. of Biological Sciences, Stanford University, Stanford, CA; <sup>3</sup>Dept. of Molecular Biophysics & Biochem, Yale Univ, New Haven, CT
- ThP 544 **Comparing the Ionization Efficiencies of Coexisting Protein Conformers in Positive Ion ESI-MS;** Mark C. Kuprowski<sup>1</sup>; Belal M. Hossain<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Canada
- ThP 545 **Conformational Changes in Proteins in Solution are Studied Using a New Membrane Electrospray Probe On-line with Electrospray Mass Spectrometer Analysis;** David G. Welkie<sup>1</sup>; Thomas P. White<sup>1</sup>; Craig M. Whitehouse<sup>1</sup>; <sup>1</sup>Analytica of Branford, INC., Branford, CT
- ThP 546 **Role of Protein Oxidation in Amyloid Fibril Formation Assemblies;** Simin D. Maleknia<sup>1</sup>; Natalia Reixach<sup>3</sup>; Joel N. Buxbaum<sup>3</sup>; <sup>1</sup>Griffith University, Brisbane, AUSTRALIA; <sup>2</sup>Sciformatics, Sydney, AUSTRALIA; <sup>3</sup>Scripps Research Institute, La Jolla, CA

### PROTEOMICS: LABELING AND AFFINITY METHODS

- ThP 547 **The “N-terminome”: Fingerprinting the In Vivo Activity of Processing Peptidases in *E. coli*;** John C. Timmer<sup>1</sup>; Wenhong Zhu<sup>2</sup>; Mari Enoksson<sup>2</sup>; Eric Wildfang<sup>2</sup>; Andy Tao<sup>3</sup>; Guy S. Salvesen<sup>2</sup>; <sup>1</sup>Molecular Pathology Program, UCSD, La Jolla, CA; <sup>2</sup>Burnham Institute for Medical Research, La Jolla, CA; <sup>3</sup>Purdue University, West Lafayette, LA
- ThP 548 **Identification of Proteolytic Cleavage Sites by Quantitative Proteomics;** Mari Enoksson<sup>1</sup>; Melanie Ivancic<sup>2</sup>; Jiangwei Li<sup>2</sup>; John Timmer<sup>1</sup>; Eric Wildfang<sup>1</sup>; Guy Salvesen<sup>1</sup>; Andy Tao<sup>2</sup>; <sup>1</sup>Burnham Institute for Medical Research, La Jolla, CA; <sup>2</sup>Purdue University, West Lafayette, IN
- ThP 549 **Development of a Mass Spectrometric Approach for Studying Mitochondrial Thiol Proteins;** Jing Wang<sup>1</sup>; Kevin Marley<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 550 **Identification and Characterization of Ligand-Dependent Estrogen Receptor Multi-Protein Complexes Using Tandem Affinity Purification and LC-MS/MS;** Jessica C. Clark<sup>1</sup>; P. Lee Ferguson<sup>1</sup>; <sup>1</sup>University of South Carolina, Columbia, SC
- ThP 551 **Carbonylated Proteins Probed by a Hydrazide-Functionalized Isotope-Coded Affinity Tag (HICAT);**



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- Bingnan Han<sup>1</sup>; Fred Stevens<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, Oregon
- ThP 552 **A Dual-Tagging Proteomic Approach that Integrates Stable-Isotope Labeling, Affinity Purification, and Mass Spectrometry Reveals Links between DNA Repair and Cytokinesis;** Yu-Chun Du<sup>1</sup>; Jianhong Zhou<sup>1</sup>; Zhiyuan Shen<sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>University of New Mexico School of Medicine, Albuquerque, NM
- ThP 553 **Mass Defect Labeling of Cysteine for Improving Peptide Assignment in Shotgun Proteomic Analyses; MALDI-FTMS versus ESI-FTMS;** Hilda Hernandez<sup>1</sup>; Sarah Niehauser<sup>1</sup>; Vijay Gawandi<sup>1</sup>; Robert S. Phillips<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- ThP 554 **Quantitative Proteomic Analysis of Clostridium thermocellum Using 15N-metabolic Labeling;** Xinping Liu<sup>1</sup>; Herbert J. Strobel<sup>1</sup>; Jennifer C. Combs<sup>1</sup>; Bert C. Lynn<sup>1</sup>; <sup>1</sup>University of Kentucky, Lexington, KY
- ThP 555 **Pyrene: a LDI-TOF Mass-tag Surfboard for the 337 nm Wave;** Mikhail S. Shchepinov<sup>1</sup>; Aleksei Ustinov<sup>1</sup>; Irina Astakhova<sup>1</sup>; Pablo Bernad<sup>1</sup>; Vladimir A. Korshun<sup>1</sup>; <sup>1</sup>Trident Technologies, Oxford, UK
- ThP 556 **Application of Reactive Desorption Electrospray Ionization (R-DESI) to Biomolecules;** Demian R. Ifa<sup>1</sup>; Justin M. Wiseman<sup>1</sup>; Nick Manicke<sup>1</sup>; Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- ThP 557 **Localization of Actin-Interacting Proteins to the Phagosome of Human Neutrophils and RAW 264.7 Macrophages;** Angelique K Florentinus<sup>1</sup>; John Marshall<sup>1</sup>; Andy Jankowsky<sup>1</sup>; <sup>1</sup>Ryerson University, Toronto, ON, Canada
- ThP 558 **A Photostable Derivatizing Reagent for MALDI Mass Spectrometry of Tryptophan-Containing Peptides and Proteins;** Chunyan Li<sup>1</sup>; Vijay Gawandi<sup>1</sup>; Adam Protos<sup>1</sup>; Phanneth Som<sup>1</sup>; Robert S. Phillips<sup>1</sup>; I. Jonathan Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- ThP 559 **Elucidating Androgen Receptor Interacting Protein Networks using Quantitative Mass Spectrometry;** Rohini J Jasavala<sup>1</sup>; Armann A Andaya<sup>1</sup>; Harryl Martinez<sup>1</sup>; Anne-Claude Gringas<sup>2</sup>; David K. Han<sup>3</sup>; Michael E Wright<sup>1</sup>; <sup>1</sup>University of California Davis Genome Center, Davis, CA; <sup>2</sup>Samuel Lunenfeld Research Institute, Toronto, Canada; <sup>3</sup>University of Connecticut, Farmington, CT
- ThP 560 **Detection and Identification of S-glutathiolated proteins in Endothelial Cells exposed to Oxidants by a Biotin-labeling: Liquid Chromatographic and MS Method;** Nicolas Clavreul<sup>1</sup>; Claire Daully<sup>1</sup>; Hua Huang<sup>1</sup>; Maha Sethuraman<sup>1</sup>; Marc McComb<sup>1</sup>; Catherine Costello<sup>1</sup>; Richard Cohen<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA
- ThP 561 **Protein Targets of Oxidative Stress in Cardiac Mitochondria;** Juan Chavez<sup>1</sup>; Woon-Gye Chung<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 562 **Developing Soluble Dendritic Polymers for Quantitative Proteomics;** Minjie Guo<sup>1</sup>; W. Andy Tao<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- ThP 563 **Quantification of Protein Expression in Human Serum Samples Collected From Normal and Cancerous Patients Using Top Down iTRAQ Technology;** Mahbod Hajivandi<sup>1</sup>; Xiquan Liang<sup>1</sup>; John Leite<sup>1</sup>; Steve Guertin<sup>2</sup>; Brian Williamson<sup>2</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>Invitrogen, Carlsbad, California; <sup>2</sup>Applied Biosystems, Framingham, Massachusetts

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- ThP 564 **A Modified SILAC Approach: a Case-Study in Tyrosine Phosphorylation;** Alejandro Zimman<sup>1</sup>; Yongming Xie<sup>1</sup>; Evangelia Komisopoulou<sup>1</sup>; Joseph Loo<sup>1</sup>; Thomas Graeber<sup>1</sup>; Judith A. Berliner<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- PROTEOMICS: DETECTION OF BIOMOLECULES**
- ThP 565 **LC-MALDI Profiling and Marker ID by in situ Digestion and MS/MS;** Sven Brand<sup>1</sup>; Stephanie Hahner<sup>1</sup>; Arndt Asperger<sup>1</sup>; Detlev Suckau<sup>1</sup>; Markus Meyer<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, D
- ThP 566 **Partial Ion Current Normalization of Mass Spectra and Biomarker Reproducibility;** Maxim Tsybin<sup>1</sup>; Julia Grigorieva<sup>1</sup>; Ed Rothhoff<sup>1</sup>; Heinrich Roder<sup>1</sup>; <sup>1</sup>Efecta Technologies, Steamboat Springs, CO
- ThP 567 **Top-Down Analysis of Proteins by ISD-MALDI-TOF for Biomarker Discovery;** Marcus Macht<sup>1</sup>; Sven Brand<sup>1</sup>; Markus Meyer<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany
- ThP 568 **Using MS/MS Databases to Find Biomarker Protein Clips;** Conor P. Mullens<sup>1</sup>; Stephan B.H. Bach<sup>1</sup>; Robert J. Christy<sup>2</sup>; John Kalns<sup>2</sup>; Linda Nagore<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, TX; <sup>2</sup>Hyperion Biotechnology, San Antonio, TX
- ThP 569 **Metal Profiling of Human Serum Using Size Exclusion Chromatography Hyphenated to Inductively Coupled Plasma-Mass Spectrometry;** Rudolf Grimm<sup>1</sup>; Dominic Hare<sup>2</sup>; Philipp Doble<sup>2</sup>; Robert Moritz<sup>2</sup>; Richard Simpson<sup>2</sup>; Michael Dawson<sup>2</sup>; Rod Minett<sup>1</sup>; Val Spikmans<sup>2</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, CA; <sup>2</sup>University of Technology, Sydney, Australia; <sup>3</sup>Ludwig Institute of Cancer Research, Melbourne, Australia
- ThP 570 **Comparative Analysis of Complex Proteomes for Biomarker Discovery Employing Differential Isotopically-labeled Acetylation Followed by LC/LC-FTMS on a 12 T Instrument;** Cameron O. Scarlett<sup>1</sup>; Ryan M. Danell<sup>2</sup>; Michael Easterling<sup>3</sup>; J. Paul Speir<sup>3</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>Danell Consulting, Greenville, NC; <sup>3</sup>Bruker Daltonics, Billerica, MA
- ThP 571 **Identification of Differentially Expressed Peptides Using a Combination of MALDI and nanoLC ESI-FTMS;** Lennard J. Dekker<sup>1</sup>; Andreas Römpf<sup>2</sup>; Ioana Taban<sup>3</sup>; Guido Jenster<sup>1</sup>; Willem Boogerd<sup>4</sup>; Hans Bonfrer<sup>4</sup>; Bernhard Spengler<sup>2</sup>; Ron Heeren<sup>3</sup>; Peter Sillevs Smitt<sup>1</sup>; Theo Luider<sup>1</sup>; <sup>1</sup>ErasmusMC, Rotterdam, The Netherlands; <sup>2</sup>Justus Liebig University Giessen, Giessen, Germany; <sup>3</sup>FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands; <sup>4</sup>The Netherlands Cancer Institute, Amsterdam, The Netherlands
- ThP 572 **Integrative Proteomic-Genomic Kinetic Analysis of HIV-1 infected CD4<sup>+</sup>-T-cells by Label-Free, Targeted Mass Spectrometry and Microarray Analyses;** Eric Y Chan<sup>1</sup>; Lee Weng<sup>2</sup>; Jennifer N Sutton<sup>3</sup>; Sean C Proll<sup>1</sup>; Andrew D Keller<sup>2</sup>; James C Wallace<sup>1</sup>; Leo E Bonilla<sup>3</sup>; Michael G Katze<sup>1</sup>; <sup>1</sup>Dept. of Microbiology, University of Washington, Seattle, WA; <sup>2</sup>Rosetta Biosoftware, Seattle, WA; <sup>3</sup>BRIMS Center, Thermo Electron Corp., Cambridge, MA
- ThP 573 **The Importance of High Precision Retention Times in LC/MS of Biomarkers;** Peter Kent<sup>1</sup>; Lori Ann Upton<sup>1</sup>; Eric Kemp<sup>1</sup>; Kerry Nugent<sup>1</sup>; <sup>1</sup>Michrom Bioresources, Inc., Auburn, CA
- ThP 574 **Pattern Recognition Mass Spectrometry for Disease Diagnosis;** Philip S. Mayer<sup>1</sup>; Bryan Prazen<sup>2</sup>; Tennille Baileykaze<sup>1</sup>; Brian Pratt<sup>2</sup>; Erik Nilsson<sup>2</sup>; Tomas Vaisar<sup>1</sup>;



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- <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Insilicos, Seattle, WA
- ThP 575 **Relative Quantitation and Validation of Proteins Determined to be Differentially Expressed from High-Throughput DNA Microarrays Using LC/MS/MS;** Sahana Mollah<sup>1</sup>; Matthew M. Champion<sup>1</sup>; Tapani Ronni<sup>2</sup>; Sam Ho<sup>2</sup>; Sinisa Dovatz<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Department of Pediatrics, University of Wisconsin, Madison, WI
- ThP 576 **LC/MSMS Study of Benzo[a]pyrene-7,8-quinone Adduction to Globin Tryptic Peptides and N-Acetylaminic Acids;** Witold M. Winnik<sup>1</sup>; Narayanan Balu<sup>2</sup>; William T. Padgett<sup>1</sup>; Stephen C. Nesnow<sup>1</sup>; <sup>1</sup>US EPA, RTP, NHEERL, ECD, Research Triangle Park, NC; <sup>2</sup>NRC Postdoctoral Associate (Now at BASF Inc.), Research Triangle Park, NC
- ThP 577 **Reproducibility of Protein Profiling by Solid Phase Extraction and Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry;** Anne Kjærgaard Callesen<sup>1</sup>; Jonna Skov Madsen<sup>2</sup>; Per E. Jørgensen<sup>2</sup>; Torben A. Kruse<sup>2</sup>; Søren Cold<sup>2</sup>; Ole Mogensen<sup>2</sup>; Werner Vach<sup>1</sup>; René dePont Christensen<sup>1</sup>; Ole Nørregaard Jensen<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Odense University Hospital, Odense, Denmark
- ThP 578 **Biomarker Discovery Combining High Mass Accuracy MS-based Profiling with Targeted MS/MS;** Christine A. Miller<sup>1</sup>; David Deng<sup>1</sup>; Patrick D. Perkins<sup>1</sup>; Bryan D. Miller<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 579 **Withdrawn**
- ThP 580 **Separation of Released and Intracellular 3T3-L1 Adipocyte Proteins by Affinity MALDI Plates;** Lucia A. de Jesus<sup>1</sup>; Andre P. Seale<sup>1</sup>; Jeong Heon Lee<sup>1</sup>; Mi Young Ha<sup>2</sup>; Yangsun Kim<sup>1</sup>; <sup>1</sup>Proteonik Inc., Ansan, South Korea; <sup>2</sup>Microbiotech Center, Ansan, South Korea
- ThP 581 **Auditory Proteomics of Mouse Model for Usher Syndrome 1F;** Mark R. Chance<sup>1</sup>; Shuqing Liu<sup>1</sup>; Ming-Zhong Sun<sup>1</sup>; Daniel Chen<sup>1</sup>; Qing Y. Zheng<sup>1</sup>; Kumar Alagramam<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH
- ThP 582 **Top-Down Proteomics by 12T-FTICR-MS for Characterizing Protein Biomarkers Discovered by SELDI;** Severine A. Patat<sup>1</sup>; Brendan McMorran<sup>2</sup>; Cameron O. Scarlett<sup>1</sup>; Claire Wainwright<sup>3</sup>; Brandon Wainwright<sup>2</sup>; Christoph H. Borchers<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>University of Queensland, Brisbane, Australia; <sup>3</sup>Royal Children's Hospital, Brisbane, Australia
- ThP 583 **The Proteomic Alterations of Rat Mitochondria Caused by Chronic Alcoholism;** Liang Shi<sup>1</sup>; Yuan Wang<sup>1</sup>; Xiaolei Li<sup>1</sup>; Jianmin Shao<sup>1</sup>; Kang Zhao<sup>1</sup>; Ningzhi Xu<sup>1</sup>; Aruni Bhatnagar<sup>2</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>Beijing Genomics Institute, Beijing, China; <sup>2</sup>Division of Cardiology, University of Louisville, Louisville, KY
- ThP 584 **Comparison of Mitochondrial Proteomes from Different Mouse Tissues;** Yuan Wang<sup>1</sup>; Liang Shi<sup>1</sup>; Xiaolei Li<sup>1</sup>; Jianmin Shao<sup>1</sup>; Kang Zhao<sup>1</sup>; Ningzhi Xu<sup>1</sup>; Siqi Liu<sup>1</sup>; <sup>1</sup>Beijing Genomics Institute, CAS, Beijing, China
- ThP 585 **Determining iTRAQ Experiment Variability and Biomarker False-Positive Rates Due to sample Preparation and Label Bias in Plasma by LC-MALDI MS/MS;** Phil Jakubowski<sup>1</sup>; Leanne B. Ohlund<sup>1</sup>; Axel Bergman<sup>2</sup>; Derek S. Smith<sup>1</sup>; Monica Elliott<sup>1</sup>; Darryl B.

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- Hardie<sup>1</sup>; <sup>1</sup>University of Victoria, Victoria, Canada; <sup>2</sup>iCAPTURE, Vancouver, Canada
- ThP 586 **Wavelet based Feature Extraction in the Analysis of Clinical Proteomics Mass Spectra;** Frank M. Schleif<sup>1</sup>; Michael Kuhn<sup>1</sup>; Thomas Elssner<sup>1</sup>; Jens Decker<sup>1</sup>; Herbert Thiele<sup>1</sup>; Mathias Lindemann<sup>2</sup>; Henning Thielemann<sup>2</sup>; Peter Maass<sup>2</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Univ. of Bremen, Center of Industrial Mathematics, Bremen, Germany
- ThP 587 **Identification of Human Microsomal Protein Targets of Reactive Electrophiles;** Nah-Young Shin<sup>1</sup>; F. Peter Guengerich<sup>1</sup>; Daniel C. Liebler<sup>1</sup>; <sup>1</sup>Vanderbilt University School of Medicine, Nashville, TN
- ThP 588 **High-Molecular Weight Protein Depletion Strategy for Enhanced MALDI-TOF MS Serum Peptide Profiling;** Thomas Elssner<sup>1</sup>; Isabell Thomas<sup>1</sup>; Ines Schäfer<sup>1</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Leipzig, Germany
- ThP 589 **Withdrawn**
- | PROTEOMICS: MEDICAL APPLICATIONS |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ThP 590                          | <b>Benchmarking of Differentiating Human and Mouse Embryonic Stem Cells by FT-MS;</b> <u>Jeroen Krijgsveld</u> <sup>1</sup> ; Dennis Van Hoof <sup>2</sup> ; Martijn W. Pinkse <sup>1</sup> ; Robert Passier <sup>2</sup> ; Christine L. Mummery <sup>2</sup> ; Albert J.R. Heck <sup>1</sup> ; <sup>1</sup> Utrecht University, Utrecht, The Netherlands; <sup>2</sup> Hubrecht Laboratory, Utrecht, The Netherlands                                                                                                                                                          |
| ThP 591                          | <b>Serum Glycomics of CDG and Galactosemic Patients;</b> Luisa Sturiale <sup>1</sup> ; Rita Barone <sup>1</sup> ; <u>Domenico Garozzo</u> <sup>1</sup> ; <sup>1</sup> CNR ICTP, Catania, Italy                                                                                                                                                                                                                                                                                                                                                                                 |
| ThP 592                          | <b>A Proteomic Approach for Evaluating the Effects of Proanthocyanidins on Rotenone-Induced Toxicity in SH-SY5Y Neuroblastoma Cells;</b> <u>Cristobal L. Miranda</u> <sup>1</sup> ; Woon-Gye Chung <sup>1</sup> ; Hui-Jing Li <sup>1</sup> ; Jan F. Stevens <sup>1</sup> ; Claudia S. Maier <sup>1</sup> ; <sup>1</sup> Oregon State University, Corvallis, OR                                                                                                                                                                                                                 |
| ThP 593                          | <b>Changes in Cell Surface and Soluble Proteins Induced by TGF-<math>\beta</math> in Liver Cancer Cells Determined Using a Label-Free Approach;</b> <u>Bin Deng</u> <sup>1</sup> ; Hong Wang <sup>1</sup> ; Laura Beretta <sup>1</sup> ; Samir Hanash <sup>1</sup> ; <sup>1</sup> Fred Hutchinson Cancer Research Center, Seattle, WA                                                                                                                                                                                                                                          |
| ThP 594                          | <b>Proteomics Approach to Fructose-Induced Fatty Liver and Type 2 Diabetes;</b> <u>Lihe Zhang</u> <sup>1</sup> ; Steven Ringquist <sup>1</sup> ; H. Henry Dong <sup>1</sup> ; <sup>1</sup> Children's Hospital of Pittsburgh, Pittsburgh, PA                                                                                                                                                                                                                                                                                                                                   |
| ThP 595                          | <b>Proteins Associated with Cisplatin Resistance in Ovarian Cancer Cells Identified by Quantitative Proteomics Technology and Integrated with mRNA expression levels;</b> Jennifer Stewart <sup>1</sup> ; James White <sup>1</sup> ; Xiaowei Yan <sup>1</sup> ; Leroy Hood <sup>1</sup> ; <u>Biao Yang Lin</u> <sup>1</sup> ; <sup>1</sup> Inst for Systems Biology, Seattle, WA                                                                                                                                                                                               |
| ThP 596                          | <b>Proteomic Comparison of Mouse Pancreatic Islet Cells Using 2-D PAGE and MALDI-TOF/TOF to Identify Proteins Associated with Type 2 Diabetes;</b> <u>Mark Scalf</u> <sup>1</sup> ; Mark Gray-Keller <sup>1</sup> ; Jessica L. Jarecki <sup>1</sup> ; Angela Tebon-Oler <sup>1</sup> ; Mary E. Rabaglia <sup>1</sup> ; Grzegorz Sabat <sup>1</sup> ; Michael R. Shortreed <sup>1</sup> ; Brian L. Frey <sup>1</sup> ; Michael S. Westphall <sup>1</sup> ; Alan D. Attie <sup>1</sup> ; Lloyd M. Smith <sup>1</sup> ; <sup>1</sup> University of Wisconsin-Madison, Madison, WI |
| ThP 597                          | <b>An Improved Peptide Profiling Strategy to Find Biomarkers for Breast Cancer;</b> <u>David H. Hawke</u> <sup>1</sup> ; Bing Zhang <sup>1</sup> ; Haitau Zhao <sup>1</sup> ; Jianhua Hu <sup>1</sup> ; Keith A. Baggerly <sup>1</sup> ; Francisco J. Esteva <sup>1</sup> ; Ryuji Kobayashi <sup>1</sup> ; <sup>1</sup> UT-M.D. Anderson Cancer Center, Houston, TX                                                                                                                                                                                                            |
| ThP 598                          | <b>Quantitative Proteomic Analysis of Diabetic Mouse Pancreatic Islets by Differential Isotope Labeling and Mass Spectrometry;</b> <u>Ying Yang</u> <sup>1</sup> ; Hongfang Lu <sup>1</sup> ; Ling                                                                                                                                                                                                                                                                                                                                                                             |

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- Xu<sup>1</sup>; Michael Wheeler<sup>1</sup>; <sup>1</sup>University of Toronto, Toronto, Canada
- ThP 599 **Global Quantitative Comparison of the Cellular Proteomes of Endothelial Cells from Consomic Rat Strains Under Normoxia and Hypoxia;** Shama P. Mirza<sup>1</sup>; Molly C. Pellitteri<sup>1</sup>; Erika Keyes<sup>1</sup>; Maria Warren<sup>1</sup>; Dani Didier<sup>1</sup>; Julia Hayter<sup>1</sup>; Brian D. Halligan<sup>1</sup>; Andrew S. Greene<sup>1</sup>; Michael Olivier<sup>1</sup>; <sup>1</sup>Medical College of Wisconsin, Milwaukee, Wisconsin
- ThP 600 **Proteomics-Based Approach for Accelerated Identification of Single Nucleotide Polymorphisms;** Maureen K. Bunker<sup>1</sup>; Benjamin J. Cargile<sup>1</sup>; Joel R. Sevinsky<sup>1</sup>; James L. Stephenson<sup>1</sup>; <sup>1</sup>Research Triangle Institute, Research Triangle Park, NC
- ThP 601 **Matrix-Assisted Laser Desorption Ionization/Time-of-Flight Mass Spectrometry as A Rapid and Sensitive Detection Method of Occult Blood in Feces;** Chen-I Wu<sup>1</sup>; Pei-Chang Wu<sup>2</sup>; Ching-Chou Tsai<sup>2</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan; <sup>2</sup>Chang Gung Memorial Hospital-Kaohsiung, Kaohsiung County, Taiwan
- ThP 602 **The Role of Proteasome in Neurodegenerative Disease Using Proteomics Approaches;** Beniam T Berhane<sup>1</sup>; Ghania Ait-Ghezala<sup>1</sup>; Claud-Henry Volmar<sup>1</sup>; Elaina Margenthaler<sup>1</sup>; Fiona Crawford<sup>1</sup>; Mike Mullan<sup>1</sup>; <sup>1</sup>Roskamp Institute, Sarasota, FL 34243
- ThP 603 **Heat Shock Prevents the Nucleocytoplasmic Shuttling of hsc70s in Mammalian Cells;** Mohamed Kodiaha<sup>1</sup>; Cathy Quan<sup>1</sup>; Neola Matusiewicz<sup>1</sup>; Ursula Stochaj<sup>1</sup>; Bernard F. Gibbs<sup>1</sup>; <sup>1</sup>McGill University, Montreal, Canada
- ThP 604 **Identification of Surface Exposed Tumor Associated Antigens in Breast Cancer Cells by Comparative Shotgun Proteomics;** Eberhard Durr<sup>1</sup>; Lori C Roth<sup>1</sup>; Mark A Miller<sup>1</sup>; Timothy J Toner<sup>1</sup>; Debbie D Nahas<sup>1</sup>; Nancy M Dougherty<sup>1</sup>; Michael Chastain<sup>1</sup>; Joseph G Joyce<sup>1</sup>; Loren D Schultz<sup>1</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA
- ThP 605 **Assessing Proteome Changes in Tumor Margins by Tissue Profiling Mass Spectrometry;** Stacey R. Oppenheimer<sup>1</sup>; Deming Mi<sup>1</sup>; Melinda Sanders<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University School of Medicine, Nashville, TN
- ThP 606 **Comparative Proteomic Analysis of Cancer Cells Growing in Normal Medium and in Medium Depleted in Methionine, Using MALDI/TOF and Nano-ESI;** Alireza Pak<sup>1</sup>; Michel Boutin<sup>1</sup>; Ying Xu<sup>1</sup>; Marie-Anne Maubert<sup>1</sup>; Carlos Afonso<sup>1</sup>; Françoise Fournier<sup>1</sup>; Anne Greffard<sup>2</sup>; Yannick Pilatte<sup>2</sup>; David Machover<sup>3</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris 6, Paris, France; <sup>2</sup>U504 INSERM, Villejuif, France; <sup>3</sup>Hôpital Paul Brousse, Villejuif, France
- ThP 607 **A Proteomic Approach to Study both Viral and Host Gene Expression in Marek's Disease Virus-infected Chicken Embryo Fibroblast Cells;** Mialy F. Ramarosan<sup>1</sup>; Erik J. Soderblom<sup>1</sup>; James F. Ruby<sup>1</sup>; Hsiao-Ching S. Liu<sup>1</sup>; Michael B. Goshe<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC
- ThP 608 **A Proteomic Approach to the Study of Systemic Amyloidosis;** Francesca Lavatelli<sup>1</sup>; David H. Perlman<sup>1</sup>; Mark E. McComb<sup>1</sup>; Roger Theberge<sup>1</sup>; David C. Seldin<sup>1</sup>; Lawreen H. Connors<sup>1</sup>; Giampaolo Merlini<sup>2</sup>; Martha Skinner<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>IRCCS Policlinico San Matteo, Pavia, Italy

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- ThP 609 **Relative Protein Expression in Normal Bronchoalveolar Lavage Fluid (BALF) Quantified via Shotgun Proteomics and Stable Isotope Free Methods;** Jinzhai Chen<sup>1</sup>; Lynn M. Schnapp<sup>2</sup>; Soyoung Ryu<sup>2</sup>; David R. Goodlett<sup>2</sup>; <sup>1</sup>Fred Hutchison Cancer Research Center, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- ThP 610 **Proteomic Studies of Fluoxetine Induced Neurogenesis in Female Rats;** Linda M Paulson<sup>1</sup>; Thorsten Klint<sup>2</sup>; Peter Eriksson<sup>1</sup>; <sup>1</sup>Institute of neuroscience and Physiology, Goteborg, Sweden; <sup>2</sup>Clinical Development, NeuroSearch A/S, Ballerup, Denmark
- ThP 611 **Exploring the Human Urine Proteome: Males, Females and Pregnant Women;** Yi-Ting Chen<sup>1</sup>; Chao-Yun Tsao<sup>1</sup>; Jen-Ming Li<sup>1</sup>; Chih-Yen Tsai<sup>1</sup>; Su-Feng Chiu<sup>1</sup>; Tzuling Tseng<sup>1</sup>; <sup>1</sup>Industrial Technology Research Institute, Hsinchu, Taiwan
- ThP 612 **Screening Slow Tight-Binding Glycosidase Inhibitors Using Nanoparticle Immobilized Enzymes;** Yet-Ran Chen<sup>1</sup>; Guo-Hsing Tseng<sup>1</sup>; Chin-Wen Ho<sup>2</sup>; Po-Chiao Lin<sup>1</sup>; Chun-Cheng Lin<sup>1</sup>; Chun-Hung Lin<sup>2</sup>; Yu-Ju Chen<sup>1</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan
- ThP 613 **Glycoprofiling of the Human Salivary Proteome;** Melissa A. Sondej<sup>1</sup>; Patricia A. Denny<sup>2</sup>; Yongming Xie<sup>1</sup>; Prasanna Ramachandran<sup>1</sup>; Yan Si<sup>2</sup>; Jona Takashima<sup>2</sup>; David T. Wong<sup>1</sup>; Joseph A. Loo<sup>1</sup>; Paul C. Denny<sup>2</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>USC School of Dentistry, Los Angeles, CA
- ThP 614 **Comprehensive Mass Spectrometric Characterisation of Purified Lipid-Anchored Growth Hormone Extracellular Domain;** Brian K. Stall<sup>1</sup>; Helen V. Montgomery<sup>2</sup>; Caroline Bowles<sup>3</sup>; Ian Wilkinson<sup>3</sup>; D. Watts<sup>3</sup>; Richard J.M. Ross<sup>3</sup>; Koichi Tanaka<sup>4</sup>; <sup>1</sup>Shimadzu Biotech, Columbia, Maryland; <sup>2</sup>Koichi Tanaka Mass Spec research Laboratory, Manchester, United Kingdom; <sup>3</sup>University of Sheffield, Sheffield, United Kingdom; <sup>4</sup>Shimadzu Corporation, Kyoto, Japan
- ThP 615 **Identifying Growth Inhibitors from Pulmonary Artery Endothelial Cells;** Haven Baker<sup>1</sup>; Cristhian D. Ochoa<sup>2</sup>; Debra A Quinn<sup>2</sup>; William Hancock<sup>1</sup>; <sup>1</sup>Barnett Institute and Northeastern University, Boston, MA; <sup>2</sup>Mass General Hospital & Harvard Medical School, Boston, MA

## PROTEOMICS: QUANTITATION TECHNIQUES IV

- ThP 616 **Quantitative Mass Spectrometric Analysis of Visual Cycle Protein Interactions;** Xiaorong Gu<sup>1</sup>; John S Crabb<sup>1</sup>; Maria Nawrot<sup>2</sup>; John C Saari<sup>2</sup>; John W Crabb<sup>1</sup>; <sup>1</sup>Cleveland Clinic Foundation, Cleveland, OH; <sup>2</sup>University of Washington, Seattle, WA
- ThP 617 **Using iTRAQ Technology to Identify and Quantify Low Abundant Proteins in Complex Samples;** Marijan Gucek<sup>1</sup>; Robert N. O'Meally<sup>1</sup>; Robert N. Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins University, School of Medicine, Baltimore, MD
- ThP 618 **Statistical Methods for Accurate iTRAQ Quantification;** George Michailidis<sup>1</sup>; Peter J Ulitz<sup>1</sup>; Eric S Simon<sup>1</sup>; Philip C Andrews<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- ThP 619 **Validation Studies of Proteolytic <sup>18</sup>O Labeling Method Using Lys-C and Trypsin;** Chandra Sekhar Rao Kadiyala<sup>1</sup>; Dagmar Hajkova<sup>1</sup>; Masaru Miyagi<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND
- ThP 620 **Optimized Proteomic Analysis of a Mouse Model of Cerebellar Dysfunction Using Amine-Specific Isobaric Tags;** Jun Hu<sup>1</sup>; Jin Qian<sup>1</sup>; Oleg Borisov<sup>1</sup>; Sanqiang Pan<sup>2</sup>; Yan Li<sup>1</sup>; Tong Liu<sup>1</sup>; Longwen Deng<sup>1</sup>; Kenneth

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- Wannemacher<sup>1</sup>; Michael Kurnellas<sup>1</sup>; Christa Patterson<sup>1</sup>; Stella Elkabes<sup>1</sup>; Hong Li<sup>1</sup>; <sup>1</sup>University of Medicine and Dentistry of New Jersey, Newark, NJ; <sup>2</sup>Jinan University, Guangzhou, China
- ThP 621 **To Label or Not to Label ? – A Comparison of PCA and iTRAQ Labelling for Studying Invasive Breast Cancer;** Devanand M Pinto<sup>1</sup>; Kenneth A Chisholm<sup>1</sup>; Moulay Alaoui-Jamali<sup>2</sup>; Christie Hunter<sup>3</sup>; Lyle Burton<sup>4</sup>; <sup>1</sup>National Research Council (Canada), Halifax, Canada; <sup>2</sup>McGill University, Montreal, Canada; <sup>3</sup>AB/SCIEX, Foster City, CA; <sup>4</sup>MDS-SCIEX, Toronto, Canada
- ThP 622 **Relative Protein Quantitation of 20S Proteasomes Using iTRAQ Labeling;** Katharina Janek<sup>1</sup>; Monika Schmid<sup>2</sup>; Peter Jungblut<sup>2</sup>; Ulrike Kuckelkorn<sup>1</sup>; Peter-Michael Kloetzel<sup>1</sup>; <sup>1</sup>Charite-Medical School of Humboldt University, Berlin, Germany; <sup>2</sup>Max Planck Institute for Infection Biology, Berlin, Germany
- ThP 623 **Quantitative Analysis of (Phospho) Synaptic Proteomes from Mutant Mice;** ka wan li<sup>1</sup>; Oleg Klychnikov<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; Stephan Miller<sup>3</sup>; Augustus B Smit<sup>1</sup>; <sup>1</sup>Vrije Universiteit, Amsterdam, Netherlands; <sup>2</sup>Applied Biosystems, Darmstadt, Germany; <sup>3</sup>The Scripps Research Institute, La Jolla, CA
- ThP 624 **Absolute Quantitative Expression Profiling of Cytochromes P450 Isoforms using Amine Reactive Tags;** Brian L Williamson<sup>1</sup>; Scott Daniels<sup>1</sup>; Christie Hunter<sup>2</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>Applied Biosystems, CA, Foster City, CA
- ThP 625 **Protein quantitation using a novel 8-plex set of Isobaric peptide labels;** Philip Ross<sup>1</sup>; Dey Subhakar<sup>1</sup>; Pillai Sasi<sup>1</sup>; Scott Daniels<sup>1</sup>; Brian Williamson<sup>1</sup>; Matthew Willets<sup>1</sup>; Tony Hunt<sup>1</sup>; Babu Purkayastha; Darryl Pappin<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA
- ThP 626 **The pH Dependency of <sup>18</sup>O Atom Incorporation into the C-terminal Carboxyl Group of Peptides by Lysyl Endopeptidase and Trypsin;** Dagmar Hajkova<sup>1</sup>; K.C.Sekhar Rao<sup>1</sup>; Masaru Miyagi<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND
- ThP 627 **Relative Quantification of the Primary Hematopoietic Stem Cell Proteome and Transcriptome Reveals Post-Translational Regulation of Stem cell Fate;** Richard D. Unwin<sup>1</sup>; David Blinco<sup>1</sup>; Duncan L. Smith<sup>1</sup>; Claire Wilson<sup>2</sup>; Crispin Miller<sup>2</sup>; Ewa Jaworska<sup>1</sup>; Andrew Pierce<sup>1</sup>; Elaine Spooncer<sup>1</sup>; Anthony D. Whetton<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>Paterson Institute for Cancer Research, Manchester, UK
- ThP 628 **iTRAQ and cICAT Based Comparative Proteomics of an Arabidopsis Protease Mutant; Consequences for Chloroplast Protein Homeostasis and Clp Complex Composition;** Andrea Rudella<sup>1</sup>; Giulia Friso<sup>1</sup>; Klaas J. van Wijk<sup>1</sup>; <sup>1</sup>Plant Biology, Cornell University, Ithaca, NY
- ThP 629 **Identification and Quantification of Mitochondrial Proteins from SS and SSBN13 Rat Heart Using Mass Spectrometry and 18O Labeling;** Julia R Hayter<sup>1</sup>; Andrew S Greene<sup>1</sup>; <sup>1</sup>Medical College of Wisconsin, Milwaukee, WI
- ThP 630 **Integration of O-18 Labeling and Solution Isoelectric Focusing in a Shotgun Analysis of Mitochondrial Proteins;** Jinshan Wang<sup>1</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD
- ThP 631 **A Comparative Study of Neurite Outgrowth with Nerve Growth Factor and an Immunophilin Ligand Using iTRAQ and Tandem Mass Spectrometry;** Tong Liu<sup>1</sup>; Veera D'mello<sup>1</sup>; Longwen Deng<sup>1</sup>; Jun Hu<sup>1</sup>; Michael Ricardo<sup>1</sup>; Sanqiang Pan<sup>1</sup>; Xiaodong Lu<sup>1</sup>; Raymond Birge<sup>1</sup>;

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- Hong Li<sup>1</sup>; <sup>1</sup>University of Medicine and Dentistry of New Jersey, Newark, NJ
- ThP 632 **Identification and Quantitation of Proteins Secreted From the ESX-1 Secretory Apparatus of Mycobacterium tuberculosis Using Isobaric Mass Tags and LC/MS/MS;** Matthew M. Champion<sup>1</sup>; Patricia A. DiGiuseppe<sup>2</sup>; Jeffrey S. Cox<sup>2</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>University of California, San Francisco, CA
- ThP 633 **Comparative Secreted Proteome of Botrytis cinerea Grown on Multiple Plants Cell Wall Extracts;** Punit K. Shah<sup>1</sup>; James A. Atwood III<sup>1</sup>; Maria Davis<sup>2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center UGA, Athens, GA; <sup>2</sup>The University of Alabama in Huntsville, Huntsville, Al
- ThP 634 **160/180 Labeling Quantitative Analysis of Tryptically Digested Mouse Serum Using Liquid Chromatography Coupled with MALDI MS and MS/MS;** Marten E. Snel<sup>1</sup>; Richard Tyldesley-Worster<sup>1</sup>; Greg S. Cavey<sup>2</sup>; P. Davidson<sup>2</sup>; James I. Langridge<sup>1</sup>; Therese McKenna<sup>1</sup>; D. Monsma<sup>2</sup>; C. Webb<sup>2</sup>; <sup>1</sup>Waters, Manchester, United Kingdom; <sup>2</sup>Van Andel Research Institute, Grand Rapids, MI
- ThP 635 **Relative Quantitation of Yeast Proteins Labeled with Isobaric Tags and Fractionated by SDS-PAGE;** Steven R. Guertin<sup>1</sup>; Marjorie Minkoff<sup>1</sup>; Brian Williamson<sup>1</sup>; Subhasish Purkayastha<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA
- ThP 636 **Application of Liquid-Based Two Dimensional Protein Fractionation (PF 2D) to Proteomic Quantification Using Mass Spectrometry;** Wells W. Wu<sup>1</sup>; Guanghui Wang<sup>1</sup>; Rong-Fong Shen<sup>1</sup>; <sup>1</sup>NHLBI, National Institutes of Health, Bethesda, MD
- ThP 637 **Study of Asymmetric Cell Division Using Multiplexed Quantitative Proteomics;** Philip Ross<sup>1</sup>; Esteban Toro<sup>2</sup>; Xunming Chen<sup>1</sup>; Jennifer Campbell<sup>1</sup>; Leticia Britos<sup>2</sup>; Lucy Shapiro<sup>2</sup>; Darryl Pappin<sup>1</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>Beckman Institute, Stanford University, CA
- ThP 638 **Temporal Proteomic Analysis of Systemic Inflammation upon Lipopolysaccharide Administration;** Tao Liu<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; Marina A. Gritsenko<sup>1</sup>; Steve E. Calvano<sup>2</sup>; Stephen F. Lowry<sup>2</sup>; Wenzhong Xiao<sup>3</sup>; Lyle L. Moldawer<sup>4</sup>; Ronald J. Moore<sup>1</sup>; Samuel O. Purvine<sup>1</sup>; Matthew E. Monroe<sup>1</sup>; Ronald W. Davis<sup>3</sup>; Ronald G. Tompkins<sup>5</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 Medicine and Dentistry of New Jersey, New Brunswick, NJ; <sup>3</sup>Stanford University School of Medicine, Palo Alto, CA; <sup>4</sup>University of Florida College of Medicine, Gainesville, FL; <sup>5</sup>Harvard Medical School, Boston, MA
- ThP 639 **A Novel Approach for Protein Expression Profiling of Mouse Prostate;** Sanjeev Bhardwaj<sup>1</sup>; Eric Winstall<sup>2</sup>; Marjorie Minkoff<sup>1</sup>; Christian Lessard<sup>2</sup>; Danielle Caron<sup>2</sup>; Sylvie Bourassa<sup>2</sup>; Isabelle Kelly<sup>2</sup>; Fernand Labrie<sup>2</sup>; Guy Poirier<sup>2</sup>; Robert Faure<sup>2</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>Centre de recherche du CHUL, Université Laval, Québec, Canada
- ThP 640 **Discovery of Early Stage Protein Biomarkers for Metastatic Breast Cancer using iTRAQ(TM) Reagents and QqTOF technology;** Christie L Hunter<sup>1</sup>; Devanand Pinto<sup>2</sup>; Kenneth Chisholm<sup>2</sup>; Moulay Alaoui-Jamali<sup>3</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>NRC, Halifax, Canada; <sup>3</sup>McGill University, m, Canada

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- ThP 641 **Quantitative Proteomics Using IEF-LCMSMS**; Peter J. Ulintz<sup>1</sup>; Philip C. Andrews<sup>1</sup>; Eric S. Simon<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- ThP 642 **Multi-dimensional Orthogonal Separation and iTRAQ®; Reagent Tracking: A Genome-wide "Tagless" Strategy for Isolation and Detection of Soluble Bacterial Protein Complexes**; Ming Dong<sup>1</sup>; Mark Biggin<sup>1</sup>; Katherine Williams<sup>2</sup>; Scott E. Dixon<sup>3</sup>; Lee Lisheng Yang<sup>1</sup>; Susan J. Fisher<sup>3</sup>; Steven C. Hall<sup>3</sup>; Jian Jin<sup>1</sup>; H. Ewa Witkowska<sup>3</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>Applied Biosystems, Foster City, CA; <sup>3</sup>UCSF, San Francisco, CA
- ThP 643 **The Integration of Stable Isotope Labeling Methods with Gel-Based Technologies: Solutions for the Quantification of Membrane Proteins**; Amir Rahbar<sup>1</sup>; Michael Lassman<sup>1</sup>; Nikolai Lebedev<sup>1</sup>; Brandy White<sup>1</sup>; Frances Ligler<sup>1</sup>; <sup>1</sup>U. S. Naval Research Laboratory, Washington, DC
- ThP 644 **Expression Proteomics of Xenopus Laevis Brain Cells After Exposure to T4 Synthesis Inhibitors Using iTRAQ® and 2D-PAGE Technologies**; LeeAnn Higgins<sup>1</sup>; Lorraine B. Anderson<sup>1</sup>; Bruce A. Witthuhn<sup>1</sup>; Joseph J. Korte<sup>2</sup>; Joseph Tietge<sup>2</sup>; Sigmund J. Degitz<sup>2</sup>; Jose Serrano<sup>2</sup>; <sup>1</sup>University of Minnesota, St. Paul, MN; <sup>2</sup>USEPA, ORD/NHEERL/MED, Duluth, MN
- ThP 645 **iTRAQ Coupled with Immobilized Metal Affinity Chromatography for Quantitative Phosphopeptide Analysis**; Yurong Guo<sup>1</sup>; Austin Rowshan<sup>1</sup>; Jennifer Van Eyk<sup>1</sup>; Joe GN Garcia<sup>2</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>University of Chicago, Chicago, IL
- ThP 646 **Optimizing Parameters in Linear Ion Trap with PQD Functionality for Simultaneous Protein Identification and Quantitation from Complex Mixtures Using iTRAQ**; Yingying Huang<sup>1</sup>; Terry Zhang<sup>1</sup>; Reiko Kiyonami<sup>1</sup>; Keith Waddell<sup>1</sup>; <sup>1</sup>Thermo Electron Corporation, San Jose, CA; <sup>2</sup>BG Medicine, Waltham, MA
- ThP 647 **iTRAQ Based Comparative Proteomics of an Arabidopsis SRP54 Mutant Defective in Chloroplast Protein Sorting**; A. Jimmy Ytterberg<sup>1</sup>; Heidi Rutschow<sup>1</sup>; Klaas J. van Wijk<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY

### PROTEOMICS: PHOSPHORYLATED APPLICATIONS

- ThP 648 **Deciphering the Prokaryotic Ser/Thr/Tyr Phosphoproteome: The Case of *Bacillus subtilis***; Boris Macek<sup>1</sup>; Ivan Mijakovic<sup>2</sup>; Jesper V. Olsen<sup>1</sup>; Florian Gnäd<sup>1</sup>; Chanchal Kumar<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max-Planck-Institute of Biochemistry, Munich, Germany; <sup>2</sup>Technical University of Denmark, Copenhagen, Denmark
- ThP 649 **Phosphorylation Site Determination of BZR1 in Arabidopsis**; Shenheng Guan<sup>1</sup>; Srinivas Gampala<sup>2</sup>; David A. Maltby<sup>1</sup>; Zhi-Yong Wang<sup>2</sup>; Alma L. Burlingame<sup>1</sup>; <sup>1</sup>University of California, San Francisco, CA; <sup>2</sup>Carnegie Institution, Stanford, CA
- ThP 650 **Identification of Phosphorylation Sites in Numb, Miranda and Lgl by Atypical Protein Kinase C**; Eric Bonneil<sup>1</sup>; Zohra Rahmani<sup>2</sup>; Roland Leborgne<sup>2</sup>; Francois Schweisguth<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>IRIC Université de Montréal, Montréal, QC; <sup>2</sup>CNRS Ecole Normale Supérieure, Paris, France
- ThP 651 **Mass Spectrometry Analysis of the Human Werner Syndrome Protein**; Angie Sibounheuang<sup>1</sup>; Gennifer Merrihew<sup>1</sup>; James Thompson<sup>1</sup>; Raymond J. Monnat, Jr.<sup>1</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 652 **The Phagosomal Phosphoproteome**; Matthias Trost<sup>1</sup>; Michel Desjardins<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>Université de

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- Montréal, IRIC, Montréal, Canada; <sup>2</sup>Université de Montréal, Pathology & Cell biology, Montréal, Canada
- ThP 653 **Investigation of the Possible Involvement of Myosin III Oxidation in the Photoresponse of *Limulus polyphemus* Photoreceptors**; Helene L. Cardasis<sup>1</sup>; Stanley M. Stevens Jr.<sup>1</sup>; Scott H. McClung<sup>1</sup>; Karen Kempler<sup>1</sup>; John R. Eyler<sup>1</sup>; David H. Powell<sup>1</sup>; Barbara-Anne Battelle<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL
- ThP 654 **Quantitative Analysis of Phosphotyrosine Signaling Networks triggered by CD3 and CD28 co-stimulation in Jurkat cells**; Ji-Eun Kim<sup>1</sup>; Forest M. White<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology, Cambridge, MA
- ThP 655 **Identification of Novel Phosphorylation Sites on the 20S Yeast Proteasome Subunits**; Karen H. LeBlanc<sup>1</sup>; Ying-ying Yang<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University CA Irvine, Irvine, CA
- ThP 656 **Quantitative and phosphoprotein-Specific MS-Based Proteomic Approach to Unravel Mechanisms Underlying Plasticity of Olfactory Neurons in *Mus musculus***; Heike Piechura<sup>1</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>Medical Proteom-Center, Ruhr-University Bochum, Bochum, Germany; <sup>2</sup>Ruhr-University Bochum, Bochum, Germany
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