The 48th ASMS CONFERENCE on MASS SPECTROMETRY and ALLIED TOPICS

ASMS

Long Beach
California
June 11 – 15, 2000
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Welcome to the 48th ASMS Conference on Mass Spectrometry and Allied Topics. Conference sessions are in the following locations:

**PLENARY SESSIONS** are in the Terrace Theater, the round building on Ocean Blvd behind the convention center, across Ocean Blvd form the Westin Hotel. There will be coffee available in front of the Terrace Theater, 7:30 – 8:00 am (prior to the plenary sessions).

**ORAL SESSIONS** A, B, C, and D are in the convention center. A and B are in the ballroom on the second level. C and D are in Room 104, which is on the lobby level at the end of the convention center closest to the Hyatt Hotel. Sessions E and F are in the Hyatt Hotel Ballroom on the third level.

**POSTERS AND EXHIBITS** are in Exhibit Hall B directly down the escalator from the main lobby of the convention center.

**SUNDAY TUTORIAL LECTURES.** The tutorial session is 5:00 pm, Sunday, in the ballroom, second level of the convention center.

5 – 5:45 pm  
Tomas Baer, *University of N. Carolina*  
Ion Energetics & Computational Chemistry

5:45 – 6:30 pm  
David Smith, *University of Nebraska*  
H/D Exchange and Protein Structure

**REFRESHMENTS.** Light refreshments and cash lunches are available in Exhibit Hall B and in the main lobby of the convention center.

**SHUTTLE BUSES.** Buses are provided to and from the convention center and the following hotels:

**ROUTE 1**  
West Coast  
Queen Mary

**ROUTE 2**  
Airport Holiday Inn  
Airport Marriott

Buses will run continuously from 7:00 am – 10:30 pm.

**ORAL PRESENTATIONS.** 35 mm slide projectors and overhead projectors will be used for oral sessions. A projectionist will be present, but speakers should advance their own slides using the control on the podium. Presenters must arrive 30 minutes prior to the start of the session to turn in loaded slide trays. Presenters have been advised to use landscape orientation for slides. Overhead projectors are also available. Speakers who choose to use overhead projection must have someone available to change transparencies as the projector is located on the floor and the speaker podium is on the stage.

**SLIDE PREVIEW ROOM.** Slides may be previewed in Room 204 of the convention center. Room 204 is on the second level directly up the escalator from the main lobby. The room will be open 3:00 to 7:00 pm on Sunday and 7 am to 5 pm Monday through Thursday. Trays will be available to load slides and to review their orientation and sequence.

**POSTER PRESENTATIONS.** Posters must be in place by 8:00 am on the day scheduled and removed between 6 – 6:30 pm. Thursday posters must be removed between 3 – 3:30 pm. REFER TO THE POSTER NUMBER IN THIS FINAL PROGRAM FOR BOARD ASSIGNMENTS. Authors are expected to supply their own push pins to mount their posters.

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

**WORKSHOPS.** Workshops are scheduled on Monday and Tuesday afternoons, 5:30 – 6:30 pm. They are located in the convention center.

**INTEREST GROUP MEETINGS.** Interest Group meetings are scheduled during the lunch break, 12:15 – 1:30 pm. Anyone interested in the topics are encouraged to buy a lunch and bring it to the meeting rooms that are set with tables and chairs.

**TUESDAY**

- Room 101 A  
  Flavor & Foodstuffs
- Room 101 B  
  Surface Science
- Room 201 A  
  FTMS
- Room 201 B  
  Fundamentals

**WEDNESDAY**

- Room 101 A  
  Metal Ion Chemistry
- Room 101 B  
  Laboratory Managers
- Room 102 A  
  Energy & Petrochemicals
- Room 201 A  
  History
- Room 201 B  
  Polymeric Materials

**EMPLOYMENT CENTER.** The Employment Center is located in Room 203, second level of the convention center. Candidates may register with the center beginning at 3 pm on Sunday. You must have at least 20 copies of your résumé. The center will be open Monday through Wednesday, 8:30 am to 5:00 pm, and Thursday 8:30 am to 3 pm. Employers may come to Room 203 to review a searchable database of candidates and schedule interviews. Interview booths are located in Room 202. The center is being coordinated by David A. Weil of 3M Company.

**CONFERENCE PROCEEDINGS.** The conference proceedings will be published on CD ROM after the conference. Manuscripts on diskette must be submitted by 12:30 pm on Tuesday. The submission office is located in Room 103 A of the convention center.

**CORPORATE HOSPITALITY SUITES.** Corporate member hospitality suites are located in the Hyatt, Westin, and Renaissance Hotels. Please refer to page 6 for locations.

**CORPORATE POSTERS.** Corporate member posters are located in the Exhibit Hall B.
SPECIAL EVENTS FOR REGISTRANTS.
- Sunday, 7:00 – 9:00 pm. Welcome Mixer, Main Lobby of the Convention Center.
- Thursday, 5 – 5:45 pm. The Chemistry of Pyrotechnics, Terrace Theater.
- Thursday, 6:00 - 9:30 pm. Conference Finale and Fireworks, $10 per person, Rainbow Lagoon, behind the Hyatt Hotel. Join us to celebrate the end of a successful meeting and say goodbye ‘til next year.

COMPANION HOSPITALITY. There is a continental breakfast for companions 9:30 – 11:30 am on Monday and Tuesday, Room 102 C, first level of the convention center.

CONFERENCE REGULATIONS.
- Name badges are required for all conference sessions, including the exhibit hall and the employment center.
- NO SMOKING is permitted in any conference area.
- The placement of advertising in the meeting area is strictly limited to Corporate Members. There are poster boards in the main lobby for corporate member notices. No signs on easels are permitted.
- No hardware, terminals, accessories, or any items for sale may be displayed in any area of the conference, except in corporate exhibit booths.
- There may be no organized activities (even off-site) other than those sponsored by ASMS during conference week.
- No corporate or institutional logos may appear on slides or posters in technical sessions.

CONFERENCE CLOSING EVENT
The closing event celebrates another great conference and is held in appreciation of all who are participating in the 48th Annual Conference. Dinner will be an elegant summer evening buffet. We will close with a bang! The following companies have made it possible to provide this outstanding event for the nominal ticket price of $10.

Our sincere thanks to each of them.

Micromass

PE Biosystems
Agilent Technologies
Bruker Instruments
Isotec
Kratos Analytical
NuGenesis Technologies (formerly Mantra Software)
Precision Instruments
Protana A/S
SGE, Inc.
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<th>Name</th>
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<tr>
<td>President</td>
<td>Robert J. Cotter</td>
<td>Johns Hopkins University, Baltimore, MD</td>
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<td>Vice President for Programs</td>
<td>Richard M. Caprioli</td>
<td>Vanderbilt University, Nashville, TN</td>
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<td>Vice President for Arrangements</td>
<td>Alfred L. Yergey</td>
<td>NIH, Bethesda, MD</td>
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<td>Secretary</td>
<td>Stephen A. Lammert</td>
<td>Oak Ridge Natl Laboratory, Oak Ridge, TN</td>
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<td>Treasurer</td>
<td>Vicki H. Wysocki</td>
<td>University of Arizona, Tucson, AZ</td>
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<td>Member at Large Publications</td>
<td>Susan T. Weintraub</td>
<td>Univ. of Texas Health Science Ctr., San Antonio, TX</td>
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<td>Member at Large Measurements &amp; Standards</td>
<td>John A. Chakel</td>
<td>Hewlett-Packard Laboratories, Palo Alto, CA</td>
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<td>Member at Large Education</td>
<td>Jon Amster</td>
<td>University of Georgia, Athens, GA</td>
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<tr>
<td>Past President</td>
<td>Veronica M. Bierbaum</td>
<td>University of Colorado, Boulder, CO</td>
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<tr>
<td>Executive Director</td>
<td>Judith A. Sjoberg</td>
<td>ASMS, 1201 Don Diego Avenue, Santa Fe, NM 87505</td>
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<td>(505) 989-4517, Fax: (505) 989-1073, e-mail: <a href="mailto:asms@asms.org">asms@asms.org</a></td>
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<tr>
<td>Staff</td>
<td>Cindi Lilly</td>
<td>Miquela Ortiz, David Shack</td>
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<td>Analytical Lab Managers</td>
<td>David L. Hachey, Vanderbilt University</td>
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<td>Timothy R. Baker, Procter &amp; Gamble Co., Dominic M. Desiderio, Univ of Tennessee Sch of Medicine</td>
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<td>Desorption Ionization</td>
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<td>C. Samuel Hsu, Exxon Research &amp; Engineering</td>
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<td>Mary T. Rodgers, Wayne State University</td>
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<td>Ross C. Willoughby, Chem-Space Associates</td>
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<td>Charles Barinaga, Battelle, PNNL</td>
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<td>LC/MS &amp; Related Topics</td>
<td>Michael P. Balog, Waters Corporation</td>
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<td>Metal Ion Coordination Chem</td>
<td>Gary D. Willett, University of New South Wales</td>
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<td>TOF MS</td>
<td>Werner E. Ens, University of Manitoba</td>
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<td>David C. Muddiman, Virginia Commonwealth Univ.</td>
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<td>Astilomar Conference</td>
<td>Julie A. Leary (Chair)</td>
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<td>Peter J. Todd, Michelle V. Buchanan, P. Jane Gale</td>
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**CORPORATE MEMBERS**

Be sure to visit the corporate suites, exhibit booths and posters. Suites are located in the Hyatt, Westin and Renaissance Hotels. The publisher’s library is in the convention center. The corporate posters and exhibit booths are located in Exhibit Hall B of the convention center.

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<td>Spectroscopy/LCGC N. America</td>
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<td>Thermo Bioanalysis</td>
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<td>Varian, Inc.</td>
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<td>Vydac/The Separations Group</td>
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<td>Waters</td>
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<td>Whatman, Inc</td>
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PROGRAM ACKNOWLEDGEMENTS

Richard M. Caprioli, Vice President for Programs
Susan Weintraub, Member at Large for Publications

STUDENT ASSISTANTS

Graduate students are assisting with all aspects of the conference, including registration, oral and poster sessions, submission of manuscripts for the Proceedings, and the employment center. The students each receive a stipend to assist with their conference expenses.

PROGRAM COMMITTEE

Ian Blair
David E. Clemmer
Catherine E. Costello
Dominic Desiderio
Richard H. Griffey
Gary Groenewold
C. Samuel Hsu
Kermit K. Murray
Susan Richardson
Michael S. Story
Gary J. Van Berkel

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Mary T. Rodgers
Ross Willoughby
Award for a Distinguished Contribution in Mass Spectrometry

The ASMS Award for a Distinguished Contribution in Mass Spectrometry recognizes a focused singular achievement in or contribution to fundamental or applied mass spectrometry. The year 2000 award is presented to Dr. Boris Aleksandrovich Mamyrin, Ioffe Physical Technical Institute, St. Petersburg, Russia, for the invention and development of the ion mirror ("reflectron") for time-of-flight mass spectrometry.

Mamyrin's development of the electrostatic ion mirror ranks as one of the most innovative and important advances in mass analyzer design over the past 50 years. Early work with time-of-flight analyzers in the 1950's revealed that the large initial energy spread of the ions produced in the extraction zone considerably limited the theoretically possible resolution of these instruments. In the 1960's and 1970's, Mamyrin developed the single stage mirror with first-order time focusing, as well as the two-stage mirror, shorter in length but providing second-order time focusing and greatly improved mass resolution in time-of-flight mass spectrometers.

The ion mirror or "Mamyrin reflectron" has since played a pivotal role in elevating the time-of-flight analyzer from an instrument of modest resolution to the high-resolution analyzer of choice for a wide variety of diverse applications in biological, pharmaceutical, and industrial polymer laboratories. Such instruments are making contributions of great consequence to scientific investigations in these disciplines.

The award will be presented at 8:00 am on Tuesday in the Terrace Theater.

The Biemann Medal

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 year 2000 award is presented to Professor Julie Ann Leary from the University of California, Berkeley, for her characterization of the role of metal ion coordination in the mass spectrometry of peptides and oligosaccharides, and for her ingenious applications of mass spectrometry to the stereochemical analysis of molecular species in the gas phase.

Dr. Leary's early investigations of anomericity and linkage position in oligosaccharides led to her use of metals and metal-ligand systems for distinguishing relative and absolute stereochemistry in the gas phase using mass spectrometry. Dr. Leary has shown that MS$^+$ can be used to unambiguously differentiate each of the four isomeric hexoses, hexosamines, and N-acetyl hexosamines when using her novel metal-ligated methodology. An important side project of this work has been the stereospecific synthesis of the diethylenetriamine-bridging saccharides, four of which have been accepted by the National Cancer Institute's Anti-Cancer Drug Discovery Program and are currently undergoing testing as potential chemotherapeutic agents. This symbiosis of synthesis and mass spectrometry is impressive in light of the fact that some of the metal-ligand-monosaccharide compounds have been characterized by X-ray crystallography and Dr. Leary has been able to show that their stereochemical differences are retained in the gas phase during MS analysis. The stereochemical analysis and determination of retention of configuration in the gas phase using electrospray ionization is an area of current research. Dr. Leary not only has conducted these important studies, but she is also directly responsible for the operation and maintenance of the Chemistry Department's Analytical Facilities (NMR, X-ray diffraction, microanalysis, computer graphics, and mass spectrometry).

The Biemann Medal will be presented at 8:00 am on Wednesday in the Terrace Theater.
RESEARCH AWARDS

sponsored by
ThermoQuest Corporation

John Klassen
University of Alberta

sponsored by
PE Biosystems

Igor A. Kaltashov
University of Massachusetts

sponsored by
Micromass

Elaine Marzluff
Grinnell College

CALL FOR YEAR 2001 RESEARCH AWARD PROPOSALS

OBJECTIVE To promote academic research by young scientists in mass spectrometry.

ELIGIBILITY Open to academic scientists within four years of joining the tenure track faculty of 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. A vita
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, 2000. Send to:
ASMS, 1201 Don Diego Avenue, Santa Fe, NM 87505

FISCAL The awards of up to $25,000 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 • asms@asms.org
PROGRAM HIGHLIGHTS

SUNDAY  TUTORIAL LECTURES, Convention Center Ballroom
5:00 pm Tomas Baer, University of North Carolina
“Ion Energetics & Computational Chemistry”
5:45 pm David Smith, University of Nebraska
“H/D Exchange and Protein Structure”

7:00 – 9:00 pm  Welcome Mixer, Convention Center

Plenary Lectures will be presented in the Terrace Theater. The Terrace Theater is located outside and behind the convention center on Ocean Blvd.

MONDAY – THURSDAY
7:30 – 8:00 am “Wake-Up” coffee will be served in front of the Terrace Theater (prior to the Plenary Session).

MONDAY  PLENARY LECTURE, Terrace Theater
8:00 am Chris McKay, NASA Ames Research Center
“The Search for Life on Mars and Beyond”

TUESDAY  PRESENTATION OF THE AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY AND PLENARY LECTURE, Terrace Theater
8:00 am Boris A. Mamyrin, Technical Institute, St Petersburg, Russia

WEDNESDAY  PRESENTATION OF THE BIEMANN MEDAL AND PLENARY LECTURE, Terrace Theater
8:00 am Julie A. Leary, University of California at Berkeley

WEDNESDAY  ASMS GENERAL MEETING, Convention Center Ballroom B
5:15 - 6:00 pm Research Award presentations
Acknowledgment of the retiring Board members
ASMS News

THURSDAY PLENARY LECTURE, Terrace Theater
8:00 am Jack Holl, Kansas State University
“Comparing Frontier Utopias: The Land of Oz and the National Laboratory System”

THURSDAY PLENARY LECTURE, Terrace Theater
5:00 pm Jerrald Laib, Naval Special Warfare Command
“The Chemistry of Pyrotechnics”

THURSDAY  CONFERENCE FINALE – DINNER and FIREWORKS, Rainbow Lagoon
6:00 – 9:30 pm Tickets required: $10 each.
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<th>SUNDAY</th>
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<td><strong>7:30 am</strong>&lt;br&gt;Wake-Up Coffee&lt;br&gt;Terrace Theater&lt;br&gt;The Terrace Theater is located outside and behind the convention center on Ocean Blvd.&lt;br&gt;&lt;br&gt;<strong>8 – 8:45 am</strong>&lt;br&gt;PLENARY&lt;br&gt;Terrace Theater&lt;br&gt;Chris McKay&lt;br&gt;NASA Ames Research Center&lt;br&gt;The Search for Life on Mars and Beyond</td>
<td><strong>8:45 – 10:15 am</strong>&lt;br&gt;POSTERS &amp; EXHIBITS&lt;br&gt;Exhibit Hall B&lt;br&gt;&lt;br&gt;Authors of odd numbered posters present&lt;br&gt;&lt;br&gt;MPA-Spray ionization (004-061)&lt;br&gt;MPB-Trapped Ions (062-092)&lt;br&gt;MPC-Drugs &amp; Metabolism: Metabolite Identification (093-105)&lt;br&gt;MPD-Drugs &amp; Metabolism: LC/MS/MS Quantitation in Plasma, Blood or Serum (106-149b)&lt;br&gt;MPE-Proteins – Basics (150-212)&lt;br&gt;MPP-Combinatorial Chemistry (213-220)&lt;br&gt;MPG-Non-Covalent Complexes (221-246)&lt;br&gt;MPI-Lipids (247-268)&lt;br&gt;MPI-Nucleic Acids (269-294)&lt;br&gt;MPI-Computer Applications (295-320)</td>
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**12:15 – 1:30 pm**<br>Lunch Break<br>Cash lunches are available in the convention center

| **5 – 6:30 pm**<br>TUTORIALS<br>CC Ballroom<br>Tomas Bacr,<br>University of North Carolina<br>Ion Energetics & Computational Chemistry<br>David Smith,<br>University of Nebraska<br>H/D Exchange and Protein Structure |

| **7 – 9 pm**<br>WELCOME MIXER<br>Convention Ctr |

| **3:00 – 5:00 pm**<br>ORAL SESSIONS<br>CC Ballroom A<br>MOA-Bacterial Taxonomy, Phenotyping & Protoomics<br>CC Ballroom B<br>MOB-Energy & Petrochemicals I<br>CC Room 104 A<br>MOC-Non-Covalent Interactions<br>CC Room 104 C<br>MOD-Synthetic Polymers & Chromatography<br>Hyatt Ballroom A<br>MOE-Laser Desorption<br>Hyatt Ballroom F<br>MOF-Relating Gas Phase Ions to Surface Structure |

<p>| <strong>5:30 – 6:30 pm</strong>&lt;br&gt;WORKSHOPS&lt;br&gt;Convention Ctr&lt;br&gt;Ballroom B&lt;br&gt;High Throughput TOF&lt;br&gt;Room 104 A&lt;br&gt;Fundamentals &amp; Biochemistry&lt;br&gt;Room 104 C&lt;br&gt;Quadrupole Ion Traps: Problem Solving in Basic &amp; Applied Research, A Student Perspective |</p>
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<td>Boris A.</td>
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<td>10:15 am – 12:15 am</td>
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<td>TOA-Protein-Protein Interactions</td>
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<td>TOC-Computer Applications</td>
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<td>TOC-DNA &amp; Protein Analysis by MALDI</td>
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<td>LC/MS Sample Introduction &amp; Separation Strategies</td>
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<td>Data Handling for High Throughput &amp; High Volume Analysis</td>
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<td>WPA-Instrumentation (004-054b)</td>
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<td>Molecule Reactions (055-097)</td>
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<td>WPC-Laser Desorption/ Ionization / Applications (098-151)</td>
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<td>WPD-Drugs &amp; Metabolism: LC/MS/MS Quantitation in Biological Fluids (152-169)</td>
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<td>WPE-Drugs &amp; Metabolism: High Throughput Methods (170-206)</td>
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<td>WPF-Proteins - Methods Development (207-265d)</td>
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<td>WPH-High Throughput (295-325)</td>
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<td>WOC-Environmental: New Problems I</td>
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<td>WOD-High Throughput/ Automation/ Robotics</td>
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<td>WOF-Ion Activation/ Dissociation: CID, ECD, SID of Peptides &amp; Proteins</td>
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<td>WOC-Environmental: New Problems II</td>
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<td>WOF-Molecular Dynamics of Ion Desorption</td>
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### Program Overview - Thursday

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<td>ThPA-Genomic Analysis (004-019)</td>
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<td>ThPB-Proteins - Structure/Func; Microorganisms and Plants (020-097)</td>
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<td>ThPC-Toxicology (098-124)</td>
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<td>ThPD-Drugs &amp; Metabolism: New Methods (125-165)</td>
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<td>THPE-Environ Analysis II (166-195)</td>
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<td>ThPF-Separations/MS - New Instrumentation &amp; General Methods (196-236)</td>
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<td>ThPG-Organic (237-262)</td>
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<td>ThPI-Ion Activation (263-309)</td>
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<td>ThPI-Isotope Ratio MS (310-316)</td>
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<td>10:15 am</td>
<td>RAL SESSIONS</td>
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<td>ThOA-Glyco-conjugates</td>
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<td>ThOB-Toxicology &amp; Pharmacology II</td>
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<td>CC Room 104 A</td>
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<td></td>
<td>ThOC-Strategies for Analysis of Complex Mixtures I</td>
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<td>CC Room 104 C</td>
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<td>ThOD-Analysis of Natural Products</td>
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<td>Hyatt Ballroom A</td>
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<td>ThOE-TOF Analyzers</td>
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<td>Hyatt Ballroom F</td>
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<td>ThOF-Mechanisms of Peptide Ion Fragmentation</td>
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<tr>
<td>12:15 pm</td>
<td>Lunch Break</td>
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<td>Authors of even numbered posters present</td>
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<td>Cash lunches are available in the convention center</td>
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<tr>
<td>1:30 pm</td>
<td>POSTERS &amp; EXHIBITS</td>
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<td>Exhibit Hall B</td>
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<td>Authors of even numbered posters present</td>
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<td>3:00 pm</td>
<td>ORAL SESSIONS</td>
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<td>ThOA-Molecular Analysis in Clinical Medicine</td>
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<td>ThOB-Pharmaceutical Development</td>
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<td>ThOC-Strategies for Analysis of Complex Mixtures II</td>
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<td>CC Room 104 C</td>
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<td>ThOD-Forensic Applications</td>
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<td>5 pm</td>
<td>PLenary</td>
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<td>Jerrald Laib, Naval Special Warfare</td>
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<td>Command The Chemistry of Pyrotechnics</td>
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<td>5–6 pm</td>
<td>Terrace Theater</td>
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<tr>
<td>6–9:30 pm</td>
<td>Conference Finale</td>
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<td>Rainbow Lagoon Behind the Hyatt</td>
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### DNA SEQUENCING, POLYMORPHISM, AND DAMAGE ANALYSIS “ENDING” IN RNA

**Chair:** David C. Muddiman  
**Conv. Ctr. Ballroom A, 2nd level**

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<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors/Institutions</th>
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<tbody>
<tr>
<td>MOA am 10:15</td>
<td>Sequencing DNA via Electrospray Ionization and Ion/Ion Chemistry in a Quadrupole Ion Trap; Scott A. McLuckey; James L. Stephenson, Jr.; Gregory B. Hurst; Purdue University, West Lafayette, IN; Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<tr>
<td>MOA am 10:35</td>
<td>Broad-based Genotyping of Short Tandem Repeat Loci Using ESI-FTICR Mass Spectrometry; James C. Hann; Allison P. Null; David C. Muddiman; Virginia Commonwealth University, Richmond, VA</td>
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<tr>
<td>MOA am 10:55</td>
<td>Measuring and understanding the differences in DNA damage resulting from normal oxidative processes and low levels of ionizing radiation; Olivier L. Blum; David S. Wunschel; Mary Lipton; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA</td>
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<tr>
<td>MOA am 11:15</td>
<td>Analysis of DNA Photoproduts by Coupled Enzymatic Digestion/Mass Spectrometry: Structure Determination, Quantification, and Application; Yinseng Wang; John-Stephen Taylor; Michael L. Gross; Washington University, St. Louis, MO</td>
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<tr>
<td>MOA am 11:35</td>
<td>Oxidative Damage of DNA by Peroxidase-Mediated Bromination; Zhongzhou Shen; Weijia Wu; Yonghong Chen; Shomenath Mitra; Yanwu Yang; Jun Qin; Stanley L Hazen; Cleveland Clinic Foundation, Cleveland, OH; Cleveland State University, Cleveland, OH</td>
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<tr>
<td>MOA am 11:55</td>
<td>Identification of the mass silent modification, pseudouridine, in RNA by chemical derivatization and mass spectrometric analysis; Patrick A. Limbach; Beniam Berhan; Kemberly G. Pattease; Lenore P. Rodicio; Louisiana State University, Baton Rouge, LA; University of Miami, Coral Gables, FL</td>
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### INDUSTRIAL POLYMERS

**Chair:** Kevin G. Owens  
**Conv. Ctr. Ballroom B, 2nd level**

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<th>Time</th>
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<th>Authors/Institutions</th>
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<tr>
<td>MOB am 10:15</td>
<td>The Characterisation of Poly(Methyl Methacrylate) Polymers Generated by Atom Transfer Radical Polymerisation (ATRP); Anthony T Jackson; Christopher D Borman; Derek J Irvine; Martin R Green; Robert H Bateman; SSG, ICI R&amp;T Centre, Cleveland, UK; Ineos Acrylates, Cleveland, UK; Micromass UK Ltd, Manchester, UK</td>
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<tr>
<td>MOB am 10:35</td>
<td>MALDI-TOF Analysis of Electroactive Macromolecular Systems; Tracy D. McCrory; Robin L. McCrory; Charles O. Noble; Claudia M. Cardona; Angel E. Kaifer; Louisiana State University, Baton Rouge, LA; University of Miami, Coral Gables, FL</td>
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<td>MOB am 10:55</td>
<td>MALDI Mass Spectrometry of Quinoxaline Homo- and Copolymers; Chrys Wesdemiotis; Michal J. Police; Daniel J. Klein; Frank W. Harris; The University of Akron, Akron, OH</td>
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<td>MOB am 11:15</td>
<td>Matrix Clusters and Polymer-Matrix Adducts in the MALDI Analysis of Polystyrene; Robert J. Goldschmidt; Charles M. Guttman; NIST Polymers Division, Gaithersburg, MD</td>
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<tr>
<td>MOB am 11:35</td>
<td>Comparison of MALDI-CID Data Obtained for Synthetic Polymers in Sector-oa-TOF and Quadrupole-oa-TOF Instruments; James H Sriverins; Anthony T Jackson; Robert S Bordoli; Martin R Green; Robert H Bateman; SSG, ICI R&amp;T Centre, Cleveland, UK; Micromass UK Ltd, Manchester, UK</td>
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<td>MOB am 11:55</td>
<td>MALDI-PSD mass spectra of low molecular weight ethoxylated polymers; Scott D. Hanton; Kevin G. Owens; Air Products and Chemicals, Inc., Allentown, PA; Drexel University, Philadelphia, PA</td>
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<td>Session Title</td>
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<tr>
<td><strong>NEW APPLICATIONS OF ESI</strong></td>
<td>Richard B. Cole</td>
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<td>Conv. Ctr. Room 104A, lobby level</td>
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<td>MOC am 10:15 Metalloproteins Oxidation and Reduction: A Study by ESI-FTICR</td>
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<td>Mass Spectrometry; I. Jonathan Amster¹; Keith A Johnson¹; Brian</td>
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<td>Shira¹; James L. Anderson¹; University of Georgia, Athens, GA</td>
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<td>MOC am 10:35 Development of a general mass spectrometric method for</td>
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<td>determination of enantiomeric composition; Gabriela Grigorean¹; Carlito B.</td>
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<td>Lebrilla¹; University of California, Davis, CA</td>
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<td>MOC am 10:55 Measurement of Binding Selectivities by ESI-IMS and an</td>
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<td>Extraction Method; Jennifer S. Brodkin¹; Sheryl Blair¹; Esther Kempen¹;</td>
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<td>Michelle Reyzer¹; University of Texas, Austin, TX</td>
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<td>MOC am 11:15 Analysis of Enzyme Kinetics using Electrospray-Ionization</td>
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<td>Mass Spectrometry; Andrew J. Norris¹; Julian P. Whitelegge¹; Kyrn</td>
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<td>F. Faull¹; Tatsushi Toyokuni²; UCLA, Los Angeles, CA</td>
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<td>MOC am 11:35 Bridging the Genome and the Proteome: A Mass Spectrometry</td>
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<td>Equivalent of the Western Blot; David Arnott¹; Genentech, Inc., South San</td>
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<td>Francisco, CA</td>
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<td>MOC am 11:55 Mass-Directed Fractionation of Compound Libraries by Packed</td>
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<td>Column Supercritical Fluid Chromatography Electrospray Ionization Mass</td>
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<td>Spectrometry; Daniel B. Kassel¹; Michael Barber¹; Tao Wang¹; DuPont</td>
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<td>Pharmaceuticals, San Diego, CA</td>
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| **NEW METHODS IN PROTEIN ANALYSIS**                                        | Bradford W. Gibson     |
| Conv. Ctr. Room 104C, lobby level                                          |                        |
| MOD am 10:15 A quantitative method for proteome-wide analysis of          |                        |
| phosphorylation; Hui Lin Zhou¹; Julian Watts¹; Ruedi Aebersold¹; Univ.    |                        |
| of Washington, Seattle, WA                                                 |                        |
| MOD am 10:35 Analysis of Protein Phosphorylation by Element-specific       |                        |
| Phosphorous Detection by LC-ICP-MS and LC-ESI-MS; Wolf D. Lehmann³;        |                        |
| Mathias Wind; Michael Edler; Michael Linscheid; Norbert Jakubowski; Horst  |                        |
| Wesch; Andreas Schlosser; Ruediger Pipkorn; Dirk Bossemeyer; German Cancer  |                        |
| Research Center; Heidelberg; Institute of Applied Spectrochemistry; Dortmund; |                        |
| Institute of Analytical and Environmental Chemistry, Berlin, Germany      |                        |
| MOD am 10:55 Rapid and Sensitive Protein Identification by ESI-IMS using   |                        |
| a Fully Integrated Microchip-Based Electrospray Device; Gary A. Schultz²; |                        |
| Sheng Zhang¹; Simon J. Prosser¹; Thomas N. Corso¹; Avidel Taheri¹; Advanced |                        |
| BioAnalytical Services, Inc., Ithaca, NY                                   |                        |
| MOD am 11:15 Protein Fold Identification Using Experimental Constraints     |                        |
| Derived from Intramolecular Cross-links and Mass Spectrometry; Gavin D.   |                        |
| Dollinger; Ning Tang; Malin M Young; Judith C. Hempel; Connie M. Oshiro;   |                        |
| Eric W. Taylor; Irwin D. Kuntz; Bradford W. Gibson; Chiron Corporation;    |                        |
| Emeryville, CA; University of California, San Francisco, CA                |                        |
| MOD am 11:35 Monitoring the expression of membrane proteins in microorganisms |                        |
| using a novel electrophoretic approach prior to MALDI- and ESI-MS; Carol   |                        |
| L. Nilsson¹; Thomas Larsson¹; Elisabet Gustafsson¹; Kajsa Thoren¹; Karl-   |                        |
| Anders Karlsson¹; Pia Davidsonson¹; Goteborg University, Sweden            |                        |
| MOD am 11:55 Strategy for quantitative and high throughput proteomics;     |                        |
| Richard D. Smith¹; Gordon A. Anderson¹; Mary S. Lipton¹; Yufeng Shen¹;    |                        |
| Harold R. Udeeth¹; Timothy D. Veenstra¹; Ljiljana Pasa Toiic¹; PNVL,        |                        |
| Richland, WA                                                               |                        |

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### MONDAY MORNING ORAL SESSIONS IN THE HYATT HOTEL

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Authors/Institutions</th>
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<tbody>
<tr>
<td><strong>ION TRAPS: APPLICATIONS AND EXPLORATIONS</strong>&lt;br&gt;Hyatt Regency Ballroom A, 3rd level</td>
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<tr>
<td>MOE am 10:15</td>
<td><strong>HI-RES: A Novel Approach to Ion Ejection on the Quadrupole Ion Trap Capable of Resolving Isobars and Multiply-charged Isotopic Envelopes up to a +15 Charge State</strong>&lt;br&gt;Joseph J. Mulholland¹; Richard A. Yost¹; University of Florida, Gainesville, FL</td>
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<td>MOE am 10:35</td>
<td><strong>A New Multiplexed MS/MS Method for Ion Trapping Instruments</strong>&lt;br&gt;Kenneth L. Ray¹; Gary L. Glish¹; University of North Carolina, Chapel Hill, NC</td>
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<td>MOE am 10:55</td>
<td><strong>Improvements in Ion Trap Operation</strong>&lt;br&gt;Michael A. Schubert¹; Andreas Brekenfeld¹; Bruker Daltonik GmbH, Bremen, Germany</td>
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<td>MOE am 11:15</td>
<td><strong>Quadrupole Ion Trap/Ion Mobility Spectrometry: Gas-Phase Mobility Studies of Amino Acid and Amine/Polyether Non-Covalent Inclusion Complexes</strong>&lt;br&gt;John R. Griffiths¹; Colin S. Creaser¹; Brian M. Stockton²; Nottingham Trent University, Nottingham, UK; SmithKline Beecham Pharmaceuticals,Tonbridge, Kent, UK</td>
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<td>MOE am 11:35</td>
<td><strong>PA Scale Estimation of Modified Uridine from Dissociation of Hydrogen-Bound Heterodimer Constituted with Amino-acid Partners Prepared in ESI/ITMS</strong>&lt;br&gt;Jean Claude Tabet¹; Sandra Alves¹; Francoise Fournier¹; Claude Pepe¹; Melanie Quelquejeu¹; Jean Marc Valery¹; Université Pierre et Marie Curie, Paris, France</td>
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<td>MOE am 11:55</td>
<td><strong>Impact of the Broadband Isolation Waveform in Ion Trap Tandem Mass Spectrometry</strong>&lt;br&gt;Bert C. Lynn¹; Kwenga Sichilongo²; Brandy R. McCrceight¹; Mississippi State University, MS State, MS; Mississippi University for Women, Columbus, MS</td>
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<td><strong>KINETIC MECHANISMS FOR ION/ MOLECULE REACTIONS</strong>&lt;br&gt;Hyatt Regency Ballroom F, 3rd level</td>
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<td>MOF am 10:15</td>
<td><strong>A New Instrument for Measuring Ion Molecule Kinetics at Elevated Pressures: The Turbulent Ion Flow Tube (TIFT)</strong>&lt;br&gt;Albert A. Viggiano¹; Susan T. Arnold¹; John V. Seeley²; Air Force Research Laboratory, (VFSP), Hanscom AFB, MA; Oakland University, Rochester, MI</td>
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<td>MOF am 10:35</td>
<td><strong>Bond Dissociation Energies of Metal Ion M&quot;</strong>, Ligand L Complexes ML &quot;n&quot; and their Biochemical Significance**&lt;br&gt;Paul Kepner¹; Michael Peshek¹; Arthur T. Blades¹; University of Alberta, Edmonton, Canada</td>
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<td>MOF am 10:55</td>
<td><strong>A Distonic Ion Approach to Understanding the Reactivity of meta-Benzene</strong>&lt;br&gt;Eric D. Nelson¹; Alexander Artau¹; Jason M. Price¹; Christopher J. Petzold¹; Hilkka I. Kettunen¹; Purdue University, West Lafayette, IN</td>
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<tr>
<td>MOF am 11:15</td>
<td><strong>Ion Molecule Reactions of Metal-Coordinated Polyglycol Distonic Radical Cations with Reactive Gaseous Reagents</strong>&lt;br&gt;Jody M. Talley¹; Michael J. Police¹; Chrys Weseemundi¹; The University of Akron, Akron, OH</td>
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<td>MOF am 11:35</td>
<td><strong>Isotope and Temperature Effects on the Low-Pressure Association Reactions of Dimethyl Ether with Protonated Dimethyl Ether: An FT/ICR-MS Study</strong>&lt;br&gt;Travis D. Fridgen¹; Terry B. McMahon¹; University of Waterloo, Waterloo, ON, Canada</td>
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<tr>
<td>MOF am 11:55</td>
<td>**Gas-phase Hydrogen Deuterium Exchange Reactions of Model Peptides: Conformational Analyses by FT-ICR; T. Solouki¹; R. Fort¹; A. Alomary¹; A. Fattah¹; University of Maine, Orono, ME</td>
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</tbody>
</table>
### Bacterial Taxonomy, Phenotyping and Proteomics

Chair: Jackson O. Lay  
Conv. Ctr. Ballroom A, 2nd level

**MOA pm 03:00** The Characterization of Bioaerosols Using in situ Thermal Hydrolysis/Methylation-Mass Spectrometry (THM-MS); Kent J. Voorhees\(^1\); Angelo J. Madonna\(^1\); David Updegraph\(^1\); Ted L. Hadfield\(^1\); John David\(^2\); Colorado School of Mines, Golden, CO; US Army/AFIP, Washington, DC

**MOA pm 03:20** Comparison of Py-MS, MALDI-TOF/MS, and Molecular Methods for Rapid Classification of Vibrio parahemolyticus Outbreak Strains; Jon G. Wilkes\(^1\); Ricky Holland\(^1\); Manuel Holcomb\(^1\); Jackson O. Lay, Jr.\(^1\); Susan McCarthy\(^1\); NCTR/FDA, Jefferson, AR; CFSPAN/FDA, Dauphin Island, AL

**MOA pm 03:40** Mass spectrometric characterization of phenotypic variations in protein and carbohydrate expression in pathogenic *Haemophilus ducreyi*; N. Karoline Schefler\(^1\); Arnold M. Falick\(^2\); Steven C. Hall\(^2\); Anthony A. Campagnari\(^2\); Bradford W. Gibson\(^3\); University of California, San Francisco, CA; PE Biosystems, Foster City, CA; State University of New York, Buffalo, NY

**MOA pm 04:00** *E. coli* Proteomics and the Bacteriological Sex Factor; Jonathan A. Karty\(^1\); James P. Reilly\(^1\); Indiana University, Bloomington, IN

**MOA pm 04:20** Comparison of the Hundred Most Abundant Proteins of Two Strains of *Helicobacter pylori* by 2-DE and MALDI-MS; Peter R Jungblut\(^1\); Stephanie Lamer\(^1\); Gaby Haas\(^1\); Dirk Bumann\(^1\); Thomas F Meyer\(^1\); Max-Planck-Institute for Infection Biology, Berlin, Germany

**MOA pm 04:40** Factors Affecting Microorganism Identification by Mass-Based Searching of Proteome Databases; Catherine Fenselau\(^1\); Plamen A. Demirev\(^1\); Jeffrey S. Linn\(^2\); Fernando J. Pineda\(^2\); University of Maryland, College Park, MD; Johns Hopkins University, Laurel, MD

### Energy and Petrochemicals (Part I)

Chairs: C. Samuel Hsu and Dean V. Davis  
Conv. Ctr. Ballroom B, 2nd level

**MOB pm 03:00** Characterization of Basic Nitrogen Compounds in Diesel Fuels by Fractionation and Mass Spectrometry; Chang S. Hsu\(^1\); Gary J. Deichert\(^1\); Doug J. Abbott\(^2\); ExxonMobil Research & Engineering Co., Annandale, NJ; Esso Petroleum, Abingdon, England

**MOB pm 03:20** Determination of Soil Surface-Bound P AH’s in Hydrocarbon-Contaminated Soils by Aerosol Mass Spectrometry; Ryan P. Rodgers\(^1\); Alexandru C. Lazar\(^1\); Peter T. A. Reilly\(^1\); William B. Whittem\(^1\); J. Michael Ramsey\(^1\); Oak Ridge National Laboratory, Oak Ridge, TN

**MOB pm 03:40** Applications of Low Energy Charge Exchange Chemical Ionization in the Analysis of Hydrocarbons; Burnaby Manson\(^1\); Brian M. Wagner\(^2\); Gordon R. Nicol\(^1\); University of Delaware, Newark, DE

**MOB pm 04:00** Real-Time Monitoring of Aromatic Air Pollutants using a Mobile TGA LPCI/MS/MS; Nicholas S. Karella\(^1\); Qiang Feng Chen\(^1\); Gary B. DeBrou\(^1\); Ontario Ministry of Environment, Toronto, Canada

**MOB pm 04:20** Source Characterization of Coal Combustion Particulate Emissions Investigated by Single Particle Chemical Analysis; David T. Suss\(^1\); Phil J. Silva\(^1\); Kimberly A. Prather\(^1\); Zohir Chowdury\(^1\); Paul Mayo\(^1\); Glen R. Cass\(^1\); David Wagner\(^1\); JoAnn S. Lighty\(^1\); Adel F. Sarofim\(^2\); University of California, Riverside, CA; California Institute of Technology, Pasadena, CA; Georgia Institute of Technology, Atlanta, GA; University of Utah, Salt Lake City, UT

**MOB pm 04:40** Identification and Weathering of Arson Accelerants and Hydrocarbon Fuels in Complex Matrices by Electron Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Christine A. Hughes\(^1\); Erin N. Blumer\(^1\); Alan G. Marshall\(^2\); Ryan P. Rodgers\(^1\); Michael A. Freitas\(^3\); Florida State University, Tallahassee, FL; Oak Ridge National Laboratory, Oak Ridge, TN; Ohio State University, Columbus, OH

### 5:30 – 6:30 pm

**Workshop: High-Throughput TOF**  
Chair: Werner E. Ens  
Conv. Ctr. Ballroom B, 2nd level
## MONDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

### NON-COVALENT INTERACTIONS
Chair: Richard Griffey

**Conv. Ctr. Room 104A, lobby level**

**MOD pm 03:00** Monitoring the Assembly of Macromolecular Complexes Using nano-ES and TOF Analysis; Carol Y Robinson1; Mark A Tito1; Marcus Fandrich1; Adam A Rostom1; Oxford University, Oxford, UK

**MOD pm 03:20** Design of High-Affinity Ligands for RNA Using Mass Spectrometry Based Screening; Steven A. Hofstadler1; Kristin A. Sannes-Lowery1; Jared J. Druder1; Eric E. Swayne1; Richard H. Griffey1; IBIS Therapeutics, Carlsbad, CA

**MOD pm 03:40** Mass Spectrometry Approaches for Studying Protein Complexes and their Topographies; Joseph A. Loo1; Patrick McConnell1; Sherrie R. Tafuri1; Parke-Davis Pharmaceutical Research, Ann Arbor, MI

**MOD pm 04:00** Binding of Small Hydrophobic Ligands to Proteins Investigated by Electrospray Mass Spectrometry; Igor A. Kaltashov1; Hui Xiao1; Lila M. Gierasch1; Stephen J. Eyles2; University of Massachusetts, Amherst, MA

**MOD pm 04:20** Characterization of the IcIR protein and its complex with two different dsDNA fragments; Lynda J. Donald1; Harry W. Duckworth1; Werner Ens1; Kenneth G. Standing1; University of Manitoba, Winnipeg, Canada

**MOD pm 04:40** Electrospray ionization mass spectrometry of drug-DNA noncovalent complexes: Is the solution-phase structure maintained in the gas phase?; Valerie Gabelica1; Frederic Rosu1; Claude Houssier1; Edwin De Paauw1; James Langridge2; Alan Millar2; University of Liège, Belgium; Micromass Ltd., Manchester, UK

### SYNTHETIC POLYMERS AND CHROMATOGRAPHY
Chair: Scott D. Hanton

**Conv. Ctr. Room 104C, lobby level**

**MOD pm 03:00** GPC-MAIDI-TOF Analysis of a,w-Bis(4-hydroxybutyl) Polydimethylsiloxanes; E. Peter Maziarcz1; X. Michael Liu1; Edmond T. Quinn1; Yu-Chin Lai1; Dan Ammon1; George L. Grobe1; Bausch & Lomb, Rochester, NY

**MOD pm 03:20** ESI and Tandem Mass Spectrometry of Mixed Polyesters; William J. Simonsick1; Laszlo Prokai2; DuPont Marshall R & D Laboratory, Philadelphia, PA; University of Florida, Gainesville, FL

**MOD pm 03:40** Sequence analysis of copolymers by ESI FTMS; Sander Koster1; Marc C. Duursma1; Jaap J. Boon1; Chris G. de Koster2; Michel W.F. Nielen3; Ron M.A. Heeren1; FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands; DSM Research, Geleen, The Netherlands; Akzo Nobel Chemicals Research, Arnhem, The Netherlands

**MOD pm 04:00** Molecular characterization of hyperbranched polymers by SEC with multiple detection; Chris G. de Koster1; Erik Gelade1; Nico Meijerink1; Rolf van Benthem1; Huub Henderickx1; DSM Research, The Netherlands

**MOD pm 04:20** Analysis of Amine Chain Extenders by Selective Hydrolysis / Electrospray LC/MS; Robert A. Ludick1; Rohm & Haas, Woodstock, IL

**MOD pm 04:40** SEC-ESI/MS of Synthetic Polymers using an Ion trap; Arnd Ingendoh1; Matthias Pelzing2; Petra Pallloch2; Ulrich Schlusen2; Werner Pettau2; Bruker Daltonik, Bremen, Germany; Bruker Saxonia, Leipzig, Germany; Byk Chemie, Wesel, Germany

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### WORKSHOP: FUNDAMENTALS AND BIOCHEMISTRY
Chair: Mary Rogers

**Conv. Ctr. Room 104A**

**5:30 – 6:30 pm**

### WORKSHOP: QUADRUPOLE ION TRAPS: PROBLEM SOLVING IN BASIC AND APPLIED RESEARCH, A GRADUATE STUDENT PERSPECTIVE
Chair: Jennifer Brodhelt

**Conv. Ctr. Room 104C**

**5:30 – 6:30 pm**
## MONDAY AFTERNOON ORAL SESSIONS IN THE HYATT HOTEL

<table>
<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Chair</th>
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<tbody>
<tr>
<td>03:00</td>
<td>Laser-induced Acoustic Desorption/Chemical Ionization Studies of Nonvolatile Organic Molecules</td>
<td>David H. Russell</td>
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<td>Laser-induced Acoustic Desorption/Chemical Ionization Studies of Nonvolatile Organic Molecules</td>
<td>James Párez; Luis E. Ramirez-Arizmendi; Leonard P. Guler; Eric D. Nelson; Hilkkka I. Kenttämaa; Christopher J. Petzold; Purdue University, West Lafayette, IN</td>
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<tr>
<td>03:20</td>
<td>Optimization of MALDI Sample Preparation for Photofragment TOF Peptide Sequencing</td>
<td>Gary Groenewold</td>
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<td>Optimization of MALDI Sample Preparation for Photofragment TOF Peptide Sequencing</td>
<td>Justin M. Hettick; David L. McCurdy; Damon C. Barbacci; David H. Russell; Texas A&amp;M University, College Station, TX</td>
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<tr>
<td>03:40</td>
<td>Infrared MALDI of DNA Using Frozen Mixed Matrices</td>
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<td>Infrared MALDI of DNA Using Frozen Mixed Matrices</td>
<td>Steven J. Lawson; Mark W. Little; Kermit K. Murray; Emory University, Atlanta, GA</td>
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<td>04:00</td>
<td>Reductive Hydrogenation of Cytosine by 2,5-Dihydroxybenzoic Acid</td>
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<td>Reductive Hydrogenation of Cytosine by 2,5-Dihydroxybenzoic Acid</td>
<td>John M. Koonen; David H. Russell; LBMS, Texas A&amp;M University, College Station, TX</td>
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<td>04:20</td>
<td>Experimental examination of the thermodynamic basis of MALDI</td>
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<td>Victor L. Talkoza; Richard J. Jacob; Alma L. Burlingame; Michael A. Baldwin; University of California, San Francisco, CA</td>
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<td>04:40</td>
<td>Modeling Infrared Matrix-Assisted Laser Desorption Ionization (IR-MALDI) Dynamics of Oligonucleotides in Succinic Acid Matrix</td>
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<td>Modeling Infrared Matrix-Assisted Laser Desorption Ionization (IR-MALDI) Dynamics of Oligonucleotides in Succinic Acid Matrix</td>
<td>Akos Vertes; Sándor Kristyan; George Washington University, Washington, DC</td>
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<td>The Characterization of Multi-fluorinated and CF₂-terminated SAM films by ion-surface reactions</td>
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<td>The Characterization of Multi-fluorinated and CF₂-terminated SAM films by ion-surface reactions</td>
<td>Darrin L. Smith; Vicki H. Wysocki; T. Randall Lee; University of Arizona, Tucson, AZ; University of Houston, Houston, TX</td>
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<td>Correlation between Gas-Phase Aluminum Oxyanions and Surface Hydration</td>
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<td>Correlation between Gas-Phase Aluminum Oxyanions and Surface Hydration</td>
<td>Jill R. Scott; Anita K. Gianotto; Gary S. Groenewold; J. B. Wright; INEL, Idaho Falls, ID; Battelle Memorial Institute, Bel Air, MD</td>
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<td>Characterization of Photooxidized Monolayers and Bilayers on Au by Secondary Ion Mass Spectrometry</td>
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<td>Characterization of Photooxidized Monolayers and Bilayers on Au by Secondary Ion Mass Spectrometry</td>
<td>Robert D. English; Michael J. Van Stipdonk; Rajaram C. Sabapathy; Richard M. Crooks; Emilie A. Schweikert; Texas A&amp;M University, College Station, TX</td>
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<td>Combining DIOS-Mass Spectrometry and FT-Infrared Spectroscopy for the identification of small molecular weight compounds</td>
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<td>Francis Bitsch; Serge Moss; Pierre Acker; Gary Stuzdak; Novartis Pharma AG, Switzerland; The Scripps Research Institute, La Jolla, CA</td>
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<td></td>
<td>The Effect of Different Laser Sources on Analysis of Self-Assembled Monolayers by Laser Desorption Time-of-Flight MS</td>
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<td>The Effect of Different Laser Sources on Analysis of Self-Assembled Monolayers by Laser Desorption Time-of-Flight MS</td>
<td>Weihtong Gong; Ingrid Fritsch; Charles L. Wilkins; University of Arkansas, Fayetteville, AR</td>
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<td>Cluster Projectiles in SIMS: Probing the Relationship between Secondary Ions and Surface Composition</td>
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<td>Cluster Projectiles in SIMS: Probing the Relationship between Secondary Ions and Surface Composition</td>
<td>Michael J. Van Stipdonk; Emilie A. Schweikert; Wichita State University, Wichita, KS; Texas A&amp;M University, College Station, TX</td>
</tr>
</tbody>
</table>
7:30 – 8:00 am  “Wake-Up Coffee” in front of the Terrace Theater
TUESDAY MORNING PLENARY LECTURE IN THE TERRACE THEATER
8:00 am  Award for a Distinguished Contribution in Mass Spectrometry
Boris A. Manyrin, Technical Institute, St Petersburg, Russia

8:45 – 10:15 am  POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR
Authors of odd numbered posters present

TUESDAY MORNING ORAL SESSIONS IN THE CONVENTION CENTER

<table>
<thead>
<tr>
<th>TIME</th>
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<tbody>
<tr>
<td>10:15</td>
<td>Mapping functional intracellular signaling pathways using mass spectrometry</td>
<td>Dave Anderson; Weigun Li; Tong Lin; Tarikere Gururaja; Rigel Inc., South San Francisco CA</td>
</tr>
<tr>
<td>10:35</td>
<td>Dissection of the BRCA1 signaling pathway with mass spectrometry</td>
<td>L Qin; Y. Wang; D. Cortez; S Elledge; Houston, TX</td>
</tr>
<tr>
<td>10:55</td>
<td>Proteins of the Golgi Complex</td>
<td>Malcolm A. Ward; Jyoti Choudhary; Helen Byers; Lu Yu; Walter P Blackstock; Adele Rowley; GlaxoWellcome Research and Development Ltd., Stevenage, UK</td>
</tr>
<tr>
<td>11:15</td>
<td>Proteomics of Human Nucleolus</td>
<td>Jens S. Andersen; Matthias Mann; Aklillesh Pandey; Bernhard Küster; Carol E. Lyon; Yan-wah Lam; Anthony Leung; Arch Fox; Angus I. Lamond; University of Southern Denmark, Odense, Denmark; MDS-Protana A/S, Odense, Denmark; University of Dundee, Dundee, Scotland</td>
</tr>
<tr>
<td>11:35</td>
<td>A Comprehensive Characterization of the T Cell Antigen Receptor Complex Composition by Micro-Capillary Liquid Chromatography Tandem Mass Spectrometry</td>
<td>Rosemary K. Boyle; Manfried Heller; David R. Goodlett; Julian D. Watts; Ruedi Aebersold; University of Washington, Seattle, WA; Geneva University Hospital, Geneva, Switzerland</td>
</tr>
<tr>
<td>11:55</td>
<td>Identification of Phosphorylated Peptides Associated with Class I MHC Molecules and Implications for Immunotherapy</td>
<td>Victor H. Engelhard; Donald F. Hunt; Scott B. Figueroa; Angela L. Zarlengo; Forest M. White; Jeffrey Shabanowitz; University of Virginia, Charlottesville, VA</td>
</tr>
</tbody>
</table>

ACCELERATING PHARMACEUTICAL DISCOVERY – PART I SCREENING

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<tr>
<td>10:15</td>
<td>Evaluation of Frontal Affinity Chromatography Mass Spectrometry (FAC-MS) as a Universal Binding Assay for Drug Discovery</td>
<td>Michele A. Kelly; Philip J. Rosner; William Zembrowski; David Beebe; Larry Mylari; Peter Oates; Nora Chan; Darren Lewis; David Schriemer; Pfizer Central Research, Groton, CT; INH Technologies, Calgary, Alberta, Canada</td>
</tr>
<tr>
<td>10:35</td>
<td>A Fully Integrated and Automated Approach to the Design, Synthesis, and Characterization of 'Drug-Like' Libraries</td>
<td>John J. Isbell; Rongda Xu; Daniel B. Kassell; Csaba Nemes; DuPont Pharmaceuticals Research Labs, San Diego, CA</td>
</tr>
<tr>
<td>10:55</td>
<td>Validation of Solubility Measurements Using Ultra-Filtration Liquid Chromatography Mass Spectrometry (UF-LC/MS)</td>
<td>Lawrence P. Wemmer</td>
</tr>
<tr>
<td>11:15</td>
<td>High Throughput Metabolic Structure Elucidation Strategies in Drug Discovery</td>
<td>Robyn A. Rourke; Rongda Xu; Daniel B. Kassell; DuPont Pharmaceutical Research Laboratories, San Diego, CA</td>
</tr>
<tr>
<td>11:35</td>
<td>The role of accurate mass MS measurement in metabolite identification</td>
<td>Nigel J. Clarke; Kathleen A. Cox; Diane Hindgen; Walter A. Korfmacher; Schering-Plough Research Institute, Kenilworth, NJ</td>
</tr>
<tr>
<td>11:55</td>
<td>A Novel Four-Column Parallel Chromatography System for Gradient SRM LC/MS Bioanalytical Analyses</td>
<td>Colleen K. Van Pelt; Thomas N. Corso; Gary A. Schultz; Stephen Lowes; Jack Henion; Advanced BioAnalytical Services, Inc., Ithaca, NY</td>
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</tbody>
</table>

INTEREST GROUP MEETINGS

Anyone interested in the topics are encouraged to buy a cash lunch and bring it to the meeting rooms where there are tables and chairs for informal discussion.

<table>
<thead>
<tr>
<th>TIME</th>
<th>ROOM</th>
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<tbody>
<tr>
<td>12:15</td>
<td>101 A</td>
<td>Flavor and Foodstuffs</td>
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<td>101 B</td>
<td>Surface Science</td>
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<td>12:15</td>
<td>201 A</td>
<td>FTMS</td>
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<tr>
<td>12:15</td>
<td>201 B</td>
<td>Fundamental</td>
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</table>
**TUESDAY MORNING ORAL SESSIONS IN THE CONVENTION CENTER**

**COMPUTER APPLICATIONS**  
Chair: Terry Lee  
*Conv. Ctr. Room 104A, lobby level*

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOC am</td>
<td>10:15 A High-Throughput Computational Platform for Efficient, Reliable Protein Identification and Proteomic Studies</td>
<td>Wen Yu1; Scott D. Patterson1; Roland Luethy1; Amgen, Inc, Thousand Oaks, CA</td>
</tr>
<tr>
<td>TOC am</td>
<td>10:35 Finding Post-Translational Protein Modifications via MS/MS</td>
<td>Pavel Pevzner1; Vlad Danck1; Zufar Mulyko1; Chris Tang1; USC, Los Angeles, CA; Millennium Pharmaceuticals, Cambridge, MA</td>
</tr>
<tr>
<td>TOC am</td>
<td>10:55 The Use of Advanced Mathematical Algorithms to Enhance the Identification of Proteins</td>
<td>Keith A. Waddell1; Jon P. DeGnore1; Melanie X. Lin1; Tony G. Ferrige1; M. Robert Alecio1; R. Stuart Ray1; X. Kate Zhang1; PE Biosystems, Framingham, MA; PPL, Isleham, Camb, England; Genzyme Corp., Framingham, MA</td>
</tr>
</tbody>
</table>

**ELEMENTAL ANALYSIS**  
Chair: Douglas C. Duckworth  
*Conv. Ctr. Room 104C, lobby level*

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<thead>
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<tbody>
<tr>
<td>TOC am</td>
<td>10:15 High Mass Resolving Power Elemental Analysis of Conduction and NonConduction Materials by Radio Frequency Glow</td>
<td>John R. Tyler1; Stanley Stevens1; Johnny Evans1; Paula Cable1; University of Florida, Gainesville, FL; Lee University, Cleveland, TN; Westinghouse Savannah River Company, Aiken, SC; Westinghouse Savannah River Company, Aiken, SC</td>
</tr>
<tr>
<td>TOC am</td>
<td>10:35 Isotopic Ratio Measurements of Geological Samples Using Laser Ablation in a Quadrupole Ion Trap Mass Spectrometer</td>
<td>Michael L. Alexander1; Maggie E. Taylor2; Cardell Greg3; Pacific NW National Lab, Richland, WA; Jet Propulsion Laboratory, Pasadena, CA</td>
</tr>
<tr>
<td>TOC am</td>
<td>10:55 The Use of Source Monitoring to Improve Accuracy of GDMS Quantified Analysis Software</td>
<td>Edward J. Pugh1; Gary S. V. Coles1; Viv J. Womer1; University of Wales, Swansea, UK; Corus Group Plc, UK</td>
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<td>FTMS</td>
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TUESDAY MORNING PLENARY LECTURE IN THE TERRACE THEATER
8:00 am Award for a Distinguished Contribution in Mass Spectrometry
Boris A. Mamyrin, Technical Institute, St Petersburg, Russia

8:45 – 10:15 am POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR
Authors of odd numbered posters present

TUESDAY MORNING ORAL SESSIONS IN THE HYATT HOTEL

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<th>ESI: NEW INSTRUMENTATION AND METHODS</th>
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<tbody>
<tr>
<td><strong>Hyatt Regency Ballroom A, 3rd level</strong></td>
</tr>
<tr>
<td><strong>Chair: Gary J. Van Berkel</strong></td>
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</tbody>
</table>

**TOE am 10:15**
Improved detection sensitivity in ES MS by a new capillary design: basic principles; Guenter Klesper¹; Gregor Fusshoeller¹; Heike Klesper¹; CARBOTEC GmbH, Germany

**TOE am 10:35**
Investigations of single isolated droplets with net charge: (i) A source of ions and (ii) a wall-less chemical reaction chamber; George R. Agnes³; Xiao Feng³; Elizabeth Chua³; Michael J. Bogan³; Simon Fraser University, Burnaby, B.C., Canada

**TOE am 10:55**
Playing Ping-Pong with Electrospayed Droplets: An Investigation into the Dynamics and Mechanism of Droplet Breakup in Electrosprays; James N. Smith¹; Richard C. Flagan¹; Jesse L. Beauchamp¹; California Institute of Technology, Pasadena, CA

**TOE am 11:15**
Lowering the limits of detection in ESI: Reduction of background noise with high-field asymmetric waveform ion mobility spectrometry (FAIMS); Roger Guevremond¹; Pierre Thibault¹; David A. Barnett¹; Barbara Ellis¹; Randy W. Purves²; National Research Council of Canada, Ottawa, ON, Canada; PE Scien, Concord, ON, Canada

**TOE am 11:35**
Development of Corona Discharge Charge Reduction Electrospray Mass Spectrometry for Analysis of Complex Biopolymer Mixtures; Daniel D. Ebeling¹; Michael S. Westphall¹; Mark Scalf¹; Lloyd M. Smith¹; University of Wisconsin, Madison, WI

**TOE am 11:55**
Microcalorimeter Detector for Biopolymer Mass Spectrometry; M. W. Rabin¹; G. C. Hilton¹; John M. Martinis¹; National Institute of Standards and Technology, Boulder, CO

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<tr>
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<tr>
<td><strong>Chair: Peter B. Armentrout</strong></td>
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</tbody>
</table>

**TOF am 10:15**
Dynamics of Competitive Fragmentation and Electron Emission of Photoactivated Metal Clusters; Kent M. Ervin¹; Vassil A. Spasov¹; Yang Shi¹; University of Nevada, Reno, NV

**TOF am 10:35**
Coordination Chemistry of Solvated Silver Cations; Brigitte S. Fox¹; Martin K. Beyer¹; Uwe Achatz¹; Stefan Joos¹; Gereon Niedner-Schatteburg¹; Vladimir E. Bondybey²; Technische Universität München, Germany; UC Berkeley, CA

**TOF am 10:55**
The Discovery and Investigation of Multiply Charged Anionic Metal Clusters; Lutz Schweikhard¹; Alexander Herlert¹; Manuel Vogel¹; Inst. f. Physik, Johannes Gutenberg University, Mainz, Germany

**TOF am 11:15**
Laser Ablation Mass Spectrometry of Binary Clusters: An Investigation of their Relative Stabilities and Reactivities with a Focus on Chromium Sulfide Clusters; Gary D. Willett¹; Ian G. Dance¹; Keith J. Fisher¹; Zhen Guo¹; Fanao Kong³; Liu Peng³; Qihe Zhu³; The University of New South Wales, Sydney, Australia; Chinese Academy of Science, Beijing, P.R. China

**TOF am 11:35**
*Ab initio* Study of Argon-HCO⁺ clusters: Insight into Size Dependent Cluster Ion Properties; Kelly O. Sullivan¹; Gregory I. Gellene¹; Creighton University, Omaha, NE; Texas Tech University, Lubbock, TX

**TOF am 11:55**
Solvation of Singly Charged Polyatomic Ions in Polycomponent Vapors; John B. Fenn¹; Zhan Dongliang¹; Virginia Commonwealth University, Richmond, VA

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TUESDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

FATTY ACIDS AND POLAR LIPIDS
Chair: J. Thomas Brenna
Conv. Ctr. Ballroom A, 2nd level

TOA pm 03:00 Quantitative Measurement of the Second Messenger Ceramide by ESI-MS/MS Revealed Elevated Ceramide Level in Plasma of Patients with Coronary Heart Disease; Gerhard Liebisch¹; Wolfgang Drobnik²; Markus Reil¹; Bernd Lieser¹; Gerd Schmitz³; Klaus Gempe²; Klaus-Dieter Gerbitz²; Inst. for Clin. Chemistry, Univ. of Regensburg, Regensburg, Germany; Inst. Clin. Chemistry, Hospital Munich Schwabing, Munich, Germany

TOA pm 03:20 Screening for inherited disorders of fatty acid metabolism by electrospray tandem mass spectrometry; David W. Johnson¹; Women’s and Children’s Hospital, Adelaide, Australia

TOA pm 03:40 Unambiguous Determination of Very Long Chain Fatty Acid Containing Phospholipids in Rat Retina by HPLC/ESI-MS; Hee-Yong Kim¹; Karl Kevalla¹; National Institutes of Health, Rockville, MD

TOA pm 04:00 Identification of Novel Omega-Oxidised Metabolites of 5-Oxo-6,8,11,14-Eicosatetraenoic Acid; John M. Heyko²; Robert C. Murphy³; National Jewish Medical and Research Center, Denver, CO

TOA pm 04:20 Effects of extracellular acidification on phospholipid composition of neuronal cells studied by quantitative nano-electrospray ionization tandem mass spectrometry; Kristine Glunde¹; Dieter Leibfritz¹; Wolf D. Lehmann³; University of Bremen, Bremen, Germany; German Cancer Research Center, Heidelberg, Germany

TOA pm 04:40 Quantitative Profiling of Polar Lipids Using Isotopic Labeling and a Hybrid Quadrupole Time-of-Flight Mass Spectrometer; Andrej Shvychenko¹; Kim Ekroos²; Igor Chernushevich²; Kai Simons³; European Molecular Biology Laboratory, Heidelberg, Germany; MPI of Molecular Cell Biology and Genetics, Dresden, Germany; PE SCIEX, Toronto, Canada

ACCELERATING PHARMACEUTICAL DISCOVERY – PART II
Chairs: Timothy R. Baker and Walter A. Korfmaner
Conv. Ctr. Ballroom B, 2nd level

TOB pm 03:00 Higher Throughput Metabolite Identification in Drug Discovery: Current Capabilities and Future Trends; Kathleen A. Cox¹; Nigel J. Clarke²; Diane Rindgen³; Walter A. Korfmaner⁴; Schering Plough Research Institute, Kenilworth, NJ

TOB pm 03:20 Rapid Analysis of Biological Samples Using Packed Column Supercritical Fluid Chromatography/Mass Spectrometry; Daniel G. Morgan¹; Lloyd W. Frick¹; Glaxo Wellcome Inc., Research Triangle, NC

TOB pm 03:40 The Use of Indexed Multi-probe Electrospray Technology for Quantitation in Support of Drug Discovery ADME Screens; D. L. Hiller¹; R. O. Cole²; Pfizer, Groton, CT

TOB pm 04:00 Techniques for Increasing the Throughput of Flow Injection Mass Spectrometry; Kenneth L. Morand³; Thomas M. Burt⁴; Brian T. Regg⁴; Procter & Gamble Pharmaceuticals, Mason, OH

TOB pm 04:20 Fourier Transform Ion Cyclotron Resonance Mass Spectrometry as a High Throughput Screen for Identifying RNA Binding Ligands; Kristin A. Sannes-Lowery¹; Jared J. Drader¹; Richard H. Grifey³; Steven A. Hofstadler³; Ibis Therapeutics, Carlsbad, CA

TOB pm 04:40 Automated Dual LC/MS/MS with Cassette Analysis Markedly Increases Throughput and Accelerates Drug Discovery; Stephen A. Wring¹; Larry S. Birkemo¹; Joseph W. Polli¹; Daniel G. Morgan¹; Jonathan B. Morgan¹; Lloyd W. Frick¹; Glaxo Wellcome Inc., RTP, NC

5:30 – 7:10 pm
SPECIAL SESSION – GC/MS: THE HONEYMOON YEARS
Chair: Ross C. Willoughby
Conv. Ctr. Ballroom B, 2nd level

5:30 Early GC/MS at the Dow Chemical Company, Fred McLafferty
5:50 The Ephemeral Effusion Separator for GC/MS, J. Throck Watson
6:10 GC/MS in the Cure of Disease, Sanford Markay
6:30 Early Data processing Strategies, Ronald A. Hites
6:50 GC/MS and the Formation of Finnigan, Michael Story
1:30 – 3 pm POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR
Authors of even numbered posters present

TUESDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

DNA AND PROTEIN ANALYSIS BY MALDI
Chair: Barbara S. Larsen
Conv. Ctr. Room 104A, lobby level

TOC pm 03:00 A Quantitative Method for Measuring the Stability of Unpurified Proteins from Rates of H/D Exchange Using MALDI Mass Spectrometry; Michael C. Fitzgerald1; Kendall Powell1; Sina Ghaemmaghami1; Terrence G. Oas1; Duke University, Durham, NC

TOC pm 03:20 A Rapid Method to Sequence "In-Solution" Digested Proteins Using MALDI/IM/SID-o-TOF/MS; Katrin Fuhrer2; Albert Schultz2; Earle G. Stone1; Kent Gillig1; Brandon Ruotolo1; Zee Yong Park1; David H. Russell1; Ionwerks, Houston, TX; Texas A&M University, College Station, TX

TOC pm 04:00 Applications of the MALDI-QqTOF Mass Spectrometer: its high sensitivity, high resolution, high mass accuracy, and high throughput make it a powerful tool for protein identification; Kenneth G. Standing; Alexander V. Loboda; Andrej Shevchenko; Anna Shevchenko; Yi-Min She; Steve Haber; Werner Ens; University of Manitoba, Canada; European Molecular Biology Laboratory, Germany; Cereal Research Centre, Agriculture and Agrifood, Canada

TOC pm 04:20 A Quantitative Method for Measuring the Stability of Unpurified Proteins from Rates of H/D Exchange Using MALDI Mass Spectrometry; Michael C. Fitzgerald1; Kendall Powell1; Sina Ghaemmaghami1; Terrence G. Oas1; Duke University, Durham, NC

TOC pm 04:40 A Rapid Method to Sequence "In-Solution" Digested Proteins Using MALDI/IM/SID-o-TOF/MS; Katrin Fuhrer2; Albert Schultz2; Earle G. Stone1; Kent Gillig1; Brandon Ruotolo1; Zee Yong Park1; David H. Russell1; Ionwerks, Houston, TX; Texas A&M University, College Station, TX

PROCESS MONITORING
Chair: Mark A. LaPack
Conv. Ctr. Room 104C, lobby level

TOC pm 03:00 Development and application of on-line process analytical methods based on selective ionisation mass spectrometry; Ralf Zimmermann1; Ralph Dorfner1; Fabian Mühlg1; Thorsten Hauler1; Klaus Haffner1; Thomas Ferge2; Antonius Kettrup2; Chahan Yeretzian2; GSF-Forschungszentrum, Germany; Nestec Ltd., Switzerland

TOC pm 03:20 Membrane Introduction Mass Spectrometry (MIMS) with Analyte-Selective, Tailored Membranes; Todd M. Allen1; Andrew J. Griggs2; Richard B. Timmons3; Charles W. Wilkerson3; Los Alamos National Laboratory, Los Alamos, NM; University of Texas, Arlington, TX

TOC pm 03:40 Parameterization for Process Analysis of Complex Mixtures: Which Peaks to Monitor?; Kelsey D. Cook1; Kevin H. Bennett1; University of Tennessee, Knoxville, TN

TOC pm 04:00 Stopped-Flow-ESI MS: A New Method for Studying Reaction Kinetics in Solution; Beata M. Kolakowski1; Douglas A. Simmons1; Lars Konermann1; The University of Western Ontario, London, ON, Canada

TOC pm 04:20 On-Line Miniaturized Protein Digestion/Pep tide Separation/Electrospray Ionization Mass Spectrometry for Proteome Analysis; Jia Xu1; Jun Gao2; Cheng S. Lee1; University of Maryland, College Park, MD

5:30 – 6:30 pm WORKSHOP: LC/MS SAMPLE INTRODUCTION AND SEPARATION STRATEGIES
Chair: Michael P. Balogh
Conv. Ctr. Room 104A

5:30 – 6:30 pm WORKSHOP: DATA HANDLING FOR HIGH-THROUGHPUT AND HIGH VOLUME ANALYSIS
Chair: Jon P. DeGnore and Timothy R. Baker
Conv. Ctr. Room 104C
### NEW (PERHAPS NOT FULLY TESTED) DESIGNS – PART I

Chairs: R. Graham Cooks and Michael W. Senko

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>TOE pm 03:00</td>
<td><strong>Fourier Transform Mass Spectrometry in a Linear Quadrupole Ion Trap</strong>: Michael W. Senko; Jae C. Schwartz; Alan E. Schoen; John E.P. Syka; Thermoquest Corporation, San Jose, CA</td>
<td></td>
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<tr>
<td>TOE pm 03:20</td>
<td><strong>Improved Performance Obtained on the Toroid Ion Trap Mass Analyzer Using Asymmetric Electrodes</strong>: Stephen A. Lammert; Cyril V. Thompson; Marcus B. Wise; Oak Ridge National Laboratory, Oak Ridge, TN</td>
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<tr>
<td>TOE pm 03:40</td>
<td><strong>Array of Coupled 3D RF Ion Traps (not Paul Traps) for MSn</strong>: Bruce Reinhold; University of New Hampshire, Durham, NH</td>
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<tr>
<td>TOE pm 04:00</td>
<td><strong>Microscale Ion Traps: 2-Dimensional Arrays</strong>: Peter T. A. Reilly; Oleg Kornienko; William B. Whitten; J. Michael Ramsey; Oak Ridge National Laboratory, Oak Ridge, TN; Merck Research Laboratories, North Wales, PA</td>
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<tr>
<td>TOE pm 04:20</td>
<td><strong>A Spatially Dispersive, Non-Scanning Miniature Cylindrical Ion Trap Array</strong>: Ethan R. Badman; R. Graham Cooks; Purdue University, W. Lafayette, IN</td>
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<td>TOE pm 04:40</td>
<td><strong>Multiple reflection energy-isochronous time-of-flight mass spectrometers for high mass resolving powers</strong>: Hermann Wollnik; Antonio Casares; Alexander Kholomeev; II Phys. Institute, Justus-Liebig University, Giessen, Germany; Max-Planck Institute für Aeronomie (MPfI), Kaut.-Lindau, Germany</td>
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### ION STRUCTURE AND ENERGETICS

Chair: Scott Gronert

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<thead>
<tr>
<th>Time</th>
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<th>Authors</th>
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<tr>
<td>TOF pm 03:00</td>
<td><strong>Large Anhydrous Polyalanine Ions: The First Fold Stabilizes a Hinged Helix-Coil</strong>: Anne E. Counterman; David E. Clemmer; Indiana University, Bloomington, IN</td>
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<tr>
<td>TOF pm 03:20</td>
<td><strong>Gas-Phase Solvation of Amino Acid-Cation Complexes: The Stabilization of Zwitterions</strong>: Rebecca A. Zoekusch; Evan R. Williams; University of California, Berkeley, CA</td>
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<td>TOF pm 03:40</td>
<td><strong>Nitronic Acid Radical and Wheland Intermediates</strong>: Frantisek Turecek; Miroslav Polasek; University of Washington, Seattle, WA</td>
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<tr>
<td>TOF pm 04:00</td>
<td><strong>Structure and Energetics of Highly Strained Radical Anions (C₅H₅⁻) Derived from the Reaction of Norbornadiene with O²</strong>: Shuju Kato; Rebecca L. Hoeningman; Weston T. Borden; Charles H. DePuy; Veronica M. Bierbaum; University of Colorado, Boulder, CO; University of Washington, Seattle, WA</td>
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<tr>
<td>TOF pm 04:20</td>
<td><strong>Photoclectron spectroscopy and gas phase thermochemistry of the methyl peroxy anion (CH₃OO⁻)</strong>: Stephen J.Blanksby; Tanya M Ramond; Gustavo E Davico; W Carl Lineberger; G Barney Ellison; University of Colorado, Boulder, CO</td>
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<tr>
<td>TOF pm 04:40</td>
<td><strong>Absolute Binding Energies of Silver Cations to Small Ligands Determined Using Threshold CID Experiments</strong>: Houssain El Arbi; Tamer Shoeb; Yun Ling; Alan, C. Hopkinson; Michael, K. W. Siu; York University, Toronto, Canada</td>
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<td>7:30 – 8:00 am</td>
<td>“Wake-Up Coffee” in front of the Terrace Theater</td>
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<td>8:00 am</td>
<td>Biemann Medal</td>
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<td>Julie A. Leary, University of California at Berkeley</td>
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<td>8:45 – 10:15 am</td>
<td>POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR</td>
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<td>Authors of odd numbered posters present</td>
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**WEDNESDAY MORNING ORAL SESSIONS IN THE CONVENTION CENTER**

**STRUCTURAL IMMUNOLOGY**
Chair: Kevin Downard

<table>
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<tr>
<th>Time</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>WOA am 10:15</td>
<td>Mass Spectrometric Epitope Mapping of Specific Monoclonal Antibodies against Matrix Metalloproteinase 19 (MMP-19), a Target Antigen of Rheumatoid Arthritis; Markus Kohlmann; Birgit Kolb; Cornelia Kolb; Radislav Sedlacek; Michael Przybyski; Universität Konstanz, Konstanz, Germany</td>
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<tr>
<td>WOA am 10:35</td>
<td>A peptidomic approach to investigate the defense reactions in Drosophila melanogaster; Philippe Bulet; Laurence Sabatier; Maurice Charlet; Lionel Cavicchioli; Alain Van Dorsseleer; Jules Hoffmann; CNRS, Strasbourg, France</td>
</tr>
<tr>
<td>WOA am 10:55</td>
<td>Affinity Capture and MALDI-MS of Cytokines from Mouse Serum; Gregory B Hurst; Stephen J Kennel; Linda J Foote; Michelle V Buchanan; Oak Ridge National Laboratory, Oak Ridge, TN</td>
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</tbody>
</table>

**TOXICOLOGY AND PHARMACOLOGY – PART I**

**WOB am 10:15** Structural Identification of a Crystalline Drug Metabolite in Tissue Sections Using MALDI-TOF MS and MALDI-FTMS; Richard D. Burton; Laura J. Miesbauer; Jane Fagerland; Alex Buol; Figen A. Seiler; Joseph Neilly; Dean Hickman; Abbott Laboratories, Abbott Park, IL

**WOB am 10:35** Identification of in vivo and in vitro metabolites of an NK1 receptor antagonist, CJ-11,972 by LC/MS/MS; Kevin Colizza; Chandra Prakash; Pfizer Central Research, Groton, CT

**WOB am 10:55** Species-Specific Formation of a Glutathione Conjugate of Efavirenz and its Role in Producing Nephrotoxicity in Rats; Abdul F. Mutlib; DuPont Pharmaceuticals Company, Newark, DE

**WOB am 11:15** Analysis of human metabolites of chemical warfare agents in urine using GC/MS/MS; John R. Barr; Dana B. Barr; Maria Ospina; W. Jack Driskell; Vincent L. Maggio; Ralph D. Whitehead Jr.; Terrance H. Jones; Donald G. Patterson Jr.; Larry L. Needham; Centers for Disease Control and Prevention, Atlanta, GA

**WOB am 11:35** A low-energy biomedical gas chromatograph-accelerator mass spectrometer for online detection of H2 and H3; John S. Wishnow; Paul L. Skipper; John T. Mehl; Steven R. Tannenbaum; Barbara J. Hughley; Robert E. Klinkowstein; Ruth E. Shefer; MIT, Cambridge, MA; Newton Scientific, Inc., Cambridge, MA

**WOB am 11:55** High-throughput LC-MS method development for bio-analysis; William D. van Dooren; Dick van der Lagermaat; Frans Schouten; Rob J. Vreken; Elwin R. Verheij; Jan van der Geest; Kees Ensing; TNO Pharma, Zeist, The Netherlands; MIP Technologies AB, Lund, Sweden

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**INTEREST GROUP MEETINGS**

Anyone interested in the topics are encouraged to buy a cash lunch and bring it to the meeting rooms where there are tables and chairs for informal discussion.

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<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Topic</th>
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<tr>
<td>12:15 – 1:30 pm</td>
<td>Room 101 A</td>
<td>Iron Metal Chemistry</td>
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<td>12:15 – 1:30 pm</td>
<td>Room 101 B</td>
<td>Laboratory Managers</td>
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<td>12:15 – 1:30 pm</td>
<td>Room 102 A</td>
<td>Energy &amp; Petrochemicals</td>
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<td>12:15 – 1:30 pm</td>
<td>Room 201 A</td>
<td>History</td>
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<tr>
<td>12:15 – 1:30 pm</td>
<td>Room 201 B</td>
<td>Polymeric Materials</td>
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</table>
 environmentally: New Problems, Diverse Approaches – Part I
Chair: Ed Furlong and Susan Richardson
Conv. Ctr: Room 104A, lobby level

WOC am 10:15 The application of MALDI-TOF mass spectrometry to the analysis of Cryptosporidium parvum: Martin A. Claydon1; David J. Eavason1; Keith Hall2; John Watkins3; Manchester Metropolitan Univ, Manchester, UK; Hall Analytical, Manchester, UK; Ctr f Research into Environment & Health, Leeds, UK

WOC am 10:35 Uptake of Chloroform in Showers: Frank M. Benoît1; Health Canada, Ottawa, Canada

WOC am 10:55 Detection of Microcystins Using Electrospray Ionization - High-Field Asymmetric Waveform Ion Mobility Spectrometry - Mass Spectrometry: Kenneth L. Froese; Barbara Ells; Steve E. Hruday; David Barnett; Roger Guevremond; Randy Purves, University of Alberta, Edmonton, Canada; National Research Council, Ottawa, Canada; MDH-Sciex, Concord, Canada

WOC am 11:15 Application of High-Performance Liquid Chromatography/Electrospray Ionization-Mass Spectrometry (HPLC/ESI-MS) to Analysis of Pharmaceuticals in Surface Water at Nanogram-Per-Liter Concentrations: Edward T. Furlong1; Jeffery D. Cuthill1; Stephen L. Werner1; Mark R. Burkhard1; U.S. Geological Survey, Denver, CO

WOC am 11:35 The use of LC/MS, LC/IR and LC/NMR for the identification of low volatile compounds formed during the alpha-pinene/ozone reaction: Schrädel Wolfgang; Geiger Jutta; Godejohann Markus; Hoffmann Thorsten; Margraf Ulli; Nigge Walter; Inst for Spektrochemie, Berlin and Dortmund, Germany; Bruker Analytik, Rheinstetten, Germany

WOC am 11:55 Relevant Polar Organic Pollutants Present in the Aquatic Environment: Investigating the Biodegradation at Picomolar Concentrations utilizing GC-MS and LC-MS/MS: Thomas Peter Knepper1; Peter Eichhorn1; Jutta Mueller1; Friedhelm Kurrenbrock2; Frank Sachse1; Inst for Water Research and Technology, Wiesbaden; Werke Koehn AG, Koen; Technologyzentrum Wasser, Karlsruhe, Germany

High Throughput/Automation/Robotics
Chair: David Sparkman
Conv. Ctr: Room 104C, lobby level

WOC am 10:15 An expert virtual instrument (EVI) approach to data dependent mass spectral analyses: Terry D. Lee1; John Pearcy1; Curtis Croker1; Douglas Stahl1; City of Hope, Duarte, CA

WOC am 10:35 Development and Throughput Improvement of Paclitaxel Bioanalytical LC-MS by Sharing the Detector between Two HPLC Systems: Min S. Chang1; Huong Mai1; Anita T. Shen1; Qin C. Ji1; Takakoi El-Shourbagy1; Abbott Laboratories, Abbott Park, IL

WOC am 10:55 Reaction Monitoring Using Open-Access LC/MS in a Discovery Pharmaceutical Environment: e-Mailing Data Reports: Larry M. Mallis1; Ani B. Sarkhian1; William L. Watts, Jr.1; Kate Bathurst1; George P. Hammond, V1; John Van Antwerp1; Ed Aig1; Eric Streckfuss2; Julius S. Aguila1; Wyeth-Ayerst Research, Radnor, PA; Waters Corporation, Morris, NJ

WOC am 11:15 Automated Data Processing for LC/MS Purity Analysis of Multicomponent Mixtures from Hybrid Combinatorial Libraries: Mark E. Bean1; Robert M. Sanchez1; Todd L. Graybill1; Walter P. Johnson1; Mark E. Hensley1; Michael L. Moore1; Ralph A. Rivero1; SmithKline Beecham Pharmaceuticals, King of Prussia, PA

WOC am 11:35 Determining Optimum Instrument Parameters for Mass Based Fraction Collection in Drug Purification by HPLC: Douglas E. McIntyre1; Christine A. Miller1; Agilent Technologies Inc., Palo Alto, CA

WOC am 11:55 Automated Characterization of Expressed Proteins by Mass Spectrometry: James H. Bourel1; Richard Vandlen1; John T. Stults1; Genentech Inc., South San Francisco, CA

Interest Group Meetings
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12:15 – 1:30 pm Room 101 A Ion Metal Chemistry
12:15 – 1:30 pm Room 101 B Laboratory Managers
12:15 – 1:30 pm Room 102 A Energy & Petrochemicals
12:15 – 1:30 pm Room 201 A History
12:15 – 1:30 pm Room 201 B Polymeric Materials
NEW (PERHAPS NOT FULLY TESTED) DESIGNS – PART II

Chairs: Michael W. Senko and R. Graham Cooks
Hyatt Regency Ballroom A, 3rd level

WOE am 10:15 High-field asymmetric waveform ion mobility spectrometry using mixed carrier gases: A new approach to “ion chromatography” in the gas-phase; David A. Barnett1; Barbara Ellis1; Roger Guevremont1; Randy W. Purves2; National Research Council of Canada, Ottawa, ON, Canada

WOE am 10:35 An Innovative EI Ion Source for Mass Spectrometry; Mingda Wang1; Ed Cirimele1; Agilent Technology, Palo Alto, CA

WOE am 10:55 In-Source Photodissociation of Ions Produced by MALDI; Murray Johnston1; Eric Van Ingen1; Cheryl Blasie1; Todd Epstein1; David Kane1; Alyza Szajna1; University of Delaware, Newark, DE

WOE am 11:15 A Micromachined Radio-Frequency Ion Filter for Mass Spectrometry with Atmospheric Pressure Ionization Sources; Gary A. Eiceman1; Erkin G. Nazarov1; Raanan A. Miller2; New Mexico State University, Las Cruces, NM; Draper Laboratory, Boston, MA

WOE am 11:35 Impact Desolvation of Electrosprayed Clusters (IDEC) – a New Ionization Method for the Mass Spectrometry of Big Molecules; Peter Williams1; Sergei A. Aksyonov1; Arizona State University, Tempe, AZ

WOE am 11:55 A Miniature Superimposed E x B Sector Field Mass Spectrometer; Dennis L. Polla1; Jorge A. Diaz1; W. Ronald Gentry1; Clayton F. Giese1; University of Minnesota, Minneapolis, MN

ION ACTIVATION/DISSOCIATION: CID, ECD, SID OF PEPTIDES AND PROTEINS

Chair: Vicki H. Wysocki
Hyatt Regency Ballroom F, 3rd level

WOF am 10:15 Can You Get Conformational Information from a Dissociation Experiment?; Evan R. Williams1; Eric F. Strittmatter1; Rebecca A. Jockusch1; Andrew Lemoi1; University of California, Berkeley, CA

WOF am 10:35 Collisional Heating of Bradykinin Ions in Quadrupole Ion Traps via Ion Acceleration and Bath Gas Temperature Variation; Douglas E. Goeringer1; David J. Butcher1; Keiji G. Asano1; Scott A. McClellay2; Oak Ridge National Laboratory, Oak Ridge, TN, Western Carolina University, Cullowhee, NC; Purdue University, West Lafayette, IN

WOF am 10:55 ESI-FTICR tandem mass spectrometry in the determination of internal energy relaxation rates of macromolecules; Ron M.A. Hoeren1; Marc C. Duursma1; Laszlo Drabos1; Karoly Vekey1; FOM Institute for Atomic and Molecular Physics, Amsterdam The Netherlands; Hungarian Academy of Sciences, Budapest, Hungary

WOF am 11:15 Activated Ion Electron Capture Dissociation of Large Biomolecules; David M. Horn1; Ying Ge1; Fred W. McLafferty1; Cornell University, Ithaca, NY

WOF am 11:35 SID versus CID: A Comparison of Peptide Sequencing Information Content of MS/MS Spectra; Lori L. Smith1; Vicki H. Wysocki1; University of Arizona, Tucson, AZ

WOF am 11:55 Investigations into the Influence of Impact Velocity and Ion Mass on the Surface-Induced Dissociation of Large Ions; Donald E. Riederer1; Lisa L. Haney1; Andrew R. Hilgenbrink1; University of Missouri, Columbia, MO

INTEREST GROUP MEETINGS

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12:15 – 1:30 pm Room 201 B Polymeric Materials
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<th>Time</th>
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<tr>
<td>03:00</td>
<td>Interfacing High pH Anion Exchange Chromatography with the LCQ Ion Trap Mass Spectrometer for On-Line Profiling of Neutral and Sialylated N-Linked Oligosaccharides; Jason C. Rouse; Anne-Marie Strang; Chuanliang Liu; Mark R. Hardy; Hubert A. Scoble; Genetics Institute, Andover, MA</td>
<td>WOA pm</td>
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<tr>
<td>03:20</td>
<td>Sequencing of tri- and tetraantennary N-glycans containing sialic acid; Dijana Sagi; Harald S. Conradt; Manfred Nimtz; Jasna Peter-Katalinic; Institute for Medical Physics and Biophysics, Münster, Germany; Gesellschaft für Biotechnologische Forschung, Braunschweig, Germany</td>
<td>WOA pm</td>
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<td>03:40</td>
<td>Detailed Characterization of the Complex Glycosylation Pattern of Recombinant Proteins; Bruno Domon; Nelly Viseux; Xiaoping Hronowski; Biogen, Inc., Cambridge, MA</td>
<td>WOA pm</td>
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<tr>
<td>04:00</td>
<td>Rapid Profiling and Structural Elucidation of Neutral Oligosaccharide Library by FTMS; Carlito B. Lebrilla; Ken Tseng; Jerry L. Hedrick; Juliette Seeley; University of California, Davis, CA</td>
<td>WOA pm</td>
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<td>04:20</td>
<td>Structural Analysis of Sulfated Glycosaminoglycans Using Electrospray Quadrupole and Fourier Transform Mass Spectrometry; Joseph Zaja; Peter T. O'Connor; Catherine E. Costello; Boston University School of Medicine, Boston, MA</td>
<td>WOA pm</td>
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<td>04:40</td>
<td>Monitoring the Stepwise Decomposition of Hyluronan by Hyaluronidase in Pleural/Peritoneal Effusions from Patients with Malignant Mesothelioma Using Negative Electrospray MS; John Roboz; Lin Deng; Longhua Ma; Demetra Silides; Mount Sinai School of Medicine, New York, NY</td>
<td>WOA pm</td>
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<td>03:00</td>
<td>Direct Speciation of Nitrogen-Containing Aromatics in Extra Heavy Crude by Electrospray Ionization Fourier Transform Mass Spectrometry; Kuangnan Qian; Ryan P. Rodgers; Christopher L. Hendrickson; Mark R. Emmett; Alan G. Marshall; ExxonMobil Research Engineering, Annandale, NJ, NHMFL, Florida State University, Tallahassee, FL</td>
<td>WOB pm</td>
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<td>03:20</td>
<td>Nitro-PAH and Nitroaromatic Analysis by Direct Formation of Negative Ions; Robert B. Cody; Kent J. Voorhees; JEOL USA, Inc., Peabody, MA; Colorado School of Mines, Golden, CO</td>
<td>WOB pm</td>
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<td>03:40</td>
<td>Quantitative Determination of Polar and Ionic Compounds in Petroleum Fractions by APCI and ESI MS; Stel G. Roussis; Jim W. Fedora; Imperial Oil, Sarnia, Canada</td>
<td>WOB pm</td>
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<tr>
<td>04:00</td>
<td>Membrane Introduction Mass Spectrometry, Fundamental Pervaporation Studies and Applications; Patricia I. Calderon; Michael Guilhaus; Khalil Sharara; Jaleh Mansouri; Anthony Fane; Phillip Crisp; The University of New South Wales, Sydney, Australia</td>
<td>WOB pm</td>
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<tr>
<td>04:20</td>
<td>Thermal Desorption Particle Beam Mass Spectrometry as a Novel Tool for Secondary Organic Aerosol Analysis; Herbert J. Tobias; Kenneth S. Docherty; Derek E. Beving; Paul J. Ziemann; University of California, Riverside, CA</td>
<td>WOB pm</td>
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<tr>
<td>04:40</td>
<td>Crude Oil and Hydrocarbon Polymer Analysis Using Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry (MALDI-MS) with Nonpolar Matrices; Stephen F. Macha; Chad Robins; Patrick A. Limbach; Scott D. Hanton; Kevin G. Owens; Louisiana State University, Baton Rouge, LA; Air Products and Chemical, Inc., Allentown, PA; Drexel University, Philadelphia, PA</td>
<td>WOB pm</td>
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1:30 – 3 pm POSTER SESSION IN EXHIBIT HALL B, CONVENTIONCTR
Authors of even numbered posters present

WEDNESDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

ENVIRONMENTAL: NEW PROBLEMS, DIVERSE APPROACHES – PART II
Chairs: Ed Furlong and Susan Richardson
Conv. Cit. Room 104A, lobby level

WOC pm 03:00 Identification of Chlorinated Dimethoxystilbene Isomers and Homologues in Bleached Paper Products; Ronald A. Hites1; Jeffery G. McDonald1; Indiana University, Bloomington, IN

WOC pm 03:20 Analysis of alkylphenols and alkylphenol ethoxylate surfactants in the environment using high performance size exclusion chromatography with electrospray mass spectrometry detection; P. Lee Ferguson1; Charles R. Iden1; Bruce J. Brownawell1; State U. of New York, Stony Brook, NY

WOC pm 03:40 Rapid Analysis of Herbicides in Environmental Waters by On-Line SPE/LC/MS/MS; Michael S. Gardner1; Robert D. Vaykner1; Stephanie K. Padilla1; Michelle Spruill1; Research Triangle Institute, RTP, NC

WOC pm 04:00 Aerosol Time-of-Flight Mass Spectrometry for the Analysis of Single Particles and Particle Evolution during SCOS97; Sylvia H. Pastor1; Anne M. Johnson1; Kimberly A. Prather1; University of California, Riverside, CA

WOC pm 04:20 Ultrahigh-Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for the Characterization of Humic Substances; Michael A. Freitas1; Xu Zang1; Patrick G. Hatcher1; Ohio State University, Columbus, OH

WOC pm 04:40 Identification of Chlorine Dioxide Drinking Water Disinfection By-Products Formed at High Bromide Levels; Susan D. Richardson1; Alfred D. Thruston, Jr.1; Chaim Rav-Acha2; Victor Glezer2; U.S. Environmental Protection Agency, Athens, GA; Israel Ministry of Health, Tel-Aviv, Israel

IMAGING MASS SPECTROMETRY
Chair: Peter J. Todd
Conv. Cit. Room 104C, lobby level

WOD pm 03:00 Direct Imaging of Tissue Sections by MALDI Mass Spectrometry; Richard M. Caprioli1; Markus Stoeckli1; Pierre Chaurand1; Vanderbilt University, Nashville, TN

WOD pm 03:20 Imaging Drugs in the Mammalian Brain Using MALDI-TOF Mass Spectrometry; Jeremy Norris1; Johan Eriksson2; Per Andre3; Sarah Baxter1; Richard Caprioli1; Vanderbilt University, Nashville, TN; University of Uppsala, Sweden

WOD pm 03:40 Mass Spectrometric Imaging of Neurons and Porous Si; Rebecca A. Kruse1; Rebecca W. Garden1; Stanislav S. Rubakhin1; Jonathan V. Sweedler1; University of Illinois, Urbana, IL; University of Virginia, Charlottesville, VA

WOD pm 04:00 Imaging Two-Step Laser Mass Spectrometry (L2MS) for Characterization of Environmentally Relevant Samples; James L. Ely1; John H. Callahan1; Herbert H. Nelson1; Andrew P. Baronavski1; Parmely H. Pritchard1; Naval Research Laboratory, Washington, DC

WOD pm 04:20 Secondary Ion Mapping of Ca in Bone; Peter J. Todd1; Carl A. McCandlish1; John M. McMahon1; Oak Ridge National Laboratory, Oak Ridge, TN

WOD pm 04:40 Elemental Profiling of Individual Aerosol Particles; William D. Reents1; Michael J. Schabel1; Bell Labs, Lucent Technologies, Murray Hill, NJ/LC/MS
**INSTRUMENTATION/METHODS**
Chair: Robert D. Voeksner

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<th>Time</th>
<th>Presentation</th>
<th>Speaker(s)</th>
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<tr>
<td>WOE pm 03:00</td>
<td>Rapid Bioanalytical Method Development with Prospekt IIIM On-line Solid Phase Extraction and LC/MS/MS; Honggang Bi¹; Roger N. Hay; Robert Casten; Otto Hamingh; Mark van Gils; Parke-Davis Pharmaceuticals, Ann Arbor, MI</td>
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<td>WOE pm 03:20</td>
<td>Evaluation of Non-Porous Membrane Extraction as a Sample Preparation Method and its effect on the Variability of the Electrospray Ionization Response for Selected Compounds; Frank G Mullins; Sally Hannam</td>
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<td>WOE pm 03:40</td>
<td>Use of the Capillary-EI Liquid Chromatography-Mass Spectrometry Interface in the Analysis of Samples of Pharmaceutical and Environmental Interest; Pierangela Palma¹; Achille Cappiello¹; Giorgio Famigliani¹; Filippo Mangani¹; Michael P. Balogh¹; Univ. di Urbino, Urbino, Italy; Waters Corporation, Milford, MA</td>
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<td>WOE pm 04:00</td>
<td>Fast LC-MS for Peptide Mass Mapping, Protein Analysis and Identification of Post-Translational Modifications Using API TOF MS; Staffan Renlund¹; Henrik Wadensten¹; Jonas Aström; Johan Ericsson¹; Simon Ekman²; Ulla Engström²; Lars Rönström²; Bruce Andrien, Jr.; Erol E. Gulcick³; Amersham Pharmacia Biotech, Uppsala, Sweden; Ludwig Institute for Cancer Research, Uppsala, Sweden; Analytica of Branford, Branford, CT</td>
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<td>WOE pm 04:20</td>
<td>Sequential sample injection for rapid analysis of protein digests by chip-based capillary electrophoresis/mass spectrometry; Jianjun Li¹; Pierre Thibault¹; Can Wang⁵; Jed D. Harrison⁵; National Research Council of Canada, Ottawa, ON, Canada; University of Alberta, Edmonton, AB, Canada</td>
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<td>WOE pm 04:40</td>
<td>Reproducible 100 Attomole Peptide Detection Limit by Use of Nano-LC Micro-ESI FT-ICR MS; Terri L. Constantopoulos¹; Mark R. Emmett¹; Christopher L. Hendrickson¹; Alan G. Marshall¹; NHMFL, Florida State University, Tallahassee, FL</td>
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**MOLECULAR DYNAMICS OF ION DESORPTION**
Chair: Barbara Garrison

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<th>Time</th>
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<tr>
<td>WOF pm 03:00</td>
<td>An Overview of Desorption Mechanisms; Michael Karas</td>
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<td>WOF pm 03:20</td>
<td>Photoacoustic Analysis of the Desorption Process in IR-MALDI-MS; Klaus Dreisewerd⁵; Christoph Menzel⁵; Franz Hillenkamp⁵; Lalit M. Kukreja⁵; Univ. of Münster, Münster, Germany; Centre for Advanced Technology, Indore, India</td>
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<td>WOF pm 03:40</td>
<td>Microscopic mechanisms of laser ablation of organic solids; Leonid V. Zhigilev¹; Barbara J. Garrison¹; Penn State University, University Park, PA</td>
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<tr>
<td>WOF pm 04:00</td>
<td>UV MALDI Ionization Mechanisms: Recent Developments; Richard Knochenmuss¹; Breuker Kathrin¹; Akos Vertes¹; Gary Kinsel¹; Dennis Marynik¹; Aike Stortelder¹; Renato Zenobi²; ETH Zurich, Zurich, Switzerland; Geo. Washington Univ., Washington DC, U. Texas, Arlington, TX</td>
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<td>WOF pm 04:20</td>
<td>Intensities and energy distributions of charged particles emitted from positional isomers of dihydroxybenzoic acid during irradiation at 2.9 microns; David R Ermer¹; Michael R Papantonakis¹; Michelle Baltz-Knorr¹; Richard F Haglund, Jr.; Vanderbilt University, Nashville, TN</td>
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<td>WOF pm 04:40</td>
<td>Influence of Analyte Volatility on Molecular Ejection Processes in Laser Ablation; Yaroslava G. Yingling¹; Leonid V. Zhigilev¹; Barbara J. Garrison¹; Antonis Koubenakis²; Savas Georgiou²; The Pennsylvania State University, University Park, PA; Institute of Electronic Structure and Laser, Crete, Greece</td>
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7:30 – 8:00 am “Wake-Up Coffee” in front of the Terrace Theater

THURSDAY MORNING PLENARY LECTURE IN THE TERRACE THEATER

8:00 am Jack Holl, Kansas State University

Comparing Frontier Utopias: The Land of Oz & the National Laboratory System

8:45 – 10:15 am POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR

Authors of odd numbered posters present

THURSDAY MORNING ORALS SESSIONS IN THE CONVENTION CENTER

GLYCOCONJUGATES
Chair: Catherine E. Costello

Conv. Ctr. Ballroom A, 2nd level

ThOA am 10:15 Comparative Analysis of Cerebrosides and Glycosylinositol Phosphorylceramides from Pathogenic and Non-pathogenic Fungi by ESI-MS and Low-energy Tandem ESI-MS/CID-MS of Lithium Adduct Ions; Steven B. Levery1; Marcos S. Toledo2; Ron Lou Doong3; Matthew Fuller4; Anita H. Strauss5; Helio K. Takahashi6; University of Georgia, Athens, GA; Universidade Federal de Sao Paulo, Sao Paulo, Brazil

ThOA am 10:35 Characterization of neutral glycosphingolipids (GSLs) by MALDI FTMS using SORI-CID; Ekaterina Mirgorodskaya1; Catherine E. Costello1; Boston University, Boston, MA

ThOA am 10:55 Fucosylation Analysis of a Complex Ganglioside Mixture from Human Granulocytes by Negative Ion Nano-ESI-Quadrupole-Time-of-Flight Mass Spectrometry; Wolfgang Metelmann; Johannes Müthing; Jasna Peter-Katalinic; Institute for Medical Physics and Biophysics, Münster, Germany

ThOA am 10:55 Matrix-assisted laser desorption/ionisation mass spectrometry of sulphated N-linked glycans released from SDS-PAGE separated glycoproteins; Susan F. Wheeler1; Maren von der Ohe2; Melitta Schachner3; David R. Wing4; David J. Harvey5; GlycoStyle Institute, University of Oxford, Oxford, United Kingdom; Zentrum für Molekulare Neurobiologie, Hamburg, Germany

ThOA am 11:15 Identification of unusual carbohydrate residues on campylobacter flagellin and implication for other glycoproteins; Pierre Thibault1; John F. Kelly; Susan M. Logan; Jean Robert Brisson; N. Martin Young; David C. Watson; Cheryl P. Ewing; John F. Kelly; Susan M. Logan; Jean Robert Brisson; N. Martin Young; David C. Watson; Cheryl P. Ewing; National Research Council, Ottawa, Ontario, Canada; Naval Medical Research Center, Rockville, MD

ThOA am 11:55 Characterization of Poly lactosamine Containing Lipooligosaccharides from Glycosyltransferase Knockout Mutants from Haemophilus ducreyi; Birgit Schilling1; Melanie Filiatrault1; Anthony A. Campagnari2; Bradford W. Gibson3; University of California, Santa Barbara, CA; University of New Mexico, Albuquerque, NM

TOXICOLOGY AND PHARMACOLOGY – PART II

Chairs: Ian A. Blair and Brahm Prakash

Conv. Ctr. Ballroom B, 2nd level

ThOB am 10:15 Molecular Toxicology: The Role of Mass Spectrometry in an Integrated Approach; Kenneth B. Tomer1; Christoph Borchers2; Cynthia Afsari3; J. Carl Barrett1; Maribel Bruno1; Alex Merrick1; Emil Nuwaysir1; Richard Paules1; Nigel Walker1; NIH, Bethesda, MD

ThOB am 10:35 Lipid Peroxidation-Mediated Covalent Modifications to DNA; Sean Hwa Lee1; Diane Rindgen1; Roy H. Bible, Jr2; Elisabeth Hajdu3; Ian A. Blair1; University of Pennsylvania, Philadelphia, PA; Searle, Skokie, IL

ThOB am 10:55 Quantitation of the heterogeneous aromatic DNA adducts N-(deoxyguanosin-8-yl)-2-amino-3-methylindazole[4,5-5]quinoline and N-(deoxyguanosin-8-yl)-4-aminoazobiphenyl in vivo using capillary LC/ESI/MS/MS; John R. Soglia1; Robert J. Turesky2; Fred F. Kadlubar1; Paul Vourou3; Northeastern University, Boston, MA; Nestec, Switzerland; NCTR, Jefferson, AR

ThOB am 11:15 Determination of 3'-Azido-3'-Deoxythymidine (AZT) Incorporation into Fetal DNA in vivo Using LC-ESI/MS/MS; Mona I. Churchwell1; Jia-Long Fang1; Frederick A. Beland1; William Slikker Jr.1; Daniel R. Doerge1; Nat. Ctr. Tox. Res., Jefferson, AR

ThOB am 11:35 Identification of Cytochrome P450 Active Site Residues by Mass Spectrometry; Luke K. Lightning1; Allan E. Rettie3; William F. Trager1; Jeffrey P. Jones2; Magang Shou2; Thomas H. Rushmore3; Thomas F. Mrdberg4; Michael P. Pritchard1; University of Washington, Seattle, WA; Washington State University, Pullman, WA; Merck Research Laboratories, West Point, PA; Biomedical Research Centre, Dunedin, UK

ThOB am 11:55 Identification of the Major Metabolite of 2,5-bis(5-Hydroxymethyl-2-thienyl)uran, an Antitumor Agent, in the S-9 Subcellular Fraction of Dog Liver Cells; Lawrence R. Phillips1; Maria I. Rivera; Sherman F. Stinson; Tracy Daw; Jean L. Jorden; Kaye Upadhyay; National Cancer Institute, Frederick, MD; Scientific Applications International Corporation, Frederick, MD
THURSDAY MORNING ORAL SESSIONS IN THE CONVENTION CENTER

STRATEGIES FOR ANALYSIS OF COMPLEX MIXTURES – PART I

Chairs: John F. Holland and Donald G. Patterson
Conv. Cir. Room 104A, lobby level

ThOC am 10:15 High-Speed GC-TOFMS Analysis of Environmental Toxicants Using Programmable Column Selectivity and Fast Temperature Programming; Carrie Coutant 1; Richard Sacks 1; Tincuta Veroticu 1; University of Michigan, Ann Arbor, MI

ThOC am 10:35 Comprehensive Two-Dimensional GC-TOFMS for Enhanced Analysis of Environmentally Significant Mixtures; James Grainger 1; Donald G. Patterson Jr. 1; Jean-Marie Dimancola 1; Centers for Disease Control and Prevention, Atlanta, GA

ThOC am 10:55 High Throughput Electrospray and MALDI-MS Using Microfluidic Separation Devices; Barry L. Karger 1; Bailin Zhang 1; Tomas Rejtar 1; Ping Hu 1; Eugene Moskovets 1; Jan Preisler 1; Franta Forcin 1; Barnett Institute, Northeastern Univ., Boston, MA

ThOD am 11:15 Metabolic Profiling by Mass Spectrometry as a Tool for Plant Functional Genomics; Oliver Fiehn 1; Peter Dörmann 1; Thomas Altmann 1; Lothar Willmitzer 1; Joachim Kopka 2; Richard N. Trethewey 1; Max-Planck Inst. Molec. Plant Physiol., Potsdam, Germany; Metanomics, Berlin, Germany

An Approach to Identify the Peptide Portion of Biological Sources Exhaustively Using Integrated Mass Spectrometric Methods; Markus Kellmann 1; Danilo Kardel 1; Kemper Birgit 1; Zucht Hans-Dieter 1; Juergens Michael 1; BioVisioN GmbH & Co KG, Hannover, Germany

The Application of Unique Software Algorithms to Manage Matrix Interferences in Complex GC-MS Analyses; Richard C. Parry 1; Kevin McNitt 1; John Hauck 1; Slava Artiaev 1; Evaldo De Armas 1; Nancy Myers 1; LECO Corporation, St. Joseph, MI

ANALYSIS OF NATURAL PRODUCTS

Chair: Randall K. Julian
Conv. Cir. Room 104C, lobby level

ThOD am 10:15 Development of LC/MS and LC/MS/MS methods for direct quantification of rhamnolipids in a P. aeruginosa culture; Francois Lepine 1; Eric Deziel 1; Sylvain Milot 1; Richard Villemeur 1; INRS-Institut Armand-Frappier, Laval, Quebec, Canada

ThOD am 10:35 Structural motifs in glycosylated conotoxins that inhibit glycosidase activity; A.G. Craig 1; W. Low 1; J. Kang 1; T. Norberg 1; The Salk Institute; Swedish University of Agricultural Sciences

ThOD am 10:55 Pulsed Ultrafiltration Mass Spectrometric Screening of Botanical Extracts and Combinatorial Libraries for Ligands of Human Estrogen Receptors; Chungang Gu 1; Dejan Nikolic 1; Jianghua Liu 1; Judy L. Bolton 1; Richard B. van Breemen 1; University of Illinois College of Pharmacy, Chicago, IL

ThOD am 11:15 Multidimensional LC/MS for the identification of natural product lead compounds; Jeffrey R. Gilbert; Andrew W. Carr; R. Thomas Williamson; Eleanor L. Chapin; Paul Lewer; William Gerwick; Dow AgroSciences LLC, Indianapolis, IN; Oregon State University, Corvallis, OR

ThOD am 11:35 Mass spectrometry techniques for structural characterization of a new class of cyclic lipopeptides; Yothib Hathout 1; Yen-Peng Ho 1; Victor Ryzhov 1; Plamen Demirev 1; Catherine Fensealu 1; UMCP, College Park, MD

ThOD am 11:55 Advances in the application of LC-MS to mixture analysis in natural products discovery; Richard F. Higgs, Jr. 1; Randall K. Julian, Jr. 1; Matthew D. Hilton 1; Lilly Research Laboratories, Indianapolis, IN
7:30 – 8:00 am  “Wake-Up Coffee” in front of the Terrace Theater
THURSDAY MORNING PLENARY LECTURE IN THE TERRACE THEATER
8:00 am  Jack Holl, Kansas State University
Comparing Frontier Utopias: The Land of Oz & the National Laboratory System”

8:45 – 10:15 am  POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR
Authors of odd numbered posters present

THURSDAY MORNING ORAL SESSIONS IN THE HYATT HOTEL

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<th>Time</th>
<th>Session Title</th>
<th>Chair</th>
<th>Location</th>
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<tbody>
<tr>
<td>ThOE am 10:15</td>
<td><strong>Performance Evaluation of Improved MALDI TOF-TOF MS System</strong>; Marvin Vestalⁱ; Jennifer Campbellⁱ; Kevin Haydenⁱ; Peter Juhászⁱ; PE Biosystems, Framingham, MA</td>
<td>Werner E. Ens</td>
<td>Hyatt Regency Ballroom A, 3rd level</td>
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<td>ThOE am 10:35</td>
<td><strong>Rapidly Switchable MALDI/ESI QqTOF-MS</strong>; Andrew N. Krutheiskyⁱ; Wenzhu Zhangⁱ; Brian T. Chait⁴; Rockefeller University, New York, NY</td>
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<td>ThOE am 10:55</td>
<td><strong>Multiple Reflection ESI TOF Mass Spectrometer: Theory and Results</strong>; Melvin A. Park⁴; Bruker Daltonics, Inc., Billerica, MA</td>
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<td>ThOE am 11:15</td>
<td><strong>A New Concept to Increase Dynamic Range Using Multi-Anode Detectors</strong>; Marc Goni⁴; Katrin Fuhrer⁴; Michael Ugarov⁴; Albert J. Schultz⁴; Ionwerks Inc., Houston, TX</td>
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<td>ThOE am 11:35</td>
<td><strong>A high resolution orthogonal TOF with selectable drift length</strong>; John B. Hoyes⁴; Robert H. Bateman⁴; Jason L. Wildgoose⁴; Micromass, UK</td>
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<td>ThOE am 11:55</td>
<td><strong>Two-Dimensional Mass Spectrometry with a MALDI Quadrupole-TOF Instrument</strong>; Werner Ens⁴; Alexander Loboda⁴; Victor Spicer⁴; Kenneth G Standing⁴; University of Manitoba, Winnipeg, Canada; MDS Sciex, Concord, Ontario, Canada; Daltonik GmbH, Bremen, Germany</td>
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<td>ThOF am 10:15</td>
<td><strong>Mass Spectrometric Evidence for Mechanisms of Fragmentation of Charge-Derivatized Peptides</strong>; Nalini Sadagopan⁴; J.T. Watson⁴; Michigan State University, East Lansing, MI</td>
<td>Chryste Westemniotis</td>
<td>Hyatt Regency Ballroom F, 3rd level</td>
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<td>ThOF am 10:35</td>
<td>**Investigation of Charge Remote Fragmentation Mechanisms in Fixed Charge Peptides Derivatized with Tris(2,4,6-trimethoxyphenyl) phosphine (TMPP); Linda Brecl⁴; Chungang Gu⁴; George Tsapralis⁴; Vicki Wysocki⁴; University of Arizona, Tucson, AZ</td>
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<td>ThOF am 10:55</td>
<td><strong>Specific fragmentation and structure of protonated dipeptides containing both basic and acidic amino acids: An ab initio and MS/MS study</strong>; Bela Paizs⁴; Zoltan Szlavik⁴; Sandor Suhai⁴; Balazs Hargittai⁴; Arpad Somogyi⁴; German Cancer Research Center, Heidelberg, Germany; University of Arizona, Tucson, AZ</td>
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<td>ThOF am 11:15</td>
<td><strong>Side Chain Effects on the Fragmentation of Deprotonated Peptides Containing Aspartic Acid and Glutamic Acid</strong>; Talat Yalcin⁴; Carolyn J. Cassady⁴; University of Alabama, Tuscaloosa, AL</td>
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<td>ThOF am 11:35</td>
<td><strong>Another Selective Cleavage in Peptides: A Common Mechanism for the Formation of Complementary b/y or b/y Ions at Protonated Histidine</strong>; George Tsapralis⁴; Vicki H. Wysocki⁴; University of Arizona, Tucson, AZ</td>
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<td>ThOF am 11:55</td>
<td><strong>The mechanism of C-terminal cleavages in the alkali metal ion complexes of peptides</strong>; Scott Gronert⁴; Wan Yong Feng⁴; Abdul Warres⁴; San Francisco State University, San Francisco, CA; University of California, Davis, CA</td>
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### THURSDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

#### MOLECULAR ANALYSIS IN CLINICAL MEDICINE
**Chair:** Mark W. Duncan  
Conv. Ctr. Ballroom A, 2nd level

- **ThOA pm 03:00**  
  **Surface Enhanced Laser Desorption / Ionization (SELDI) Approaches for Biomarker Discovery and Characterization:**  
  Scot R. Weinberger²; Tai-Tung Yip¹; Maggie Merchant¹; Alexander Loboda¹; Werner Ens³; Ken G. Standing³; Ciphergen Biosystems, Inc., Palo Alto, CA; Sciex, Concord, Ontario, Canada; University of Manitoba, Winnipeg, Canada

- **ThOA pm 03:20**  
  **Following Cancer Progression by MALDI Mass Spectrometry:**  
  Pierre Chaurand¹; Naoya Masunori¹; Tanja Z. Thomaš¹; Susan Kasper¹; Beverly B. Dague¹; Scott Shappell¹; Taiji Tsukamoto¹; Robert J. Matusik¹; Richard M. Caprioli¹; Vanderbilt University, Nashville, TN; Sapporo University, Japan

- **ThOA pm 03:40**  
  **Affinity Assisted Micro-Scale Protein Structure Analysis:**  
  Rong-Wang²; Brian T. Charl¹; Seong-Hun Kim¹; Sangram S. Sisodia²; The Rockefeller University, New York, NY; The University of Chicago, Chicago, IL

- **ThOA pm 04:00**  
  **Mass spectrometric immunoassay for parathyroid hormone related protein (PTHrP):**  
  Kefei Zheng¹; Jeffery D. Rivera¹; John S. Voge³; Bruce A. Buchholz²; Douglas W. Burton¹; Leonard J. Defos²; David A. Herold¹; Robert L. Fitzgerald¹; VA Med Center/University of California, San Diego, California; Lawrence Livermore National Laboratory, Livermore, CA

- **ThOA pm 04:20**  
  **Lipid protection of cerebroside sulfate activator protein against proteolysis:**  
  Kym E. Eau⁴; Richard L. Stevens¹; Howard Umemoto¹; Syed S. Ahmed¹; Julian P. Whitelegge¹; Claire Fluharty¹; Arvan Fluharty¹; UCLA, Los Angeles, CA

- **ThOA pm 04:40**  
  **Analysis of Human Tear Samples by Mass Spectrometry:**  
  Kim Fung¹; Carol Morris²; Mark Duncan¹; University of Colorado Health Sciences Center, Denver, CO; Ciba Vision Corporation, Atlanta, GA

#### PHARMACEUTICAL DEVELOPMENT
**Chairs:** Michael J. Hayes and Swapan K. Chowdhury  
Conv. Ctr. Ballroom B, 2nd level

- **ThOB pm 03:00**  
  **High-Throughput LC/MS/MS Analysis of Clinical Samples:**  
  J. Henion¹; H. Zhang¹; J. Onorato¹; Y. Deng¹; T. Wachs¹; Cornell University, Ithaca, NY

- **ThOB pm 03:20**  
  **The Use of a Quadrupole Orthogonal Acceleration Time-of-Flight for Bioanalytical Method Development and Validation in a GLP Environment:**  
  Patrick J. Rudewicz²; Liyu Yang¹; Robert P. Clement¹; Schering-Plough Research Institute, Kentwood, NJ

- **ThOB pm 03:40**  
  **Formation and Reactivity of Acyl Glucuronides Assessed by LC/MS/MS:**  
  Cornelis E.C.A. Hop¹; Martin Rabe¹; Zhen Wang¹; Jianmei Pang¹; Kwan H. Leung¹; Ronald B. Franklin¹; Merck Research Laboratories, Rahway, NJ

- **ThOB pm 04:00**  
  **Application of Turbulent Flow Chromatography Tandem Mass Spectrometry for the High Throughput Analysis of Major Drug Metabolizing Cytochrome P450 Enzyme Activities:**  
  H. K. Lim¹; M. R. Anari¹; K. Chan¹; E. A. Dierkes¹; S. E. Ball¹; C. Tio¹; J. Kao¹; J. A. Scatina¹; F. S. Abbott¹; D. Kwok¹; Wyeth-Ayerst Research, Princeton, NJ; University of British Columbia, Vancouver, BC, Canada; Biopharmaceutical Research Inc., Burnaby, BC, Canada

- **ThOB pm 04:20**  
  **Simultaneous Coupling of HPLC to ICP-MS and ESI-TOF-MS for the Rapid Identification and Quantification of Drug Metabolites in Rat Urine:**  
  Jose Castro-Perez¹; Fadi Abou-Sharka¹; Ashley B. Sage¹; Ian D. Wilson²; Jeremy Nicholson²; John Lindon¹; Graeme Scarfe³; Micromass UK Ltd., Manchester, UK; AstraZeneca Pharmaceuticals, Cheshire, UK; Imperial College of Science Technology & Medicine, London, UK

- **ThOB pm 04:40**  
  **Sensitive Detection and Characterization of Repifermin by SELDI Protein Chip™ Time-of-Flight Mass Spectrometry:**  
  Tina S. Morris¹; Markus Buergin¹; Brian Mansfield¹; Reiner Gentz¹; Scot R. Weinberger¹; Maggie Merchant¹; Alexander Loboda¹; Ken G. Standing¹; Werner E. Ens¹; Human Genome Sciences Inc., Rockville, MD; Ciphergen Biosystems Inc., Palo Alto, CA; University of Manitoba, Winnipeg, Canada
1:30 – 3 pm POSTER SESSION IN EXHIBIT HALL B, CONVENTION CTR
Authors of even numbered posters present

THURSDAY AFTERNOON ORAL SESSIONS IN THE CONVENTION CENTER

STRATEGIES FOR ANALYSIS OF COMPLEX MIXTURES – PART II

Chairs: John F. Holland and Donald G. Patterson
Conv. Ctr. Room 1044, lobby level

ThOC pm 03:00 Beyond 2-D Gels: Multidimensional Separations for Proteomics; John T. Stults1; David Arnott1; Genetech, Inc., South San Francisco, CA

ThOC pm 03:20 Ion Mobility/Time-of-Flight Analysis of Combinatorial Libraries: Rapid Assessment of Purity and Affinity Screening; Catherine A Srebalus Barnes1; David E Clemmer1; Indiana University, Bloomington, IN

ThOC pm 03:40 Fast analysis of protein digest mixtures by MALDI/IM/ToF/MS; Brandon T. Ruotolo1; Kent J. Gillig1; Earl G. Stone1; Zee Yong Park1; David H. Russell1; Texas A&M University, College Station, TX.

ThOC pm 04:00 High Throughput Bioassay-Guided Fractionation – A Practical Enabling Technique for Determining the Active Component in Screening Hits from Exploratory Combinatorial Libraries and Other Mixtures; Douglas W. Phillipson1; Linda S. Rusnak1; David A. Haggerty1; K. Eric Milgram1; Alexander I. Yanovsky1; William P. Farrell1; Michael J. Greig1; Xiaohong Xiong1; Mark L. Proufke2; Alarex Division of Agouron Pharmaceuticals, Inc., San Diego, CA; Parke-Davis Division of Warner-Lambert Co., Ann Arbor, MI

ThOC pm 04:20 High-Throughput Quantitative Analysis of Complex Protein Mixtures; Timothy L. Griffin1; David K. M. Han1; Kenneth C. Parker2; Steven P. Gyg1; Beate Rist1; Rudi Aebersold1; University of Washington, Seattle, WA; PE Biosystems, Framingham, MA

ThOC pm 04:40 Detection of low- to sub-femtomole amounts of native proteins present in complex biological mixtures via biomolecular interaction analysis mass spectrometry (BIA/MS); Dobrini Nedelkova1; Randall W. Nelson1; Kemmons A. Tubbs1; Intrinsic Bioprobes Inc., Tempe, AZ

FORENSIC APPLICATIONS
Chair: Brian Eckenrode
Conv. Ctr. Room 104C, lobby level

ThOD pm 03:00 Mass Spectrometric Analysis of Chemical Warfare Agents and their Degradants with a Modular Field-Transportable Forensic Laboratory; Shauna M. Darby1; Michael W. Wensing1; Earl Austin1; James C. Peterson1; Monica J. Hey1; Dennis J. Reutter2; Battelle, Edgewood, MD, U.S. Army SBCCOM, Edgewood, MD

ThOD pm 03:20 Forensic Applications of Tandem Mass Spectrometry in the Investigation of Sudden Infant Death (SID); Donald H Chace1; James C. DiPerna1; Edwin W. Naylor1; Neo Gen Screening, Pittsburgh, PA

ThOD pm 03:40 Forensic Applications of Desorption/Ionization Mass Spectrometry in the Analysis of Ink on Paper - Who, What, When, Where and Why?; Donna M. Grim1; John Allison1; Jay Siegel1; Michigan State University, East Lansing, MI

ThOD pm 04:00 Rapid Bacterial Identification Based on MALDI Time-of-Flight Mass Spectrometry with Automated Data Analysis; Karen L. Wahl1; Kristin H. Jarman1; Nancy B. Valentine1; Sharon E. Cebula1; Catherine E. Petersen1; Adam J. Saenz1; Mark T. Kingsley1; Pacific Northwest National Laboratory, Richland, WA

ThOD pm 04:40 Chromatogram Matching as a GC/MS Tool for Automated Identification of Accelerants in Arson Studies; Nick Bukowski1; John A Lucey2; Scott T Harrison2; ThermoQuest, Manchester, UK; Michigan State Police, Grayling, MI
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<tr>
<td>ThOE pm 03:00</td>
<td>Accurate Mass Measurement: Taking Full Advantage of Nature's Isotopic Complexity; Alan G. Marshall; Christopher L. Hendrickson; Fei He; Guillaume van der Rest; Ryan P. Rodgers; Erin N. Blumer; Kuangnan Qian; Florida State University, Tallahassee, FL; ExxonMobil Research Engineering, Annandale, NJ</td>
<td>Jon Amster</td>
<td>Hyatt Regency Ballrooms A, 3rd level</td>
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<td>ThOE pm 03:20</td>
<td>Broadband ion accumulation with an internal source MALDI FTICR-MS; Todd H Mize; I Jonathan Amster; University of Georgia, Athens, GA</td>
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<td>ThOE pm 03:40</td>
<td>DeCAL: A new method for more accurate mass measurements based on mass deconvolution; Gordon A. Anderson; James E. Bruce; Michael D Brands; Lijian Pasa-Tolic; Richard D Smith; Pacific Northwest National Laboratory (PNNL), Richland Washington; Merck Research Laboratories, West Point, PA</td>
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<td>ThOE pm 04:00</td>
<td>Characterization of Miniature ICR Cells; Karl P. Wanezek; Andreas Rappmund; Inorg. &amp; Phys. Chemistry, Bremen, Germany</td>
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<tr>
<td>ThOE pm 04:20</td>
<td>Hydrogen Radical-Polyatomic Ion Reactivity Probed by FTICR Mass Spectrometry; Pimpen A. Demirci; University of Maryland, College Park, MD</td>
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<tr>
<td>ThOE pm 04:40</td>
<td>A New MALDI Source for FTMS with Pulsed In-Source Collision Gas and In-Source Ion Accumulation; Gokhan Baykus; Roland Jertz; Matthias Witt; Gerhard Weiss; Bruker</td>
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<tr>
<td>ThOF pm 03:00</td>
<td>A Study of Cluster Ions of Salts of Polyatomic Acid Groups and of Multivalent Metals: A Probe into Electrospray Ionization Processes; Chunyan Hao; Raymond E. March; Trent University, Peterborough, ON, Canada</td>
<td>Robert C. Dunbar</td>
<td>Hyatt Regency Ballroom F, 3rd level</td>
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<tr>
<td>ThOF pm 03:20</td>
<td>Charge Reduction Electrospray Mass Spectrometry; Mark Scal; Michael S. Westphall; Lloyd M. Smith; University of Wisconsin-Madison, Madison, WI</td>
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<tr>
<td>ThOF pm 03:40</td>
<td>Ion-Ion Reactions in the Gas Phase: Deprotonation and Dissociation of Peptides and Protein; Guiwen Xu; Robert McIver; UC, Irvine, CA</td>
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<td>ThOF pm 04:00</td>
<td>Rapid Screening of Mouse Hemoglobin by Ion/Ion Recombination Mass Spectrometry; T. Gregory Schafer; Keiji G. Asano; Benjamin J. Cargile; Eugene M. Rinchik; Scott A. McLuckey; James L. Stephenson, Jr.; Oak Ridge National Laboratory, Oak Ridge, TN; Purdue University, West Lafayette, IN</td>
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<tr>
<td>ThOF pm 04:20</td>
<td>Electron-Ion Reactions of Multiply-charged Polypeptides; Roman A. Zubarev; Bogdan A. Budnik; Michael L. Nielsen; University of Southern Denmark, Odense, Denmark</td>
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<tr>
<td>ThOF pm 04:40</td>
<td>Interdependent Manipulation of Critical Electrospray Parameters: Control over In-source Dissociation Processes, Ion-Molecule Reactions and a Means of Influencing Energy Deposition into Produced Ions; Sergiu P. Paliu; John R. Eyrle; University of Florida, Gainesville, FL</td>
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MONDAY POSTERS

7:30 – 8:00 am
SET UP POSTERS, Exhibit Hall B

8:45 – 10:15 am
POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.

1:30 – 3:00 pm
POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.

6:00 – 6:30 pm
REMOVE POSTERS. Please leave posters for the full day.

MPA 001
Historical Highlights of the Early Days of SIMS; Bryan L. Benz\(^1\); Sarnoff Corporation, Princeton, NJ

MPA 002
Mass Spectrometry in an Adversarial Context: A Proposal for Demonstrating Method Fitness; Robert Betham, Joe Boisj, John Chakel, Jane Gale, David Heller, Steven Musser, Phil Price, Stephen Stein

SPRAY IONIZATION, 004 - 061

MPA 004
A Robust PEEK Barium Titanate Ion Source for Electrospray Mass Spectrometry; Murray Hacker\(^1\); SangHyun Park\(^2\); Univ. of Washington, Seattle, WA

MPA 005
Determination of Polar Lipid Composition in Single Fish and Shrimp Egg Cell by Direct Electrospray Probe/Mass Spectrometry; Chih-Pin Ku\(^1\); Jing-Yueh Jeng\(^1\); Jentia Shiea\(^1\); National Sun Yat-Sen Univ., Kaohsiung, Taiwan

MPA 006
Improved Spray Stability for Capillary LC/MS of Proteins Using the Fales Modification; Kevin D. White\(^1\); Reginald W. Bennett\(^1\); Steven M. Musser\(^1\); Trixi Uebereide\(^1\); Center for Food Safety and Applied Nutrition, FDA, Washington, DC; University of Hamburg, Institute of Food Chemistry, Germany

MPA 007
Distinguishing the Constant Current and Constant Voltage Modes of Electrospray Ionization; Ma'an Hazem Amad\(^1\); Nadja Cech Lindley\(^1\); University of New Mexico, Albuquerque, NM

MPA 008
Ionization Mechanism Studies of Atmospheric Pressure Chemical Ionization (APCI). Is APCI a Transformed Chemical Ionization (CI)?; Xiao Yu\(^1\); Donghui Cui\(^1\); Merck & Co., West Point, PA

MPA 009
Characterization of the Atmospheric Pressure Ionization Mass Spectrometric Process Obtained Using a Fused Silica Emitter with the High Voltage Applied Upstream; Per J. R. Sjöberg\(^1\); Leif Nyholm\(^1\); Karin E. Markides\(^1\); Analytical Chemistry, Uppsala University, Uppsala, Sweden

MPA 010
Pulsation and Mode Switching in Modulated and AC Electrosprays; Marina C. Galleija\(^1\); Jennifer M. Gaunt\(^1\); Akos Vertes\(^1\); George Washington University, Washington, DC

MPA 011
Fourier Analysis of Current Oscillations in Electrosprays; Jennifer M. Gaunt\(^1\); Akos Vertes\(^1\); George Washington University, Washington, DC

MPA 012
Fluorescence Measurements of Denatured Proteins within Electrospray Droplets; Joel H. Parks\(^1\); Sandra E. Rodriguez-Cruz\(^1\); Joseph T. Knouz\(^1\); The Rowland Institute for Science, Cambridge, MA

MPA 013
Probing Protein Structure with Oxygenated Radicals in a New Electrospray Ion Source; Simin D. Malekina\(^1\); Mark R. Chance\(^1\); Kevin M. Downard\(^1\); Albert Einstein College of Medicine, Bronx, NY

MPA 014
Atmospheric Pressure Photionization: A New Ionization Technique For LC/MS; Damon B. Robb\(^1\); Andries P. Bruins\(^1\); Thomas R. Covey\(^1\); University of Groningen, Groningen, The Netherlands; Sciex, Concord, ON, Canada

MPA 015
Atmospheric Pressure Photionization (APPI) for High Sensitivity LC/MS in Bioanalysis; Andries P. Bruins\(^1\); Damon B. Robb\(^1\); Harrie A.M. Peters\(^2\); Peter L. Jacobs\(^2\); University of Groningen, Groningen, The Netherlands; Orgaon, Oss, Netherlands

MPA 016
Oxidation of Aniline Derivatives in the Electrospray Emitter; Kepji Asamo\(^1\); Vilmos Kertesz\(^2\); Gary Van Berkel\(^3\); Haitong Deng\(^2\); Oak Ridge National Laboratory, Oak Ridge, TN; Albert Einstein College of Medicine, Bronx, NY

MPA 017
Electrolytic Deposition of Metals onto the High Voltage Contact in an ES Emitter; Gary J. Van Berkel\(^1\); Oak Ridge National Laboratory, Oak Ridge, TN

MPA 018
Adduct Ion Formation of Nitro-Compounds in Electrospray Ionization-Fourierion Ion Trap Mass Spectrometry; Richard F. Reich\(^1\); Joseph E. McClellan\(^1\); Richard A. Yost\(^1\); University of Florida, Gainesville, FL

MPA 019
Characterization by ESI-MS of Neutral Fullerenefunctionalized dendritic branches; Helene Nierengarten; Delphine Felder; Emmanuelle Leize; Jean-Francois Nierengarten; Jean-Francois Nicoud; Alain Van Dorsseleer; LSMBO, ULP, Strasbourg, France; GMO, IPCMS, Strasbourg, France

MPA 020
Monitoring of Thermally Initiated Reactions Online by Electrospray Ionization Mass Spectrometry; Jens Griep-Raming\(^1\); Juergen O. Metzger\(^1\); University of Oldenburg, Germany

MPA 021
Nitrogen-fixing molecular transformation during electrospray ionization; Shigeru Sakamoto; Tsuneo Imanoto; Kentaro Yamaguchi; Chemical Analysis Center, Chiba University, Japan

MPA 022
ESI Detection of Inherently Nonresponsive Butadiene Diepoxide by Peptide Binding; Jennifer R. Krone\(^1\); Nadja Cech Lindley\(^1\); Christie G. Enke\(^1\); University of New Mexico, Albuquerque, NM

MPA 023
Predicting Electrospray Response from Chromatographic Retention Time; Nadja Cech Lindley\(^1\); Jennifer R. Krone\(^1\); Christie G. Enke\(^1\); University of New Mexico, Albuquerque, NM

MPA 024
Controlling the Charge State of Peptides in Electrospray Ionization Mass Spectrometry; Gary N. Lawson\(^1\); Henry M. Fales\(^1\); National Institutes of Health, Bethesda, MD

MPA 025
Solvent Influence on Ion Distribution within Electrospray Droplets; C. Fredrik Bökman\(^1\); Per J. R. Sjöberg\(^1\); Dan Bylund\(^1\); Karin E. Markides\(^1\); Uppsala University, Uppsala, Sweden

MPA 026
Transition Metal Ion-Assisted Kinetic Resolution of Amino Acids and Dipeptides: A Model System for Chiral Recognition in the Gas Phase; W. A. Tao\(^1\); Duxi Zhang\(^1\); Kim J. Koch\(^1\); R. Graham Cooks\(^1\); Purdue University, West Lafayette, IN

MPA 027
The Relative Importance of Charge Saturation and Solution Properties to Electrospray Ionization Response; Richard C. King\(^1\); Carmen L. Fernandez-Metzler\(^1\); Cynthia Miller-Stein\(^1\); Merck Research Laboratories, West Point, PA

MPA 028
A pH - Controller for ESI Mass Spectrometry Applied to Textile Dyes; Peter Kesner\(^1\); Gerhard Matz\(^2\); Thomas Zey\(^2\); Michael Kuhfeld\(^2\); ecb-ONLINE Analysentechnik, Schwerin, Germany; TU Hamburg-Harburg, Hamburg, Germany; Brucker-Daltonik, Bremen, Germany

MPA 029
Enhancement of Salt Tolerance by Newly Developed Droplet-Fused Electrospray Mass Spectrometry;
MONDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

Jentsaie Shieh1; Der-Yeuo Chang2; National Sun Yat-Sen Univ., Kaohsiung, Taiwan

MPA 030  Fluoride Attachment To Improve Negative Ion Electrospray Mass Spectrometry; Thomas L. Hatfield1; Robert D. Voecks2; Cleston M. Lange3; David P. Zimmerman3; 3M Environmental Laboratory, St. Paul, MN; Research Triangle Institute, RTP, NC; Braun Interpace Corporation, Minneapolis, MN

MPA 031  The Influence of Size Selectivity on the Solution of Alkali Metal Ions and Dimerization of Novel Bis(Benzo Crown Ethers) by ESI-Quadrupole Ion Trap Mass Spectrometry; Sheldon M. Williams1; Jennifer S. Brodbelt1; University of Texas, Austin, TX

MPA 032  A Novel Competitive Method for the Determination of Solution Binding Constants by Electrospray Ionization Mass Spectrometry; Esther C. Kempen1; Jennifer S. Brodbelt1; Meanmap Song1; University of Texas, Austin, TX

MPA 033  Determination of Alkali Metal Binding Selectivities of Novel Caged Crown Ethers by ESI QIT-MS; Michelle L. Rezvez1; Jennifer S. Brodbelt1; The University of Texas, Austin, TX

MPA 034  Electrospray Ionization Mass Spectrometry of Novel Sodium Ion Binding Molecules; Michael L. Gross1; Hossein Shabany1; Charles A. Groechen1; Michael A. Grayson1; George Gokel1; Robert Behm1; Washington University, St. Louis, MO

MPA 035  Complexes of Ru(II) with 1,4,7,10 Tetrathiacyclododecane and Nitrogen Containing Ligands: A Study by Electrospray Mass Spectrometry; Francisco L. Amado1; Cristina M. Barros1; M. Graca Santa-Marques1; Pedro M. Domingues1; Antonio J. Ferrer-Corred1; Joao Madureira1; Teresa M. Santos1; Vitor Felix1; University of Aveiro, Aveiro, Portugal

MPA 036  ESI/MS Investigation of Cluster Ions of Alkali Chloride and Sodium Salts: Effects of Ionic Radius, Cone Voltage and pH; Jeffrey C. Smith1; Steven P. Rafferty1; Raymond E. March1; Chanyan Han1; Timothy R. Crole1; Trent University, Peterborough, ON, Canada

MPA 037  Evolution of Electrospray Droplets in a Fourier Transform Ion Cyclotron Mass Spectrometer; Matt A. Lasater1; Carla A. P. Armorgan1; David A. Laude1; University of Texas, Austin, TX

MPA 038  Characterization of Peptide-Anion-Adducts by Nano-ESI QIT MS; Andrea Schmidt1; Michael Karas1; Instr. Anal. Chem., J. W. Goethe University, Frankfurt/Main, Germany

MPA 039  MS/MS Characterization of Procartidin Compounds Using Electrospray Ion Trap Mass Spectrometry; Richard C. Fleming1; Rebecca M. O'Malley1; David F. Fitzpatrick1; Betsey Bing1; University of South Florida, Tampa, FL

MPA 040  On the Origin of DNA Monomer Peaks in Nano Electrospray Mass Spectra of DNA Duplex Solutions; John C. Jurchen1; Anthony T. Ivarone1; Evan R. Williams1; University of California, Berkeley, CA

MPA 041  Investigation of Protolytic Dissociation Constants of Citric Acid by Electrospray Mass Spectrometry; Zoltan Takacs1; Gabor Bunkocz2; Karoly Vekey1; Institute of Chemistry, Hung. Acad. Sci., Budapest, Hungary; Eotvos Lorand University of Sciences, Budapest, Hungary; Institute of Chemistry, Hung. Acad. Sci., Budapest, Hungary

MPA 042  A New Interface with a Linear Quadrupole Ion Guide for an Electrospray-Ion Trap Mass Spectrometer System; Byungchul Cha1; Michael Blades1; Donald Douglas1; University of British Columbia, Vancouver, Canada

MPA 043  An atmospheric pressure MALDI probe for use with ESI source interfaces; Ryan M. Daniel1; Gary L. Glish2; University of North Carolina, Chapel Hill, NC

MPA 044  Tip flow restrictor for stable electrohydrodynamic spray of aqueous electrolytes in vacuum; Sergei A. Aksyonov1; Peter Williams3; Arizona State University, Tempe, AZ

MPA 045  Polyaniline: A New Coating for Nanospray Emitters for Improved Durability; Thomas P. White1; Sarah A. Lorenz1; E. Peter Maziarz2; Troy D. Wood3; State University of New York at Buffalo, Buffalo, NY; Bausch and Lomb Healthcare, Rochester, NY

MPA 046  Thermal Spray is Back: A Modified APCI Interface on LC/MS/MS for the Quantitation of Famotidine in Human EDTA Plasma; Ritha Najah1; Paul Brown1; Alan Duerk1; Patrick Lin1; MDS Harris, Inc., Lincoln, NE

MPA 047  Development of Electrospray/Atmospheric Sampling Glow Discharge Ionization; Christine N. Dalton1; Gary L. Glish1; University of North Carolina, Chapel Hill, NC

MPA 048  Development of a Microliter Flow Rate Atmospheric Pressure Chemical Ionization (APCI) Liquid Phase Separation/Mass Spectrometry Interface; David J. Hort1; Larry D. Bowers1; Indiana University Medical Center, Indianapolis, IN

MPA 049  Simple Modification of the HP 1100 Electrospray Nebulizer to Accommodate Low Flow Rates Liquid Chromatography; Alain Carrier1; RTP Pharma Inc., Montreal, Canada

MPA 050  Ion transmission through multi-capillary inlet and ion funnel interface; Taeman Kim1; Kess Jang1; Aleksy Tolmachev1; Harold R. Udsen1; Richard D. Smith1; Environmental Molecular Sciences Laboratory, Richland, WA

MPA 051  LC-MS with Supersonic Molecular Beams; Aviv Amirav1; Ori Granot1; Tel Aviv University, Tel Aviv, Israel

MPA 052  Zero Adjustment Device for Nano-Spray and Micro-Spray Ionization; Hoong Wang1; Melvin Park1; Sunna Aizaal1; Bruker Daltonics Inc., Billerica, MA

MPA 053  A new ES capillary design for improved detection sensitivity: detailed characterization of the analytical qualities; Günter Klesper1; Heike Klesper1; Gregor Fusshoeller1; CARBOTECH GmbH, Germany

MPA 054  A True Nanoelectrospray Ion Source Compatible with On-Line HPLC Systems; Matthias S. Wilms1; Kast Juergen1; European Molecular Biology Laboratory (EMBL), Heidelberg, Germany

MPA 055  High throughput protein identification using a multisprayer equipped with disposable nanoLC needles; Devanand M. Pinto1; Tom Covey1; Daniel Flegys1; MDS-SCIEX, Toronto, Canada; MDS-Ocata, Toronto, Canada
<table>
<thead>
<tr>
<th>Time</th>
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**MONDAY POSTERS**

### MPA 056
Quantitation of okadac acid by LC-MS/MS on an ion trap MS fitted with a custom constructed ESI source; Mark Busman1; Debra Petipain1; NOAA-NOS, Charleston, SC

### MPA 057
Device for Acquiring Alternating ESI and APCI HPLC Mass Spectral Data on an API Time-of-Flight Mass Spectrometer; Keiko Tabei1; Barry Hausner2; Frank Lambert1; Warren Yeisley1; Miguel Maccio1; Marshall M. Siegel1; Wyeth-Ayerst Research, Pearl River, NY

### MPA 058
High Throughput Protein Analysis Using Multi-ESI-Sprayer, Multi-Atmospheric-Pressure-Inlet Mass Spectrometry; Mehdz Moini1; Longfei Jiang1; University of Texas, Austin, TX

### MPA 059
Polymer-based Microchips Interfaced to a Nanoelectrospray Source and a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer; Zhaoming Meng1; Shize Qi1; Steven A. Soper1; Patrick A. Limbach1; Louisiana State University, Baton Rouge, LA

### MPA 060
An Automated Microchip-Based Electrospray Device for High Throughput MS Analysis; Gary A. Schultz1; Thomas N. Corso1; Simon J. Prosser1; Sheng Zhang1; Avidah Tashri1; Advanced BioAnalytical Services, Inc., Ithaca, NY

### MPA 061
An API-MS Microsprayer for Sampling from Chips, Multi-Well Plates and Surfaces; Jack Henion1; Timothy Wachs1; Yuzhong Deng1; Cornell University, Ithaca, NY

### TRAPPED IONS, 062 - 092

### MPB 062
Multiple-Stage Mass Analysis of Complex Oligosaccharide Antibiotics in a Quadrupole Ion Trap; P. L. Bartner1; G. Chen1; B. N. Pramanik1; P. Shipkova1; A. K. Saksea1; V. Girjavallabh1; M. L. Gross1; Schering-Plough Research Institute, Kenilworth, NJ, Washington University, St. Louis, MO

### MPB 063
Radial stratification of ions as a function of m/z ratio in collisional cooling frequency multipole as ion guides or ion traps; Alexsey Tolmachev1; Richard Harkevicius1; Christophe Masselon1; Gordon Anderson1; Sergey Rako1; Ljiljana Pas-To11; Eugene Nikolaev1; Mikhail Belov1; Harold Udseth1; Richard D. Smith1; Pacific Northwest National Laboratory, Richland, WA

### MPB 064
Chemical Mass Shifts in the RF Quadrupole Ion Trap: The Effect of Nonlinear Fields and Elastic and Dissociative Collisions on Absolute Ejection Times, Peak Shapes and Mass Measurement Accuracy; Wolfgang Plass1; J. Mitchell Wells1; R. Graham Cooks1; Purdue University, West Lafayette, IN

### MPB 065
Chemical analysis of single microparticles using a quadrupole ion trap; David A. Kirkwood1; Anthony J. Stace1; University of Sussex, England

### MPB 066
Multipass Light Scattering Optics for the Atmospheric Pressure Interface of an Aerosol Sampling Ion Trap Mass Spectrometer; Douglas G. J. Weir1; Michael L. Alexander1; Stephan E. Barlow1; Battelle Pacific NW National Lab, Richland, WA

### MPB 067
Detection of Biomarkers Using Post-Column Metal Complexation ESI-MS; Mary B. Setfield1; Meensup Song1; Jennifer S. Brodbelt1; University of Texas, Austin, TX

### MPB 068
Reducing the Capacitance of a Miniature Cylindrical Ion Trap; Thomas F. Meaker1; Bert C. Lynn1; Mississippi State University, MS

### MPB 069
Automatic CID Optimization with FNF Technology for Enhanced Ion Trap LC/MS/MS Analysis of Peptide Mixtures; Steven T. Finnin1; Craig A. Walla1; Sharon Lau1; Peter B. Grosshans1; Hitachi Instruments, Inc., San Jose, CA

### MPB 070
Practical Aspects of Obtaining Higher Resolution on an API Quadrupole Ion Trap and the Implications for Accurate Mass Measurements; Jae C. Schwartz1; Tina Hemenway1; Finnigan Corporation, San Jose, CA

### MPB 071
Atmospheric Pressure Matrix-Assisted Laser Desorption Ionization (AP-MALDI) with an Ion Trap Mass Spectrometer; John H. Callahan1; Marsha C. Galicic2; Akos Vertes2; Naval Research Laboratory, Washington, DC, George Washington University, Washington, DC

### MPB 072
Development of a Research-Grade Quadrupole Ion Trap Mass Spectrometer with Microelectrospray Ionization Interface; Kevin J. McHale1; Richard A. Yost1; University of Florida, Gainesville, FL

### MPB 073
An IR-MALDI Quadrupole Ion Trap Mass Spectrometer for High Mass Analysis; Vladimir M. Doroshenko1; Timothy P. Lippa1; Nelli I. Taranenko1; Coorg R. Prasad2; Robert J. Cotter2; Mass Technologies, Burlingtonville, MD; Science & Engineering Services Inc., Burlingtonville, MD; The Johns Hopkins University, Baltimore, MD

### MPB 074
Investigation of collision-induced fragmentation of laser desorbed ions using ion trap tandem mass spectrometry; Kyouseok Song1; Kwanghee Hong1; Hyungki Cha1; Jongmin Lee1; Changwoo Lee1; Korea Atomic Energy Research Institute, Taegon, Korea

### MPB 075
Behavior of Multiply-Charged Myoglobin in the Gas Phase toward Dissociation in Ion Trap Mass Spectrometer; Carlos Afonso1; Francoise Fournier2; Patrick Breton2; Jean-Claude Tabet2; CEB, Vert-le-Petit, France; Universite Pierre et Marie Curie, Paris

### MPB 076
Mass Instability in a Linear Segmented Quadrupole Ion Trap in the Presence of High Space Charge; Eugene N. Nikolav1; Mikhail E. Belov1; Alexey V. Tolmachev1; Richard D. Smith1; On leave from the Inst. of Energy Probl. of C.P., Moscow, Russia; Pacific Northwest National Laboratory, Richland, WA

### MPB 077
Investigation of Protein Conformers Separated by FAIMS Using Energy Loss Methods; Randy W. Purves1; Barbara Ellis1; David A. Barnett2; Roger Guevremont2; PE Sciex, Concord, ON, Canada; National Research Council of Canada, Ottawa, ON, Canada

### MPB 078
Selective Ion Accumulation Based on RF-Only Resonant Dipolar Excitation in the Presence of High Space Charge; Ken J. Auberry1; Mikhail E. Belov1; Evgenii N. Nikolav2; Richard D. Smith2; Pacific Northwest National Laboratory, Richland, WA; Inst. of Energy Problems of Chemical Phys., Moscow, Russia

### MPB 079
Multishot Acquisition and Stitched Pulse Sequences for Selected Ion Accumulation; Peter B. O'Connor1; Ekaterina Mirgorodskaya1; Catherine E. Costello1; Boston University, Boston, MA
MONDAY POSTERS

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MPB 080  Direct Optical Spectroscopy of Gas-Phase Molecular Ions Trapped and Mass-Selected by Ion Cyclotron Resonance: Laser Induced Fluorescence Excitation Spectrum of Hexafluorobenzene (C₆F₆); Yang Wang; Christopher L. Hendrickson; Alan G. Marshall; NHMFL, Florida State University, Tallahassee, FL

MPB 081  Ion-Ion Interaction in Magnetical Traps; Robert Malek; Karl P. Wanezek; University of Bremen, Bremen, Germany

MPB 082  Tandem Mass Spectrometry of Intact Proteins: Dissociation to Database Searching; James L. Stephenson Jr.; Benjamin J. Cargile; Scott A. McLuckey; Oak Ridge National Laboratory, Oak Ridge, TN; Purdue University, West Lafayette, IN

MPB 083  Quadrupole Mass Filtered External Accumulation for Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Christopher L. Hendrickson; John P. Quinn; Mark R. Emmett; Alan G. Marshall; National High Magnetic Field Lab, Tallahassee, FL

MPB 084  A SIMION Collision Algorithm to Simulate Individual Ion-Neutral Collision Events and Investigate Ion Loss in an FTICR Trapped Ion Cell; C Richard Arkin; D. A. Laude; University of Texas, Austin, TX

MPB 085  Chemical analysis of complex environmental samples by FT ICR MS; Elizabeth Stevenson; Renato Zenobi; Swiss Federal Institute of Technology, Zurich, Switzerland

MPB 086  Sub-ppm local frequency shifts in FTICR mass spectrometry; Christophe Masselon; Aleksy V. Tolmachev; Vsevolod S. Rakov; Ljiljana Pasa-Tolic; Richard Harkewicz; Gordon A. Anderson; Evgenij N. Nikolaev; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA; On leave from Inst of Energy Problems Chem. Phys., Moscow, Russia

MPB 087  Combined External and Internal Ion Accumulation: Improved Detection Limit for Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Ahmed Almawry; Touradj Solouki; University of Maine, Orono, ME

MPB 088  How Does High Resolution ES-FTICR-MS under Broadband Conditions Enhance Characterization of Protein and Peptide Mixtures?; Robert L. Hettrich; Michelle V. Buchanan; Oak Ridge National Lab, Oak Ridge, TN

MPB 089  Master Equation Analysis of Ion-Molecule Complexation in the Zero Pressure Limit; Adam S. Rust; William D. Price; Marshall University, Huntington, WV

MPB 090  Evaluation of a Novel Central Trapping Electrode Cell for FTICR Mass Spectrometry and Ion Accumulation for LC-ESI/FTICR; Chad M. Ostrander; C. R. Arkin; David A. Laude; University of Texas, Austin, TX

MPB 091  Complications in Ion-Trap MS/MS Experiments Due to Undesirable Rearrangement or Ion-Molecule Reactions; Xinzhen (Jane) Xiang; Rong Feng; Rosie Chang; Brigitte Segmuller; James Weber; H. Marlon Zhong; Birdella Kenney; Ahmed Abdel-Magid; R. W. Johnson Pharmaceutical Research Institute, Spring House, PA

MPB 092  Ion Trap LC/MS® Study of an Unusual Acetyl Migration Reaction in The Gas Phase and NMR Study of the Parallel Reaction in the Solution Phase; Rong Feng; Xinzhen (Jane) Xiang; Brigitte Segmuller; James Weber; H. Marlon Zhong; Ahmed Abdel-Magid; R. W. Johnson Pharmaceutical Research Institute, Raritan, NJ

DRUGS & METABOLISM: METABOLITE IDENTIFICATION, 093 - 105

MPB 093  The importance of good chromatography in LC/MS/MS: identification of an unreported metabolite of Propafenone in man; Munoz Yongrandi; Alain Desroches; Martin Jutras; Micheal Mancini; Martine Allard; MDS Neopharm, Blainville, Canada

MPB 094  A Multiple Radio- and Stable-Isotopic Labeling Approach for Evaluating the Metabolism of Omapatrilat in Bile Duct Cannulated Rats; Ramaswamy A. Iyer; James G. Mitroka; Bimal K. Malhotra; Stephen C. Waller; Sam Bonacorsi; J. Kent Rin Bernardino; Kishin J. Kripalani; Bristol-Myers Squibb PRI, Princeton, NJ

MPB 095  Analysis and Identification of the In-Vitro Drug Metabolism of the Antiparkinsonian Drug Selegiline by LC/MS/MS; Jeffrey Selken; Jennifer McCaffery; Steve Neitzel; Diane Tutko-Francisco; PPD Discovery, Madison, WI; PPD Development, Morrisville, NC

MPB 096  Human Excretion of Urinary Metabolites of RJR-2403; Gary D. Byrd; Johnnie R. Hayes; Jackie M. Greene; William S. Caldwell; Targacept, Inc., Winston-Salem, NC

MPB 097  Characterization of N-Deacetylated Ketoconazole Metabolites Produced by a Recombinant Human FMO System Using Triple Quadrupole and QqQ TOF Instruments; Jeffrey D. Miller; Rosita I. Rodriguez; Sai Y. Chang; Takeo Sakuma; Chuan Lu; Albert Li; PE Biosystems, Framingham, MA; Oregon State University, Corvallis, OR; MDS Sciex, Concord, ON, Canada; In Vitro Technologies, Baltimore, MD

MPB 098  Characterization of Imidazole Ring Cleaved Metabolites of 1-Phenyl-2-Methyl-Imidazole by LCQ Ion Trap; Zhuang Miao; Chandra Prakash; Pfizer Central Research, Groton, CT

MPB 099  Biotransformation of SU006685 in vivo and in vitro; Qingling Zhang; Tracy Lou; Cho Tang; Cheng Yang; Jiuhamas Sukburhong; Shamsi Raeissi; Mike Van Petten; Joshua Haznedar; Laura Shawver; Lida Antonian; Sugen, Inc., South San Francisco, CA

MPB 100  Metabolite Identification of Iloperidone and Major Metabolites in Human Liver Slices by Liquid Chromatography Tandem Mass Spectrometry Methods; Elizabeth Brahnam; Robert Tullman; Laura Guarducci; Alban Allenoff; Kirk Bordeaux; Laurie Johanson; Volker Fischer; Novartis Pharmaceuticals, Hanover, NJ

MPB 101  Rapid Screening Method for Detection of Acidic and Neutral Drugs in Urine Using Liquid Chromatography and Mass Spectrometry; Wayne Skinner; Scott D. Stanley; University of California, Davis, CA

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MONDAY POSTERS

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8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

MPC 102  Characterization of omega-oxidation of PNU-108342 using a combination of MS and 19F-NMR; L James Vrbana; Bruce A. Thornburgh; Paul E. Fagerness; Richard L. Voorman; Gwendolyn D. Fate; Pharmacia & Upjohn, Kalamazoo, MI

MPC 103  Metabolism of GnRH Analog antagonist Abarelix in Rats; Gondi N Kumar; John C. Le; Shekman Wong; Christopher Molinaux; Robert McGarr; Anup Zutshi; Christopher Sproul; Sharon Turner; David Lau; John Young; Amgen Inc., Thousand Oaks, CA; Praecis Inc, Cambridge, MA; Battelle Inc., Columbus, OH

MPC 104  Evaluation of a New Orthogonal Spray Benchtop Ion Trap Mass Spectrometer for the Identification of Bile Acid Metabolites; Linda L. Lopez; Michael Zumwalt; Agilent Technologies, Inc., Palo Alto, CA

MPC 105  Mass Spectrometric Characterization of Metabolites Derived from Tegaserod, a New Therapy in Development for Gastrointestinal Motility Disorders, by LC-MS, H/D-Exchange Experiments and Exact Mass Measurements; Markus Zollinger; Ulrike Glänzel; Bruno Inverardi; Robert Dannecker; K. Olaf Boernson; Novartis Pharma AG, Basel, Switzerland

DRUGS & METABOLISM: LC/MS/MS QUANTITATION IN PLASMA BLOOD OR SERUM, 106 – 149b

MPD 106  Quantitative Analysis of Cyclosporin A using Negative Ion Electrospray Mass Spectrometry; Lawrence R. Hopkins; Elaen D. Korshinski; Gordon McKay; University of Saskatchewan, Saskatoon, SK, Canada

MPD 107  Quantitative Determination of HIV-1 Protease Inhibitors and their Metabolites in Patients Serum/Plasma by Tandem LC-MS/MS; Sonny Gunawan; Marshall P. Griswold; Douglas G. Kahn; Consolidated Laboratory Services, Van Nuys, CA

MPD 108  Determination of scopolamine in human serum and microdialysis samples by liquid chromatography-tandem mass spectrometry; Reinhard Oertel; Ulrike Ebert; Klaus Richter; Wilhelm Kirch; Institute of Clinical Pharmacology, TU Dresden, Dresden, Germany

MPD 109  Examination of matrix-induced ionization suppression in quantitative LC/MS-MS analysis; Frederick E. Wolf; Keyang Xu; Krys Miller; Amgen Inc., Thousand Oaks, CA

MPD 110  A Rapid and Sensitive HPLC/MS/MS Method for the Determination of Bucillamine in Human Blood; Francis Beaudry; Dave Proulx; Milton Furtado; Marcus Horwitz; Lawrence Horwitz; Joseph Cap; Phoenix International, Montreal, Canada; University of California, Los Angeles, CA; University of Colorado School of Medicine, Denver, CO

MPD 111  Determination of 21-Hydroxy Deflazacort in Human Plasma by HPLC/APCI/MS/MS. Application to Bioequivalence Study; Demian R. Iff; Maria E. Moraes; Manuel O. Moraes; Vincenzo Santagada; Giuseppe Caliendo; Gilberto De Nucci; University of Sao Paulo, Brazil; University of Ceara, Brazil; University of Naples Federico II, Italy

MPD 112  Development and Validation of an HPLC-MS/MS Method for the Determination of Atorvastatin and its Metabolites in Human Serum; Yizhong Zhang; Lorella Di Donato; Charles Grandmaison; Robert Masse; Phoenix Life Sciences International, Montreal, Canada

MPD 113  Sensitive LC/MS/MS Bioanalytical Method for Nicotine in a non-sterile environment; Alain Desroches; Manon Vandenbrouck; Evgeni Fedorov; Michaeal Mancini; Martine Allard; MDS Neo-Pharm, Blainville, QC, Canada

MPD 114  A High Performance Liquid Chromatographic Mass Spectrometric Method for the Determination of Rimantadine in Human Plasma; John Simpson; Harry Demirdjian; Francis Beaudry; Phoenix International Life Sciences, Montreal, Quebec, Canada

MDP 115  Determination of Adefovir in Human Plasma by LC/MS/MS; Alain Hardy; Sylvain Feron; Milton Furtado; Francis Beaudry; Stanley C. Gill; David Tinnermeier; Phoenix International, Montreal, Canada; Gilead Sciences Inc., Boulder, CO

MPD 116  Determination of 5-Aminosalicylic Acid Concentrations in Whole Blood by LC/MS/MS Using Derivatization as a Chromatographic Aid; Peter J. Stoffelmann; C. Michelle Dunaway; LaShonda Anderson; Kenneth R. Wehmeyer; Charles Cruz; Timothy R. Baker; Procter & Gamble Pharmaceuticals, Mason, OH

MPD 117  An Improved Rapid LC-MS/MS Method for Quantitation Detection of Thymosin Alpha-1 (TA-1) in Human Serum; Cynthia W. Tuthill; Alfred Rudolph; Yang Li; Beijing Tan; Thomas J. Fitzgerald; Stephen R. Beck; Yong-Xi Li; SciClone Pharmaceuticals, Inc., San Mateo, CA; Ricerca, LLC, Painesville, OH

MPD 118  Quantifiable level of the produg Fenofibrate found in human plasma, using a sensitive LC/MS/MS method; Francois Pedneau; Michaeal Mancini; Alexander Pimenov; Manon Vandenbrouck; Martine Allard; Martine Allard; MDS Neo-Pharm, Blainville, QC, Canada

MPD 119  The Rapid Analysis of Selegiline and Seven Metabolites Using On-Line Column Switching and Electrospray LC/MS/MS; Edward J. Daly; Donald Chun; Themis Flarakos; Mark L. J. Reimer; Phoenix International Life Sciences, Saint-Laurent, Canada

MPD 120  Quantification of OSU-6162 and a N-desalkyl Metabolite in Plasma by HPLC-MS/MS following TCA Protein Precipitation: A Comparison of Two Instrument Platforms; Joe Palandra; Brian A. Staton; Eric M. Shobe; Timothy G. Heath; Jim Cregan; Suzanne Walton; Jennifer Morris; Amy Pearsall; Pharmacia & Upjohn, Kalamazoo, MI; PPD Development, Richmond, VA

MPD 121  A Rapid and Sensitive LC-ESI/MS/MS Method for the Determination of Misoprostol Acid in Human Plasma; Lynda Letarte; Dino Cicci; Michel Coutu; Rudolf Guibaud; Phoenix International, Montreal, Canada

MPD 122  Determination of MRE0470, an analog of adenosine, by LC/MS/MS in human plasma; Kevin Sils; John Simpson; Milton Furtado; Medco Research, Inc., Research Triangle Park NC; Phoenix International Life Sciences, Montreal, Canada
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<th>Time</th>
<th>Session Details</th>
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<td>7:30 – 8:00 am</td>
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**MONDAY POSTERS**

**MPD 123**
A High Performance Liquid Chromatographic Mass Spectrometric Method for the Determination of Phenyltin in Human Plasma by Automated Sample Extraction (TOMTEC™); Piers Gaudette1, Rudolf Guibault1, Michel Coutu1; Phoenix International Life Sciences Inc, Montreal, Canada

**MPD 124**
A Rapid and Sensitive HPLC/MS/MS Method for the Determination of Felodipine in Human Plasma; Alan Arsenault1, Genevieve Plante1; Phoenix International Life Science Inc., Ville St-Laurent, Montreal, Canada

**MPD 125**
Development of a Sensitive LC-ESI-MS/MS Method for the Determination of Hydrophilic Compound MX-68 in Human Plasma, Using Short Column with Low Ion Suppression; Keisuke Uchida1, Yoshinori Ashi1, Masayuki Iiizaka1, Kiminori Sai1, James MeBland1, Chugai Pharmaceutical Co., Ltd., Gotemba, Shizuoka, Japan; Chugai Pharma Europe Ltd, London, UK

**MPD 126**
A method for the quantitative determination of methylmalonic acid in plasma by LC/MS/MS stable isotope dilution analysis; Mark J. Magera1, Jean M. Lacey1, Janice K. Helgeson1, Dietrich Matern1, Piero Rinaldo1; Biochemical Genetics Laboratory, Mayo Clinic, Rochester, MN

**MPD 127**
LC/MS/MS Analyses and Initial Clinical Pharmacology Study of a Traditional Chinese Medicine for Chronic Renal Failure Treatment; Xiaoyun Wang1, Takeo Sakuma1, Yan Xue1, Tonghui Zhou1; PE-Sciex, Concord, Ontario, Canada; Peking Union Medical College, Beijing, China

**MPD 128**
Validation of an HPLC/MS/MS Method for the Determination of Metoprolol and Alpha-hydroxy metoprolol in human plasma; Mohammad Hamzavi1, John Ulrich1, Danie Schlatter1, Anthony Chilton1; Magellan Research & Bioanalytical, RTP, NC

**MPD 129**
A Rapid Approach to Resolve a Matrix Effect in a Complex Mixture of Analytes; Patrick Bennett1, Brad Coopersmith2, Marc Browning3, Jennifer Cragger3, Edward Brewer3, Jerry Brisson3, Steven L. Bramer3; NACI & Northwest Bioanalytical, Princeton, NJ

**MPD 130**
The application of antioxidants to analyze extracts of an unstable compound by LC-APCI/MS/MS; Lawrence P. Colwell1, Gino M. Salturo1; Merck Research Laboratories, Raritan, NJ

**MPD 131**
Development of an HPLC-MS/MS Method for the Determination of Nefazodone, Hydroxynefazodone and Chloro-piperoxyl in Human Plasma; Gerard Dussault1, Danielle Lachance1, Yves G. Leblanc1; Charles Grandmaison1, Loretta Di Donato1; Phoenix International Life Sciences, Montreal, Canada

**MPD 132**
Development and Validation of an LC-MS/MS Method for the Determination of Oxybutynin and Desethyloxybutynin in Human Plasma; Serge Bourg1, Gerard Dussault1, Yves G. Leblanc1; Charles Grandmaison1, Loretta Di Donato1; Phoenix International Life Sciences, Montreal, Canada

**MPD 133**
Quantitation of Estrogen Metabolites in Plasma by Electron Capture Atmospheric Pressure Chemical Ionization Mass Spectrometry; Alejandro Gutierrez1, Gurkeerat Singh1; Peter O'Dwyer1; Ian A. Blair1; University of Pennsylvania, Philadelphia, PA

**MPD 134**
Pharmacokinetic Profile for Etoposide and its Catechol Metabolite in Pediatric Cancer Patients Determined by LC/ESI/MS/MS; Naiyu Zheng1, Shaojun Pang2, Carolyn Felc3, Ray Boston3, Ian A. Blair1; University of Pennsylvania, Philadelphia, PA; Bristol-Meyers Squibb Pharmaceutical Research Inst., New Brunswick, NJ; Children's Hospital of Philadelphia, Philadelphia, PA

**MPD 135**
Quantitative analysis of a tri-chlorinated compound and its metabolite in serum samples using LC/MS/MS: The need for chromatographic separation; Peter Lodengrad1, Bilin Chou1, Matthew Baumgardner1, Yang Wang1, Genentech, Inc., South San Francisco, CA

**MPD 136**
Complete Serum Concentration vs. Time Profile in a Small Experimental Animal Using Minute Blood Sampling via Venous Catheter followed by LC-MS-MS; Martin Jorgensen1, Connie Sanchez1, H. Landbeck A/S, Valby, Denmark

**MPD 137**
Characterization of Metabolites of the D4 Antagonist CI-1030 in Dog, using LC-MS and LC-MS/MS; Laura A. Egna1, Kimberly Lapham1, Rasmay E. Talat2, Raghu Ramnathan1; Parke-Davis Pharmaceutical Research, Ann Arbor, MI

**MPD 138**
Determination of Tramadol and its Metabolites in Plasma by Liquid Chromatography and Electrospray Ionization Tandem Mass Spectrometry; Ann Zhu1, Voong S. Ong1, Danlin Wu1, Purdue Pharma, Ardsley, NY

**MPD 139**
Validation of a method for the enantiomeric determination of (R)-warfarin and (S)-warfarin in human plasma using high-performance liquid chromatography with triple quadrupole mass detection; Paula K. Ring1, Xiangyu Jiang1, Carmilla Midtlien1; Covance Laboratories Inc., Madison, WI

**MPD 140**
Quantitation of FTC in Human Plasma Using LC/MS/MS: A Comparison of the Ion Trap versus the Triple Quadrupole: John P. Walsh1, John A. Begley1, Feng Wang1; Triangle Pharmaceuticals, Inc., Durham, NC

**MPD 141**
Determination of Triazolam and its Two Metabolites in Human Plasma by APC1 Tandem LC/MS/MS; Huaibing He1, Mary L. Manier1, Jiemin Wang1, Deborah W. Robinson1, Alastair J. Wood1, David L. Hackey1; Vanderbilt University, Nashville, TN

**MPD 142**
Drug Stability Studies Using On-Line Extraction and LC/MS/MS Analysis; Anjula Pamidimukkala1, Roger Blain1, Natalya Khelemskaya1, Surendra Bansal1, Louis Renzetti1; Hoffmann-LaRoche, Nutley, NJ

**MPD 143**
A Validated Normal-Phase Chiral LC/MS/MS Method for a Drug Candidate from Plasma; John R. Kage1, Tresavon D. Parker III1, Roger Hayes1, David T. Rossi1; Primedica Corp., Worcester, MA; Parke-Davis, Ann Arbor, MI

**MPD 144**
Quantitative Determination of Free Thiol-containing Organic Compounds in Rat Plasma by LC-MS/MS; Jun Shen1, Jih-Lie Tseng1, Marilyn Lam1, Babu Subramaniam1; Berlex Biosciences, Richmond, CA

**MPD 145**
The Effects of Drug Conjugates in the LC-MS/MS Quantitation of Animal Plasma Samples; Walter Yu1;
MONDAY POSTERS

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Phil Enriquez1; Axys Pharmaceuticals, South San Francisco, CA

MPD 146  Determination of SCH 351754 and SCH 18908 in Rat and Monkey Plasma by LC-ESI/MS/MS; Yves G. Leblanc1; Danielle Lachance1; Yizhong Zhang1; Charles Grandmaison1; Themis Flarakos3; Josephine Lim2; Bhavana Kantesar1; Robert Clement2; Phoenix International Life Sciences, Montreal, Canada; Schering Plough Research Institute, Kenilworth, NJ

MPD 147  On-Line and Off-Line SPE Extractions for LC-MS/MS Analysis of Memantine in Rabbit and Human Plasma; Lisa Borbridge1; David Loureiro1; Andrew Acheampong1; Allergan, Inc., Irvine, CA

MPD 148  Analysis of Animal Cassette Dosing and Pooled Plasma for Sulfonil-3-phenylbutanoic Acids by LC/MS/MS with Turbulent Flow On-Line Plasma Extraction; John P. Pirro2; Daniel T. Pentek2; Renato J. Sciallis3; Du-Shieng Chien4; Bayer Corporation, West Haven, CT

MPD 149  Simultaneous Validation of an LC/MS/MS Method for the Quantitation of Loradamine and Metabolite in Four Preclinical Species Using a Multiplexed Electro-spray Triple Quadrupole Mass Spectrometer; Liyu Yang1; Robert P. Clement1; Patrick J. Rudewicz1; Schering-Plough Research Institute, Kenilworth, NJ

MPD 149b  Comparative Pharmacokinetic Profiles of Paxitaxel and Metabolites from Two Different Intravenous Formulations in the Dog; Travis Culley1; Michael S. Alexander1; James D. McChesney2; Steve J. Bannister2; James H. Rudy3; Catherine Romine3; LC Resources, McMinnville, OR; NaPro Biotherapeutics, Inc., Boulder, CO

PROTEINS – BASICS, 150 - 212

MPE 150  A Combination of Chemical Derivatization Techniques for Improving Protein Identification in Proteomics; Francesco Branca1; Anna Butt1; Simon Hubbard1; Rob Beynon1; Stephen Oliver1; Simon Gaskell1; UMIST, Manchester, UK; University of Liverpool, Liverpool, UK; University of Manchester, Manchester, UK

MPE 151  Derivatization and Postsource Decay MALDI Mass Spectrometry for Definitive Protein Identification in Proteomics Research; Thomas W. Kough1; Martin P. Lacey1; Angela M. Fieno1; Raymond A. Grant1; Yiping Sun1; Mark D. Bauer1; Karen B. Begley1; The Procter and Gamble Company, Cincinnati, OH

MPE 152  Mass Spectrometric Identification of Proteins from Laser Capture Microdissected Tissue; Laura C. Lawrie1; Stephanie Curran1; Phillip Cash1; John E. Fothergill1; Graeme I. Murray1; Aberdeen University, Aberdeen, Scotland, UK

MPE 153  Analysis of Biological Samples and Functionalyzed Surfaces with MALDI MS and Scanning Microprobe MALDI MS; Werner Bouschen1; Christian Hoffmann1; Gunter Tovar1; Bernhard Spengler1; Inst. Phys. Chem., Univ. Würzburg, Würzburg, Germany; Fraunhofer Inst. for Interf. Engin. and Biotech., Stuttgart, Germany

MPE 154  Electrophoretic mobility-based sequencing for protein identifications by non-aqueous CE/MS; HiroshiTakahama1; Yazuishi Ishihama1; Yoshikawa Oda1; Naoki Asakawa1; Eisai Co. Ltd., Ibaraki, Japan

Two Dimensional Electrophoretic/Chromatographic Separations with Electrospray Ionization Mass Spectrometry for High Throughput Proteome Analysis; Hengying Gao1; Yuefeng Shen1; Timothy D. Veenstra2; Richard D. Smith1; Pacific Northwest National Laboratory, Richland, WA

MPE 155  Comparing Ga(III)-IMAC Methods for Selective Extraction and MALDI/TOF MS Characterization of Phosphopeptides; Douglas Olson1; Andrew R. Ross2; Michael J. Chalmers3; Simon J. Gaskell4; NRC Plant Biotechnology Institute, Saskatoon, Canada; UMIST, Manchester, UK

MPE 157  Site-Specific Protein Cleavage by Copper(II)-1,4,7-triazacyclononane dichloride (CuTACN): Isolation and Identification of Protein Fragments by SDS-PAGE and MALDI-TOF; Gregory M. Polzin1; Judith N. Burstyn1; University of Wisconsin, Madison, WI

MPE 158  In-Situ Chemical Cleavage for Rapid and Sensitive Protein Identification; Kuo-Liang Hsia1; Christine A. Sittineri2; Lydia M. Nuwaysir3; David H. Hawke3; Steven O’Neill4; David R. Dupont4; PE Biosystems

MPE 159  High Temperature Protein Mass Mapping Using a Thermophilic Protease; Steven J. Bark1; Gary Szupek1; The Scripps Research Institute, La Jolla, CA

MPE 160  Quantitative Evaluation of the Efficiency of in-gel Digestion of Proteins by Isotopic Labeling and Mass Spectrometry; Anna Shevchenko1; Matthias Wilk1; Andrej Shevchenko1; European Molecular Biology Laboratory, Heidelberg, Germany

MPE 161  Mass Spectrometry Provides No Evidence for Disulfide Cleavage by Formic Acid; Kris P. Tjon1; Kym F. Faul1; Richard L. Stevens1; Julian P. Whitelegg1; University of California, Los Angeles, CA

MPE 162  Rapid Identification of Proteins by MS and MS/MS on a MALDI-QSTAR; Breit G. Larsen1; Lorne Taylor2; Dan Figyes3; Mike Tyers1; Samuel Lunenfeld Research Institute, Toronto, Canada; MDS Oecet, Toronto, Canada

MPE 163  Strategies for optimizing peptide mapping by MALDI-MS; Gary Ward1; Steven L. Cohen1; P.K. Tsai1; Merck Research Laboratory, West Point, PA

MPE 164  A Novel Approach to Analyze Membrane Proteins and Peptides by Mass Spectrometry; Steven L. Cohen1; Gary Ward1; Brent Oswald1; P.K. Tsai1; Merck Research Laboratory, West Point, PA

MPE 165  Quantitative Protein Charge State Distributions at Various pH and Flow Regimes; Brian T. Cooper1; Michael F. Streeter1; UNC, Charlotte, NC

MPE 166  Energetics of Heme Unit Dissociation from Heme Proteins: Evidence of the Correlation between Charge States and Conformational States of Proteins in ESI/ITMS Analyses; Gregg Pratt1; Fred L. King1; West Virginia University, Morgantown, WV

MPE 167  From Mass to Mass - Deconvoluting ESI Spectra; Julio C. Paolovan1; David P. Fenyo1; Brian T. Chait1; Rockefeller University, New York, NY

MPE 168  Effects of Solvent on the Maximum Charge and Charge State Distributions of Protein Ions Formed by Electrospray Ionization; Anthony T. Javaron1;
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John C. Jurchen1; Evan R. Williams1; University of California, Berkeley, CA

MPE 169  Analysis of Proteins from 2D-Gels by MALDI-TOF MS and LC-ESI-TOF MS; Manfred Raids1, Gerald Reit2, Angelika Görg3, Jonas Aaström4, Henrik Wadenstein5, Staffan Renlund6, Ameersham Pharmacia Biotech, Freiburg, Germany; TU Munich, Freising, Germany; Ameersham Pharmacia Biotech, Uppsala, Sweden

MPE 170  Mass Spectrometry and N-Terminal Sequencing in Proteomics; Martin P. Hornshaw1, Volker Kroft1, Utz Fischer2, PE Biosystems, Germany; Max Planck Institute, Germany

MPE 171  Assignment of the Four Disulfide Linkages in the Knotted Peptide Sullcin by Cyanylation/Mass Mapping; Jianfeng Qi1, Jack Throck Watson1, Michigan State University, East Lansing, MI

MPE 172  Using Negative Ion MS/MS in an Ion-trap to Confirm a Trisulfide Structure in Recombinant Human Growth Hormone; Long Truong1, Victor Ling1, Genentech Inc, South San Francisco, CA

MPE 173  A Systematic Approach to the Determination of Disulfide Bonds in Complex Proteins; Joseph P. Nawrocki1, Sonja Hess1, Lewis K. Pannell1, National Institutes of Health, NIDDK, LBC, Bethesda, MD

MPE 174  Analysis of Peptides and Proteins Containing Nitrotyrosine by Matrix-Assisted Laser Desorption Ionization (MALDI) Time-of-Flight Mass Spectrometry; Aaron Sarver1, Karoline Scheffler1, Martin Shetlar1, Bradford W. Gibson1, University of California, San Francisco, CA

MPE 175  Fourier Transform Mass Spectrometry to Characterise and Monitor Nitrated Proteins with Specific Reference to Renal Transplantation; Helen J. Cooper1, Peter J. Derrick1, John Heptinslall1, David Walton1, University of Warwick, Coventry, UK; Coventry University, Coventry, UK

MPE 176  Characterization of S100-Protein Nitration Products Using Electrospray Mass Spectrometry; Mark J. Raftley1, Carolyn L. Geczy1, University of NSW, Australia

MPE 177  Determination of the Site of Cysteine-Nitrosylation in Proteins by Electrospray Tandem Mass Spectrometry; Ivan Haller1, Steven S. Gross1, Gang Hao1, Linjun Xie1, Weill Medical College of Cornell University, New York, NY

MPE 178  Investigation of tyrosine nitration by mass spectrometry; Ann-So菲 N Petersson1, Dario E. Kalumee2, Kenneth Caidah3, Peter Roepstorff4, Sahlgrenska University Hospital, Gothenburg, Sweden; University of Southern Denmark, Odense, Denmark

MPE 179  Oxidation of Apolipoprotein B-100 in LDL; Jim Wang1, Chao-yuh Yang1, Charles V. Smith1, Jun Qin1, Baylor College of Medicine, Houston, TX; Rockefeller University, NY

MPE 180  Determination of Protein-Derived Free Radicals by Mass Spectrometry; Leesa J. Deterding1, Yeong-Renn Chen1, Ronald P. Mason1, Kenneth B. Tomer1, National Institute of Environmental Health Science, RTP, NC

MPE 181  Preparation of irreversibly sickled cell beta-actin from normal red blood cell beta-actin verified by liquid chromatography and off-line mass spectrometry; Ann Abraham1, F. Aladar Bencsath1, Archil Shartava1, David Kakhkashvili1, Steven R. Goodman1, University of South Alabama, Mobile, AL

Coadvecative Modification of Platelet Cell Surfaces; Jennie Koons1, Michael R. Gill1, Thomas H. Morton1, University of California, Riverside, CA

Coadvecative Modification of Platelet Cell Surfaces; Jennie Koons1, Michael R. Gill1, Thomas H. Morton1, University of California, Riverside, CA

MPE 183  Characterization of post-translational modifications of gel-isolated proteins: new techniques for in-gel digestion and CZE-MS detection; John Kelly1, Jianjun Li1, Pierre Thibault1, National Research Council of Canada, Ottawa, ON, Canada

MPE 184  Protein Phosphorylation at Serine and Threonine Analyzed by Elastase Digestion and Tandem Mass Spectrometry with Neutral Loss Scanning; Andreas Schlosser1, Ruediger Pipkorn1, Dirk Bossemeyer1, Wolf D. Lehmann1, German Cancer Research Center, Heidelberg, Germany

MPE 185  Enrichment analysis of phospho-Ser and phospho-Thyr proteins; Yoshiya Oda1, Takeshi Nagawa1, Brian T. Chait1, Eisai Co., Ltd, SFT lab., Ibaraki, Japan; The Rockefeller University, New York, NY

MPE 186  Phosphopeptide analysis using a MALDI Qq/TOF mass spectrometer; Keiryn Bennett1, Allan Stensaas2, Alexandre Podtelejnikov3, Ole N. Jensen2, MD3, Portland A/S, Odense, Denmark; University of Southern Denmark, Odense University, Odense, Denmark

MPE 187  A Rapid And Sensitive Procedure for Identification and Optimization of Peptide Substrates for Protein Kinase C; Xiaolong Zhang1, Khanh-Ha Nguyen1, Jeffrey Jackson1, Roland S. Annan1, Steven A. Carr1, SmithKline Beecham Pharmaceuticals, King of Prussia, PA

MPE 188  Phosphopeptide Mapping by Electron Capture Dissociation FT/MS; Stone D., H. Shi1, Mark E. Hemling1, Steven A. Carr1, David M. Horn2, Inge-Maria Lindt1, Fred W. McMafferty1, SmithKline Beecham Pharmaceuticals, King of Prussia, PA; Cornell University, Ithaca, NY

MPE 189  Mapping of the Phosphorylation Sites of Proteins by Precursor Ion Scan on a Quadrupole Time of Flight Mass Spectrometer (Qq/QTOF) at the Femtomole Level; George J. Scott1, Jane Zhao1, PE Sciex, Concord, Canada

MPE 190  Characterization of the pattern and sites of phosphorylation in different forms of the myristoylated alanine-rich protein kinase C substrate (MARCKS) protein; Christoph Borchers1, Cameron O. Scarlet1, Judith M. Thorn1, Perry J. Blackshear1, Kenneth B. Tomer1, St. Louis, NC

MPE 191  Mapping the Phosphorylation of Human Tau by Tau Protein Kinase II; Eric T. Lund1, Rosemary McKenna1, David B. Evans1, Satish K. Sharma1, W. Rodney Mathews1, Pharmacia & Upjohn, Kalamazoo, MI

MPE 192  Phosphorylation Mapping of a Hyper-Phosphorylated Protein from Saccharomyces cerevisiae Involved in Regulation of Mitosis; Susan L. Chen1, Michael J. Huddleston1, Steven A. Carr1, Roland A. Annan1, Wenyin Shou1, Raymond Deshaies1, SmithKline Beecham, King of Prussia, PA; California Institute of Technology, Pasadena, CA
MONDAY POSTERS

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MPE 193 Analysis of Phosphopeptides from Peptide Mixtures Using Micro-Affinity Chromatography by Mass Spectrometry; Cheryl L. Brucato1; John M. Asara2; Kerry A. Pierce3; Aleta Schnitzler4; William S. Lane4; William Kopaciewicz5; Millipore Corporation, Danvers, MA; Harvard University, Cambridge, MA

MPE 194 Examination of Phosphorylation Sites in Carbamoyl Phosphate Synthetases by Electrospray Tandem Mass Spectrometry; Christina S. Raska1; Marshall Pope1; Lee Graves1; University of North Carolina, Chapel Hill, NC

MPE 195 On Membrane Digestion of Phosphoproteins for Determination of Phosphorylation Sites by MALDI-QqTOFMS; Colin H. Lee1; Mark E. McComb2; Maciej M. B. Boromiski3; Werner Ens4; Kenneth G. Standing5; Helene Perreault6; University of Manitoba, Winnipeg, MB, Canada; presently at Boston University School of Medicine, Boston, MA

MPE 196 Identification and characterization of regulatory tyrosine phosphorylation sites in Eph receptor tyrosine kinases; Kathleen L. Binn5; Paul D. Taylor1; Tony Pawson1; Samuel Lunenfeld Research Institute, Toronto, Canada

MPE 197 Identification of Cyclin-Dependent Kinase 2 (CDK2) Glucosylation/Phosphoglucoysylation Sites Using Electrospray and Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry; Yan-Hui Liu1; Urooj Mirza1; Birenda N. Pramanik1; Lata Ramanath1; Mark Demna1; Charles McNemar1; Patricia C. Weber1; Zhen Wu1; Schering-Plough Research Institute, Kenilworth, NJ

MPE 198 Characterization of Protein Glycoforms in Cellbiohydrolase and Endogucanase from Trichoderma reesei; Joseph Pok Man Hui1; Makoto Yaguchi1; Pierre Thibault1; Theresa White1; Rene Roy2; Institute for Biological Sciences, NRC, Ottawa, Canada; Iogen Corporation, Ottawa, Canada; University of Ottawa, Ottawa, Canada

MPE 199 Screening for new types of glycosylation in the IgG molecule with nano-ESI Q-TOF using a novel strategy for glycosylation status and site determination of glycopeptides in mixtures; Boris Macek1; Gordan Lauc2; Mirna Flogel3; Jasna Peter-Katalinic1; Institute for Medical Physics and Biophysics, Miinster, Germany; Faculty of Pharmacy and Biochemistry, Zagreb, Croatia

MPE 200 Rapid Analysis of Viral Glycoproteins; Yeoung J. Kim1; Amy A. Freas1; Catherine Fenselau1; University of Maryland, College Park, MD

MPE 201 The Effect of Delayed Extraction Parameters on the Prompt Fragmentation of Labile Biomolecules in MALDI-TOF MS; James A. Blackledge1; Joseph A. Loo1; Parke-Davis, Ann Arbor, MI

MPE 202 Identification and Location of Cysteinyl Post-translational Modification of an Amyloidogenic Bence Jones Protein by MALDI and ESI Mass Spectrometry; Amarnath Lim1; Jeremy L. Wally2; Mary T. Walsh3; Catherine E. Costello4; Boston University School of Medicine, Boston, MA

MPE 203 Method for Determining the Average Degree of Substitution of o-Vanillin Derivatized Porcine Somatotropin; Thomas R. Sharp1; Ronald Morris1, George J. Horan1; Linda H. Pezzullo1; Justin G. Stroh1; Pfizer Central Research, Groton, CT

MPE 204 Characterization of plasma derived and recombinant blood coagulation factor IX by means of high resolution UV MALDI mass spectrometry and CF PSD fragment ion analysis; Omar Belguem1; Andreas Rizzi2; Guenter Allmaier3; Helen Montgomery4; Andrea Buchacher5; Katharina Pock5; Djuro Josic6; University of Vienna, Vienna, Austria; Kratos Analytical, Manchester, UK; Octapharma Pharmazeutika, Vienna, Austria

MPE 205 Detailed Characterization of Protein Glycosylation Using a Combined Approach of Nanoscale Data-Dependent LC/MS/MS and MS/MS of Methylated Oligosaccharides; Douglas M. Sheeley1; R. Kevin Blackburn1; M. Arthur Moseley2; Glaxo Wellcome Inc., RTP, NC

MPE 206 Clinical Diagnosis of Transferrin Isoforms by LC-MS; A New On-Line Assay for Analytes in Complex Matrices; H. Robert Bergen, III1; John F. O'Brien1; Kenneth L. Johnson1; Stephen Naylor1; John F. O'Brien1; Joyce A. Tinsley1; Mayo Clinic/Foundation, Rochester, MN

MPE 207 Identification of Modifications in Adult Human Lens Beta-Crystallins; Zhangli Zhang1; Jean B. Smith1; David L. Smith1; University of Nebraska, Lincoln, NE

MPE 208 Identification of the Localized Thermally Stable Regions of Human alpha-Crystallin; Azeeem S. Hasan1; Jiong Yu1; Jean B. Smith1; David L. Smith1; University of Nebraska, Lincoln, NE

MPE 209 Identification of in vivo post-translational modifications at Lys 92 of human alpha B-crystallin: distinguishing features of MS/MS fragmentation patterns for carbamylated and acetylated peptides; Veniamin N. Lapko1; David L. Smith1; Jean B. Smith1; University of Nebraska, Lincoln, NE

MPE 210 Identification of Degraded Proteins in Post-Surgery Cataracts by MALDI-TOF Mass Spectrometry; Christine Colvis1; Yvonne Douglass-Tabor1; Karen Werth1; Nancy Vieira2; Jeffrey Kowalak3; Alireza Janjani4; Alfred Yergey5; Donita Garland2; National Eye Institute, NIH, Bethesda, MD; National Institute of Child Health and Human Devel, Bethesda, MD; National Institute of Mental Health, NIH, Bethesda, MD; University of Modena, Modena, Italy

MPE 211 Amide Bond Fragmentation of Proteins during Analysis by Electrospray Ionization Mass Spectrometry-TOF; Robert W. Johnson1; Alex Buko1; Rohinton Edalji1; Richard Smith1; Abbott Laboratories, Abbott Park, IL

MPE 212 Precursor Ion Scan and SIM Analysis of Glycoprotein Using A Hybrid Quadrupole Time of Flight Mass Spectrometer (QuTOF); Jie Y. Zhuo1; Tina Settineri1; Lydia Nuwaysir2; George Scott2; PE ScieX, Concord, Ontario, Canada; PE Biosystems/PE ScieX, Foster City, CA

COMBINATORIAL CHEMISTRY, 213 - 220

MPF 213 Optimizing Quality Control of Combinatorial Libraries with SFC/MS; Manuel C. Ventura1; William P. Farrell1; Christine M. Aurigenerra1; Xiaobing Xiong1; Michael O. Osonburi1; Rodolfo Lopez Jr.1;
MONDAY POSTERS

7:30 – 8:00 am SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm REMOVE POSTERS. Please leave posters for the full day.

Michael J. Greig1; Agouron Pharmaceuticals, La Jolla, CA
MPG 214 A Universal Threshold Ionizer for High Throughput Combinatorial Library Analysis; Karl A. Hanold1; Matthew D. Evans2; Yong Liu1; Jack A. Syage1; Syagen Technology, Inc., Tustin, CA
1:30 – 3:00 pm

Automated High Throughput Structure Elucidation of Compounds from Combinatorial Libraries by Mass Spectrometry: Shared Chemical History Approach; Olga Isakova1; Nikolai Sepetov1; NanoSyn Inc, Tucson, AZ
MPG 216 LC/ELSD/MS for purity and quantity analysis in combinatorial library using a single calibration curve; Liling Fang1; Jianmin Pan1; Prashanth Mack1; Bing Yan1; Axys Advanced Technologies, Inc., South San Francisco, CA

A Novel Approach to High-Throughput Quality Control of Parallel Synthesis Libraries; Nikhil Shah1; Ken Tsutsui1; Amy Lu1; Jennifer Davis1; Randall Scheurman1; William Fitch1; Affymax Research Institute, Santa Clara, CA
MPG 217

Assessing the Stability of Combinatorial Library Synthesis Products Stored in Solution at -70°C; K. Eric Milgram1; Michael Greig1; Agouron Pharmaceuticals, San Diego, CA
MPG 218

A Rapid Screening Method for Evaluating Combinatorial Mixtures Based on Cross-Correlation of Measured and Predicted Electrospray Ionization Mass Spectra; Nathan Yates1; Drew Roberts2; Daniel Wislocki2; Patrick Griffin2; Merck Research Laboratories, Rahway, NJ
MPG 219

Phase I and Phase II Metabolism Screening of Combinatorial Libraries Using Primary Fluorescence and Secondary LC/MS Screening Techniques; John A. Josey1; Kathy A. Hahn1; Jeffrey D. Yingling1; Gary P. Hingoran1; Larry E. Burgess1; Array BioPharma, Inc., Boulder, CO
MPG 220

NON-COVALENT COMPLEXES, 221 - 246

Detection of Oligonucleotide: Ligand Complexes Using Electrospray Ionization Mass Spectrometry (DOLCE-MS); Jessica M. Robinson1; Michael J. Greig1; Agouron Pharmaceuticals, San Diego, CA
MPG 221

New Approaches to the Study of Non-Covalent DNA-Drug Complexes; Amit Kapur1; Jennifer L. Beck1; Margaret M. Shell1; University of Wollongong, Australia
MPG 222

Detection of Noncovalent Complex between alpha-Amylase and its Microbial Inhibitor Tendamistat by ESI-MS; Victor J. Nesati1; Shin Numao1; Bruce A. Collings1; Donald J. Douglas1; University of British Columbia, Vancouver, BC, Canada
MPG 223

Rescheduled as MPA 026
MPG 224

Detection of intact megadalton protein assemblies by electrospray mass spectrometry; Albert J. R. Heck1; Cees Versluis1; Willem J. H. van Berkell1; Robert H. H. van den Heuvel1; Utrecht University, The Netherlands; Wageningen University, The Netherlands
MPG 225

ESI-MS Analysis of Noncovalent Interactions within the Electron Transferring Flavoprotein; Heidi Hoard1; Linda M. Benson1; Gerald Vockley1; Stephen Naylor1; Mayo Clinic/Foundation, Rochester, MN
MPG 226

Evaluation of Ligand Binding to the Non-Covalent Transthyretin Tetramer; Margaret G. McCampong1; Paula Tito1; Jeffrey W. Kelly1; Carol V. Robinson1; OMS, University of Oxford, UK; Scripps Research Institute, La Jolla, CA
MPG 227

Binding of selected carbohydrates to apo-concanavalin A studied by electrospray mass spectrometry; Rob J. Vreekens1; William D. van Dongen1; Cornelis Versluis1; Albert J.R. Heck2; TNO Pharma, Zeist, The Netherlands; Utrecht University, Biomolecular Mass Spectrometry, Utrecht, The Netherlands
MPG 228

Identification and Structural Characterization of a Non-covalent Dimer Complex of Lung Surfactant Protein SP-C by FT-ICR-ESI-MS; Andreas Seidl1; Giuseppina Maccarrone1; Kai Bruns2; Uwe Krüger2; Klaus P. Schäfer2; Michael Przybyski2; University Konstanz, Konstanz, Germany; Byk Gulden Lomberg GmbH, Konstanz, Germany
MPG 229

Preservation and Detection of Specific Immune Complexes by Matrix-assisted Laser Desorption Ionization Mass Spectrometry; Kevin M. Downard1; Janna G. Kiselar1; Albert Einstein College of Medicine, Bronx, NY
MPG 230

Determination of Peptide-Peptide Interaction by Matrix Assisted Laser Desorption/Ionization; Amina S. Woods1; NIDA Intramural Program, NIH
MPG 231

Influence of Experimental Parameters on the Determination of Surface-Protein Retention by MALDI-MS; Gary R. Kiniel1; Jim Zhang1; Richard B. Timmons1; Haibo Qiu1; University of Texas, Arlington, TX
MPG 232

ESI-FTICR Characterization of Supramolecular Coordination Compounds; Ulla N. Andersen1; Marco Ziegler1; J. J. Miranda1; Darren W. Johnson1; Kenneth N. Raymond1; Julie A. Leary1; University of California, Berkeley, CA
MPG 233

Oligomerization of Calcium-Binding Proteins MRPI and MRP14 in the Presence of Zinc Ions: Comparison of the Non-Covalent Complexes by MALDI-MS and ESI-MS; Kerstin Strupat1; Franz Hillenkamp1; Helene Rogniaux2, Alain Van Dorsselaer3; Johannes Roth3; Thomas Vogl4; Institute for Medical Physics & Biophysics, Münster Germany; Lab. de Spectrometrie de Masse Bio-Organique, Strasbourg France; Institute of Experimental Dermatology, Münster Germany
MPG 234

Interface structure of cystatin-papain complex studied by H/D exchange and hexapole-CID with ESI-FTICR MS; Satoko Akashi1; Koji Takio1; RIKEN, Wako, Saitama, Japan
MPG 235

Determination of the Mutual Binding Sites in Binary and Ternary Complexes of p19 Tumor Suppressor Protein, Cyclin-Dependent Kinase 6, and Cyclin D2 by Solution-Phase H/D Exchange and Online HPLC ESI FT-ICR Mass Spectrometry; Fei He1; Weiqun Li1; Mark R. Emmett1; Alan G. Marshall1; Wei Zhang2; Ernest D. Laue2; Peter J. Dornaille3; NIIMPL, Florida State University, Tallahassee, FL; University of Cambridge, Cambridge, UK; DuPont Pharmaceuticals, Wilmington, DE
MPG 236
MONDAY POSTERS

7:30-8:00 am  SET UP POSTERS, Exhibit Hall B
8:45-10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30-3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00-6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

MPG 237  The Effects of pH on the Kinetic Reaction Mechanism of Myoglobin Unfolding Studied by Time-Resolved ESI MS; Konermann, Lars1; Sogbein, O. Oyebola1; Simmons A. Douglas1; University of Western Ontario, London, Canada

MPG 238  Use of mass spectrometry for the characterization of nuclear receptors and their non-covalent complexes with ligands and corepressors; Noelle Potier1; William Bourguet1; Carole Illis2; Virginie Andry2; Dino Moras2; Alain Van Dorselaer1; Laboratoire de Spectrométrie de Masse Bioorganique, Strasbourg, France; Laboratoire de Biologie Structurale, Illkirch, France

MPG 239  A Mass Spectrometric Examination of the Quaternary Structure of the Nitric Oxide Synthase Oxygenase Domain: The Effect of pH on Monomer-Dimer Equilibrium; Jeffrey C. Smith1; Stephen P. Rafferty1; Timothy R. Crole1; Raymond E. March1; Trent University, Peterborough, ON, Canada

MPG 240  New Evidence for the Location of Bicyclomycin Binding to Rho Protein in E. coli; Matthew Openshaw1; Fabien Vincent2; Mark Trautwein3; Simon J. Gaskell4; Harold Kohn5; William R. Widger6; UMIST, Manchester, UK; University of Houston, Houston, TX; University of North Carolina, Chapel Hill, NC

MPG 241  Studies on protein/ligand interaction using ESI-MS: Specific interaction between octylsulfonic acid and basic residues of lysozyme; Hideaki Ichiba1; Mitsuao Takayama1; Takehiko Yajima2; School of Pharmaceutical Sciences, Toko University, Chiba, Japan

MPG 242  Determination of Ligand Binding to Two Pockets on the Surface of the Tetanus Toxin Targeting Domain; Loren C. Zeller1; Felicie Lightstone1; Rod Ballhorn1; Dana Roe2; Sunia Afzal2; Lawrence Livermore National Laboratory, Livermore, CA; Sandia National Laboratory, Livermore, CA; Bruker Daltonics, Billerica, MA

MPG 243  Isotopic Resolution of Noncovalent Complexes of Metalloproteins; P. Kristina Taylor1; Donald M. Kurtz1; J. Jonathan Amster1; University of Georgia, Athens, GA

MPG 244  Non-Covalent Complexes of Iron-Dependent Enzymes Using Nanoflow ESI TOF Mass Spectrometry; Helena Hernandez1; Kirsty S. Hewitson1; Malkit Sam1; Christopher J. Schofield1; Peter L. Roach1; Carol V. Robinson1; Oxford University, Oxford, UK; Southampton University, Southampton, UK

MPG 245  A MALDI-Based Combinatorial Chemistry Approach for Studying the Folding and Stability of a Multimeric Protein; Bassam M. Nakhle1; Michael C. Fitzgerald1; Duke University, Durham, NC

MPG 246  Observation of non-specific protein cluster ions in MALDI: Abundances, stabilities and dynamical aspects; Vincent Livaditis1; Jean-Claude Blais2; Jean-Claude Tabet1; Université Pierre et Marie Curie, Paris, France; CNRS, Paris, France

Spectrometry-II: Carl G. Johnson1; Timothy I. Eglington1; Naohiko Ohkouchi1; Woods Hole Oceanographic Institution, Woods Hole, MA

Potent Eicosanoid Chemotactants, Oxosceratetraenoic Acids, are Generated by Eosinophil Peroxidase via Formation of Reactive Nitrogen Species; Jennifer C. MacPherson1; Stanley L. Hazen1; Cleveland Clinic Foundation, Cleveland, OH

The Long-term Reproducibility of a Biodetector Built Around a Thermal Hydrolysis-Methylation (THM) Ion Trap MS; Ming Xu1; Kent J. Voorhees1; Ted L. Hadfield1; Colorado School of Mines, Golden, CO; US Army/AFIP, Washington, DC

Characterization of Triacylglycerols in Natural Fats and Oils by Neutral Loss and Product Ion ESI-MS3; Craig A. Dorschel1; Waters Corporation, Milford, MA

Analysis of triglycerides in thirteen edible oils using LC/APCI-MS; Naoto Shimizu1; Shigeki Daishima2; Kenji Yamaguchi2; Akemi Fukushima3; Kinya Tsuchiya2; Yokogawa Analytical Systems, Japan; The Nissin Oil Mills, Japan

Cuticular wax - initial defense in the battle against pathogenic fungi; Christian Sehou1; Helge Figsärd1; Rice National Laboratory, Roskilde, Denmark

FABMS and HPLC Profiles of Fungal Lipids; Petra Miketova1; Karl H. Scharra1; K. I. M. Moore1; Alexander Jegorov2; Vladimir Matha2; University of Arizona, Tucson, AZ; Academy of Science, C. Budejovice, Czech Rep.

Interrogation of Intact Microorganisms by Static Secondary Ion Mass Spectrometry; Jani C. Ingram1; F. S. (Rick) Colwell1; R. Michael Lehman1; William F. Bauer1; Andrew D. Shaw1; INEEL, Idaho Falls, ID; Westminster Christian Academy, St. Louis, MO

Negative Regulation of Cytosolic Phospholipase A2 (cPLA2) by Melatonin Monitored by GC/NCI-MS and HPLC/ESI-MS; Beibei Li1; Hongjian Zhang1; Mohammed Akbar1; Hee-Yong Kim1; Section of MS, LMBB/NIAAA, NIH, Rockville, MD

Monitoring phosphatidylserine decarboxylation by liquid chromatography-electrospray ionization mass spectrometry; Ilonone H. Hamilton1; Hee-Yong Kim1; Laboratory of Membrane Biophysics and Biochemistry, Rockville, MD

A Rapid Method for the Accurate Assessment of Diglycerides in Environmental Matrices; Cory A. Lytle1; Ying Dong M. Gan1; David C. White1; University of Tennessee, Knoxville, TN

A Method for Direct Characterization and Quantification of Lipid Species by Atmospheric Pressure Chemical Ionization Liquid Chromatography/Mass Spectrometry; Ying Yang1; Givaudan Roure Corp., Cincinnati, OH

Small Bore HPLC Column Advantages for the Analysis of Phospholipids and Sphingolipids by LC-MS; Charles V. Bartlett1; Tom McNabb2; Keith J. Duffy1; Restek Corporation, Bellefonte, PA; Gellex Pharmaceuticals, Inc., Waltham, MA

Separation, Identification and Quantification of Phosphatidylcholines Using High Pressure Liquid Chromatography - Mass Spectrometry; Pedro
MONDAY POSTERS

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8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

**MPH 261**
Positive and Negative Electrospray Ion Trap Mass Spectrometry in the Characterization of Glycophospholipid Molecular Species and their Seasonal Changes in the Heteropteran Insects; **Petra Berkova**; **Petr Simek**; Magdalena Hodkova; University of Chemical Technology, Czech Republic; Institute of Entomology, Czech Republic

**MPH 262**
An ESI-FTICR tandem mass spectrometry study of natural and photo-oxidized egg glycerol lipids; **Oscar E. van den Brink**; **Marc C. Duursma**; Jaap J. Boon; Ron M.A. Heeren; FOM Institute for Atomic and Molecular Physics, The Netherlands

**MPH 263**
An ESI-FTMS study of the phospholipid composition of *E. coli* cell division sites; **Cecile-Marie Koppelman**; Tanneke den Blauwen; Nanne Nanninga; Marc C. Duursma; Jaap J. Boon; Ron M.A. Heeren; Swammerdam Institute for Life Sciences, UvA, Amsterdam. The Netherlands; FOM-Institute for Atomic and Molecular Physics, Amsterdam. The Netherlands

**MPH 264**
Analysis of sulfatide by ESI-MS from developing rat and MS brain; **Beth N. Marbois**; Arvan Fluharty; Sujna Raval-Fernandes; Leonhard H. Rome; Kym F. Faul; UCLA, Los Angeles, CA

**MPH 265**
Tandem-MS analysis of globotetrasyl ceramide based glycoconjugates from natural globotetrasyl ceramide; **Ling-Jie Meng**; Myl Mylvaganam; Ying Yang; Clifford A. Lingwood; University of Toronto, Toronto, Canada; The Hospital for Sick Children, Toronto, Canada

**MPH 266**
Tandem LC/MS Analysis of Cholesteryl Linoleate and Arachidonate Oxidation Products by Cationization with Silver Tetrafluoroborate in Nonpolar Solvents; **David L. Hachey**; Christine M. Havrilka; Ned A. Porter; Vanderbilt University, Nashville, TN

**MPH 267**
Identification of Unusual 7-Oxynorleucine Acid Sulfates in a Patient with Nieman-Pick Disease, Type C1; **Gunvor Alveius**; Ola Hjalmarsson; William Griffiths; Ingemar Björkhem; Jan Sjövall; Huddinge University Hospital, Huddinge, Sweden; Sahlgrenska University Hospital, Göteborg, Sweden; Karolinska Institutet, Stockholm, Sweden

**MPH 268**
Measurement of cis- and trans- Lycopenes in Human Prostate Tissue Using APCI LC-MS; **Xiaoying Xu**; Long wen Chen; Maria Stacewicz-Sapuntzakis; Phyllis E. Bowen; Richard B. van Breemen; University of Illinois at Chicago, Chicago, IL

**NUCLEIC ACIDS, 269 - 294**

**MPI 269**
Differential of Diastereomeric Benzog[hi]fluorethene Tetraols by Matrix-Assisted Laser Desorption Ionization (MALDI) and Post-Source Decay (PSD); M. Paul Chiarelli; Duane M. Huffer; Chang Hui-Fang; Cho Bongsup; Loyola University, Chicago, IL; University of Rhode Island, Kingston, RI

**MPI 270**
Analysis of the in vitro Digestion of Modified DNA to Oligonucleotides by LC-MS and LC/MS/MS; **Christine L. Andrews**; Andreas Harsch; Paul Vouros; Barnett Institute and Northeastern University, Boston, MA

**MPI 271**
MALDI-TOF-MS of Enzymatically and Chemically Cleaved RNA; **Ralf Hartner**; Julia Gross; Beatrice Spottke; Franz Hillenkamp; Inst. for Med. Physics & Biophysics, Minster, Germany

**MPI 272**
Identification of the Apurinic Sites in Modified Oligodeoxynucleotides by MALDI-TOF MS and ES-MS; **Li-Kang Zhang**; Kimberly A. Chapman; Michael L. Gross; Erocole L. Cavaleri; Eleanor G. Rognan; Washington University, St. Louis, MO; University of Nebraska, Omaha, NE

**MPI 273**
Analysis of the stereoisomers of thymine glycol by LC/MS/MS; **Charles R. Iden**; Robert A. Rieger; State University of New York, Stony Brook, NY

**MPI 274**
Detection of Halogen-Nucleoside Adducts by LC/ESI/MS/MS and GC/MS: Implications for Carcinogenesis at Sites of Inflammation; **Jaeman Byun**; Jeffrey P. Henderson; Jay W. Heinecke; Washington University, St. Louis, MO

**MPI 275**
Identification of new adducts of thymidine-3'-monophosphate, 2'-deoxyuridine-3'-monophosphate, and 2'-deoxyadenosine-3'-monophosphate with phosphoramidate mustard by electrospray LC/MS; **Zhaoyang Li**; Kenneth K. Chan; Biogen Inc., Cambridge, MA; The Ohio State University, Columbus, OH

**MPI 276**
HPLC-MS/MS Identification of Positionally Isomeric Benzo[c]phenanthrene Diol Epoxide Adducts in Duplex Oligonucleotides; **Andreas Harshc**; Jane M. Sayer; Donald M. Jerina; Paul Vouros; Northeastern University, Boston, MA; NIDDK at NIH, Bethesda, MD

**MPI 277**
Development of a liquid chromatography-mass spectrometry method for the detection of N7-(2-hydroxyethyl)guanine adducts in DNA; **Pao-Chi Liao**; Ching-Ming Li; Shu-Hui Chen; National Cheng Kung University Medical College, Tainan, Taiwan, ROC

**MPI 278**
Attomole detection and characterization of Estrogen-DNA-adducts with Nano-LC-ES MS/MS column-switching; **Jan Embrechts**; Ilse Hoes; Filip Lemiere; Walter Van Dongen; Eddy L. Emsmans; University of Antwerp (RUA), Antwerp, Belgium

**MPI 279**
A search for cross-linked DNA-adducts of melphalan: a novel Lc-exoeltro spray tandem MS approach; **Filip Lemiere**; Ilse Hoes; Jan Embrechts; Walter Van Dongen; Eddy L. Emsmans; Dirk Van Bockstaele; Zwi Berneman; University of Antwerp (RUA), Antwerp, Belgium; University of Antwerp (UA), Wilrijk, Belgium

**MPI 280**
Cyclooxygenase-induced DNA Oxidation Measured Using LC-MS-MS; **Dejan Nikolic**; Richard B. van Breemen; University of Illinois College of Pharmacy, Chicago, IL

**MPI 281**
MALDI-TOF MS sequencing of oligonucleotides containing oxidative lesions; **Natalia Y. Tretjakova**; John S. Wishnow; Steven R. Tannenbaum; MIT, Cambridge, MA

**MPI 282**
Measurement of 8-oxo-7,8-dihydro-2'-deoxyguanosine and Screening for 8-oxo-2'-deoxyadenosine in Urine by HPLC- Tandem Mass
Spectrometry; Allan Weinmann1; Dorthe Belling1; Henrik E. Poulsen1; Rigshospitalet, Copenhagen University Hospital, Copenhagen, Denmark

MPI 283 Measuring Oxidized Nucleosides in Normal and Damaged DNA Using LC-MS-MS; Yousheng Hua1; Yanan Yang1; Judi L. Bolton1; Richard B. van Bremen1; University of Illinois, Chicago, IL

MPI 284 Comparison of the CID fragmentation of normal and carba-cyclic analogs of nucleosides and the influence of a carba-cyclic nucleoside on sequence specific ions from an oligonucleotide; Robert A. Rieger1; Charles R. Iden1; State University of New York, Stony Brook, NY

MPI 285 Fragmentation Mechanism of Oligodeoxynucleotides Studied by HDX Exchange and Tandem Mass Spectrometry; Katty X. Wan1; Julia Gross2; Franz Hillenkamp2; Michael L. Gross2; Washington University, St. Louis, MO; University of Münster, Münster, Germany

MPI 286 Metastable decay of negatively charged DNA analyzed with UV-MALDI-PSD and deuterium-exchange; Julia Gross1; Katty X. Wan2; Michael L. Gross2; Franz Hillenkamp2; Institute for Medical Physics and Biophysics, Münster, Germany; Washington University, St. Louis, MO

MPI 287 UraCil - A Neutralization - Reionization M.S. and Computational Analysis; Jill K. Wolken1; Frank Turecek1; University of Washington, Seattle, WA

MPI 288 The Gas-phase Chemistry of Radical-cation Clusters of Guanosine and Deoxyguanosine with Substituted Naphtalenes and Sipapinic acid; Giovanni Sindona1; Anna Napoli1; Angelo Liguori1; Universita della Calabria, Rende, Italy

MPI 289 Antisense Oligonucleotide Separations Utilizing Capillary Electrophromatography - Electrospray Mass Spectrometry; Hans J. Gaus1; Lendell L. Cummins2; Isis Pharmaceuticals, Carlsbad, CA

MPI 290 Simultaneous determination of nucleoside and nucleotide analogs in rat plasma and human cellular extracts at nanomolar levels by using ion-pairing HPLC/Ms/MS; Pziwa N. Pong1; Zongwei Cal1; Thimyra C. Burnette1; Achintyka K. Sinhababu1; Glaxo Wellcome, RTP, NC

MPI 291 Characterization of the UV-Crosslinked E. coli Uracil-DNA Glycosylase-dT32, Nucleoprotein Interface by MALDI-MS and ESI-MS/MS; Philip R. Galten1; Dale W. Mustaugh2; Douglas F. Barofsky3; Oregon State University, Corvallis, OR

MPI 292 Multiplexed Gene Expression Analysis by MALDI-TOF Mass Spectrometry; W. Travis Berggren1; Timothy J. Griffin1; Tetsuo Takova1; Lloyd M. Smith1; University of Wisconsin, Madison, WI; Third Wave Technologies Inc., Madison, WI

MPI 293 Composition Assignment of DNA Oligomers by High Mass Accuracy MALDI Analysis; William K. Russell1; John M. Koomen1; Justin M. Hetrick1; David H. Russell1; LBMS, Texas A&M University, College Station, TX

MPI 294 Analysis of DNA up to 30kDa using ESI-ion trap Mass Spectrometry; Stephanie Hahmer1; Andrea Schneider2; Arnd Ingendoh1; Jörg Mosner2; GAG Bioscience GmbH, Bremen, Germany; Braker Daltonik GmbH, Bremen, Germany

COMPUTER APPLICATIONS, 295 - 320

MPJ 295 A novel mass spectrometry data compression algorithm; Victor V. Lalko2; Robert J. Cotter1; Johns Hopkins University, Baltimore, MD

MPJ 296 Simulation of a Unique Quadrupole Mass Filter Using SIMION 7.0; Steven M. Colby1; John D. Prestage2; Scientific Instrument Services, Inc., Ringoes, NJ; NASA Jet Propulsion Laboratory, Pasadena, CA

MPJ 297 Solvent-Assisted Intramolecular Proton Transfer (Proton Switching) in Peptides; Christopher E. Rodriguez1; Alwin Cunje1; Tamer Shoeb1; Ivan K. Chu1; Alan C. Hopkinson1; K. W. Michael Siu1; York University, Toronto, Canada

MPJ 298 NIST Search Program: Standard Corporate Method for Searching EI Databases; James L. Little1; Eastman Chemical Company, Kingsport, TN

MPJ 299 EI-Spectra evaluation using library search, PCA spectra analysis and computer assisted fragmentation prediction; Alexei Nikiforov1; Robert Mistrik2; University Vienna, Vienna-9, Austria; High Chem. Id., Bratislava, Slovakia

MPJ 300 Application of Visual Basic for Intelligent Automation of High Throughput LC-MS Analysis; Bernard K. Choi1; David M. Hereules2; Arkady I. Gusev1; Enrique L. Michelotti2; Blanca Martinez2; Tianlan Zhang3; Mark Eisenschmid4; Vanderbilt University, Nashville, TN; The Rohm and Haas Company, Spring House, PA

MPJ 301 Automation Software for Evaluation of Mass Spectral Data; Leslie G. Partridge1; Richard D. Gless1; Don R. James2; Karl J. Fisher2; Cambridge Discovery Chemistry, Richmond, CA

MPJ 302 Computer Applications Developed for Affinity Selection Mass Spectrometry; Lan Gao1; Xueheng Cheng1; HouJun Yang1; Mark Schurda1; Daniel Burns1; Abbott Laboratories, Abbott Park, IL

MPJ 303 Eva_Lution: A software tool for high-speed quantitative processing and review of LC/MS data collected from high-throughput ADMT screens; Kevin M. Whalen1; Katrina J. Rogers1; John S. Janiszewski1; Mark J. Cole1; Elbridge W. Luther1; Eva Duchoslav2; Pfizer, Groton, CT, PE SCIEX, Ontario, Canada

MPJ 304 Mass Spectrometry Software Validation for Quantitative Bioanalysis; Stephen D. Clarke1; Jeremy Cook1; Terry Norton1; Ian Smith1; Jane Shackleton1; Karen Tennant1; York Bioanalytical Solutions, York, UK

MPJ 305 The Effect of Real Time and Post-Run Data Smoothing on the Accuracy and Precision of Quantitative Data by LC/MS; Paul A. Zavoritos1; Agilent Technologies, Toronto, Canada

MPJ 306 Evaluation of Whole Protein Quantitation by Four Commercial Protein-Processing Algorithms; Adrian R. Woolfitt1; John R. Barr1; Maria Ospina1; Vince L. Maggio1; Uwe Kobold2; Centers for Disease Control, Atlanta, GA; Roche, Germany

MPJ 307 Use of Cumulative Distribution Functions to Determine Purity and Homogeneity of Proteins from MALDI-TOF Spectra; Alfred L. Yergey1; Paul S.
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**MONDAY POSTERS**

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<tr>
<td>MPJ 308</td>
<td>Deconvolution of Isotopic Distributions in MALDI and MALDI-PSD Analysis of Peptides</td>
<td>Marco Welchowski; Ralf Hoffmann; Martin Hubert; Bernhard Spengler; Biomedical Research Center, Univ. of Duesseldorf, Germany; Inst. of Laser Medicine, Univ. of Duesseldorf, Germany; University of Wuerzburg, Germany</td>
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<tr>
<td>MPJ 309</td>
<td>Rapid Analysis of Low Resolution ES-LC/MS Runs to Determine Component Molecular Weights</td>
<td>John O. Pearcy; Curtis Croker; Terry Lee; Roger Moore; City of Hope/Beckman Research Institute, Duarte, CA</td>
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<tr>
<td>MPJ 310</td>
<td>Maximizing proteomic information from MS data: Enhancements to Protein Prospector, a suite of programs for mining genomic databases</td>
<td>Richard Jacob; Peter R Baker; Leon Huang; Michael A Baldwin; UCSF, San Francisco</td>
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<td>MPJ 311</td>
<td>Effects of Isotope Distributions on the Mass Accuracy of PSD with MALDI TOF MS</td>
<td>Andrew R. Bowdler; Emmanuel Raptakis; Ian Brookhouse; Kratos Analytical Ltd, Manchester, UK</td>
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<tr>
<td>MPJ 312</td>
<td>A Computer Program for De Novo Peptide Sequencing Using MS2 and MS3 Data Acquired on an Ion Trap Instrument</td>
<td>Zhongqi Zhang; James S. McElvain; Amgen, Thousand Oaks, CA</td>
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<td>MPJ 313</td>
<td>Validation of database sequence matches using automated de novo peptide sequencing</td>
<td>Richard S. Johnson; J Alex Taylor; Immunex Corporation, Seattle, WA</td>
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<td>MPJ 314</td>
<td>Direct software interpretation of de novo sequence from ESI-MS/MS data for novel protein identification using BLAST</td>
<td>Robert Bordoli; Jon Cottrell; Eugene Kapp; James Langridge; R. Rachubinski; R. Wozniak; Jennifer Smith; John Skilling; Micromass, UK; University of Alberta, Canada; Maximum Entropy Data Consultants, UK</td>
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<td>MPJ 315</td>
<td>Analysis of Enzymatically Digested Proteins Using a 9.4 T FT-ICR Mass Spectrometer</td>
<td>Magnus Palmblad; Magnus Wetterhall; Jonas Bergquist; Karin Markides; Per Hakansson; Uppsala Universitet, Sweden</td>
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<td>MPJ 316</td>
<td>A spreadsheet approach to bacterial identification based on MALDI-TOF spectra of whole cells</td>
<td>Leslie A. Harden; Andrew Lieberman; Robert Mandrell; William F. Haddon; Western Regional Research Center, ARS, USDA, Albany, CA</td>
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<td>MPJ 317</td>
<td>Data Handling for Identification of Bacteria by Pattern Recognition Techniques</td>
<td>Martha L. Gay; Denis Andrzejevski; Frederick S. Fry; Ben J. Tall; Steven M. Musser; Food and Drug Administration, Washington, DC</td>
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<tr>
<td>MPJ 318</td>
<td>The rapid identification of microorganisms by mass spectrometry</td>
<td>Therese M. McKenna; Martin S. Lunt; Michael Morris; Martin A Claydon; John J Bright; Micromass UK Ltd, Manchester, UK; BARC Manchester Metropoli, Manchester, UK</td>
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**Public Health Laboratory, London UK; Micromass UK Ltd, Manchester UK**

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<td>MPJ 320</td>
<td>Use of a Fully Automated Peak Detection and Characterization Algorithm on Different MALDITOF-MS Data Types</td>
<td>Kristin H. Jarman; Nancy B. Valentine; Catherine E. Petersen; Karen L. Wahl; Pacific Northwest National Laboratory, Richland, WA</td>
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**TUESDAY POSTERS**

**TPA 001** Historical Highlights of the Early Days of SIMS; Bryan L. Benzé; Sarnoff Corporation, Princeton, NJ

**TPA 002** Mass Spectrometry in an Adversarial Context: A Proposal for Demonstrating Method Fitness; Robert Betham, Joe Boisson, John Chakel, Jane Gale, David Heller, Steven Musser, Phil Price, Stephen Stein

**TPA 004** Pentai fluorophenylpropiony1 Stationary Phases to Improve the HPLC/ESI/MS Analysis of Cocaine and Egonine Methyl Ester; Shane Needham; Patrick Jeanville; Keith Duff; Phyllis Brown; Pfizer Inc., CT; Restek Corp., PA; University of Rhode Island, Providence, RI

**TPA 005** Measurement of subpicomolar levels of triaminolone acetinate in human bronchoalveolar lavage fluid by gas chromatography-mass spectrometry; Walter C. Hubbard; Mark C. Liu; Carol Bickel; Robert P. Schleimer; Dominick Argenti; Don Heald; JHMI Asthma and Allergy Center, Baltimore, MD; Aventis Pharmaceuticals, Collegeville, PA

**TPA 006** A High Throughput and Automated In-Line Extraction LC-LC-MS/MS Method for the Quantitation of Nalmefene, Narlfonine, Naloxone and Naltrexone (4N) in *vivo* Studies; Yong-Xi Li; Tiang-Sheng Lu; Thomas J. Fitzgerald; Stephen R. Beck; Ricerca, LLC, Painesville, OH

**TPA 007** Measurement of Urinary Trimethylamine and Trimethylamine N-Oxide by FAB; Orval A. Marner; Luc Choiniere; Eileen Treacy; McGill University, Montreal, Canada

**TPA 008** Characterization and Quantitation with Confirmation of Six Related Penicillins with LC/MS on a Single Quadrupole Mass Spectrometer; Kevin C. Credlin; Emily Sible; Waters Corporation, Pasadena, CA

**TPA 009** Determination of the Enantiomers of Amphetamine in Human Plasma by Chiral Gas Chromatography/Mass Spectrometry; Shari L. Bozich; Bruce J. Hidy; Rand G. Jenkins; PPD Development, Richmond, VA

**TPA 010** Detection of GBH in urine without sample preparation; Philippe Moutay; Philippe Parsy; Mass Evolution, Inc., Houston, TX; I.D. Analytical Services, Poinieres, France

**TPA 011** Determination of 17a-Ethyl Estradiol Sulfates in Human Serum by Selective Enzyme Hydrolysis using Gas Chromatography/Mass Spectrometry; Bruce J. Hidy; Shari L. Bozich; Rand G. Jenkins; PPD Development, Richmond, VA

**TPA 012** Quantitative Determination of a Novel Peptide, Conantokin G, in Rat Plasma and Serum by Liquid Chromatography-Tandem Mass Spectrometry; Lixiang Jiang; Rodger L. Foltz; Michael E. Morgan; R. Tyler McCabe; Northwest Bioanalytical, Salt Lake City, UT; University of Utah, Salt Lake City, UT; Cognetix Inc., Salt Lake City, UT

**TPA 013** Cocaine N-oxide in Human Plasma: Is There a Need to Use LC/MS-MS Rather Than GC/MS for Accurate Determination of Cocaine and Benzoylecgonine?; Shen-Nan Lin; David E. Moody; Rodger L. Foltz; University of Utah, Salt Lake City, UT

**TPA 014** Quantitative enantioemic analysis of drugs via FT-ICR MS; Michelle Stone; Gabriela Grigorean; Carlito B. Lebrilla; University of California, Davis, CA

**TPA 015** Quantitative Analysis of Pyridostigmine in Guinea Pig Plasma Using LC/MS; I. Richard Smith; Ming L. Shih; Benedict R. Capacio; William D. Korte; US Army Medical Research Inst. of Chemical Defense, APG, MD; California State University, Chico, CA

**TPA 016** The Use of GC/MS to Determine the Dopamine Production of Differentiated Stem Cells; Jan R Crowley; David Gottlieb; Karen O'Malley; Julia Nash; Meenakshi Rao; Andrew St. Clair; John Turk; Washington University, St. Louis, MO

**TPA 017** LC-MS Method Development for the Investigation of NAD Formation in Cultured Cells; Jason J. Evans; S. P. Markey; Melvin P. Heyes; Cai Y. Chen; Tao-Chin L. Wang; National Institute of Mental Health, Bethesda, MD; FDA, Rockville, MD

**TPA 018** A Novel, Rapid Extraction Method to Reduce Ionization Suppression Caused by the Presence of the Dosing Vehicle in Biological Samples; Don Boo; Diane Tutko-Francisco; PPD Discovery Inc., Middleton, WI

**TPA 019** The Application of ESI-TOF for the Identification and Quantitation of the Anabolic Steroid Stanozolol and Its Metabolites in Horse Urine; Bruno Cassetta; Mark H. Allen; PE Biosystems, Monza, Italy

**TPA 020** Development of a High-Resolution Capillary Gas Chromatography/High-Resolution Mass Spectrometry Method for the Analysis of the Tobacco-specific Nitrosamine NNAL in Human Urine; Lanqing Wang; John T. Bernert; Centers for Disease Control and Prevention, Atlanta, GA

**TPA 021** Analysis of fluasterone from human plasma using solid phase extraction and gas chromatography/mass spectrometry; Jeffery D. Rivera; David A. Herold; Chienying N. Liu; Yolanta T. Kruzysnka; Jerrold M. Olefsky; Robert B. MacArthur; Robert L. Fitzgerald; VAMed Center, San Diego, CA; VA Med Center and UC, San Diego, CA; Columbia Presbyterian Medical Center, New York, NY

**TPA 022** Applications of Novel Data Dependent Experiments; Ming Yang; Nic Bloomfield; Lyle Burton; Ron Bonner; Yves Le Blanc; PE Sciex, Concord, ON, Canada

**TPA 023** High Throughput Analysis of S9 Microsomal Incubations by Multiplexed Parallel LC-MS on oao-TOF to Determine Rates of Drug Metabolism; Ashley B Sage; Jose Castro-Perez; Steve Preec; Gary Bowers; Pisal Chandrasurin; Micromass UK Ltd, Manchester, UK; GlaxoWellcome, RTP, NC

**TPA 024** LC/MS Analysis of Neurosteroids in Biological Fluids: Effect of Specific PBR Ligands on Neurosteroidogenesis; Françoise Uzabiaga; Antoine Berthemy; Anne Tuong; Stephane Rouder; Mohamed Maftouh; Badia Fazza; Jesus Benavides; Claudine PICARD; Sanofi Synthelabo, Toulouse, France; Sanofi Synthelabo, Bagnes, France
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**TPA 025** The Determination of Gabapentin in Human Serum by LC/MS; Paul A Zavitansanos, Courtney MacDonald; Agrident Technologies, Toronto Canada; St Joseph’s Health Center, London, Canada

**TPA 026** The Influence of Ammoniated Tobacco on Smoke pH and Nicotine Delivery; Clifford H. Watson; Michelle Beeson; David L. Ashley; Centers for Disease Control and Prevention, Atlanta, GA

**TPA 027** Development of High Throughput Analytical Techniques for Compound Permeability Studies Using HPLC/MS and Time-Of-Flight Mass Spectrometer; Ru Wei; Darren Wei; Lily Li; Wolfgang Goetzinger; Hongsheng Yu; James N. Kyranos; ArQuie Inc., Woburn, MA

**TPA 028** Evaluation of the Micromass LCT for Exact Mass Measurement in HPLC/MS; James N. Kyranos; Ru Wei; Lily Li; Wolfgang Goetzinger; ArQuie Inc., Woburn, MA

**TPA 029** A Novel LC/MS Mix to Expedite Method Development and Performance Check in Pharmaceutical Analysis; Liang Tang; Bill Fitch; Mike Alexander; John Dolan; Affymax Research Institute, Palo Alto, CA; LCResources, Inc., McMinnville, OR

**TPA 030** Metabolite Identification Using a LC-QqTOF System: Accurate Mass Determination Using Different Calibration Modes; Sabine Leonhardt; Gerald Gütter; Jürgen Gerdon; Wolfgang Dreher; Beate Behnke; BASF AG, Agricultural Center, Germany

**TPA 031** Rapid and Sensitive Metabolite Identification Using a Capillary LC-QqTOF System; Gerald Gütter; Sabine Leonhardt; Jürgen Gerdon; Wolfgang Dreher; Beate Behnke; BASF AG, Agricultural Center, Germany

**TPA 032** Electrospray Ionization Coupled with Time-of-Flight Mass Spectrometry For Fast Separations: When Speed Really Counts; Brian W. Pack; Rick Parry; Mary Kinsel; LECO Corporation, St. Joseph, MI

**TPA 033** Fast screening method for the detection of exogenous anabolic steroids in urine by gas chromatography/combustion/isotope ratio mass spectrometry; Rodrigo Aguilera; Donald Catlin; Thomas Chapman; UCLA Olympic Analytical Laboratory, Los Angeles, CA

**TPA 034** Identification of Metabolites in Urine Samples Using a Hybrid Quadrupole Time-of-Flight Mass Spectrometer and Direct Sample Introduction with Nanospray; Lorne M. Fell; Alina Dyndal; George Scott; Yves Le Blanc; PE Sciex, Concord, Canada

**TPA 035** Validation of a 96-Well Plate LC/MS/MS Method for the Quantitation of an Antifungal Agent in Monkey Plasma; Kenneth Roth; Jerry P. Roach; Robert P. Clement; Patrick J. Rudewicz; Schering-Plough Research Institute, Kenilworth, NJ

**TPA 036** Validation of a 96-Well Plate LC/MS/MS Method for the Quantitation of Loratadine and Metabolites in Human Plasma; Luyu Yang; Robert P. Clement; Patrick J. Rudewicz; Francis Beaudy; Charles Grandmaitre; Lorella Di Donato; Robert Mass; Schering-Plough Research Institute, Kenilworth, NJ; Phoenix International Life Sciences, Montreal, Canada

**TPA 037** Quantitative determination of BMS-186295 in human EDTA plasma; Rajesh N. Patil; Daisy B. Whigan; Bristol-Myers Squibb Pharmaceutical Research Inst, New Brunswick, NJ

**DRUGS & METABOLISM: STRUCTURAL CHARACTERIZATION, 038 – 054**

**TPB 038** Degradation of a Retinoid Analogue Characterized By Liquid Chromatography Coupled With Ion Trap Mass Spectrometry; Pa Zhang; Mathews Nunes; Johnson & Johnson CPhW, Skillman, NJ

**TPB 039** Characterization and Quantification of Impurities Found In 'over-the-counter' Melatonin; Brian L. Williamson; Jeffrey W. Finch; PE Biosystems, Framingham, MA

**TPB 040** Identification of Substance P Antagonist [14C]CJ-11,974-01 Degradation Product by NMR and Hydrogen Deuterium Exchange and Electrospray Ionization Tandem Mass Spectrometry (ESI/MS/MS); Amin M. Kamei; Chandra Prakash; Kathleen S. Zandi; Sandra A. Miller; Keith E. McCarthy; Walter W. Massefski; Pfizer Inc., Groton, CT

**TPB 041** LC/MS and GC/MS Identification of an Unknown Degradant Caused by the Maillard Reaction in a Pharmaceutical Drug Formulation: Pauline C. Chow; Thomas A. Walker; Geneva Pharmaceuticals, Brookfield, CO

**TPB 042** Characterization of amidarone metabolites and its impurities by HPLC/APCI-MS/MS; Seung-Woon Myung; Yoong-Jung Chang; Hye-Ki Min; Myungsoo Kim; TaeKyeong Kang; Eun-Ah Yoo; Yong-Hyeon Yim; Korea Institute of Science and Technology, Seoul, Korea; Sungshin Women's University, Seoul, Korea; LG Chemical Ltd., Taegon, Korea

**TPB 043** H/D-exchange as a Tool to Elucidate Fragmentation Mechanisms of Metabolites of Omeprazole in the MS/MS Mode; Lars Weidahl; Margaret Gabrielson; Neal Castagnoli, Jr.; AstaZeneca R&D Malmö, Sweden; Virginia Tech, Blacksburg, VA

**TPB 044** Tandem Mass Spectrometry Study of Naturally Occurring Anti-HIV Agent (+)-Calanolide A and Its Congeners; Matt S. Dunn; Lisa Y. Tan; Jenny L. Lin; Richard B. van Bremmer; Ze-Xi Xu; MedChem Research, Inc., Lenmont, IL; University of Illinois, Chicago, IL

**TPB 045** Analytical approaches with he-itms for structural elucidation of new drug substances and formulation support; E. Dumag; C. Van Aerden; C. Brossin; P. Lavabre; N. Cohen; L. Lecointre; IRJ-PDS Parke-Davis, Fresnes, France

**TPB 046** Investigation of Magnolol and Honokiol Fragmentation by EI-FTICR MS; Susan T. Weintraub; Richard D. Burton; Kenneth T. Matuszak; Alex M. Boku; Paul R. West; Yuji Maruyama; University of Texas Health Science Center, San Antonio, TX; Abbott Laboratories, Abbott Park, IL; Gunma University, Gunma, Japan

**TPB 047** Structure Elucidation of Tetracycline Antibiotics Using Electrospray Ionization and Multiple Stages of Mass Spectrometry; David N. Heller; FDA Center for Veterinary Medicine, Laurel, MD
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**TPC 048** Isolation and Characterization of Anti-Viral Nucleoside Compounds from the Chinese Herb *Taraxacum mongolicum*; Erika N. Ebbe1; Vincent C. X. Gao2; John M. Essigmann3; Massachusetts Institute of Technology, Cambridge, MA; Perkin Elmer Applied Biosystems, Foster City, CA

**TPC 049** Determination of 3-Methoxy-4-hydroxyphenylglycol (MHPG) Levels in Plasma of Patients Treated with Tamoxifen; Bozena Winnik1; Linda Patrick-Miller1; Brian Buckley3; EOHSI, Rutgers University, Piscataway, NJ; UMDNJ/Robert Wood Johnson Medical School, Piscataway, NJ

**TPC 050** Effects of Mobile Phase Buffer Contents on the Ionization and Fragmentation of Simvastatin in LC/MS/MS Determination; Jamie J. Zhao1; John D. Rogers1; Merck Research Laboratories, West Point, PA

**TPC 051** Deuterium Exchange and LC/MS/MS in the Identification of the Major Metabolite of Nicotinylalanine in Mice; Patrick S. Gallery1; Girish S. Gudi1; Gregg Pratt1; Fred L. King1; Julie L. Eiseman3; West Virginia University, Morgantown, WV; University of Pittsburgh Medical Center, Pittsburgh, PA

**TPC 052** Investigation of the Reaction of Estradiol-2,3-Quinone with Desoxyribonucleosides Using LC-ESI-MS and Tandem Mass Spectrometry on Model Steroids; C. Van Aerden1; L. Debrauwere2; F. Fournier2; E. Rathahao2; O. Convent3; A. Paris3; J-C. Tabet2; INRA, Toulouse, France; UMPC/Paris 6, Paris, France

**TPC 053** Structure Identification of Impurity in FTC Oral Solution by LC/MS/MS; Feng Wang1; John P. Walsh1; John A. Begley1; Triangle Pharmaceuticals Inc, Durham, NC

**TPC 054** Forced Degradation Studies of AG1549, a Potent Non-Nucleoside HIV-1 Reverse Transcriptase Inhibitor; Rodney S. Basnawat1; Barbara C. Potts1; Melissa V. Deaton-Rowinski1; Agouron Pharmaceuticals, San Diego, CA

**CARBOHYDRATES, 055 - 086**

**TPC 055** Hydrogen Abstraction from Sugars by Distonic Radical Cathions; Leonard P. Geiler1; Hilka I. Kenttamaa2; Purdue University, West Lafayette, IN

**TPC 056** Stereoelectronic Effects on Ion-Trap MS Fragmentation of Epimeric Carbohydrate Mimetics; Min Wang2; Ting Wang1; Patrick R. Jones1; University of the Pacific, Stockton, CA

**TPC 057** Partial Characterization of Glycal Dimers by APCI Mass Spectrometry - A New Class of Carbohydrate Mimics; Andreas H. Franz1; Patrick R. Jones1; Paul H. Gross3; University of the Pacific, Stockton, CA

**TPC 058** Ion Mobility Measurements of Metal Ligated Monosaccharide Diastereomers; Michael D. Leavell1; John A. Taraska2; Sara P. Gaucher1; David E. Clemmer1; Julie A. Leary2; University of California, Berkeley, CA; University of Indiana, Bloomington, IN

**TPC 059** Enhancement of Stereoelectronic Effects Using Multiply Charged Complexes of Four Monosaccharides with Transition Metal by ESI/ITMS; Valerie Carlesso1; Francoise Fournier1; Jean Claude Tabet1; LCOB, France

**TPC 060** Disaccharide Analysis: Electrophoretically Assisted ES-MS of Carbohydrate Cyclic Ferrocenyl Boronate Esters; Dudley Williams1; Terry D. Lee1; Mary K. Young1; City of Hope/Beckman Research Inst., Duarte, CA

**TPC 061** Structural Characterization of Heparin and Chondroitin Sulfate Disaccharides by ESI-MS/MS; Heather Desaire1; Julie A. Leary1; UC Berkeley, Berkeley, CA

**TPC 062** A Novel Fluorescent Tagging Procedure for the Enhanced Chromatographic Separation and Mass Spectrometric Analysis of Biologically Important Glycans; Philip B. Grace1; John K. MacLeod1; Craig Freeman1; Steven Ramsay1; The Australian National University, Canberra, Australia

**TPC 063** Negative-Ion Electrospray Mass Spectrometry of Native Neutral Oligosaccharides; Wengang Chai1; Alexander M. Lawson1; Imperial College School of Medicine, Harrow, Middlesex, UK

**TPC 064** O-Mannosylated Proteins from A. fumigatus: Fragmentation Analysis of Neutral Glycans by nanoESI-QTOF and MALDI-TOF MS; Matthias Letzel1; Simone Koenig1; Eduardo A. Leitao1; Eliana Barreto-Bergter2; Jasna Peter-Katalinic1; University of Bielefeld, Bielefeld, Germany; University of Minnesota, Minneapolis, Minnesota, Germany; University of Rio de Janeiro, Rio de Janeiro, Brasil

**TPC 065** Fragmentation of N-linked glycans ionised by electrospray on a Q-TOF mass spectrometer; David J. Harvey1; Louise Royle1; University of Oxford, Oxford, UK

**TPC 066** Construction of oligosaccharide structural database for mass spectral simulation; Yasuho Mizuno1; Tatsuhiro Sasaoka2; Toray Research Center, Japan

**TPC 067** Size Exclusion Chromatography-Mass Spectrometry (SEC-MS) of Polysaccharides; Elaine Stimson1; Michael J. Deery1; Colin G. Chappell1; DuPont UK Ltd, Cereals Innovation Centre, Cambridge, UK

**TPC 068** Analysis of Glycose Oligosaccharide in the Urine of Patients with Glycogen Storage Diseases using ESI-MS/MS; Sarah P. Young1; Yan An1; Robert D. Stevens1; David S. Millington1; Duke University Medical Center, NC

**TPC 069** Capillary Electrophoresis-Ion Trap Mass Spectrometry for Profiling and Characterizing Glycan Mixtures; Jeanine Delaney1; Lynn Gennaro2; Paul Vouros3; Northeastern University, Boston, MA

**TPC 070** Normal-Phase HPLC/ESI-MS Studies of Derivatized Glycans; Julian A. Sals1; James C. Jamieson1; Helene Percevault1; University of Manitoba, Winnipeg, MB, Canada

**TPC 071** Isoform Analysis of Polygalacturonase-inhibiting Protein by Mass Spectrometry; Lucy K. Miller-Keating1; Carl W. Bergmann2; Alan G. Darvill1; Peter Albersheim2; Ron Orlando2; Macquarie University, NSW, Australia; CCRC, UGA, Athens, GA

**TPC 072** Characterizing the Glycans of Catfish IGM by Mass Spectrometry; Maria Esteban Warren1; Joanne L. Maki1; Harry W. Dickerson1; Ron Orlando1; University of Georgia, Athens, GA

**TPC 073** Structural Characterization of the N-linked Glycans of the Recombinant Matrix Metalloproteinase-9 (MMP-9) from Human by Glycosidase Digestions and MALDI-MS; Li Zhang1; Ron Orlando1; Shahriar...
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**TPC 074**  
MALDI-TOF analysis of Asn-linked glycans found on Trypanosoma brucei variant surface glycoproteins; Angela Mehler¹; Michael A.J. Ferguson¹; University of Dundee, Dundee, UK

**TPC 075**  
Analysis of Glycans of Phosphatidyl A2 from Honeybee Venom by Capillary Electrophoresis/Electrospray Ionization Mass Spectrometry; Guo-Rong He¹; Chien-Chen Lai¹; National Taiwan University, Taipei, Taiwan

**TPC 076**  
Glycosylation Structure-Function Relationships with C. elegans; the Proteome and Glycome; J. Cesar Rosa¹; Song Ye¹; Bruce B. Reinhold¹; Vernon N. Reinhold¹; University of New Hampshire, Durham, NH

**TPC 077**  
Mass spectrometric analysis of hydroxyproline glycans; Sven Kiltz¹; Sabine Waffenschmidt¹; Helmut Muenster¹; Herbert Budzikiewicz²; Finnigan MAT GmbH, Bremen, Germany; University of Cologne, Germany

**TPC 078**  
Structural refinement of O-linked oligosaccharides by enzymatic digestion and Matrix-Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry; Yongming Xia¹; Ken Tseng¹; Jerry L. Hedrick¹; Carlito B. Lebrilla¹; University of California, Davis, CA

**TPC 079**  
C-nonsymylylation in the complement system; Steffen Hartmann¹; Daniel Hess¹; Marcel Blommers¹; Aleksandra Furmanek¹; Jan Hofsteenge¹; Friedrich Miescher Institut, Basel, Switzerland; Novartis Pharma AG, Basel, Switzerland

**TPC 080**  
Method for the Analysis and Characterization of Flavonoid and Sapogenin Glycosides in the Leaf of the Hostas Plant; Paul A. Zavattanos¹; Pujiwan Fu¹; Agilent Technologies, Toronto, Canada; Noble Laboratories, Mississauga, Canada

**TPC 081**  
Profiling Glucosamine Polymers and their Catecholamine Adducts from Insect Cuticle; James L. Kerwin¹; Cornell University, Ithaca, NY

**TPC 082**  
Mapping of the phosphocholine determinant in lipoteichoic acid from Streptococcus pneumoniae by positive and negative ion nano ESI-QTOF-MSMS; Arne L. Beckedorf¹; Werner Fischer¹; Jasna Peter-Katalinic¹; Institute for Medical Physics and Biophysics, Munich, Germany; Institute for Biochemistry, Erlangen, Germany

**TPC 083**  
Investigation of the Sialic Acid Biosynthesis Pathway in Haemophilus Using Isotope Labeling and FT-ICR MS; Sara P. Gaucher¹; Brgit Schilling¹; Nicole M. Samuels¹; Bradford W. Gibson¹; Julie A. Leary¹; University of California, Berkeley, CA; University of California, San Francisco, CA

**TPC 084**  
Applicability of MALDI-PSD in Negative Mode for Analysis of Oligosaccharides, N-Glycans and O-Glycosylated Amino Acids; Marko Jovanovic¹; Simone Koenig¹; Jasna Peter-Katalinic¹; Institute for Medical Physics and Biophysics, Munich, Germany

**TPC 085**  
Protein-carbohydrate interactions characterized by ES-FIMS; John S. Klassen¹; Elena N. Kitova¹; David R. Bundle¹; University of Alberta, Edmonton, Canada

**TPC 086**  
Investigation of Human Milk Components by Electrospray Ionization Mass Spectrometry; Jianru Stahl-Zeng¹; Ute Bahr¹; Michael Karas²; Bernd Stahl²; Marco Euler³; Gilda Georgi²; Bernd Finke²; PE Biosystems, Langen, Germany; University of Frankfurt, Frankfurt, Germany; Wissens Research Group Germany, Friedrichsdorf, Germany

**PROTEINS – BIOLOGICAL ORIGIN, 087 – 168b**

**TPD 087**  
Targeted Proteomics Techniques for the Identification of Disease State Markers in Biological Fluids; Janice L. Bleibraun¹; Robert L. Martin¹; Brenda L. Gale¹; Rebecca T. MacKenzie¹; Kenneth M. Straub¹; Roche Bioscience, Palo Alto, CA

**TPD 088**  
Using Proteomics and Mass Spectrometry to Reveal the Mechanism of Action of Fatty Acid Biosynthesis Inhibitors; Ping Du¹; Erin E. Schiller¹; Ronald Ernser¹; Rachel R. Ogorzaalek Loo¹; Nicole Dawson¹; Greg W. Kilby¹; Tracy L. Stevenson¹; Eric R. Olson¹; Ruth A. VanBogelen¹; Parke-Davis Pharmaceutical Research, Ann Arbor, MI

**TPD 089**  
Proteomic Approaches for Identifying Components of the Bovine Mitochondrial Ribosomal Small Subunit (28S) Complex; R. Kevin Blackburn¹; William Burkhart¹; Arthur Moseley¹; Emine Koc²; Linda Spremulli¹; Glaxo Wellcome, RTP, NC; University of North Carolina, Chapel Hill, NC

**TPD 090**  
Identification of Brain Proteins by Two-Dimensional Gel Electrophoresis and Mass Spectrometry in Foetuses with or without Down Syndrome; Madalina Oppermann¹; Neus Cols¹; Tomas Bergman¹; Nisse Kalkkinen¹; Roser González-Duarte¹; Hans Järnwall¹; Karolinska Institutet, Stockholm, Stockholm, Sweden; Universitat de Barcelona, Barcelona, Spain; University of Helsinki, Helsinki, Finland

**TPD 091**  
Identification of Calorie-Regulation-Related Mouse Liver Proteins by Nano-Electrospray Mass Spectrometry; Fu Shang¹; Gejing Deng¹; Thomas R. Nowell¹; Allen Taylor¹; HNRC at Tufts University, Boston, MA; AstraZeneca R & D Boston, Cambridge, MA

**TPD 092**  
Identification of Small Proteins from Mycobacterial 2-DE Gels - MALDI-MS versus ESI-MS; Eva-Christina Mueller¹; Jens Mattew²; Peter R. Jungblut³; Max Delbrueck Center for Molecular Medicine, Germany; Max Planck Institute for Infection Biology, Germany

**TPD 093**  
A New Concept to Bridge Genomics and Proteomics; Holger Eickhoff¹; Konrad Buesow²; Dolores Cahill¹; Hans Lehrach¹; Joachim Klose³; Eckhard Nordhoff³; Max-Planck-Institute for Molecular Genetics, Berlin, Germany; Humboldt University, Virchow-Klinikum, Berlin, Germany

**TPD 094**  
An Old, Yet New Isotope Tag for Comparative Proteomics; Plamen Demirev¹; Catherine Fenselau¹; Xuoding Yao¹; Amy Freas¹; Javier Ramirez¹; University of Maryland, College Park, MD

**TPD 095**  
Identification of prostate cancer specific protein markers; Yingming Zhao¹; Hongjun Shu¹; Emanuel Petricoin²; The Mount Sinai School, New York, NY; CBER/FDA, Bethesda, MD

**TPD 096**  
Large Scale Protein Identification using Automated 2D-gel Spot Excision, Digestion and Data Dependent
TUESDAY POSTERS

7:30 – 8:00 am
SET UP POSTERS, Exhibit Hall B

8:45 – 10:15 pm
POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.

1:30 – 3:00 pm
POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.

6:00 – 6:30 pm
REMOVE POSTERS. Please leave posters for the full day.

TPD 097
Proteomic analysis of soluble lysosomal proteins; Hongjun Shu 1; Robert J. Dewsnick 1; Yiming Zhao 1; E. Sarnihausen 2; B. Kösters 2; B. Simons 3; A. Haslik 3; The Mount Sinai School, New York, NY; Institut für Physiologische Chemie, Marburg, Germany

TPD 098
Sequence Analyses of Rat Liver Cytosolic Proteins Separated by Gel Electrophoresis Using MALDI Mass Spectrometry; Yi-Min Shi 1; Gu-Qi Wang 1; Frank J. Burczynski 2; Alexander Loboda 1; Werner Ens 1; Kenneth G. Standing 2; University of Manitoba, Winnipeg, Canada

TPD 099
Using Proteomics Approaches to Identify Specific Cytochrome P450 Isozymes Up-Regulated in Mouse Liver; Surinder Kaur 1; Dazhi Tang 1; Frank Buschman 1; Frank R. Masiarz 1; Larry Coussens 2; George M. Conlon 3; Glenda Polack 1; Isa Samuels 1; Kirk Johnson 1; Robert Johnson 2; Chiron Corporation, Emeryville, CA

TPD 100
Differential Scanning for De Novo Sequencing: Application for the Identification of a Complex Involved in Endocytosis; Sandrine Uttenweiler-Joseph 1; Savvas Christoforidis 1; Zinno Zerial 1; Matthias Wilk 1; European Molecular Biology Laboratory, Heidelberg, Germany

TPD 101
Analysis of the Human Plutitary Proteome; Sarka Beranova 1; Shelly D. Timmons 1; Dominic M. Desiderio 1; University of Tennessee, Memphis, TN

TPD 102
High Resolution Proteome Analysis of Membrane Proteins by 2-D Gel Electrophoresis in Combination with FT-ICR-Mass Spectrometry; Eugen N. Danov 1; Markus Kohlmann 1; Viorel Mocanu 1; Stefan Buehler 1; Kai Bruns 1; Soeren O. Deininger 1; Claudia Stuermers 1; Dieter Brdiczka 1; Michael Przybylski 1; University ofKonstanz, Germany

TPD 103
Proteomics on Full Length Membrane Proteins Using Mass Spectrometry; Johannes le Coutre 1; Julian P. Whitelegg 1; Jenny C. Lee 1; Adrian Gross 1; H. Ronald Kaback 2; Kym F. Faull 3; Howard Hughes Medical Institute, UCLA, Los Angeles, CA; The Pasarow Mass Spec Laboratory, Los Angeles, CA

TPD 104
Analysis of the Mouse Cerebellum Proteome: Selected Proteins Identified in the Lurcher Mutant; Tara Russell 1; Sarka Beranova 1; Michael J. Pabst 1; Dan Goldowitz 1; Dominic M. Desiderio 1; University of Tennessee, Memphis, TN

TPD 105
A Proteomic Approach to Understanding the Role of a Novel Aspartyl Protease 2 (Asp 2) in Alzheimer's Disease; Zhongdong Pan 1; Gregory S. Cavey 1; Richard S. Myers 1; Ronggui Shuang 1; Jinhe Li 1; Mary E. Shuck 1; Michael J. Bienkowski 1; W. Rodney Mathews 1; Pharmacal & Upjohn, Kalamazoo, MI

TPD 106
Proteome Analysis of Leukemia Cell Apoptosis Related Proteins by Two-Dimensional Gel Electrophoresis and MALDI-TOF Mass Spectrometry; Xiao-Hong Qian 1; Jing-Hong Wan 1; Jing-Lan Wang 1; Fu-Chu He 1; National Center of Biomedical Analysis, Peking, P.R. China

TPD 107
Quantitation in Proteomics: Automatic Processing of ICAT Data; Kenneth C. Parker 1; Tim Griffin 2; Steve Gygi 2; Ruedi Aebersold 2; PE Biosystems, Framingham, MA; U. Washington, Seattle, WA

TPD 108
High Throughput Profiling of Proteome from Brain Tissue Using Robotic, MALDI-TOF MS and Intelligent Data Processing Tools; Melanie Lin 1; Barbara Wolf 1; Jon DeGnore 1; Srinivasan Krishnan 1; Darryl Spencer 1; Dale Patterson 1; Keith Waddell 1; Mary Lopez 1; Elena Chernokalskaya 1; Alexander Lazarev 1; PE Biosystems, Framingham, MA; Genomic Solutions, Chelmsford, MA

TPD 109
Application of a MALDI QIT TOF Mass Spectrometer in the Analysis of Protein Digests from 2D Gels; Chris Sutton 1; Koichi Tanaka 1; Mike Dunn 1; Kratos Analytical Ltd, Manchester, UK; Harefield Hospital, Harefield, UK

TPD 110
The Application of Virtual 2D Gel Technologies to the Study of Membrane Proteins; Angela K. Walker 1; Gretchen L. McGannon 1; Gary A. Rymar 1; Heather A. Haynes 1; Mary C. Hurley 1; Philip C. Andrews 1; University of Michigan, Ann Arbor, MI

TPD 111
Comparative analysis of tryptic digestion products of PS II proteins using SA-MALDI-MS and LC-ESI-MS; Connie J. Saunders 1; Laurie K. Frankel 1; Kari B. Green-Church 1; Rama Tummala 1; Terry M. Bricker 1; Patrick A. Limbach 1; Louisiana State University, Baton Rouge, LA

TPD 112
Mass spectrometric characterisation of synthetic amyloid peptides related to Alzheimer's disease neurotoxicity; Roxana E. Cecal 1; Stefan Buehler 1; Markus Wunderlin 1; Sarah Trimpin 1; Martina Schuhmacher 1; Bontond Penke 2; Gabor Toth 2; Michael Przybylski 2; University of Konstanz, Germany; Albert-Szent-Gyorgy University, Szeged, Hungary

TPD 113
Identification and Comparative Quantitative Analysis of Secreted Proteins from Normal and Cancerous Prostate Epithelial Cells using Isotope Coded Affinity Tags; David K. M. Han 1; Timothy J. Griffin 1; Beate Rist 1; Steven P. Gygi 2; Ruedi Aebersold 2; University of Washington, Seattle, WA

TPD 114
Automated gel processing and MALDI mass spectrometry for high throughput protein studies; Dominic Gostick 1; Ronan O'Malley 1; James Langridge 1; Kevin Howes 1; Robert Bordoli 1; Jeff Brown 1; Ann-Charlotte Bergman 2; Olle Danielsson 2; Mats Eronius 2; Ayodele Aliyaji 1; Micromass UK Ltd, Manchester; Karolinska Institute, Stockholm, Sweden; Karolinska Hospital, Stockholm, Sweden

TPD 115
Peptide Mapping of the APHIS Binding Site of Cycloxygenase-2; Jennifer F. Nemeth 1; G. Phillip Hochgesang, Jr 1; Lawrence J. Marlett 1; Hugh M. Caprioli 1; Vanderbilt University Medical Center, Nashville, TN

TPD 116
Identification of arginine dimethylation sites of an RNA-binding protein using MALDI-MS and ESL-MS/MS; Peter M Gehrig 1; Larisa Belyanskaya 1; Heinz Gehrig 1; Peter E Hunziker 1; University of Zurich, Zurich, Switzerland

TPD 117
MHC class I associated peptide identification after measles virus infection employing isotope labeling and column switching nanoLC-MS/MS; Ad P.J.M. de
TUESDAY POSTERS

7:30 – 8:00 am SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm REMOVE POSTERS. Please leave posters for the full day.

TPD 118
Presentation of Minor HEL-epitopes to T-cells by Class II MHC I-At- Molecules - Identification of Post-translationally Modified Peptides; Koen van der Drift; Ilan Vidavsky; Carlos Velazquez; Emil R. Unanue; Michael L. Gross; Washington University, St. Louis, MO

TPD 119
High Resolution Comparative Mass Spectrometry for the Elucidation of the Role of Tapasin in the MHC Class I Processing Pathway; Jarrod A. Marto; John C. Luckey; Forest M. White; Angela L. Zalting; Scott B. Ficarro; Cynthia J. Bramle; Jeffrey Shabanowitz; Victor H. Engelhard; Donald F. Hunt; University of Virginia, Charlottesville, VA

TPD 120
Mass spectrometric characterization of discontinuous epitopes recognized by anti-HIV-gp120 human monoclonal antibodies; Elisabeth O. Hochleitner; Miroslav Gorny; Susan Zolla-Pazner; Kenneth B. Tomer; NIEHS, RTP, NC; New York University, New York, NY

TPD 121
Mass spectrometric identification of naturally processed HLA-DR4- and -DR1-presented epitopes from the diabetes-relevant autoantigen glutamic acid decarboxylase 65; Markus Schirle; Wieland Keilholz; Petra Sohnlein; Hubert Kalbacher; Wilfrid Richter; Stefan Stefanovic; Hans-Georg Rammensee; Institute for Cell Biology, University of Tubingen, Germany

TPD 122
Determination of the structure of recombinant HBx protein and its immunologically active epitope; Tamás Jakab; Zoltan Kele; Ilona Marczinovits; Janos Molnar; Jozsef Pal; Peter Nemeth; University of Szeged, Szeged, Hungary; University of Pecs, Pecs, Hungary

TPD 123
Mass Spectrometry Analysis of T Cell Epitopes Derived from Human Alpha-Fetoprotein; Wilson S. Meng; Lisa H. Butterfield; Antoni Ribas; Vivian B. Dissette; John A. Glaspy; William H. McBride; Kym Faull; James S. Economou; University of California, Los Angeles, CA

TPD 124
Identification of MHC class I derived peptides from in vivo malignant material and transplanted cell lines using nano-electrospray quadrupole ion trap mass spectrometry; Jennie R. Lilly; Colin S. Creasser; Philip L.R. Bonner; Seran C. Hill; Robert C. Rees; Steven Christmas; Richard Clark; Louise Norbury; Anthony I. Dod; Alejandro A. J. Madrigal; Nottingham Trent University, Nottingham, UK; University of Liverpool, Liverpool, UK; Anthony Nolan Trust, Royal Free Hospital, London, UK

TPD 125
Mass Spectrometry as a Tool for Routine Characterization and Quantitation of Post-Translational Modifications (PTMs) of Therapeutic Monoclonal Antibodies; Christine M. Holland; John N. Hope; Yuhui Wang; Cathy Klette; Mark A. Schennerman; MedImmune, Inc, Gaithersburg, MD

TPD 126
Identification of Proteins in Jurkat T Cell Lipid Rafts via Micro-Capillary HPLC Electrospray Ionization Tandem Mass Spectrometry; Priska D. von Haller; Samuel M. Donohoe; Julian D. Watts; David R. Goodlett; Rick Newitt; Ruedi Aebersold; University of Washington, Seattle, WA; Institute for Systems Biology, Seattle, WA

TPD 127
CD8 Dependence of T Cell Activation Correlates With T Cell Receptor Affinity; Gregory A. Barrett-Will; Amick Guimezanes; Pamela H. Thompson; Jeffrey Shabanowitz; Donald F. Hunt; University of Virginia, Charlottesville, VA; Centre d'Immunologie INSERM-CNRS de Marseille, Marseille, France; Millennium Pharmaceuticals, Cambridge, MA

TPD 128
Identification of a Membrane-Bound Tumor Antigen using Immunoaffinity Chromatography, MALDI-TOF-MS and Capillary HPLC-MS/MS; Kathy L. O'Connell; Katya E. McLane; Gordon A. Vehar; Elizabeth A. Luis; John T. Stults; Genentech, Inc., South San Francisco, CA; Raven Biotechnologies, Inc., San Carlos, CA

TPD 129
Identification of Protein Binding Partners of Mouse Syntactin 3 and Syntaxin 4 by Orthogonal 2-D Chromatography and Mass Spectrometry; Wei Quan Lu; Takafumi Goto; Mark Bennett; Dave Anderson; Rigel, Inc., South San Francisco, CA

TPD 130
Characterization of the in vivo activity of the beta-secretase, Asp2, by immunoprecipitation - mass spectrometry; W. Rodney Mathews; Adele E. Pauley; Mary E. Shuck; Michael J. Bienkowski; Mark E. Guney; Pharmacia & Upjohn, Kalamazoo, MI

TPD 131
Synthesis and MS Characterization of Peptide-based Polymers as Synthetic Immunogens; Hasson Rashidzadeh; Mark R. Chance; Kevin M. Downard; Albert Einstein College of Medicine, Bronx, NY

TPD 132
The Identification of Free Sulphhydrys in the Heavy Chain Variable Domain of a Recombinant Monoclonal Antibody Directed Against Human IgE; Edward T. Chin; Derf A. Lewis; Viswanatham Katta; Genentech, Inc., South San Francisco, CA

TPD 133
Identification and Sequencing of Peptides Isolated from MHC Class II I-A^b - Progress Toward Finding the Juvenile Diabetes Antigen; Ilan Vidavsky; Koen van der Drift; Michael L. Gross; Anish Suri; Osami Kanagawa; Emil R. Unanue; Washington University, St. Louis, MO

TPD 134
ESI-MS of Two Purified 14- and 15-Span Transmembrane Proteins; Eric Turk; Olivia Kim; Johannes le Coutre; Julian P. Whitelegge; Kym F. Faull; Ernest M. Wright; Univ of CA, Los Angeles, CA

TPD 135
Identification of Ubiquitination of Alpha Spectrin Using LC/MS/MS and Database Searching on an Ion Trap Mass Spectrometer; Tanuja Chaudhary; Steven R. Goodman; Ian Jardine; David G. Kakhniashvili; ThermoQuest Corporation, San Jose, CA; University of South Alabama, Mobile, Alabama

TPD 136
Identification of Posttranslationally Modified Histones; Griffiths William; Wang Yuqiu; Johnsson Jan; Karolinska Institutet, Sweden

TPD 137
Characterisation of a glutamate receptor complex by online nanoscale LC-MS/MS analysis; Vydi Choudhary; Malcolm Ward; Walter Blackstock; Seth Grant; Holger Husi; GlaxoWellcome Medicines
TUESDAY POSTERS

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Research Centre, England; Centre for Genomic Research, U. of Edinburgh, Scotland

TPD 138  Complete Sequencing of an Antibody Fab Fragment by Ion Trap Mass Spectrometry; John C. Geblet1; Maciej Adamczyk1; Jiang Wu1; Abbott Laboratories, Abbott Park, IL

TPD 139  Characterization of Proteins Expressed from Gloma Cell Lines by Use of ESI FT-ICR MS; TuKiet Lam1; Mark R. Emmett1; Christopher L. Hendrickson1; Alan G. Marshall1; Florida State University, Tallahassee, FL

TPD 140  Quantification of Constitutive (Gl)15 and Mutant (Arg)15 Forms of Ras Protein in the TG/AC Mouse; Michael J. Bar ties1; Donald Decker1; Kathy A. Brzak1; H. Lynn Kan1; B. Bhaskar Gollapudi1; Dow Chemical, Midland, MI

TPD 141  Identification of a Novel Ser O-Glucuronidation in Acidic Proline-Rich Proteins via Electrospray Tandem Mass Spectrometry; Andreas P. Jonsson1; William J. Griffiths1; Nicklas Strömberg1; Hans Järnval1; Tomas Bergman1; Karolinska Institutet, Stockholm, Sweden; Umea University, Umea, Sweden

TPD 142  Comparison of LCQ-deca Mass Spectrometer and Q-TOF Mass Spectrometer for Protein Characterizations; Rong-Rong Zhu1; Tsoyue Joanne Sun2; Kathleen L. Grant1; BASF Bioresearch Corp., Worcester, MA

TPD 143  Identification of proteins involved in differential regulation of the end-1 gene of Caenorhabditis elegans; Erin D. Field1; Jeffery Shabanowitz1; Donald F. Hunt1; Eric Witze2; Joel H. Rothman3; University of Virginia, Charlottesville, VA; University of California, Santa Barbara, CA

TPD 144  Rapid Separation and Identification of Viral Coat Proteins; Benjamin J. Cargile1; James L. Stephenson, Jr.4; Scott A. McMickey5; Oak Ridge National Laboratory, Oak Ridge, TN; Purdue University, West Lafayette, IN

TPD 145  Subtractive Analysis of High Resolution Mass Spectra and LC MS/MS for the Identification of Bacillus subtilis Sporulation Proteins; Anthony A. High1; Forest M. White1; Steffen Heim1; Antje M. Hofmeister1; Jeffrey Shabanowitz1; Donald F. Hunt1; University of Virginia, Charlottesville, VA; University of California, Berkeley, CA

TPD 146  Assessment of full complement of histone modifications reveals novel phosphorylation sites; Cynthia L. Brann1; Jennifer A. Caldwell1; Scott B. Ficarro1; Scott D. Briggs1; Brian D. Stahl1; Jeffrey Shabanowitz1; C. David Allis1; Donald F. Hunt1; University of Virginia, Charlottesville, VA

TPD 147  Electrospray LC/MS Investigation of the Mechanisms by which Nitric Oxide Donors Inhibit the Cysteine Protease Cathepsin K Activity; Chun Li1; Marc Ouellet1; David Percival1; Merck Frosst Canada & Co., Kirkland, Canada

TPD 148  Identification of clinically significant but electrophoretically silent hemoglobin variants; Dilip K Rai1; Gunvor Alvesius1; Britta Landin1; William J Griffiths1; Karolinska Institutet, Stockholm; KFC, Sweden; Clinical Chemistry, Stockholm; MBB, Sweden

TPD 149  Identification of the blocked N-terminus of baculovirus expressed His-tagged protein kinase B-beta as N-acetyl serine; John Q. Hu1; Vivian Li1; Rashid Syed1; Greg Brothers1; Robert Rosenfeld1; Wen-Tse Tseng1; Brian Varnum1; Mark Bray1; Hsiang Lu1; Mitsuru Hamu1; Angen Inc, Thousand Oaks, CA; Angen Institute, Toronto, Canada

TPD 150  Protein Profiling, Isolation and Identification Using Non-Porous RP-HPLC from Human Breast Cancer Cells with Analysis by MALDI-TOFMS and LC-MS-MS; Bathsheba E. Chong1; Rick L. Hamler1; David M. Lubman1; Fred R. Miller1; Allen J. Rosenspire1; University of Michigan, Ann Arbor, MI; Karmanos Cancer Institute, Detroit, MI; Wayne State University, Detroit, MI

TPD 151  Elucidation of Complex Disulfide Structure of Fc-Osteoprotegerin Dimer Protein by Ultra-Fast PSESI-LCMS and MALDI-PSD; John C. Le1; Lee Anne Merewether1; Grant Shimamoto1; Angen, Inc., Thousand Oaks, CA

TPD 152  A New On-Plate Microextraction Approach for Detection of Peptides by Single-Cell MALDI Mass Spectrometry; Lingjun Li1; Elena V. Romanova1; Amanda B. Hummon1; Stanislav S. Rubakhin1; Vera Y. Alexeeva1; Klaudius R. Weiss1; Ferdinand S. Vilim1; Jonathan V. Sweedler1; University of Illinois, Urbana, IL; Mount Sinai School of Medicine, New York, NY

TPD 153  The disulfide bond linkages in insulin-like growth factor binding protein-4 (IGFBP-4); Michael A. Baldwin1; Dirk Chelius2; E. Martin Spencer2; University of California, San Francisco, CA; California Pacific Medical Center, San Francisco, CA

TPD 154  The Protein Composition of the Enamel Pellicle; Zhuchen Wu1; James Grogan1; Frank Oppenheim1; Catherine E. Costello1; Boston University School of Medicine, Boston, MA; Boston University School of Dental Medicine, Boston, MA

TPD 155  Rescheduled as ThuA pm 04:40

TPD 156  Trapping of Protein-based Radicals Formed in the Metmyoglobin/Hydrogen Peroxide Reaction using DBNBS: A Mass Spectrometric Investigation; Angelo Filosa1; Ann M. English1; Concordia University, Montreal, Canada

TPD 157  de novo Sequencing of an Immune Induced Molecule of drosophila Melanogaster by Nano-Electrospray Ion Trap and MALDI-TOF Mass Spectrometry; Nukhet Cavusoglu1; Nathalie Carte1; Emmanuelle Leize1; Philippe Bulet1; Jules A. Hoffmann1; Alain Van Dorselaer1; Laboratoire de Spectrometrie de Masse Bioorganique, Strasbourg, France; Reponse Immunitaire et Dev., Strasbourg, France

TPD 158  Characterization of Selenoprotein P by MALDI-TOF MS and NanoESI-MS/MS; Shuang Ma1; Ansley Tharpe1; Kristina Hill1; Raymond Burck1; Richard Caprioli1; Vanderbilt University, Nashville, TN

TPD 159  The Anchor Structure of Cell Wall Surface Proteins in Enterococcus faecalis; Gautam Dhar1; Kym F. Faull1; Olaf Schneewind1; University of California, Los Angeles, CA

TPD 160  Peptidylglycine-alpha-hydroxylating Monooxygenase Generates Two Hydroxylated Products From Its Mechanism-based Suicide Substrate, 4-Phenyl-3-butenolic Acid; Henry M.
TUESDAY POSTERS

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6:00 – 6:30 pm
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Fales 1; William J. Driscoll 2; Simone Konig 3; Lewis K. Pannell 3; Betty A. Epper 3; Gregory P. Mueller 3; NHLBI, NIH, Bethesda, MD; Uniformed Services Univ. of the Health Sciences, Bethesda, MD; NIDDK, NIH, Bethesda, MD; Johns Hopkins School of Medicine, Baltimore, MD

TPD 161
Electrospray and CE-MS Characterization of BSA-Fatty Acid Complexes; Minshan Shou 1; Brian T. Cooper 1; UNC Charlotte, Charlotte, NC

TPD 162
Influences of the Lactam Bridge in Human Parathyroid Hormone (hPTH) Peptides on Selective Cleavages at the Aspartic Acid Residue; Nghanh C. Luu 1; Douglas P. Ridge 1; Runzhi Zhao 1; Robert McKean 1; Stephen Codorn 1; University of Delaware, Newark, DE; Rhone-Poulenc Rorer, Collegeville, PA

TPD 163
Monitoring Protein Kinase Catalyzed Reactions Using ESI-MS; Darryl L. Davis 1; Catherine M. Bentzley 1; University of the Sciences, Philadelphia, PA

TPD 164
Proteins in human liquor; Albert Siekmann 1; Wilma Dormeyer 1; Steffi Wortelkamp 1; Dirk Wotlall 1; Wilfried Kuhn 1; Helmut E. Meyer 1; Univ. Bochum, Germany; St. J osef Hospital Bochum, Germany

TPD 165
Identification of N-linked Glycoproteins, which Vary between the Normal and Cancer States, Using Prostate Cancer Cell Line LNCaP and Applying 2-D Gels, DE-MALDI MS and Database Searches; Nikitia N. Dinh 1; Dudley Williams 1; Terry Lee 1; Mary K. Young 1; BRI of the City of Hope, Duarte, CA

TPD 166
Subtractive Analysis of High Resolution Fourier Transform Mass Spectrometric Data for Identification of Cancer Related Class II MHC Peptides; Forest M. White 1; Jeffrey Shabanowitz 1; Donald F. Hunt 1; University of Virginia, Charlottesville, VA

TPD 167
ESI-MS determination of the steady-state kinetics for the reaction between ricin A-chain and HIV-1 psi-RNA hairpins; Dan Fabris 1; University of Maryland, Baltimore, MD

TPD 168
Studying germ line formation during maturation of C. elegans by differential proteome analysis of a temperature-sensitive mutant; Marcus Bartscheff 1; Bruno Ringel 1; Keith Ashman 1; Ralf Schnabel 1; Hans-Juergen Thiesen 1; Michael O. Glockler 1; University of Rostock, Rostock, Germany; EMBL, Heidelberg, Germany; Biozentrum, TU Braunschweig, Braunschweig, Germany

TPD 168b
Screening of Brain Protein Profiles in Animal Models of Parkinson’s Disease; Karl Skold 1; Johan Eriksson 1; Jonas Aestrom 1; Bengt Bjellqvist 1; Per E. Andre 1; Uppsala University, Uppsala, Sweden; Amersham Pharmacia Biotech, Uppsala, Sweden

SEPARATIONS/MS (TECHNIQUES) BIOMEDICAL APPLICATIONS, 169 – 198

TPE 169
The Use of LC/ESI/TOF/retESOFS/MS for Characterization of Oncoproteins from Human Breast Cancer Cells; Rick L. Hamler 1; Bathsheba E. Chong 1; David M. Lubman 1; The University of Michigan, Ann Arbor, MI

TPE 170
Identification of Proteins from Human Ovarian Cancer Cells Using a Two-Dimensional Liquid Phase Separation Method Followed by MALDI-TOF Mass Spectrometry; Haixing Wang 1; Maureen T. Kachman 1; David E. Misek 1; David M. Lubman 1; The University of Michigan, Ann Arbor, MI

TPE 171
The Use of Two-Dimensional Liquid Phase (IEF-Nonporous RP HPLC) Separations of Whole Cell Lysates for the Identification of Cancer Marker Proteins; Maureen T Kachman 1; Haixing Wang 1; David E Misek 1; David M Lubman 1; University of Michigan, Ann Arbor, MI

TPE 172
Capillary Electrophoresis-Electrospray Mass Spectrometry of Nucleosides and Nucleotides: Application to Phosphorylation Studies of Anti-HIV Nucleosides in Vitro; Chun-Sheng Liu 1; Woei G. Tan 1; Jyy S. Huang 1; Nan Li 1; David L. J. Tyrrell 1; Norman J. Dovichi 1; University of Alberta, Edmonton, AB, Canada

TPE 173
SRM-ESI-MS Determination of a Selected Estrogen Receptor Modulator-Related Compound and its Metabolite in Human Plasma Using High-Throughput, Sequential Injection and Chromatography; Joelle L. Onorato 1; Jack D. Henion 1; Paul M. Lefebvre 1; Jeffrey F. Kiplinger 1; Cornell University, Ithaca, NY; Gilson Center for Integrated Technology, Lincoln, RI

TPE 174
Analysis of sulfated neurosteroids in brain by capillary liquid chromatography/micro-electrospray mass spectrometry; Suayu Liu 1; Jan Sjovall 1; William J. Griffiths 1; Karolinska Institute, Sweden

TPE 175
Quantification of neurosteroids in rat plasma and brain following swim stress and allopregnanolone administration using negative chemical ionization gas chromatography/mass spectrometry; Robert L. Fitzgerald 1; Jeffery D. Rivera 1; Robert H. Purdy 1; George F. Koo 1; Monique Valle 1; IA Med Center/University of California, San Diego, CA; Scripps Research Institute, San Diego, CA

TPE 176
Determination of neuropeptides in artificial cerebrospinal fluid using column-switched micro-LC coupled to orthogonal time-of-flight mass spectrometry; My. M. Moberg 1; Jonas Bergquist 1; Karin E. Markides 1; Uppsala University, Uppsala, Sweden

TPE 177
Quantification of Bone Markers by LC/MS/MS; Maria L. Osipa 1; Cynthea Audaun 1; Adrian R. Woolfit 1; Hubert Vesper 1; Gary Myers 1; John R. Barr 1; Centers for Disease Control and Prevention, Atlanta, GA

TPE 178
Strategies for the Identification of Novel Growth Factor Receptor Binding Peptides; Adam W. Lucka 1; Douglas J. Beussman 1; Purdue University, W. Lafayette, IN

TPE 179
Oligonucleotide affinity chromatography and MALDI TOF define transcription factor complexes assembled on discrete promoter elements; A. Christie King 1; Pavel Bondarenko 1; Charlotte Mobarak 1; Sebastian Bredow 1; Lovelace Respiratory Research Institute, Albuquerque, NM; Thermo BioAnalysis Corporation, Santa Fe, NM

TPE 180
Quantitation of Androgenic and Estrogenic Steroids in Serum using Gas Chromatography and Negative Chemical Ionization Mass Spectrometry; René Bérube 1; Jacinthe Malecnant 1; Dominique Gauvin 1; Martine Blais 1; Eric Gagnon 1; Réjean Dumas 1; Marie-
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<td>6:00 – 6:30 pm</td>
<td>REMOVE POSTERS. Please leave posters for the full day.</td>
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TUESDAY POSTERS

Claude Racine 1; Josée Bourque 1; Alain Balanger 1; CHUL Research Center, Ste-Foy, Québec, Canada

**TPE 181**

Nano-HPLC as a Preparative Technique for Isolating Peptides from Proteolytic Digests for Subsequent Characterization by MALDI-TOF MS and Nanospray MS/MS; Célestin E. Dondéu 1; Don Griffin 2; Elisabeth Barofsky 2; Douglas F. Barofsky 2; Oregon State University, Corvallis, OR

**TPE 182**

Immovilized gradient Non-porous Reversed Phase HPLC Mass Spectrometry (IPG-NP RP HPLC-MS): A Novel 3-dimensional Separation Method for Generation of 3-dimensional Whole Cell Lysate Protein Profiles; Siyuan Gong 1; Daniel B. Wall 1; University of Michigan, Ann Arbor, MI

**TPE 183**

Carrier Ampholyte IEF with Electrophoresis Coupled with Nonporous RP HPLC for the Identification of Cellular Proteins by MALDI-TOF Mass Spectrometry; Siyuan Gong 1; Daniel B. Wall 1; David E. Misek 1; David M. Lubman 1; The University of Michigan, Ann Arbor, MI

**TPE 184**

Analysis of Neutral Oligosaccharides by Aminoalkyl-phase Capillary Electrochromatography/Electrospray Ionization - Ion Trap Mass Spectrometry; Amy H. Quach 1; Milos V. Novotny 1; Indiana University, Bloomington, IN

**TPE 185**

Molecular Anatomy of Bovine Cerebellum Using Multi-Dimensional HPLC Combined with ESI/TOF Mass Spectrometry; Kazuo Seto 1; Toshihiko Miki 2; Masanori Takao 2; Toshio Yamanaka 2; PE Biosystems Japan, Tokyo, Japan; Tokyo Metropolitan University, Tokyo, Japan; National Institute for Infectious Diseases, Tokyo, Japan

**TPE 186**

Alkyl Chloroformates as General Purpose Reagents for the Determination of Amino Acids, Neuroamines and Polyamines in Biological Matrices by HPLC/Atmospheric Pressure Ionization Mass Spectrometry; Petar Simic 1; Daniela Chvalova 2; Petr Husek 1; Institute of Entomology, Czech Republic; Charles University, Prague, Czech Republic

**TPE 187**

CE/MS/MS analyses of Protein Digests of Human Myelin Basic Proteins in a qIT/teTOF Mass Spectrometer; Jeonggwon Kim 1; Steve Parus 2; Robert Zand 1; David M. Lubman 1; University of Michigan, Ann Arbor, MI

**TPE 188**

Size Exclusion Chromatography-Microelectrospray Ionization Mass Spectrometry Analysis of Non-Covalent Protein Complexes; Linda M. Benson 1; Stephen Naykor 2; Mayo Clinic/Foundation, Rochester, MN

**TPE 189**

Determination of Androstrone Glucuronide and Androstane-3α,17β-diol-glucuronide in Human Plasma by Turbo-Ionspray LC-MS/MS; Patrick Bélanger 1; Dominique Paradis 1; René Berube 1; CHUL Research Center, Ste-Foy, Canada

**TPE 190**

Analysis of Underivatized Amino Acid Mixtures and Protein Digests Using HPLC/MPS-MS; Jun-Young Kwon 1; Mehdi Moimi 1; University of Texas, Austin, TX

**TPE 191**

Improved Silver Staining Protocols Compatible with Large-Scale Protein Identification; Eivind Moertt 1; Thomas N. Krogh 1; James Crawford 2; Lene Jakobsen 2; Hildur Mortensen 2; Henrik Vorum 1; Angelika Goerg 1; MDS Protana A/S, Odense, Denmark; Institute for Medical Biochemistry, Aarhus, Denmark; Technical University Munich, Freising-Weihenstephan, Germany

**TPE 192**

High Throughput Purification, Identification and Characterization of Proteins by MALDI-TOF Mass Spectrometry; Tom C. Hassel 1; Handong Li 1; John G. Dapron 1; Rick J. Mehlig 1; William K. Kappel 1; Sigma Chemical Company, St. Louis, MO

**TPE 193**

Development of an LC-MS Method for Simultaneous Determination of Retinol and all-trans, 9-cis, and 13-cis Retinoic Acid in Rat Prostate; Yan Wang 1; William Y. Chang 1; Gail S. Prins 2; Richard B. van Breemen 1; University of Illinois, Chicago, IL

**TPE 194**

Low Picoliter Volume Monolithic Columns for Online LC/MS Analysis of Proteins and Peptides; Roger E. Moore 1; Larry Licklider 2; Terry D. Lee 1; Beckman Research Institute, City of Hope, Duarte, CA; Zycos Inc., Cambridge, MA

**TPE 195**

High pH Mobile Phases for Reversed Phase HPLC-ESI/MS Peptide Mapping; Alex Apfel 1; Barry Boyes 1; John Chace 1; Bill Hancock 1; Meihao Hu 2; Xiaocheng Gu 3; Agilent Technologies, Palo Alto, CA; Peking University, Beijing, China

**TPE 196**

An Automated LC/LC/MS/MS Platform Using Binary IEX and Gradient Reverse-Phase Chromatography for Improved Proteomic Analyses; Michael Davis 1; Jill Beierle 2; Ted Bures 2; Michael McGinley 3; Jessica Mort 1; John Robinson 1; Chris Spahr 1; Scott Patterson 1; Amgen, Inc., Thousand Oaks, CA

**TPE 197**

High Performance Peptide Analysis by On-Line CE-MALDI/TOF MS; Ping Hu 1; Tomas Rejtar 2; Jan Preisler 1; Franta Foret 1; Barry L. Karger 1; Barnett Institute, Northeastern Univ., Boston, MA

**TPE 198**

Quantification of Serum Pancreatic Polypeptide by MALDI-TOF Mass Spectrometry; Martin P. Bucknall 1; Ani Amarantunga 2; George A. Smythe 2; Bernard E. Tuch 2; University of New South Wales, Sydney, Australia; Prince of Wales Hospital, Sydney, Australia.

**TPE 199**

Assessment of in vitro Permeability Across the Blood-Brain Barrier Using LC/MS/MS in Drug Discovery; Inhoo Chu 1; Fei Liu 1; Tony Soares 2; Pramila Kumari 2; Chin-Chung Lin 2; Ronald White 1; Amin A. Nomer 1; Schering-Plough Research Institute, Kenilworth, NJ

**TPE 200**

LC/MS Method for High Throughput log P/log D Profiling; Edward Kerns 1; Susan L. Petusky 2; Michael Chlenov 2; Teresa A. Kleinlop 1; Oliver McConnell 1; Wyeth Ayerst Research, Princeton, NJ

**TPE 201**

High Throughput Log D Determination Using Parallel Liquid Chromatography/Mass Spectrometry (LC/MS); Xiaoli Wang 1; Rongda Xu 2; Dean M. Wilson 1; Robyn A. Rourke 1; Daniel B. Kassell 1; DuPont Pharmaceutical Research Laboratories, San Diego, CA

**TPE 202**

Direct Determination of Early Drug Discovery Compounds in Plasma Using Mixed-Function Column Liquid Chromatography / Tandem Mass Spectrometry; Matthew Bryant 1; Jean-Marc Brisson 1; Walter Kofrniczker 1; Yunsheng Hsieh 2; Grace Gruela 2; Schering Plough Research Institute, Kenilworth, NJ

**SEPARATIONS/MS – DRUGS, 199 - 228**

**TPF 199**

**TPF 200**

**TPF 201**

**TPF 202**
TUESDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 pm  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

TPF 203  Withdrawn
TPF 204  Distribution of the Hallucinogens N,N-Dimethyltryptamine and 5-Methoxy-N,N-Dimethyltryptamine in Rat Brain Following Intraperitoneal Injection; Connie M. Davo1; Martha A. Littlefield-Chabaud1; Steven A. Barker1; Louisiana State University, Baton Rouge, LA

TPF 205  Determination of Acyclovir Metabolites in Human Serum and Cerebrospinal Fluid by LC/API/MS/MS; Showchen Hsieh1; John Dunn1; GlaxoWellcome, Research Triangle Park, NC

TPF 206  Method for LC/MS/MS Analysis of Paclitaxel and Metabolites in Plasma Using an Isotopically-Labelled Internal Standard; Michael S. Alexander1; John W. Dolan1; James D. McChesney1; Steve J. Bannister1; James H. Rudy1; Jan Zygmunt1; LC Resources, McMinnville, OR; NaPro Biotherapeutics, Inc, Boulder, CO

TPF 207  Quantitative Analysis of Indapamide in Whole Blood by LC/MS/MS; Marius Folga1; Garnet McRae1; Manju Gupta1; Orthochemia Fragiskatos1; Loreda Di Donato1; Phoenix International Life Sciences Inc., Montreal, Canada

TPF 208  Improved Analysis of Paclitaxel in Human Plasma; Garnet McRae1; Manju Gupta1; Orthochemia Fragiskatos1; Loreda Di Donato1; Phoenix International Life Sciences Inc., Montreal, Canada

TPF 209  Quantitative Analysis of Promethazine in Human Plasma Using Turbo Ionspray LC-MS-MS; James Havel1; Dr. Allan Xu1; Keystone Analytical Laboratories, North Wales, PA

TPF 210  Simultaneous Determination of SU005416 and its Metabolites in Rat and Dog Plasma by LC/MS/MS; Xiping Zhao1; Chris Yang1; Joshua Haznedar1; Greg Wagner1; Laura Shawver1; Lida Antonian1; Sugen, Inc., South San Francisco, CA

TPF 211  Identification of a Previously Unknown Low Level Degradation Product of Montelukast Sodium by Isolation, LC/MS, and LC/NMR; Rosie Visentin1; Suzanne Spagnoli1; Caroline Rousseau1; Elisabeth Sourial1; Stephanie Hall1; Laird A. Trimble1; Merck Frost Centre for Therapeutic Research, Pie-Claude, Canada

TPF 212  Analysis of R.R-Formoterol in Human Plasma by LC/MS/MS; Michael Allen1; Quao Zhan1; Christian McGhee1; Patrick Koch2; Triangle Laboratories, Inc., Durham, NC; Sgroaroc, Marlborough, MA

TPF 213  Analysis of Propofol in Beagle Plasma by High Resolution GC/MS/SIR; Qiao Zhan1; Michael Allen1; Keith Erdman2; Triangle Laboratories, Inc., Durham, NC; Abbott Laboratories, Abbott Park, IL

TPF 214  A Sensitive and Specific Automated APCI LC/MS/MS Assay for Misoprostol Acid in Human Plasma in the Picogram Range; Roger Demers1; Luca C. Matassa1; Tung Chau1; Sanj Deverajan1; MAXXAM Analytics Inc, Ontario, Canada

TPF 215  Determination of Risperidone and Hydroxyrisperidone by Direct Online Injection (Cohesive Technologies) Coupled to Scxi API 3000 MS Detection; Erick Tessier1; Adria E. Nigeebrugge1; Rudolf Guibaud1; Loreda Di Donato1; Robert Masse2; Phoenix International, Montreal, Canada

TPF 216  Development of a LC/MS/MS Assay for the Quantification of LY326869 and its Dehydrogenated Metabolite in Human Plasma; Kirk D. Knotts1; Darlene K. Satonin1; Kenneth J. Ruterbories1; Bradley L. Ackermann1; Richard L. Shugert1; Boris A. Czeskis1; Qimin Li1; Michelle M. He2; Frank J. Belas1; Eli Lilly and Company, Indianapolis, IN

TPF 217  Development of a Dual Range LC/MS/MS Assay for the Quantification of LY444657 and Two Metabolites in Rat and Monkey Serum; John H. Mullen1; Joseph L. Horn1; Elizabeth M. Watts1; Richard L. Shugert1; Michelle M. He1; Darlene K. Satonin1; Eli Lilly and Company, Indianapolis, IN

TPF 218  Development of a LC/MS/MS Assay for the Quantification of LY335979 and its Metabolite, 335995, in Human and Rat Plasma; Elizabeth M. Verburg1; Tamara R. Priest1; Darlene K. Satonin1; Ajai K. Chaudhary1; Eli Lilly and Company, Indianapolis, IN

TPF 219  Determination of degradation products from sumatriptan succinate by LC/MS and LC/MS/MS; Xiao-shui (Sophia) Xu1; Kathick Vishwanathan1; Michael G. Bartlett1; James T. Stewart1; College of Pharmacy, University of Georgia, Athens, GA

TPF 220  The need for adequate LC separation to eliminate the interference arising from nefazodone in the quantitation of its biotransformation product in plasma by direct-injection LC/MS/MS; Yuan-Qing Xia1; Daisy Whigan1; Mark L. Powell1; Mohammed Jama1; Bristol-Myers Squibb Company, New Brunswick, NJ

TPF 221  Structural Elucidation of Biodegradation Products of a Quinolone Antibiotic in Very Dilute Aqueous Waste Streams by Accurate Mass LC/MS and LC/MS/MS; Duncan K. Bryant1; Christopher J. Gripton1; Luisa Freitas Dos Santos1; Sylvia Baron3; SmithKline Beecham Pharmaceuticals, Tonbridge, Kent, UK; SmithKline Beecham Pharmaceuticals, Harlow, Essex, UK

TPF 222  Structural Characterization of Oxidative Degradation Products of a Novel Triazone Antifungal Agent by High Performance Liquid Chromatography and Electrospray Ionization Tandem Mass Spectrometry; G. Chen1; B. N. Pramanik1; W. Feng1; H. Liu1; R. Malchow1; F. Bennett1; E. Lin1; T. M. Chan1; Schering-Plough Research Institute, Kenilworth, NJ

TPF 223  Determination of Benzalkonium Chloride in Aqueous Samples Using Reverse Phase Liquid Chromatography - Electrospray Mass Spectrometry; Daniel J. Weston1; J. Graham Lawrence2; Mark D. Burford1; Ian H. Grant1; David Cooper1; Ian D. Bromlow2; Keith D. Bartle2; Unilever Research Port Sunlight, UK; University of Leeds, UK

TPF 224  Do all the deuterium labeled internal standards behave chromatographically the same as their corresponding compounds?; Wei Sun1; John Rollag1; Souhail Naghmouchi1; Patrick Lin1; MDS Harris, Inc., Lincoln, NE

TPF 225  Mass-Directed Autopurification: Optimization of Separation and Detection Chemistry; Thomas E.
TUESDAY POSTERS

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Wheat; Charles H. Phoebe; Uwe D. Neu; Waters Corporation, Milford, MA

TPF 226 Quantitative MS Analysis of Drug Mixture for High Throughput: A Comparison of LC/MS And FIA/MS; Kate Yu; Michael Balogh; Jeanne Li; Eric Block; Waters Corporation, Milford, MA

TPF 227 High Throughput Quantitation Using Indexed Multi-electrospray Technology in Support of Drug Discovery; D. L. Miller; R. O. Cole; D. Little; A. Hooper; Pfizer, Groton, CT; Micromass Inc., Manchester, UK

TPF 228 Frontal Affinity Chromatography Mass Spectrometry (FAC-MS): Method Evaluation with a Nuclear Hormone Receptor; David C. Schriemer; Nora Chan; Darren Lewis; Philip Rosner; Lise Holtz; Kieran Geoghegan; Michele Kelly; INH Technologies, Inc., Calgary, Canada; Pfizer Central Research Division, Groton, CT

SEPARATIONS: CONTAMINANTS, NATURAL PRODUCTS, 229 - 243

TPG 229 Determination of estrogens in animal feeds by negative-ion electrospray LC/MS; Ernst Pittgenauer; Thomas Aichinger; Josef Bailer; Walter Welz; Fed. Off. & Res. Agric., Vienna, Austria; Goreon Bioan. Labs, Wels, Austria

TPG 230 Detection of Isoflavonoids from Urine Using Solid-Phase Microextraction Gas Chromatography Mass Spectrometry; David Black; Mary Satterfield; Jennifer Brodbelt; University of Texas, Austin, TX

TPG 231 On-line Sample Preparation for the Automated LC-ES/MS Analysis of Soy Isoflavones in Blood; Daniel R. Doerge; Mona Churchwell; Steve Bajic; Michael McCullagh; Zora Djuric; Nat. Ctr. Tox. Res., Jefferson, AR; Finnigan MassLab, Manchester, UK; Wayne State University; Detroit, MI

TPG 232 Usefulness of High Performance Liquid Chromatography/Tandem Mass Spectrometry and Gas Chromatography/Mass Spectrometry for the Analysis of Potential Allergens in Oakmoss Absolute; Dennis F. H. Wijtten; Richard D. Hiserodt; Sharon M. Brown; Cynthia J. Musstein; IFP, Union Beach, NJ

TPG 233 Rapid quantitative screening of polyphenol compounds; Neil J. Loftus; Stephen Koczten; Susanne Schindler; Alistair Sterling; Shimadzu GmbH, Germany

TPG 234 The Analysis of Pesticide in Human Plasma Using LC-MS; Spiros Garbis; Richard van Bremen; University of Illinois, Chicago, IL

TPG 235 Profiling Saponin Glycosides in Medicago sativa (alfalfa) and Medicago truncatula Using HPLC Coupled to an Electrospray Ion-Trap Mass Spectrometer; David V. Huhman; Richard A. Dixon; Lloyd W. Sumner; The Noble Foundation, Ardmore, OK

TPG 236 A comparison of the structural information contained in the EI and CI LCMS spectra of selected chemicals and natural products; Scott Niemann; CSS Analytical Co. Inc, Shawnee, KS

TPG 237 Detection of Beneficial Components in Herbal Products by GC-MS; Mohammed Al-Tufail; Huda Hasan; John Tate; Mohammed Akram; Afrozul Haq; King Faisal Specialist Hospital, Riyadh, Saudi Arabia

TPG 238 Analysis of Tobacco Specific N-Nitrosoamines (TSNAs), NN and NNI, in Tobacco by HPLC/Particle Beam/TEA, HPLC/ESI/MS, and GC/ESI/MS; Rick D. Holland; Thomas M. Heinze; Pat Freeman; Willie M. Cooper; Aaron Kuperman; Jackson O. Lay Jr.; Stanley M. Billedeau; NCTR, Jefferson, AR

TPG 239 Liquid Chromatography/Electrospray Ionization/Mass Spectrometry Study of Sulfur Heterocycles; Walter Rudzinski; Steve Sassaman; Linette Watkins; Southwest Texas State U, San Marcos, TX

TPG 240 Ion Chromatography/Mass Spectrometry of Organic Acids in Beverages Using Electrospray Ionization in Negative Ion Mode; Robert A. Sanders; D. Rick White; Deborah K. Ewald; Patricia Hudson; The Procter & Gamble Company, Cincinnati, OH

TPG 241 Determination of Arginine and Methylated Arginines from Human Plasma by LC/MS/MS; Karthick Vishwanathan; James T. Steward; Randall Tackett; Michael G. Bartlett; The University of Georgia, Athens, GA

TPG 242 Identification of a Novel Secondary Metabolite, A Comparison of Two Generations of Mass Spectrometers; Jesse L. Balcer; Jeffrey R. Gilbert; Paul R. Graupner; Tom L. Siddall; Gary D. Crouse; Phil Fanwick; Dow AgroSciences LLC, Indianapolis, IN; Purdue University, West Lafayette, IN

TPG 243 Identification of Asian Ginseng (Panax ginseng) and American Ginseng (Panax quinquefolius) Using High Performance Liquid Chromatography Tandem Mass Spectrometry; Wenku Li; Chonggu Gu; Hongjie Zhang; Harry H. S. Fong; Richard B. van Bremen; John F. Fitzloff; University of Illinois College of Pharmacy, Chicago, IL

ENVIRONMENTAL ANALYSIS I, 244 - 283

TPH 244 Investigation of Disinfection By-products in Drinking Water Using Solid-Phase Extraction and Gas Chromatography/Mass Spectrometry; Salvador J. Pastor; Stuart W. Krasner; Howard S. Weinberg; Susan D. Richardson; Metropolitan Water District of Southern California, La Verne, CA; University of North Carolina, Chapel Hill, NC; U.S. Environmental Protection Agency, Athens, GA

TPH 245 Detection of the Nine Chlorinated and Brominated Halocarbon Acids at Part-per-Trillion Levels Using ESI-FAIMS-MS; Barbara Ellis; David A. Barrett; Roger Gueuvenmont; Kenneth Froese; Steve E. Hrudey; Randy W. Purves; National Research Council of Canada, Ottawa, Canada; University of Alberta, Edmonton, Canada; PE-Sciex, Concord, Canada

TPH 246 Solid Phase Microextraction for Trace Level Analysis of Disinfection By-products; Alicia C. Gonzalez; Stuart W. Krasner; Howard Weinberg; Susan D. Richardson; Metropolitan Water District, La Verne, CA; University of North Carolina, Chapel Hill, NC; U.S. Environmental Protection Agency, Athens, GA

TPH 247 Survey of Halonitromethanes and Iodomethanes: Disinfection By-products in Drinking water; Alfred
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**TPH 248**

**Analysis of Trace Level NMDA in Drinking Water**
- Yingbo C. Guo 1, Cordelia J. Hwang 1, Russell Chinn 1, Sylvia E. Barrett 1, Metropolitan Water District of Southern California, La Verne, CA

**TPH 249**

**Analysis of Perchlorate in Drinking Water, Human Serum, and Other Biological Matrices by LC/MS/MS**
- Enaksha Wickremesinhe 1, Emily Stauffer 1, John Flaherty 1, Centre Analytical Laboratories Inc

**TPH 250**

**Electrospray Mass Spectrometry of Stable Association Complexes for the Determination of Drinking Water Contaminants**
- Matthew L. Magnuson 1, Edward T. Urbansky 1, Catherine A. Kelty 1, US Environmental Protection Agency, Cincinnati, OH

**TPH 251**

**LC-MS/MS Analysis of Microcystins in Blue-green Algae Products**
- Benjamin P.-Y. Lau 1, David Lewis 1, Jim Lawrence 1, Barbara Niedzwiedak 1, Cathie Menard 1, Health Canada, Ottawa, Canada

**TPH 252**

**Detection of Toxins in Environmental Samples Using Py-MAB-TOF Mass Spectrometry**
- Claude Beaugrand 1, Pascal Martin 1, Anik Forest 1, Denis Faubert 1, Gabriel Sanchez 1, Michel J. Bertrand 1, MGP Instruments, Lamanon, France; Deyso Technologies, Quebec, Canada; University of Montreal, Montreal, Canada

**TPH 253**

**An Examination of Flavonoids by ESI-MS and ESI-MS/MS: Methods and Madness**
- Richard J. Hughes 1, Timothy R. Crolely 1, Yiannis Kiarisipis 1, Christopher D. Meicaff 1, Raymond E. March 1, Trent University, Peterborough, ON, Canada

**TPH 254**

**Application of FAB MS for Studying Composition and Structure of Inorganic Aquatic Sediments**
- Gennadi Pronchenko 1, Irene Korobemakova 1, Alexander Yermakov 1, Inst. of Energy Problems of Chemical Physics RAS, Moscow, Russia

**TPH 255**

**Trace Level Detection of Trichloroethylene and its Metabolites in Whole Blood**
- Stacy D. Cross 1, James V. Bruckner 1, Michael G. Bartlett 1, S. Muralidharan 1, University of Georgia, Athens, GA

**TPH 256**

**Characterization of Extractable Organochlorines from Marine Animals by Various Mass Spectrometric Techniques**
- Stacey J. Mass 1, Joe W. Kiceniuk 1, Christina S. Bottaro 1, Amara Chett 1, Louis R. Ramey 1, Dalhousie University, Halifax, Nova Scotia, Canada

**TPH 257**

**The Simultaneous Quantitation and Confirmation of Multiple Quinone Biosynthesis Inhibitors (QBI) in Rodent Chow by HPLC/ESI/MS**
- Dan A Markham 1, M. J. Bartels 1, N. R. Pearson 1, B. J. Schuster 1, M. Simo 3, Dow Chemical Company, Midland, MI

**TPH 258**

**Mass Spectrometric Methods for the Determination of Estrogens and Estrogen Metabolites in Environmental Matrices**
- Timothy R. Crolely 1, Richard J. Hughes 1, Brenda G. Koegel 1, Christopher D. Metalfat 1, Raymond E. March 1, Trent University, Peterborough, ON, Canada

**TPH 259**

**Normal Phase HPLC/APCI/MS Data-Dependent Fracton Collection of Preparatively Separated Homologues of Nonylphenol Polyoxyethylenes**
- Tim Hoffman 1, Yves Mouget 1, Jeffery Plomley 1, Patrick Crozier 3, Vincent Taguchi 1, MSD SCIX, Concord, Canada; Ontario Ministry of the Environment and Energy, Etobicoke, Canada

**TPH 260**

**Determination of Dissolved Naphthenic Acids in Natural Waters Using Negative-ion Electrospray Mass Spectrometry**
- John V. Headley 1, Kerry M. Peri 1, Duane A. Friesen 1, Marcus Winkler 1, NWRI, Environment Canada, Saskatoon, Canada; UZF Centre for Environmental Research, Magdeburg, Germany

**TPH 261**

**Quantitative Analysis of PCD/FS in Marine Sediment Samples Using HRGC/MS**
- Ki-Ho Kim 1, Min-Ho Boo 1, Ik-Hee Lee 1, Chan-Won Lee 1, Yongseong Kim 1, Sang Chun Lee 1, Kyungnam University, Masan, Kyungnam, Korea

**TPH 262**

**Quantitative Determination of Polybrominated Flame Retardants in Environmental Samples by GC/HRMS with MAB vs EI Ionization**
- Tim He 1, Michael G. Ikononov 1, Mark B. Fischer 1, Denis Faubert 1, Institute of Ocean Sciences, Sidney, Canada; Deyso Technologies, Montreal, Canada

**TPH 263**

**Determination of Brominated Flame Retardants in Environmental Matrices**
- Mohan Allee 1, David B. Sergeant 1, Jennifer M. Luross 1, Christina M. Cannon 1, National Water Research Institute, Burlington, Ontario; GLFAS, Burlington, Ontario, University of Guelph, Guelph, ON, Canada

**TPH 264**

**Determination of Tetraethylenes in Aquaculture Products by APCI-LC/MS/MS**
- Dayue Shang 1, Monica Dyck 1, Xiaoyan Jia 1, Angelo DiCesio 1, Carl Alleyne 1, Helen Nicolodakis 1, Brian Mori 1, Health Canada, Burnaby, Canada

**TPH 265**

**Sorption of tri- and diethyphosphate to mineral surfaces determined by atmospheric pressure chemical ionization Fourier-transform mass spectrometry (APCI-FTMS)**
- Patterson R. Nueske 1, Gary L. Mills 1, Savannah River Ecology Laboratory, Aiken, SC

**TPH 266**

**Identification of Erioglaucine (Brilliant Blue) as a Wastewater Marker by Liquid Chromatography/Electrospray Mass Spectrometry**
- Colleen E. Rostad 1, Jerry A. Leenheer 1, U.S. Geological Survey, Denver, CO

**TPH 267**

**Cost-effective Online Analysis of Semi-volatile Organic Compounds in Water by Automated SPE**
- Twin-PAL LVI-GC-MS; Yongtao Li 1, John George 1, Earl Hansen 1, Jerry Thomas 1, Werner Martin 1, Peter Smith 1, Environmental Health Laboratories, South Bend, IN; LEAP Technologies, Caryboro, NC

**TPH 268**

**Quantitative Determination of Two Diazinon Metabolites in Human Urine Using SPE-LC/ESI/MS**
- Nanzi Shi 1, Robert A. Yokley 1, Max W. Cheung 1, Novartis Crop Protection, Inc., Greensboro, NC

**TPH 269**

**Validation of an HPLC-LIF/UV/Electrospray Mass Method for Imidazolinone Herbicides in Aquaculture Matrices**
- John Albritten 1, Jeffrey T. Keefer 1, Stephanie Padilla 1, Michelle Spruill 1, Robert Voykner 1, Research Triangle Institute, RTP, NC

**TPH 270**

**Determination of Benomyl Residues in Various Crops using Liquid Chromatography/Electrospray
TUESDAY POSTERS

7:30 – 8:00 am SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 pm POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm REMOVE POSTERS. Please leave posters for the full day.

Ion Trap MS/MS; Lei Jin1; Frederick Q. Bramble2; Anne Pentz1; Teresa H. Johnson1; DuPont Agriculture Products, Wilmington, DE

TPH 271 The Application of Single Quadrupole Mass Spectrometers for Identification, Confirmation and Quantitation of Pesticide Residues; Emily Sibbes1; Kevin C. Crelin1; John Van Antwerp1; Waters Corporation, Dublin, CA

TPH 272 Multi Photon Ionization Mass Spectrometry of Carbamate Pesticides and Chemical Warfare Agents; Carsten Grun1; Christian Weickhardt1; Karen Toennies1; Juergen Grotemeyer1; Inst. Phy. Chem. University Kiel, Kiel, Germany

TPH 273 Determination of pesticides in plants with GC/MS in El, NCI and PCI mode, with normal and fast technique; Petra Gerhard1; Karin Friedrichs1; Shimadzu Deutschland GmbH, Duisburg, Germany; Chemisches Untersuchungsamt, Bielefeld, Germany

TPH 274 Detection and characterization of modern pesticides, their metabolites and degradation products by LC/MS/MS; Clevis J. Monasteros1; Yves Mougel1; Iryna Chervetsov1; Eva Duchoslav2; David Pekar3; Takeo Sakuma1; Luis E. Soto3; PE Sciex, Concord, ON; ASL Laboratories Inc., Vancouver, BC, Canada

TPH 275 Considerations in the Analytical Determination of the Substituted Urea Herbicide, Diuron; William E. Holmes1; Bert C. Lynn1; Earl G. Alley1; Mississippi State University, Mississippi State, MS

TPH 276 Contamination of the Caspian Sea Ecosystem with Organic Pollutants; Albert T. Lebedev1; Olga V. Poliakova1; Irina V. Dianova1; Lyudmila G. Saganova1; Moscow State University, Moscow, Russia

TPH 277 Mass Spectrometry in the Hydrosphere; David P. Fries1; R. Timothy Short1; Robert H. Byrne1; Chad E. Lembke1; Michael L. Kent1; University of South Florida, St. Petersburg, FL

TPH 278 Electrospray LC/MS Detection of S-12-(Diisopropylamino)ethyl Methylphosphonothioic Acid in Aqueous Solution; Dennis K. Rohrbaugh1; Michael W. Elley1; U.S. Army Edgewood Chemical Biological Center, APG, MD

TPH 279 Evaluation of Py-MAB-Tof as a Technique for the Detection of Explosives by Direct Analysis of Soil Samples; Anik Forest1; Pascal Martin1; Denis Faubert1; Gabriel Sanchez1; Michel J. Bertrand1; DEPHY Technologies, Quebec, Canada, University of Montreal, Montreal, Canada

TPH 280 HILIC-UV-ESI-MS for Characterization of TNT Transformation by Oxyrase; Ying Shi1; James A. Campbell2; Steven C. Goheen2; Pacific Northwest National Laboratory, Richland, WA

TPH 281 High-Throughput Screening of Chemical Weapons Related Compounds; Matthew D. Evans1; Karl A. Hanold1; Yong Liu1; Jack A. Syage1; Syagen Technology, Inc., Tuscan, CA

TPH 282 Rapid Determination of Explosives Residue by GC/MS; Mark L. Miller1; FBI Academy, FSRU, Quantico, VA

TPH 283 In vitro Metabolism Study with a Mixture of Organophosphorus Insecticides Chlorpyrifos and Diazinon; James A. Campbell1; Gary M. Meng1; Torika S. Poet1; Charles Timchalk1; Pacific Northwest National Laboratory, Richland, WA

MATERIALS AND PROCESS SUPPORT, 284 - 311

TPI 284 Analysis of Silicone Contaminants on Electronic Components by Thermal Desorption GC-MS; Eric D. Butryn1; Scientific Instrument Services, Inc., Ringoes, NJ

TPI 285 Equal intensity time of flight mass spectra of equimolar polydisperse synthetic polymers using cryodetectors; Damien Twerenbold1; Dominique Gritti1; Daniel Gerber1; Giovanni Gervasio1; Yvan Goin1; Alexandre Netuschil1; Frederic Rossel1; Dominique Schenker1; Jean-Luc Vuilleumier1; GenSpec SA & Institut de Physique, Neuchatel, Switzerland

TPI 286 Quantitative MS Analysis of Industrial Ethylene Oxide/Propylene Oxide Copolymers; Amy M. Tseng1; Rui Chen1; Nan Zhang1; Liang Li1; Nalco Chemical Company, Naperville, IL; University of Alberta, Edmonton, Canada

TPI 287 Comparison of Different MALDI-TOF MS Instruments for Analysis of Synthetic Polymers; H.C. Michelle Byrd1; Charles N. McEwen1; University of Delaware, Newark, DE; E.I. du Pont de Nemours and Co., Inc., Wilmington, DE

TPI 288 Determination of N-Nitrosamines in baby bottle rubber nipples by liquid chromatography-atmospheric pressure chemical ionization mass spectrometry; Michael P. Donegan1; William G. Sawyers1; Eric Stanislav2; PE Biosystems, Framingham, MA; West Pharmaceutical Services, Lionville, PA

TPI 289 Formulations and degradation pathways upon gamma irradiation of unknown copolymers surfactant mixtures by mass spectrometry techniques: GC-MS, FAB-MS, ES-MS/MS and MALDI-TOF; Bardia Amekrag11; Henri Virelizier1; Daniel Gaudin1; Gerard Guille1; Christophe Moulin1; Bernard Demaziere1; Ceo/Dcc/Dpe/Spex/Laso, Gif Sur Yvette, France; Evry, France

TPI 290 Characterisation of synthetic polymers by MALDI-TOF/MS: New methods of sample preparation and consequence on mass spectrum fingerprint; Aul Marie1; Jeremie Walker1; Francoise Fourrier1; Jean-Claude Tabet1; Universite Pierre et Marie Curie, Paris, France; Elf-Stocher, Lyon, France

TPI 291 Quantitative Determination of Saccharide Surfactants in Protein Samples by Liquid Chromatography Coupled with Electrospray Ionization Mass Spectrometry; Gejing Peng1; Denise Chow1; Gautam Sanyal1; AstraZeneca Research and Development Boston, Cambridge, MA

TPI 292 Development of MS/MS methodology in support of cleaning validation for pharmaceutical manufacturing; John P. Caesar1; Sigmund M. Waraszkiewicz2; Sigmund M. Waraszkiewicz2; Sigmund M. Waraszkiewicz2; AstraZeneca, Westborough, MA

TPI 293 Thermal Stability and Solvation Effect of An Inhibitor Aluminum Salt of Tris(N-nitrosophenylhydroxylamine); Frank Meng1; Juanita Parrish1; David Biro1; Sun Chemical Corporation (GP), Carlstadt, NJ
TUESDAY POSTERS

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6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

TPI 294  Fast GC/MS Identification of Sesquiterpenes; Qingmei Zha; Fernando Carrico; Serban C. Moldoveanu; Brown & Williamson Tobacco Corporation, Macon, GA

TPI 295  Unambiguous Characterisation of Synthetic Pathways by Exact Mass GC-MS Analysis using a GCT Mass Spectrometer; Anthony Newton; Martin R. Green; Peter M. Hancock; Victor Garner; Micromass UK Limited, UK; Hall Analytical Laboratories Ltd, UK

TPI 296  Structural Characterization of Copolymers (Polyesters) by GPC/FTMS; Wendy Zhong; William J. Simonsick, Jr.; Hai Ni; Mark D. Soucek; DuPont Marshall Laboratory, Philadelphia, PA

TPI 297  Thermal Desorption Mass Spectrometric Studies of Three-Dimensional Self-Assembled Monolayers; Julia E. Wingate; Gary L. Glish; Allen C. Templeton; Royce W. Murray; University of North Carolina, Chapel Hill, NC

TPI 298  Characterization of the Functional Properties of a Catalyst by Using Mass Spectral Thermodesorption Method - MSTD; Alexandre V. Mitroshin; Ada A. Poliakova; Pacific Northwest National Laboratory, Richland, WA

TPI 299  Product Analysis of Novel Anionic Polymerizations by MALDI TOF MS; Mark A. Arnould; Chrys Wesdemiotis; Youngjoon Lee; R.P. Quirk; The University of Akron, Akron, OH

TPI 300  Low-energy Collisions of Silyl Cations with an OH-Terminated Self-Assembled Monolayer Surface: Ion/Surface Reactions and Subsequent Surface Modification; Nathan A. Wake; Chris A. Evans; R. Graham Cooks; Purdue University, West Lafayette, IN

TPI 301  ESI-MS Detection of One Electron Oxidation Intermediates in Photochemical Reaction of Bis(2,2-bipyridine)diaminocerium(II) Complexes; Kazuyuki Abe; Tsutomu Abura; Tsuyoshi Fukuo; Yasuo Nakabayashi; Ryuchi Arakawa; Kansai University, Osaka, Japan

TPI 302  Fast Screening of Potential Degradates of a Novel Carbanapen Antibiotic by LC-MS; Zhongxi (Zack) Zhao; Qingxi Wang; Danielle Godshall; Xue-Zhi Qin; Eric W. Tsai; Robert A. Reed; Dominic P. Ip; Merck & Co., Inc., West Point, PA

TPI 303  Characterization of PMDA-ODA Derived Polymides Using MALDI Mass Spectrometry; Renata Murgasova; Yan Lin Zhang; David M. Hercules; James R. Edman; Vanderbilt University, DuPont Technologies

TPI 304  Characterization of Silicone Rubber Extract Using GPC and MALDI Mass Spectrometry; X. Michael Liu; E. Peter Maziarz; Paula Witham; Friend Price; David J. Heller; Bausch & Lomb, Rochester, NY

TPI 305  Silicon Alkoxides: An Electrospray Ionization-Fourier Transform Ion Cyclotron Resonance Mass Spectrometry and Tandem Mass Spectrometry Analysis of Species in Solution; Robert E. Bossio; Sean D. Callahan; Albert E. Steigman; Alan G. Marshall; Florida State University, Tallahassee, FL

TPI 306  Characterization of Cyclic Polyethiane by Electrospray Ionization Mass Spectrometry; Takehiro Watanabe; Tsuyoshi Fukuo; Kiyoshi Endo; Ryuchi Arakawa; Kansai University, Osaka, Japan; Osaka City University, Osaka, Japan; Kansai University, Osaka, Japan

TPI 307  Rules and Peculiarities of the Fragmentation of Single Amino Acids Prepared by Electrospray; Simone Koenig; Henry M. Fales; University of Muenster, Muenster, Germany; NIH, NHLBI, Bethesda, MD

TPI 308  Study of the Interactions between Long Chain Alkanes and Transition-Metal Ions and its Application in MS Analysis of Polyethylene; Rui Chen; Liang Li; University of Alberta, Edmonton, Canada

TPI 309  Electrospray Ionization Mass Spectrometry of Conducting Polymers; Anthony R. Dolan; E. Peter Maziarz; Troy D. Wood; State University of New York, Buffalo, NY; Bausch & Lomb Healthcare, Rochester, NY

TPI 310  Investigation of Poly(ethylene terephthalate) epsilon-caprolactone copolyester synthesis by SEC/MALDI-TOFMS; Martine Tessier; Jean-Pierre Bonnet; Alain Frader; Blais Jean-Claude; CNRS, Paris, France; Universite Pierre et Marie Curie, Paris, France

TPI 311  Effects of Matrix and Alkali Cation Availability on the MALDI-TOF Mass Spectra of Phosphorus-Containing Dendrimers; Jean-Claude Blais; Cedric-Olivier Turrin; Anne-Marie Carmine; Jean-Pierre Majoral; CNRS, Paris, France
WEDNESDAY POSTERS

7:30 – 8:00 am
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6:00 – 6:30 pm
REMOVE POSTERS. Please leave posters for the full day.

WPA 001
Historical Highlights of the Early Days of SIMS;
Bryan L. Bentz1; Saroff, Princeton, NJ

WPA 002
Mass Spectrometry in an Adversarial Context: A Proposal for Demonstrating Method Fitness;
Robert Betham, Joe Boison, John Chakel, Jane Gale, David Heller, Steven Musser, Phil Price, Stephen Stein

INSTRUMENTATION, 004 – 054b

WPA 004
A reflector TOF system with MS/MS capability;
Rüdiger Frey1; Aurelio LaRotta2; Armin Holl2; Claus Köster3; Jochen Franzen2; Bruker Daltonik GmbH, Bremen, Germany

WPA 005
New Instrument Developments for Automated MALDI-TOF Mass Spectrometry;
Jeffrey M. Brown1; Dominic Gostick2; Andrew Preston2; Stephen Thornton2; Garry Scott1; Jeffrey Lockett2; Therese McKenna3; Robert Bateman4; Micromass Ltd., Manchester, England

WPA 006
Duty cycle improvement for a QqTOF mass spectrometer and its use for precursor ion scans;
Igor V. Chernushchev1; Andrej A. Shevchenko2; Bruce Thomson3; SCIEX, Concord, Canada; EMBL, Heidelberg, Germany; SCIEX, Concord, Canada

WPA 007
Optimization of the Time-Dependent Field in the Ion Mirror for Delayed and Direct Ion Extraction;
Eugene Moskovets1; Barnett Institute, Northeastern University, Boston, MA

WPA 008
Use of a Second Extraction Pulse to Improve the TLF Focusing of Ions in Delayed Extraction MALDI;
Craig LaPlagette1; Edward D. Durrant1; Robert S. Brown1; U of Alaska State University, Logan, UT

WPA 009
Analytical Figure of Merit of a Multi-Pass Time-of-Flight Mass Spectrometer;
Ching Wu1; Thomas A. Dresch1; Ulrich P. Giessmann1; Melvin A. Park1; Houle Wang2; Bruker Daltonics Inc., Billerica, MA

WPA 010
A multiple reflection time-of-flight mass spectrometer (Multi-RTOF) for space applications;
Antonio Casares1; Alexandre Kholomeev2; Fred Goesmann2; Reinhard Rolf2; Helmut Rosenbauer2; Hermann Wollnik1; Io Phys. Institut, Justus-Liebig University, Giessen, Germany; Max-Planck Institute für Aeronomie (MPIE), Kran-Lindau, Germany

WPA 011
Spatial Focusing of PSD Fragment Ions in a Time-of-Flight Mass Spectrometer with a Curved Field Reflectron;
Emmanuel Raptakis1; Andrew R. Bowdl2; Frank Trundle1; Kratos Analytical Ltd., Manchester, UK

WPA 012
Optimization of the Duty-cycle of TOF-MS for Use in Separation Sciences;
David R. Russell1; Theodor Krustev1; Gareth Brenton1; Mathew A. Kennedy1; Claudi K. Ward1; Christopher M. Williams1; MSI, University of Wales Swansea, Swansea, Great Britain

WPA 013
Designing Coffee-can and Shoe-box Mirrors for Time-of-Flight Mass Spectrometers;
Jun Zhang1; Christie G. Enke1; University of New Mexico, Albuquerque, NM

WPA 014
Improved Laser and Ion Optics for SELDI and MALDI Mass Spectrometers; S. E. "But" Buttrill, Jr.; Scott Weinberger1; Ray Bryan2; Ciphergen Biosystems, Inc., Palo Alto, CA; Synergy Technology, Inc., Reno, NV

WPA 015
The Role of Radial Velocity in Signal Loss with Increasing Mass of Oligonucleotides with MALDI-TOF MS; David A. Preston1; Michael S. Westphall1; Lloyd M. Smith2; University of Wisconsin, Madison, WI

WPA 016
Novel LINAC II electrode geometry to create an axial field in a multipole ion guide; Alexandre Loboda1; Krutchinsky Andrew1; Olga Loboda2; Jim McNabb1; Vic Spencer1; Werner Ens1; Kenneth Standing1; University of Manitoba, Winnipeg, Canada

WPA 017
The Mass-Correlated Pulsed Extraction in TOF Mass Spectrometer; Andrew Bowlder1; Andrew R. Bowlder1; Robert J. Cotter1; Slava V. Kovtoun1; Kratos Analytical, Manchester, UK; Johns Hopkins University, Baltimore, MD

WPA 018
Miniaturized EI/QqTOF mass spectrometer; Yadvan D. Berkou1; Robert J. Cotter1; The Johns Hopkins University, Baltimore, MD

WPA 019
A new interface for off-line CE-MALDI-MS; Johan Godom1; Torbjorn Johnson1; Jonas Bergquist2; Rolf Ekman1; Eckhard Nordhoff4; Martin Schuerenber5; Klaus-Dieter Klopepel6; Gothenburg University, Molndal, Sweden; Uppsala University, Uppsala, Sweden; Max-Planck Institute for Molecular Genetics, Berlin, Germany; Bruker Daltonik, Bremen, Germany

WPA 020
Analysis of biological mixtures on microchips with capillary electrophoresis and matrix-assisted laser desorption/ionization (MALDI) mass spectrometry; Jie Liu1; Ken Tseng1; Carlito Lebrilla1; University of California, Davis, CA

WPA 021
Multi-in-Capillary Electrode Sheathless Interface and its Application to Analysis of Biological Mixtures Using CE-MS and cIEF-MS; Alex D. Smith1; Mehdi Moini1; University of Texas, Austin, TX

WPA 022
Design and Construction of Cryo-Cooled ICR Trap in a 3T Horizontal Bore Magnet; Hak-No Lee1; Christopher L. Hendrickson1; Alan G. Marshall1; NHMFL, Florida State University, Tallahassee, FL

WPA 023
Laser Scanning Design for a Fourier Transform Mass Spectrometer; Paul L. Tremblay1; Jill R. Scott1; INEEL, Idaho Falls, ID

WPA 024
FTICR Mass Spectrometry Employing Data-Dependent External mz Ion Selection and Accumulation; Richard Harkewicz1; Gordon A. Anderson1; Christophe Masselon1; Liljana Pasa-Tolice1; David C. Prior1; Harold R. Usdeth1; Richard D. Smith1; Pacific Northwest National Laboratory, Richland, WA

WPA 025
Selective External Accumulation of Electrospayed-Generated Ions Coupled to Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Mikhail E. Belov1; Yevgeniy N. Nikolaev2; Gordon A. Anderson1; Harold R. Usdeth1; Mikhail V. Gorskikh2; Tom Bailey1; Richard D. Smith1; EML, PNNL, Richland, WA (on leave) Institute of Energy Problems of Ch. Ph., Moscow, Russia; University of Delaware, Newark, DE

WPA 026
A Radio/Trap Supply Design that Accommodates both Trap Electric Field Compensation and Rapidly Switched Gated Trapping for In-Field MALDI Fourier Transform Mass Spectrometry; Don L. Rempel1; M. L. Gross1; Washington University, St. Louis, MO

WPA 027
Improved Deceleration of MALDI Produced Ions for the FT-ICR Spectrometry; Sven Burmester1; Karl
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<th>Time</th>
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<tr>
<td>7:30 – 8:00 am</td>
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<td>6:00 – 6:30 pm</td>
<td>REMOVE POSTERS. Please leave posters for the full day.</td>
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**WEDNESDAY POSTERS**

**WPA 028** Characteristics of Quadrupole Mass Filter Operated in the Fourth and Sixth Regions; Wei Chen¹; Don J. Douglas¹; University of British Columbia, Vancouver, Canada

**WPA 029** Transmission Characteristics of Quadrupoles to m/z 10,000; Randall E. Pedder¹; Jian Wei¹; Richard A. Schaeffer¹; ABB Automation Inc., Analytical Division - Extrel, Pittsburgh, PA

**WPA 030** Mass Range Extension in an RF-Only Quadrupole Mass Filter Using Auxiliary Excitation; Lisa M. Cousins¹; PE-SCIEX, Canada

**WPA 031** QqQqQ tandem Mass Spectrometer for the Study of Ion/Surface Collision Processes; Zheng Quyang¹; Verena Grill¹; Henry Rohrs¹; Peter D. Thomas¹; Graham Cooks¹; Purdue University, West Lafayette, IN; University of Innsbruck, Innsbruck, Austria; Washington University, St. Louis, MO

**WPA 032** Fundamental Studies of Ion Injection into the Quadrupole Ion Trap; James P. Murphy¹; Richard A. Yost¹; University of Florida, Gainesville, FL

**WPA 033** Interfacing the Orbitrap to an electron impact ion source; Alexander A. Makarov¹; HD Technologies, Manchester, UK

**WPA 034** Atmospheric Pressure MALDI - Ion Trap Mass Spectrometry; Susanne C. Moyer¹; Victor V. Laiko²; Robert J. Cotter³; Johns Hopkins University, Baltimore, MD; The Johns Hopkins University School of Medicine, Baltimore, MD

**WPA 035** Tandem TOF-Orthogonal TOF Mass Spectrometer with MALDI Ion Source; Anatoli N. Verenchikov¹; Kevin Hayden¹; Marvin L. Vestal¹; PE Biosystems, Framingham, MA

**WPA 036** Description and Performance of a Novel Tandem Quadrupole Mass Spectrometer Combining Low-Energy CID and SID; Janine De Maaijer-Gielbert¹; Michael J. Chalmers¹; Shabaz Mohammad¹; Francesco Brancia¹; Myriam Ferro¹; Simon J. Gaskell¹; Les Gora¹; Charles Smith¹; UMIST, Manchester, UK; Micromass, Manchester, UK

**WPA 037** The 'EnvirTOF': A New Electron Ionization - Orthogonal Acceleration Time-of-Flight Mass Spectrometer Designed for Process and Environmental Monitoring; Nageeb Sousou¹; Michael Guilhaus¹; The University of New South Wales, Sydney, Australia

**WPA 038** A Benchtop Mass Spectrometer Optimized for Pyrolysis-Mass Spectrometry: Py-MAB-Tof; Pascal Martin¹; Anik Forest¹; Olivier Peraldi¹; Michel J. Bertrand¹; Dehy Technologies Inc., Quebec, Canada; University of Montreal, Montreal, Canada

**WPA 039** On the mechanism of field induced high temperature microneedle growth of activated emitters used for field ionization and field desorption mass spectrometry; Gregor Fusshegger¹; Guenter Klesper¹; Heike Klesper¹; F.W. Roelgen¹; CARBOTEC GmbH, Germany; University of Bonna, Germany

**WPA 040** GC Detection with an ESI Source; Bruce F. Wilcox¹; Ma'an H. Amad¹; Nadja C. Lindley¹; Christie G. Enke¹; University of New Mexico, Albuquerque, NM

**WPA 041** Quartz Tip for Supersonic Molecular Beams in GC/EI/MS; Hiroshi Kishi¹; Toshihiro Fuji³; Oyama National College of Technology, Oyama, Tochigi, Japan; National Institute for Environmental Studies, Tsukuba, Japan

**WPA 042** Nanoscale Laser Ablation Mass Spectrometry; Raoul M. Stöcklé¹; Patrick Setz³; Volker Deckert¹; Thomas Lippert¹; Renato Zenobi¹; Swiss Federal Institute of Technology, Zurich, Switzerland; Paul Scherrer Institute, Villigen, Switzerland

**WPA 043** Helium Microwave Induced Plasma Time of Flight Mass Spectrometry; Pamela R. Keating¹; Jon W. Carnahan¹; Lee S. Sunderlin¹; Northern Illinois University, DeKalb, IL

**WPA 044** A New Electron Ionization Interface for Coupling Liquid Chromatography and Mass Spectrometry; Achille Cappiello¹; Giorgio Famigli¹; Filippo Mangani¹; Pierangela Palma¹; Univ. di Urbino, Urbino, Italy

**WPA 045** Metastable Atom Bombardment (MAB): An Ionization Source Combining the Features of EI, CI and FI; Denis Faubert¹; Marguerite Boulou²; Anik Forest³; Michel J. Bertrand³; DEPHY Technologies, Quebec, Canada; University of Montreal, Montreal, Canada

**WPA 046** Li ion attachment mass spectrometry; Toshihiro Fuji³; Nat. Institute for Environ. Studies, Tsukuba City, Japan

**WPA 047** Sodium Ion Attachment Reactions: A New Chemical Ionization Mode for Ion Trap Mass Spectrometry; Michele Sablier¹; Christian Rolando³; Toshihiro Fuji³; Univ. Pierre et Marie Curie, Paris, France; Univ. des Sciences et Technologies de Lille, France; National Institute for Environmental Studies, Japan

**WPA 048** IR-MALDI Mass Spectrometry for DNA Analysis; Nelli I. Taranenko¹; Vladimir M. Doroshenko¹; Timothy P. Lippa¹; Jun Zeng¹; Pierre Karbo³; Robert J. Cotter¹; Coorg R. Prasad¹; Mass Technologies, LLC, Burlington, MD; SESI, Burlington, MD; The Johns Hopkins University, Baltimore, MD

**WPA 049** Direct Injection High Efficiency Nebulizer for Inductively Coupled Plasma Axial Time-of-Flight Mass Spectrometry; Craig S. Westphal¹; John A. McLean¹; Billy W. Acorn¹; Lloyd A. Allen³; Akbar Montaser¹; The George Washington University, Washington, DC; Leco Corporation, St. Joseph, MI

**WPA 050** In-source sample infusion for fully automated FD MS; H. Bernhard Linden¹; Martin Maurer¹; Linden CMS GmbH, Leeste Germany; AMD Insecta GmbH, Harpstedt, Germany

**WPA 051** Performance Evaluation of a Multi-Turn Time-of-Flight Mass Spectrometer 'MULTUM Linear Plus'; Michisato Toyoda¹; Shin-ichi Yamaguchi¹; Morio Ishiura¹; Osaka University, Japan

**WPA 052** Design of a New Compact Multi-Turn Time-of-Flight Mass Spectrometer 'MULTUM II'; Michisato Toyoda¹; Itsuo Katakuse¹; Osaka University, Japan

**WPA 053** Ion Formation Efficiency in Sonic Spray Ionization (SSI); Atsumi Hirabayashi¹; Min Huang¹; Yukiko Hirabayashi¹; Hisakazu Koizumi¹; Hitachi, Central Research Laboratory, Tokyo, Japan
WEDNESDAY POSTERS

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WPA 054 Remote Operation and Monitoring of Underwater Mass Spectrometers for in situ Chemical Analysis; R. Timothy Short; John Diaz; David P. Fries; Randy Russell; University of South Florida, St. Petersburg, Florida

WPA054b Negative Ion Generation Using a MAB Source; Nancy M. Leymarie; Jean-Claude Tabet; Michel J. Bertrand; University of Montreal, Montreal, Canada; University of Pierre et Marie Curie, Paris, France

ION MOLECULE REACTIONS, 055 - 097

WPB 055 Energies of Chloride-Alkane Clustering Reactions; Tanya N. Gamble; Terry B. McMahon; University of Waterloo, Waterloo, Canada

WPB 056 Flowing Probe Pyrolysis - High Resolution Mass Spectrometry for Study of Sulfur Oxidation Products; Aaron J. Frank; Frantisek Turecek; University of Washington, Seattle, WA

WPB 057 Nборновское: The Reactivity and Thermochemistry of a Highly Strained Alkane; Dana R. Reed; Steven R. Kass; Weston T. Borden; Rebecca L. Hoenigman; Lani V. Lockett; University of Minnesota, Minneapolis, MN; University of Washington, Seattle, WA

WPB 058 Ion Chemistry of Peroxfluoroalkyl Phosphines and Silanes; Frank Lübkeaman; Karl P. Wancek; Inorg. & Phys. Chemistry, Bremen, Germany

WPB 059 Cycloaddition within an Intermediate Complex: Unimolecular Dissociation of Ionized tert-Butylvinylether; Henri-Edouard Audier; Guillaume van der Rest; Philippe Mourgues; Julia Chamot-Rooke; Jean-Pierre Denhez; DCMR-Ecole Polytechnique-CNRS UMR, Palaiseau, France

WPB 060 Dynamics Study of the Gas Phase Reactions of Fluoride Ions with Chloromethane; Laurence A. Angel; Kent M. Ervin; University of Nevada, Reno, NV

WPB 061 Experimental and computational study of the effects of methylolation on gas-phase s2O2; Bogdan Bogdanov; Terry B. McMahon; University of Waterloo, Waterloo, Canada

WPB 062 Base-promoted ester hydrolysis: mechanistic insight via oxygen-18 labeled hydroxyde; Vyacheslav N. Fishman; Joseph J. Grabowski; University of Pittsburgh, Pittsburgh, PA

WPB 063 The Reactions of O2 with Alkyl and Aryl Esters of Benzoic Acid: An NCI and FT-ICR Study; Elizabeth A. Stennaker; Eri M. Yoshida; Joshua M. Pacheco; Erik D. Woodbury; Tournaj Solouk; Bowdoin College, Brunswick, ME; University of Maine, Orono, ME

WPB 064 Cations from Tritium Decay: Neutral Products from their Gas Phase Reactions with Allyltrimethylsilane; Philip S. Mayer; Thomas H. Morton; University of California, Riverside, CA

WPB 065 The Determination of Alkane Ionization Potentials; Michael E. Laszynski; Burnaby Munson; Brian Wagner; University of Delaware, Newark, DE

WPB 066 A New Approach to the Gas-Phase Acidity of Sulfuric Acid; Cynthia A. Pommerehne; Lee S. Sunderlin; Northern Illinois University, DeKalb, IL

WPB 067 Energy effects in high temperature chemistry of O2+ and NO+ with alkylbenzenes (300-1400 K); A.J.

Midley; S. Williams; S. T. Arnold; R. A. Dressler; Y. H. Chiu; D. J. Levandier; M. R. Berman; A. A. Viggiano; R. A. Morris; Air Force Research Lab, Hanscom AFB, MA; AFOSR, Arlington, VA

WPB 068 Reactions of Gas-Phase Uranium and Uranium Oxide Ions with Pentamethylcyclopentadiene in a Quadrupole Ion Trap; Douglas C. Dickworth; John K. Gibson; Oak Ridge National Laboratory, Oak Ridge, TN

WPB 069 Analysis of explosives under complementary ionization conditions using an external ion source fitted to an ion trap mass spectrometer; Thierry Faye; Alain Brunot; Christine Fuchs; Toshhiro Fuji; Michel Sablier; Jean-Claude Tabet; University Pierre et Marie Curie LCSOB, Paris, France; CREL, Paris, France; National Institute for Environmental Studies, Japan

WPB 070 Studies of reactions of atomic and atomic oxidations using a novel ICP/SIFT/CD mass spectrometer; Diethard K. Bohme; Gregory K. Koyanagi; Vitali V. Lavrov; York University, Toronto, Canada

WPB 071 Reactions of Al and Si Oxyanions with H2S; Gary S. Greenewald; Brittany D. M. Hodges; Anthony D. Appelhans; Jill R. Scott; Glen F. Kessinger; Idaho National Engineering & Environmental Lab, Idaho Falls, ID

WPB 072 Organonitrile Adducts of Silver (I) Ion. Theoretical and Experimental Binding Energies. Correlation between Free Energies and Hammett Constants; Tamer Shoeb; K. W. Michael Sui; Alan C. Hopkinson; Houssain Elarbi; York University, Toronto, Canada

WPB 073 Reactivity and Binding Energies of Singly Charged Transition Metal Halogenide Ions to Benzene; Alex Gapeev; Robert C. Dunbar; Case Western Reserve University, Cleveland OH

WPB 074 Origin of Neutralls Implied in Ion-Molecule Reactions in an ESI/ITMS; Francois Fourrier; Valerie Carlesso; Carlos Alfonso; Jean-Claude Tabet; Helmut Schwarz; University of Berlin, Germany; LCSOB, France

WPB 075 Ion-Molecule Reactions of C5H5Fe+ and C5H6Fe+ with C1-C4 Alcohols by FT-ICR; Melvin B. Comisarow; Eva Korenkova; University of British Columbia, Vancouver, BC, Canada

WPB 076 Fulleromeric Ion Chemistry: Reactions of C60Fe+ and C59H10Fe+ in the Gas-Phase; Donna Caraman; Gregory K Koyanagi; Diethard K Bohme; Lawrence T Scott; York University, Toronto, Canada; Boston College, Chestnut Hill, MA

WPB 077 Reactivity of meta-substituted Phenyl Radicals toward Various Aromatic Substrates; Louis E. Ramirez-Arizmendi; Joseph J. Ferra; Kami K. Thoen; Hilka I. Kenttämä; Purdue University, West Lafayette, IN

WPB 078 Gas-Phase Radical-Radical Recombination Reactions; Jenny L. Heidbrink; Frances S. Amegayibor; Hilka I. Kenttämä; Purdue University, West Lafayette, IN

WPB 079 Interactions of Ions and Radicals in an FT-ICR; Amber L. Russell; Henry W. Rohrs; Don L. Rempel;
WEDNESDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B

8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.

1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.

6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

Micheal L. Gross; Washington University, St. Louis, MO

WPB 080  The First Nonclassical Distonic Ion: Fabio Cesar Gozza 1; Luiz Alberto B. Moraes 1; Marcos N. Eberlin 1; Kenneth K. Lahti 2; State University of Campinas - UNICAMP, Campinas, SP Brazil, Kent State University, Kent, OH

WPB 081  The role of the "three-point interaction" of chiral selectivity in the gas-phase reaction 
interaction; Javier Ramirez 3; Seonghee Ahn 4; Carlito B. Lebrilla 4; University of California, Davis, CA

WPB 082  Evidence for the Formation of Gas-Phase Inclusion Complexes with Cycloextrins and Amino Acids; Seonghee Ahn 4; Javier Ramirez 3; Carlito B. Lebrilla 4; University of California, Davis, CA

WPB 083  Chiral Templating Effects in a Gas Phase Ion-Molecule Reaction?; David V. Dearden 5; Eric S. Handberg 5; Brigham Young University, Provo, UT

WPB 084  Gas Phase Studies of Inclusion Complexes Involving Hydroxylated and Permyethylated Cycloextrins; Katherine A. Kellersberger 6; David V. Dearden 5; Brigham Young University, Provo, UT

WPB 085  Catalyzed Keto-Eno1 Tautomerism in the Gas Phase: An FT-ICR Study; Guillaume van der Riet 7; Philippe Mougrues 7; Julia Chamot-Rooke 7; Henri-Edouard Audier 7; Terrance B. McMahon 7; DCMR-Ecole Polytechnique-CNRS UMR, Palaiseau, France

WPB 086  Stable and Non-Interconverting Ter-Body Intermediates in the Gas Phase: Reactions of Ionized Enols with tert-Butanol; Henri-Edouard Audier 7; Guillaume van der Riet 7; Philippe Mougrues 7; Julia Chamot-Rooke 7; Terrance B. McMahon 7; DCMR-Ecole Polytechnique-CNRS UMR, Palaiseau, France

WPB 087  Addition of Water to Product Ions Formed by Low Energy CID in the Collision Cell of a Triple Quadrupole Mass Spectrometer; Mary Ellen K. Salvan 8; Mark S. Boilag 8; Jonathan L. Josephs 8; Bristol-Myers Squibb Company, New Brunswick, NJ

WPB 088  Do Amines React With Protonated Peptides in the Gas Phase to Induce Peptide Bond Cleavage via Transacylation Reactions?; Richard A. J. O'Hair 9; N. K. Androustopoulos 9; Gavin E. Reid 9; University of Melbourne; Ludwig Institute for Cancer Research

WPB 089  Binding of HI to Gas-Phase Protein Basic Sites: An ab initio Study; William D. Price 10; Saged Keshavzaran 10; Marshall University, Huntington, WV

WPB 090  Determination of Rate Constants for the Abstraction of Sodium Ions from Poly(ethylene glycol) by Crown Ether; Sara C. McGrath 11; Gary L. Glish 11; University of North Carolina, Chapel Hill, NC

WPB 091  Binding of Na+ and K+ at the MALDI matrix; Juan Zhang 11; Elizabeth Stevenson 11; Harold Baumann 11; Renato Zenobi 11; Renato Zenobi 11; Swiss Federal Institute of Technology Zurich, Switzerland

WPB 092  Ion/Molecule Reactions of Methyamine with Peptide CID Product Ions to Identify 8 Ions; Anne H. Payne 12; Gary L. Glish 11; University of North Carolina, Chapel Hill, NC

WPB 093  Incorporation of Thermal Rotation of Distonic Ions into Mobility Calculations: Drastic Effect for Heavier Buffer Gases; Alexandre A. Shwartsburg 13; Stefan V. Maskevitch 13; K.W. Michael Sui 13; York University, Toronto, Canada; Merrill Lynch Global Headquarters, New York, NY

WPB 094  Intramolecular Fluorine Migration via 4-Member Cyclic Transition States; Thomas H. Morton 14; Viet Q. Nguyen 15; Philip S. Mayer 1; University of California, Riverside, CA

WPB 095  Experimental and Theoretical Investigation of Peroxycetic and Peroxypropionic Acids: Andreas Rappmund 16; Karl P. Wanczek 17; Inorg. & Phys. Chemisty, Bremen, Germany

WPB 096  A Comparison of the Gas-Phase Reactivities of Positively and Negatively Charged Distonic Ions; Harvey A. Lardin 18; Christopher J. Petzold 18; Eric D. Nelson 19; Hilika I. Kenttamaa 20; Purdue University, West Lafayette, IN

WPB 097  The Association Reactions: HCNH+ + C2H2; HCNH+ + C2H4; Murray J. McEwan 21; Daniel B. Milligan 21; Colin G. Freeman 21; Robert Gar Macclagan 21; Paul F. Wilson 21; Vincent G. Antich 21; University of Canterbury, New Zealand; Jet Propulsion Laboratory, Pasadena, CA

LASER DESORPTION/IONIZATION APPLICATIONS, 098 - 151

WPC 098  Laser Ablation Ion Mobility Spectrometry of Polycyclic Aromatic Hydrocarbon Solids and Particles; Derek A. Lake 22; Murray V. Johnston 22; David Young 22; Gary A. Eiceman 22; University of Delaware, Newark, DE, New Mexico State University, Las Cruces, NM

WPC 099  Lifting Ions Out-of-Solutions via Aerosol Laser Evaporation Mass Spectrometry; Tomas Baer 23; Ephraim Woods 23; Yurii Dussanetik 23; Jay Raval 23; Roger Miller 23; University of North Carolina, Chapel Hill, NC

WPC 100  Development of the compact time-of-flight mass spectrometer; Jongmin Lee 24; Kyuseok Song 24; Hyungki Cha 24; Seongha Park 24; Yong-Ill Lee 25; Korea Atomic Energy Research Institute, Taejon, Korea; Changwon University, Changwon, Korea

WPC 101  Petroleum/water drilling mud pia mica particulate analysis by laser microprobe ms and data reduction utilizing wavelets and infomatics; Ronny C. Robbins 26; U.S. Army, APG, MD

WPC 102  Aspects of Desorption/Ionization of Porous Silicon (DIOS) Mass Spectrometry; Zhouxin Shen 27; John, J. Thomas 27; Jing Wei 27; Kras Broo 27; John, E. Crowell 27; M.G. Finn 27; Gary Siudzak 27; UCSD, La Jolla, CA; The Scripps Research Institute, La Jolla, CA

WPC 103  Desorption/Ionization on Porous Silicon (DIOS) for Proteomics; John J. Thomas 27; Zhouxin Shen 27; Jing Wei 27; John Crowell 27; Gary Siudzak 27; The Scripps Research Institute, La Jolla, CA; UCSD, La Jolla, CA; Novartis Institute, La Jolla, CA

WPC 104  Spark-Processed Silicon in Desorption/Ionization on Silicon Time-Of-Flight Mass Spectrometry; Mark A. Villoria 28; David H. Powell 28; Benjamin W. Smith 28; James D. Winefordner 28; University of Florida, Gainesville, FL

WPC 105  Desorption Ionization on Silicon (DIOS) for the Analysis of Small Organic Molecules; Peter Kittinos 29; Douglas M. Sheelely 29; Robert L. Johnson 29; Glaxo Wellcome R&D, RTP, NC
WEDNESDAY POSTERS

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REMOVE POSTERS. Please leave posters for the full day.

WPC 106
The surface activity effect in surface-assisted laser desorption ionization (SALDI) mass spectrometry; Yuh-Chieh Chen; Tsu Chi College of Medicine and Humanities, Hualien, Taiwan

WPC 107
Reproducibility in MALDI-TOF MS Measurement: Improvements in Sample Substrate; Shin-ichiuro Kawabata; Makoto Gonda; Shimadzu Corporation, Japan

WPC 108
10-100 fold Sensitivity Increase for MALDI MS; Martin Schürenberg; Eckhard Nordhoff; Albert Sickmann; Suckau Detlev; Bruker Daltonik GmbH, Bremen, Germany; Max-Planck-Institute for Molecular Genetics, Berlin, Germany; Ruhr-University, Bochum, Germany

WPC 109
The Potential of SPE-MALDI-TOF-MS in Routine Bioanalysis; Kenny Watson; Stephen Plessance; GlaxoWellcome, Park Road, Ware, Herts, UK

WPC 110
Solvent Extraction with a Nanoliter Droplet Combined with Microspot MALDI TOF Mass Spectrometry; Bernd O. Kellner; Liang Li; University of Alberta, Edmonton, Canada

WPC 111
The Use of Surfactant-aided Matrix-assisted Laser Desorption/Ionization Mass Spectrometry for Peptide Mapping Experiments; Rama Tummala; Lisa M. Ballard; Gary A. Breaux; Kari B. Green- Church; Patrick A. Limbach; Louisiana State University, Baton Rouge, LA; Ohio State University, Columbus, OH

WPC 112
MALDI-TOF/MS Using Inorganic Particle Matrix for Small Molecule Analysis; Tomoyo Kinumi; Mitsuo Takayama; Haruki Niwa; National Institute of Infectious Diseases, Tokyo, Japan; Toho University, Chiba, Japan; University of Electro-Communications, Tokyo, Japan

WPC 113
Characterization of Novel Thin Film Matrices for Peptide Mixture Analysis; Karen R. Jonscher; Robert C. Murphy; National Jewish Medical and Research Center, Denver, CO

WPC 114
A MALDI-TOF-MS Method for Studying Peptide H/D Exchange; Martha M. Vestling; Melissa J. Lucero; Faisal A. Syed; Samuel H. Gellman; University of Wisconsin, Madison, WI

WPC 115
Matrix-assisted laser desorption/ionization (MALDI) mass spectrometry with re-engineered 2,5-dihydroxybenzoic acid derivatives; Sajid Bashir; Rodger Mutter; Anastassios E. Giannakopoulos; Martin Wills; Peter J. Derrick; University of Warwick, Coventry, UK

WPC 116
UV-MALDI: Fluorescence Spectroscopy of Crystalline Matrices; Hans-Christian Liedemann; Robert W. Redmond; Franz Hillenkamp; Harvard Medical School, Boston, MA; University of Münster, Germany

WPC 117
Confocal laser scanning microscopy (CLSM) as a suitable imaging technique for studies of the analyte distribution in MALDI standard preparations; Verena Horneff; Andre Forssmann; Kerstin Strupat; Franz Hillenkamp; Ulrich Kubitscheck; Institute for Medical Physics and Biophysics, Münster, Germany

WPC 118
Successful MALDI Analysis: Interaction or Incorporation of Analyte and Matrix?; Anja Pfenninger; Matthias Glueckmann; Michael Karas; J.W. Goethe University, Frankfurt/Main, Germany

WPC 119
Similarities of ECD and ISD as a hint for electron capture in MALDI; Ralf Krüger; Michael Karas; Peter Juhász; J.W. Goethe University, Frankfurt/Main, Germany; PE Biosystems, Framingham, MA

WPC 120
Imaging of the ion velocity in the plume produced by UV-MALDI; Matthias Glueckmann; Michael Karas; J. W. Goethe University, Frankfurt/Main, Germany

WPC 121
Some experimental evidence of cluster desorption as precursor in the ion production in MALDI; Gerard Bolbach; Alain Brunot; Jean-Claude Tabat; Isabelle Fourrier; Univ P & M Curie, LCSOB, Paris, France

WPC 122
Influence of Gas-Phase Ionization/Desolvolation Processes on the Charge State Distribution of Multiply-Charged Proteins Desorbed by MALDI; Francck-Janeld Wind; Sandra Alves; Francoise Fourrier; Jean-Claude Tabat; DGA/CAB, Vert le Petit, France; LCSOB University Pierre et Marie Curie, Paris, France

WPC 123
Signal Suppression Effects in the MALDI Analysis of Peptide Mixtures: The Role of Intrinsic Charge; Michael Z. Wang; Michael C. Fitzgerald; Duke University, Durham, NC

WPC 124
Matrix and Structural Effects on Selectivity of Polyethers for Alkali Ion Complexation in MALDI; Yingqi Wang; H Rashidzadeh; Baochun Guo; Chemistry Department, Cleveland State University, Cleveland, OH

WPC 125
Phthalic Anhydride Derivatization for Mass Spectrometric Analyses of Low Molecular Weight Alkoxylated Surfactants; David M. Parees; Scott D. Hanton; Air Products and Chemicals, Inc

WPC 126
Characterization of Polyolefin Copolymers by MALDI Mass Spectrometry; Frederick J. Cox; Murray V. Johnston; Kuangnan Qian; Dennis G. Peiffer; University of Delaware, Newark, DE; ExxonMobil Research and Engineering, Annandale, NJ

WPC 127
Detection of Polystyrene Molecules with Molecular Weight up to 3.9 Million Daltons by MALDI Mass Spectrometry; Hsiu-Jung Hsu; Jentia Sheu; Nat’l Sun Yat-Sen Univ., Kaohsiung, Taiwan

WPC 128
Investigation of Bacteria from Toilet Seats and Restroom Door Handles Using Thermal Hydrolysis/Methylation-Mass Spectrometry (THM-MS) and Matrix Assisted Laser Desorption Ionization (MALDI); Angelo J. Madonna; Kent J. Voorhees; Ted L. Hadfield; John David; Colorado School of Mines, Golden, CO; US Army/AFIP, Washington, DC

WPC 129
The Effects of Sterilization Methods on the MALDI Spectrum of Pathogenic Bacteria; Denis Andrzejelewski; Farukh Khambati; Steven Musser; U.S. Food and Drug Administration, Washington, DC

WPC 130
Potential Subtyping of Methicillin Resistant Staphylococcus aureus Using Intact Cell MALDI; Kathleen Lewis; Kathryn A. Ralphson; Chris Sutton; Valerie Edwards-Jones; Andrew J. Fox; Kratos Inc., Chesterfield, NY; Kratos Analytical Ltd, Manchester, UK; Manchester Metropolitan University, Manchester, UK; Manchester Public Health Laboratory, Manchester, UK
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<th>Time</th>
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<td>7:30 – 8:00 am</td>
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<td>6:00 – 6:30 pm</td>
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### WEDNESDAY POSTERS

**WPC 131** Matrix-Free Identification of Bacillus Spore Species Using Laser Desorption and TOF-MS: Joel N. Lillam; Matthias Frank; Eric E. Gard; Joanne M. Horn; Christopher Hack; Joanne M. Horn; Simon E. Labov; Kevin Langry; Frank Magnotta; Kenneth A. Stajon; W. Henry Benner; Lawrence Livermore National Laboratory, Livermore, CA; Lawrence Berkeley National Laboratory, Berkeley, CA;

**WPC 132** Evaluation of Factors Contributing to Peak Broadening in the Characterization of Intact Spores and Cells Using MALDI-TOF MS: Javier Ramirez; Yetrioth Hauthou; Catherine Fenselau; University of Maryland, College Park, MD

**WPC 133** Rapid Identification of USP Objectionable Microorganisms in Pharmaceutical Ingredients by MALDI-TOF Mass Spectrometry: Huiping Chen; Gerald Marino; Anthony M. Cundell; Marshall M. Siegel; Wyeth-Ayerst Research, Pearl River, NY; Wyeth-Ayerst Pharmaceuticals, Pearl River, NY


**WPC 135** Application of MALDI-TOF/MS for the Verification of Sulfur Mustard Exposure: Michael C. Babin; Karen M. Ricketts; Michelle Gazaway; Peter L. Norton; Rudy Macalalal; Elvis O. Price; Ming L. Shih; US Army MRIDC, APG, MD

**WPC 136** A Quadrupole Ion Trap Mass Spectrometer Instrument for the Mapping of Pharmaceutical Compounds in Intact Tissues: Joshua J Coon; Frederick J Treendle; Richard A Yost; University of Florida, Gainesville, FL

**WPC 137** A MALDI-QIT-ToF for High MS and MS/MS: Koich Tanaka; Chris Sutton; Eiho Kawahito; Li Ding; Kratos Analytical Ltd., Manchester UK; Shimadzu Research Laboratory (Europe) Ltd., Manchester UK

**WPC 138** Practical aspects for MALDI FTMS of glycoconjugates and glycosyphilipids: Catherine E. Costello; Ekaterina Mirkorogodeska; Peter B. O'Connor; Boston University, Boston, MA

**WPC 139** Laser Induced Electron Capture Fourier Transform Mass Spectrometry: Jie Yao; Poguang Wang; Xin Zhang; Roger W. Giese; Northeastern University, Boston, MA

**WPC 140** MALDI-FTMS of Cyclic and Star-shaped Arrays of Metalloporphyrins: Titus A. Janni; Albert Gossauer; Olivier Mongin; Gokhan Baykut; Matthias Witt; Fribourg University, Switzerland; Bruker Daltonik, Bremen, Germany

**WPC 141** Direct Observation of MALDI Ion Behavior Using Simultaneous Excitation and Detection for FTICR Mass Spectrometry: Michael A. Fiorentino; Sarah E. Hopkins; David A. Laude; University of Texas, Austin, TX

**WPC 142** Comparison of SIMS and MALDI-PSD for Peptide Sequencing: Yangsun Kim; Yeonhee Lee; Bolyun Park; Chunsuk Cho; Eun Joo Song; Kong-Joo Lee; Ewha Women University, Seoul, Korea; Korea Institute of Science and Technology, Hyundai Pharm. Ind. Co., Ltd, Bucheon, Korea

**WPC 143** High Mass Accuracy in MALDI-TOF without Internal Standards: Stephen C. Davis; Alexander A. Makarov; Grant Cameron; HD Technologies, Manchester, UK; Genomic Solutions, Huntington, UK

**WPC 144** Improved Coverage of Protein Amino Acid Sequence from Enzymatic Digests with MALDI/TOF-MS: Zohra Oluneva; Damon C. Barbacci; Gerardo A. Brucker; Stanford Research Systems, Sunnyvale, CA

**WPC 145** A Comparative Study of MALDI-PSD and MALDI-CID Fragmentation for Structural Elucidation of Synthetic Polyglycopes: Sarah Trimpin; Harm-Anton Klok; Franz J. Mayer-Posner; Hans-Joachim Riede; Max-Planck Institute for Polymer Research, Mainz, Germany; Bruker Daltonik GmbH, Bremen, Germany

**WPC 146** Protein Identification using MALDI and a quadrupole time of flight (MALDI Q-ToF) hybrid tandem mass spectrometry: Robert Bateman; Robert Bordoli; Andrew Organ; Klaus Schneider; Micromass, UK; SmithKline Beecham Pharmaceuticals, UK

**WPC 147** A Comparison of IR-MALDI and UV-MALDI In-Source Decay of Peptides and Proteins: Robert S. Brown; Edward E. Durrant; Utah State University, Logan, UT

**WPC 148** IR-MALDI Response from Various Absorption Modes: Michael R. Papantonakis; David R. Ermer; Michelle Balz-Knorr; Richard F. Haglund, Jr.; Vanderbilt University, Nashville, TN

**WPC 149** Infrared MALDI with a Compact Tunable Optical Parametric Oscillator: Mark W. Little; Kermit K. Murray; Eli Margalith; Emory University, Atlanta, GA; OPETEK, Inc., Carlsbad, CA

**WPC 150** Infrared Matrix-assisted Laser Desorption/Ionization with Orthogonal Injection TOF Mass Spectrometry: Maciej P. Bromirski; Alexander Loboda; Werner Ens; Kenneth G. Standing; University of Manitoba, Winnipeg, Canada

**WPC 151** Surface Morphology Variations in MALDI-TOF-Mass Spectrometry Samples Prepared by Various Techniques Examined by Scanning Electron Microscopy: William R. Blair; Charles M. Guttman; Anthony A. Giuseppetti; National Institute of Standards and Technology, Gaithersburg, MD; ADAHF-Paffenberger Research Center

### DRUGS & METABOLISM: LC/MS/MS QUANTITATION IN BIOLOGICAL FLUIDS, 152 - 169

**WPD 152** Development of TurbifionSpray LC/MS/MS: A Specific Sensitive and Rapid Method for Free Cortisol in Human Urine: Tian P. Wang; Paul Bright; Wellington Paul; Quest Diagnostics, Van Noy, CA

**WPD 153** The profiling of N-acetylcysteine conjugate of 3-keto-4-ene VPA in humans, guinea pigs, and rats: Y. Sashi Gopaul; Roland Burton; Kevin Farrell; Frank S. Abbott; UBC, Vancouver, BC, Canada

**WPD 154** Determination of Total Carnitine, Carnitine, Acetyl Carnitine and Pivaloyl Carnitine using LC/MS/MS Analysis in Human Plasma, Serum and Urine: Milton Furtado; John Chapdelaine; Troy Bradley
WEDNESDAY POSTERS

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Francis Beaudry 1; Michael D. Mayer 2; Darcy J. Mulford 2; Phoenix International, Montreal, Canada; TAP Holdings Inc., Deerfield, MI

WPD 155 Derivatization of Corticosterone as a Biomarker to Obtain a Lower Limit of Quantification Using HPLC/ESI-MS/MS; C. Michelle Dunaway 1; Mary K. Durr 2; Peter J. Stoffolano 2; Kenneth R. Wehmeyer 3; Timothy R. Baker 4; Procter & Gamble Pharmaceuticals, Mason, OH

WPD 156 The matrix effect evaluation in the LC/MS analysis of microsomal incubation products; Joanna J. Zheng 1; Eric Lynch 2; Steve Unger 2; DuPont Pharmaceutical Company

WPD 157 Analysis of flavonoids using liquid chromatography in combination with electrospray (tandem) mass spectrometry; Chris J. van Platerink 1; Theo P.J. Mulder 2; P.J. Wijnand Schuyt 2; Hans M.M. Ameloot 3; Unilever Research Vlaardingen, The Netherlands

WPD 158 LC/MS/MS Quantitation of Phenytoin in Rat Plasma and Bile to Evaluate the Effect of Dosing Vehicle and Bile Flow on Absorption Rate; Lucinda H. Cohen 1; Annie Zheng 2; Elke Lipka 3; Karen Gajda 4; David T. Rossi 5; Purka-Davis Pharmaceutical Research, Ann Arbor, MI

WPD 159 Less is Better: LC/MS/MS Quantitation in Cerebrospinal Fluid without Sample Preparation; Susan E. Hill 1; Neil J. Hayward 2; James E. Vath 3; Proaxis Pharmaceuticals, Inc.

WPD 160 Quantification of Risperidone (RIS) and 9- Hydroxyrisperidone (9-OH-RIS) in Saliva; Lynn Gennaro 1; A. S. Fang 2; I. Utkin 3; M. G. Aman 3; N. Gerber 4; P. Vourou 5; Barnett Institute, Boston, MA; Childrens Hospital, Columbus, OH

WPD 161 Separation and Quantitative Analysis of Butylated Acylcarbinol Isomers by HPLC/ESI-MS/MS; Giuseppe Giordano; Piero Rinaldo; Alberto B. Burlina; C.L. Yu; Mauro Natarello; Franco Zaccello; Padua University; Padua, Italy; Mayo Clinic, Rochester, MN; Yale University, New Haven, CT

WPD 162 In vivo Production of 3-Nitro-4-hydroxybenzoate, a Marker of Peroxynitrite Formation during Cerebral Ischemia; Jane A. Montgomery 1; Line Ste-Marie 2; Daniel Boismenta 3; Orval A. Mamer 4; CHUM Research Center, Notre-Dame Hospital, Montreal, Canada; McGill Biomedical Mass Spectrometry Unit, Montreal, Canada

WPD 163 Development and Validation of a Method for the Determination of Sibutramine and Desmethyldiethylamine in CaCo-2 Cell Culture Media by Liquid Chromatography - Tandem Mass Spectrometry (LC/MS/MS); Sadayappan V. Rahavendran 1; Phillip J. Tzetzlbaum 2; Robert S. Hasi 3; Covance Laboratories, Madison, WI; Sepacor Inc., Marlborough, MA

WPD 164 Determination of CYP1A2 Activity by ESI/MS of Caffeine Metabolite Profiles in Human Urine; Girish S. Gudi 1; Cem Yucesoys 2; Patrick S. Callery 3; Timothy S. Tracy 4; West Virginia University, Morgantown, WV

WPD 165 Quantitation of Anesthetic Agents in Rat Plasma by ESI-Ion Trap MS; Andrea Schneider 1; Andrea Kiehle 1; Arnd Ingendohr 1; Bruker Daltonik, Bremen, Germany

WPD 166 Quantitative LC/MS/MS method for lactone and lactonizable hydroxy acids: [M+H]+ vs. [M+NH4]+ as a precursor ion vis-a-vis the need for Q1 unit mass resolution or chromatographic separation; Zheng Qunyang 1; Mohammed Jamal 2; Mark Powell 3; Bristol-Myers Squibb, New Brunswick, NJ

WPD 167 Rapid Quantitation of Multiple Analytics in Biological Matrices Using Liquid Chromatography / LCQ Ion Trap: Applications in Neuropeptide Y (NPY) Antagonist Series In Discovery Pharmacokinetics Support; Lei Zhang 1; Jim Meyer 2; John Laycock 3; Stanley Mallard 1; Mike Hayashi 1; Krys Miller 1; Angen, Inc., Thousand Oaks, CA

WPD 168 Sample pooling and on-line desalting to accelerate throughput of in vitro permeability screening; Richard Lam 1; Yvonne Pan 1; Shireen Ahmed 2; Jinbin Li 3; David Lau 4; Feng-Yin Hsieh 5; Angen, Thousand Oaks, CA

WPD 169 Quantitative Analysis of Multiply Charged Species in Biological Samples Using LC/MS/MS Instrument Combined with Automated On-Line Extraction; Casey C. Hao 1; Yves Le Blanc 1; PE Scies, Concord, Canada

DRUGS & METABOLISM: HIGH THROUGHPUT METHODS, 170 - 206

WPD 170 High-Throughput LC/MS Analysis of ADME Screen Samples: An Integrated Module Approach; Katrina J. Rogers 1; Kevin M. Whalen 1; John S. Janiszewski 1; Mark J. Cole 2; Pfizer Inc, Groton, CA

WPD 171 HPLC-MS/MS Determination of a GABA/BZ Site Compound and its Metabolite in Human Plasma Using Semi-Automated Sample Preparation; Li Lin 1; John Hsieh 2; Mark Rose 2; Eric Woolf 3; Bogdan Matuszewski 1; Merck Research Laboratories, West Point, PA

WPD 172 Increased Throughput in Bio-Analytical HPLC- MS/MS Quantitation Using Dual Spray Technology; Lance P. Gauld 1; Donna L. Miller 2; Roderic O. Cole 3; Adam H. Brockman 1; Pfizer Central Research, Groton, CT

WPD 173 Development and Validation of a Metabolite Assay in Rat and Mouse Plasma Using On-line SPE LC/MS/MS; Hesham Ghobarah 1; Julie C. Flynn 2; John D. Laycock 3; Krys J. Miller 4; Angen, Inc., Thousand Oaks, CA

WPD 174 Cross Validation and High Throughput Implementation of Clinical Assay Using State-of-the-Art Equipment and Procedures; Julie C. Flynn 1; John D. Laycock 3; Krys J. Miller 4; Angen, Inc., Camarillo, CA

WPD 175 The Development of a Delayed Parallel Separation LC/MS/MS System with Parallel On-Line Extraction for High-Throughput Screening of Drug Candidates in Biological Matrices; Jing-Tao Wu 1; DuPont Pharmaceuticals, Newark, DE

WPD 176 Miniaturized Affinity Ultrafiltration for High Throughput Drug Screening and Residue Analysis; Yun Jiang 1; Pen-Cheng Wang 2; Cheng S. Lee 1; University of Maryland, College Park, MD

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<th>WEDNESDAY POSTERS</th>
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**WPE 177**
A High Throughput High Performance Liquid Chromatographic Mass Spectrometric Method for the Determination of Delavirdine in Human Plasma; Harry Demerdjian¹; John Simpson²; Francis Beaudry³; *Phoenix International Life Sciences, Montreal, Canada*

**WPE 178**
Optimization of Rapid Pharmacokinetic Screening in the Rat Using HPLC-APCI-MS/MS and Semi-Automated Sample Preparation; Samuel B. Wainhaus¹; Greg Tucker¹; Matthew Bryant¹; Neeta Juvkar¹; Kimberly Dunn-Meynelli¹; Walter Korfmarher¹; Ronald E. White¹; Schering-Plough, Kenilworth, NJ

**WPE 179**
Parallel Capillary Ultra-High Flow Rate Liquid Chromatography with Mass Spectrometric (MS/MS) Detection for Rapid, Direct and Sensitive Determination of Pharmaceuticals in Plasma at Extremely High Throughput; David N. Mallett¹; David Little²; Robert S. Plumb²; Martin K. Baylis³; Glaxo Wellcome Research and Development, Stevenage, UK; Micromass, Manchester, UK

**WPE 180**
Increased throughput for in-vitro drug metabolism screening using 384-well plate format for LC-MS/MS analysis; Johnny Cardenas¹; Darcy Nelson¹; Dennis A. Percira¹; Rod O. Cole¹; Adam H. Brockman¹; Pfizer Inc., Groton, CT

**WPE 181**
Application of the Eight Channel Multiplexed Electrospray to High-Throughput in vitro ADME Screens; Susan M. Chesson¹; Jessica P. Collins¹; Jeffrey L. Dage¹; Aventis Pharmaceuticals Inc., Bridgewater, NJ

**WPE 182**
LC/MS/MS Screening for beta-blockers and beta-agonists in urine with automated sample preparation; Borislav Starcevic¹; Emma Di Stefano¹; Don H. Catlin¹; UCLA Olympic Analytical Laboratory, Los Angeles, CA

**WPE 183**
Validation of a Fully Automated Method for GW275X and Two Metabolites Using a Custom Built Zymark-Tecan Robotics System and PROSPEKT On-line SPE- LC/MS/MS; Mark G. Woodward¹; Gary D. Bowers¹; Jack Chism¹; Lisa St John-Williams¹; Glenn Smith¹; Bioanalysis and Drug Metabolism, GlaxoWellcome Inc., RTP, NC

**WPE 184**
A High Throughput Solid Phase Extraction LC-MS/MS Method for Simultaneous Analysis of Amprenavir, Ritonavir and ABT-378; Ray Wisebold¹; Qin C. Ji¹; Matt Rieser¹; Hope T. Skribba¹; Anita T. Shen¹; Bill LaBeau²; Min S. Chang¹; Tawakol El-Shourbagyi¹; Abbott Laboratories, Abbott Park, IL

**WPE 185**
Investigation of Direct Injection/On-Line Guard Cartridge Extraction/Tandem Mass Spectrometry with Positive/Negative Polarity Switch for High-Throughput Bioanalysis; Hai-Zhi Bu¹; Philip Teitelbaum¹; Song Lin¹; Covance Laboratories, Inc., Madison, WI

**WPE 186**
High Throughput Dual Columns to Support Fully Validated Methods Using LC/MS/MS; Genevieve Plante¹; Rudolf Guibal¹; Phoenix International Life Sciences Inc., Ville St-Laurent, Canada

**WPE 187**
MS/MS Method Improvements for High Throughput Bioanalytical Support of Low Doses of Ilotropine and its Metabolites; Michael J. Hayes¹; Tim Bedman¹; Jack Lohn¹; Francis L. S. Tse¹; Novartis, East Hanover, NJ

**WPE 188**
Increase Throughput on Pharmacokinetic Screening with On-line Extraction-HPLC/MS/MS; Hideji Fujjwara¹; Jerry Muhammad¹; Melissa A. Lewis¹; Randy McKeé¹; James P. Doorn¹; Chante M. Boden¹; Tiffany Duffin¹; Kevin L. Duffin¹; Monsanto Co., St. Louis, MO

**WPE 189**
High Throughput/High Sensitivity LC/MS/MS Approaches to the Analysis of Highly Potent Pharmaceuticals in Biological Fluids; Shaojun Pang¹; Celia D’Arienzo¹; P. Jane Gale¹; Stanley Murakami¹; Robert Bethem²; Bristol-Myers Squibb, New Brunswick, NJ; Alta Analytical Laboratory, El Dorado Hills, CA

**WPE 190**
MS/MS Method Improvements to Accelerate the Development of STI571, an Anti-Lukemia Drug; Lakshmi Khemani¹; Michael J. Hayes¹; Tim Bedman¹; Francis L. S. Tse¹; Novartis, East Hanover, NJ

**WPE 191**
Development and Validation of a Rugged Quantitative LC/MS/MS Method for the Determination of CP-122,721 in Human Saliva; Robert L. Walsky¹; Michael J. Avery¹; Pfizer INC, Groton, CT

**WPE 192**
High Throughput LC/MS Permeability Screening Using Caco-2 Cells; Stephen Lowes¹; Colleen K. Van Pelt¹; Jack Henion¹; Cindy Seliger¹; Lee Henderson¹; Advanced BioAnalytical Services, Inc., Ithaca, NY; Viral Therapeutics, Inc., Ithaca, NY

**WPE 193**
Automated High Throughput Permeability Assessment Using Caco-2 Cell Membranes and LC/MS; Rongda Xu¹; Csaba Nemes¹; Daniel B. Kassel¹; DuPont Pharmaceuticals Research Labs, San Diego, CA

**WPE 194**
The Utility of Mass Spectrometric Detection in the Determination of Drug Permeability through Phospholipid Membranes; Eric H. Block¹; Kate Yu¹; Michael Balogh¹; Beverly Kenney¹; Alex Adveef²; Cynthia Berger²; Waters Corporation, Milford, MA; pION Corporation, Cambridge, MA

**WPE 195**
High Throughput Quantitation and Metabolite Identification Using Liquid Chromatography/API-TOF Mass Spectrometry; Edward Takachi¹; Brian Boucher¹; Robert Deutschman¹; John Peltier¹; PE Biosystems, Framingham, MA

**WPE 196**
A Novel Approach for LC/MS Analysis of Caco-2 Transport Samples Utilizing a Dual Cartridge Backflush System; Joseph A. Tweed¹; James P. Bulgarelli¹; Mark G Qian¹; DuPont Pharmaceuticals Company, Wilmington, DE

**WPE 197**
Development and Validation of a High Throughput Tamotoe 96 Well Plate Method for the Determination of Fexofenadine in Human Plasma by LC/MS/MS; Christian Lemoine¹; Yves G. Leblanc³; Charles Grandmaison¹; Lorella Di Donato¹; Phoenix International Life Science, Montreal, Canada

**WPE 198**
Multi-Analysis and Semi-Automated Sample Preparation for Faster Brain Penetration Assays in Drug Discovery using LC/MS/MS; Kwok-lung Ng¹; Shiyong Wang¹; Cymbeline Nardo¹; Gregory Tucker¹; Matthew Bryant¹; Walter Korfmarher¹; Schering Plough Research Institute, Kenilworth, NJ
WEDNESDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
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WPE 199  Metabolite Identification Using Fast Gradient HPLC; Philip R. Thaler; Cornelis E.C.A. Hop; Leslie Romanyszyn; Sai Chang; Merck Research Laboratories, Rahway, NJ; PE Biosystems, Framingham, MA

WPE 200  Biocolloidal Strategies for Application of HPLC-MS/MS/MS To Support Drug Development: From Lead Identification to Clinical Studies; Timothy G. Heath; Eric M. Shobe; Tracy L. Chingino; Marta G. Williams; Joe Paliandra; Pharmacia & Upjohn, Kalamazoo, MI

WPE 201  High Throughput Cytochrome P450 Inhibition Assays Using Parallel LC/MS Methodologies; Kelly M. Jenkins; Robyn A. Rourke; Rongda Xu; Daniel B. Kassel; DuPont Pharmaceuticals Research Laboratories, San Diego CA

WPE 202  Automated and Streamlined Biocolloidal Analytical Sample Processing for Supporting Clinical Pharmacokinetic (PK) Studies by LC/MS/MS; Rena Zhang; Jamie Zhao; J. Douglas Rogers; Merck & Co., West Point, PA

WPE 203  Increased Throughput Using a Dual Prospekt System; Charles D. James; John A. Dunn; Otto Halming; Glaxo Wellcome Inc., Res. Triangle Park, NC; Spark Holland BV, Enmen, The Netherlands

WPE 204  SPE LC-MS/MS Assays for Quantitation of Brimonidine in Rabbit Aqueous Humor; Ning Qin; Dom Vitarella; Andrew Aechempong; Allergan, Inc., Irvine, CA

WPE 205  96-Well Plate Online Plasma Injection (Cohesive Technologies) for the Determination of Quinapril and Quinaprilat with Select API III MS Detection; Adil El Haddad; Erich Tesner; Rudolf Guilbaud; Lorella Di Donato; Robert Massé; Phoenix International, Montreal, Canada

WPE 206  Ultra High Throughput Preclinical Pharmacokinetic Studies using 96-Well Plate Filtration Technology with On-Line Column Switching and LC/MS/MS Analysis; Ari Gittis; Themis Flarakos; Mathieu Lahaye; Mark L.J. Reimer; Phoenix International Life Sciences, Saint-Laurent, Canada

PROTEINS – METHODS DEVELOPMENT

WPF 207  Native PAGE- NP RP HPLC: A Two-Dimensional Separation Method for Biomarker Screening of Cancer Cell Lines; Kimberly A. O’Neil; Batshabea E. Chong; David M. Lubman; Fred R. Miller; Allen J. Rosenspire; University of Michigan, Ann Arbor, MI; Wayne State University, Detroit, MI

WPF 208  Extraction of Intact Proteins from PVD Membranes; Cheryl A. Blasie; Barbara S. Larsen; University of Delaware, Newark, DE; E. I. Du Pont de Nemours and Company, Wilmington, DE

WPF 209  High Throughput Proteome Analysis Using Isoelectric Focused Affinity Tags and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Thomas P. Conrads; Beatte Rist; Gordon A. Anderson; Christophe D. Masselon; Timothy D. Veenstra; Reudi Aebersold; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA; University of Washington, Seattle, WA

WPF 210  Potential of the MALDI Quadrupole TOF instrument in Proteomics Research; Matthias Mann; Angus King; Thomas Krogh; Ole Vorm; Alexander Loboda; Ken Standing; Igor Chernushevich; Alexandre V. Podtelejskii; Protana A/S, Odense, Denmark; Univ Manitoba, Manitoba; Sciex, Toronto, Canada; Univ Southern Denmark, Odense, Denmark

WPF 211  Recovery of Intact Proteins From SDS Gels For Top-Down Proteomics; Julian P. Whitelegg; Blas Cerda; David Horn; Ying Ge; Kathrin Brueker; Ryan Young; David Holowka; Barbara Baird; Fred McLafferty; Cornell University, Ithaca, NY

WPF 212  Evaluation of a SDS Analogue for 2-D Gel Separation and MALDI/TOF MS Mapping of Proteins using Automated Spot Cutting and in-gel Digestion Procedures; Andrew R. S. Ross; James I. Langridge; Duncan Smith; Simon J. Gaskell; NRC Plant Biotechnology Institute, Saskatoon, Canada; Microman, Manchester, UK; UMMIST, Manchester, UK

WPF 213  Nano-electrospray and real-time database searches; Juri Rappisber; Jens S. Andersen; Matthias Mann; Kenneth Budin; Carsten Pedersen; Peter Mortensen; University of Southern Denmark, Odense, Denmark; MDS-Protana A/S, Odense, Denmark

WPF 214  Mass spectrometry enables direct protein identification in large genomes; Bernhard Kuster; Peter Mortensen; Kenneth Budin; Jens Andersen; Alexandre Podtelejskii; Akhilesh Pandey; Juri Rappisber; Hanno Steen; Matthias Mann; MDS Protana A/S, Odense, Denmark; Univ Southern Denmark, Odense, Denmark

WPF 215  Fishing for novel human genes. Mass spectrometry as a tool for gene prediction; Alexandre V. Podtelejskii; Jens Andersen; Matthias Mann; Peter Mortensen; Bernhard Kuster; P.I.L. CEIB, University of Southern Denmark, Odense, Denmark; MDS Protana A/S, Odense, Denmark

WPF 216  An Improved Silver-Stain Method for 2D Gel Electrophoresis Reduces Background Staining and Dramatically Increases the Total Number of Proteins that are Visualized; Robert R. Becker; Edward S. Unstot; Dominic M. Desiderio; University of Tennessee, Memphis, TN

WPF 217  Evaluation of Two-Dimensional Gel Electrophoresis Based Proteome Analysis Technology; Steven P. Gigi; Garry L. Corthals; Yanni Zhang; Yvan Rochon; Ruedi Aebersold; University of Washington, Seattle, WA; Garvan Institute of Medical Research, Australia; Fred Hutchinson Cancer Research Center, Seattle, WA

WPF 218  Simplified sample preparation for peptide mass mapping: In-gel digestion on the MALDI probe; Ole N. Jensen; Allan Stensballe; University of Southern Denmark, Odense University, Odense, Denmark

WPF 219  Protein Identification from a Single Proteolytic Fragment Using High Mass Accuracy and Constrained Database Searching; Jonathan Amster; Julia S. Swancz; Todd H. Mize; Anne O. Summers; University of Georgia, Athens, GA

WPF 220  Identification and Characterization of Proteins from In-gel Digest using Non-Nanoscale LC/MS/MS; Paul C. Goodley; Agilent Technologies, Palo Alto, CA

WPF 221  Characterization of Native, SDS, and 2-D Gel Electrophoresis Separated Proteins by
Electrophoretic Capture Bioreactive MALDI-TOF MS; Tommy L. Ashton; Allen Bieber; Peter Williams; Arizona State University, Tempe, AZ

WPF 222

Automation of a Proteomic Approach to Drug Discovery: An Analytical Laboratory Perspective; Tracey I. Stevenson; Ping Du; Robert Lepley; Mutsumi Yoshida; Joseph Maceri; Terri Dyke; Stephen Rapundalo; Greg W. Kilby; Parke-Davis Pharm. Res., Div. of Warner-Lambert Co., Ann Arbor, MI

WPF 223

The Effect of Combined High Mass Measurement Accuracy and MS/MS in Proteomics with MALDI-and ESI-FT-ICR Mass Spectrometry; Matthias Witt; Gokhan Baykut; I. Paul Speir; James E. Bruce; Theresa Wood; Bruker Daltonik GmbH, Bremen, Germany; Bruker Daltonics Inc., Billerica, MA; Merck and Company Inc., West Point, PA

WPF 224

Probing Delinovus camelidus Proteome by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Lilijana Pasa-Tolivic; Gordon A. Anderson; David J. Anderson; Richard Harkewicz; Mary S. Lipton; Christophe D. Masselon; Kim K. Peden; Yufeng Shen; Timothy D. Veenstra; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA

WPF 225

Gas Phase Edman Degradation of Peptides for Protein Identification by Two-Dimensional Electrospray Ionization FT-ICR MS/MS; Guillaume van der Rest; Fei He; Alan G. Marshall; Simon Hubbard; Simon Gaskell; NIMRFL, Florida State University, Tallahassee, FL; U. Manchester Institute of Science & Technology, Manchester, U.K.

WPF 226

Identification of Proteins by Peptide-Mass Fingerprinting and Sequence-Tagging with Nanoelectrospray Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Yoshiyuki Kosaka; Tomoko Takazawa; Kazuaki Kubota; Takemichi Nakanuma; Sankyo Co., Ltd., Tokyo, Japan

WPF 227

Tryptic peptide mapping and amino acid variation of recombinant L-asparaginase II by LC/ESI/MS and in-source CID; Jun Han; Longsheng Sheng; Zhongyuan Yang; Dengkui An; Guangzhou Institute for Drug Control, Guangzhou, China

WPF 228

Hydroyl Radical Mediated Modification of Amino Acid Residues in Probing Protein Peptide Interactions; Benedetta Nagella Nakanuma; Michael B. Goshe; Vernon B. Anderson; Case Western Reserve University, Cleveland, OH

WPF 229

Characterization of Cysteine Residues and Disulfide Bonds in Proteins by LC/ESI/MS/MS and LC/ESI- MS/MS/MS; Tien-Yang Yang; Scott Thomas; Rajesh K. Joshi; Hui Yan; Irene Tom; Bruce A. Macher; San Francisco State University, San Francisco, CA

WPF 230

Site-specific nitration of tyrosine in human serum albumin by peroxynitrites; Saraswathi Mandapat; Kaisheng Jiao; Paul L. Skipper; Steven R. Tannenbaum; John S. Wishnok; Massachusetts Institute of Technology, Cambridge, MA

WPF 231

Characterization of the Endogenous Phosphorylation Sites in Beta-Elimination/Ethanol-Modified Squid NF220 by Proteolytic Digestion, LC/ESI/MS/MS and Database Searching; Howard Jaffe; Pushkar Sharma; Philip Grant; Harish C. Pant; LNC, NINDS, NIH, Bethesda, MD

WPF 232

Increased Proteome Coverage Using a Novel Peak Trapping Interface for Nanoscale Capillary LC/MS/MS Analysis of Complex Peptide Mixtures; Arthur Moseley; Kevin Blackburn; Hans Vissers; Robert Bordoli; Glaxo Wellcome, RTP, NC, LC Packings, Amsterdam, The Netherlands; Micromass, Manchester, UK

WPF 233

Quantitation of Myosin Using Electrospray Ionization Mass Spectrometry; Eric E. Niederkoifer; Urban A. Kiernan; Sergey A. Aksonov; Peter Williams; Arizona State University, Tempe, AZ

WPF 234

Mass Determination of Intact Alpha-chain Hemoglobin Adducts to within 0.2 Da Using Mass Peak Profiling from Selected Ion Recording Data (MPPSRD) with Electrospray Ionization; Xiaoming Zhao; Andrew H. Grange; G. Wayne Sovocool; U.S. EPA, Las Vegas, NV

WPF 235

Covariant Modification and LCMS of Glucokinase to Identify ATP Active Site and Protein Conformation; Troy D. Wood; Craig P. Duensing; Thermoquest Scientific Services, Riveira Beach, FL; State University of New York at Buffalo, Buffalo, NY

WPF 236

Study Sites of Biotinylation of IL-18 by LC/MS and LC/MS/MS; Tsuyuki Joanne Sun; Rong-Rong Zhu; Renee Miller; Kathleen L. Grant; BASF BioResearch Corp., Worcester, MA

WPF 237

Automated High-Throughput Parallel LC/MS for Fast Characterization of Proteins and Peptides; Bingbing Feng; Anan Patel; Zoming Wu; Jennifer Dally; Carol C. LePage; J. Randall Seamon; SmithKline Beecham Pharmaceuticals, King of Prussia, PA

WPF 238

Microespray ESI in the cone-jet mode followed by charge reduction and differential mobility analysis in protein chemistry: from non-covalent protein complexes to intact viruses; Guenter Allmair; Gerold Bacher; Dieter Blas; Wladyslaw Szymanski; Stan Kaufman; University of Vienna, Vienna, Austria; TSI Inc., St. Paul, MN

WPF 239

Microfabricated Device and Method for High-Throughput ESI-MS Analysis of Proteolytic Digestion Fragments; Julia M. Lazar; Roswitha S. Ramsey; J. Michael Ramsey; Oak Ridge National Laboratory, Oak Ridge, TN

WPF 240

Site-Specific Identification of IsoAspartic Acid Residues by Protein Isoaspartyl Methyltransferase/LC-MS/MS Analysis; Paul S. Russo; John V. Amari; Susan E. Abbatiello; Thomas J. Porter; Jason C. Rousse; Hubert A. Scoble; Genetics Institute, Andover, MA

WPF 241

Protein Identification by Automated Nanospray Mass Spectrometry Zoom Scan Walking; Matt J. Sweeney; Christoph W. Tuck; Matt Sweeney-Mass Spec Consulting, San Jose, CA; UC San Francisco, Howard Hughes Medical Institute, San Francisco, CA

WPF 242

The Development and Application of an Automated NanoLC/MS/MS System for Proteomic and Peptidomic Sample Analysis; Dawn D. Buie; James A. Carroll; Jennifer R. Kiesel; Kevin L.
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WPF243  Novel nanoflow gradient generator coupled with micro-LEC-ESI-MS/MS for protein identification; Thierry Le Billon; Daniel Figeys; MDS-Ocata, Toronto, Canada

WPF244  Comparison of Nanoelectrospray and Liquid Chromatography for Mass Spectrometric Sequencing of Low Amounts of Proteins on a Hybrid Quadrupole-Time of Flight Instrument; Juergen Kaas; Matthias Wilms; EMBL Heidelberg, Germany

WPF245  Using Multidimensional Microscale HPLC with Nanoflow/MS/MS as an Alternative to 2D PAGE with Nanoflow/MS/MS for Characterization of Complex Protein Mixtures; Mark Carrier; Shawn Duffy; Kerry Nugent; Jaim Mylchreest; David Kage; Tanuja Chaudhary; W. Jenny Kung; Suzanne Miyamoto; Anthony Martinez; Microm BioResources, Auburn, CA; Thermosquest, San Jose, CA; UC Davis Medical Center, Sacramento, CA

WPF246  Distinguishing Recombinant Monoclonal Antibodies by In-source Fragmentation and Delayed Extraction MALDI-TOF/MS; Viswanatham Katta; Rej J. Harris; Genetech, Inc., South San Francisco, CA

WPF247  Protein-Dodecyl Sulfate Binding and Cation Suppression in ESI-MS; Harsha P. Gunawardena; Brian T. Cooper; UNC, Charlotte, NC

WPF248  HPLC/MS/MS Analysis of ADP-Ribosylated Fluorescent Tagged Peptide Used to Quantitate Pertussis Toxin; Terry D. Cyr; Alan J. Menzies; Gerry Calver; Jean C. Ethier; Larry W. Whitehouse; Therapeutic Products Programme, Health Canada, Ottawa, Canada

WPF249  Collision Cross Sections of Apometallothioneins and Metal-Containing Metallothioneins Probed by a Segmented Quadrupole Mass Spectrometer; Yun Ling; Gholamreza Jahavary; K. W. Michael Siau; York University, Toronto, Canada; PE Sciex, Concord, Canada

WPF250  Microtiter Volume CE Fraction Collection Coupled with In-Capillary Digestion and MALDI-MS for Protein Identification; Andrea G. Kiceniuk; Bernd O. Keller; Liang Li; University of Alberta, Edmonton, Canada

WPF251  Protein Concentration and Enzyme Digestion on Micro-Beads for MALDI-TOF Peptide Mass Mapping of Proteins from Dilute Solutions; Alan A. Doucette; David Craft; Liang Li; University of Alberta, Edmonton, Canada

WPF252  In-Column Protein Concentration, Sample Clean-Up and Enzyme Digestion of Dilute Proteins for MALDI-TOF Peptide Mass Mapping of Proteins; David R Craft; Alan Doucette; Liang Li; University of Alberta, Canada

WPF253  Reaction Monitoring of Succinylation of Collagen with Matrix-Assisted Laser Desorption Ionization Mass Spectrometry; Jeong-Hwa Lee; Chul-Ho Jun; Jong-Shin Yoo; Sung-Ho Kim; Shin-Young Yun; Hwal Sub; Soonchunhyang University; Asan, South Korea; Yonsei University, Seoul, South Korea; Korea Basic Science Institute, Taejon, South Korea

WPF254  Detection and Quantification of b-2-Microglobulin Using Mass Spectrometric Immunoassay (MSIA); Kemmons A. Tubbs; Dobrin Nedelkov; Randall W. Nelson; Intrinsic Biobprobes Inc., Tempe, AZ

WPF255  Characterization of Conigrated Globin Variants from Electrophoresis Gel by Mass Spectrometry; Akun Li; Hua Lin; Henry Fales; Neal Epstein; National Institutes of Health, Bethesda, MD

WPF256  Peptide sequence information derived by pronase digestion and ammonium sulfate in-source decay MALDI-TOF; Lisa A. Mazzilli; Tamara R. Golden; Robert J. Cotter; Amina S. Woods; Johns Hopkins University School of Medicine, Baltimore, MD

WPF257  A robust, detergent-friendly method for the analysis of integral membrane proteins; Martine Cadene; Brian T. Chait; Rockefeller University, New York, NY

WPF258  Characterization of Integrins and Associated Proteins Using MALDI Tandem Mass Spectrometry; Igor Galich; David Puff; Jay Krishnan; Alexandre Loboda; Werner Ens; Kenneth G. Stauding; John A. Wiltkin; University of Manitoba, Winnipeg, Canada

WPF259  Peptide sequencing and protein identification using a novel tandem TOF/TOF mass spectrometer; Katalin F. Medzhizhadsyky; Jennifer M. Campbell; Lan Huang; Van Hoang; Michael A. Baldwin; Alma L. Burlingame; University of California, San Francisco, CA; PE Biosystems, Framingham, MA

WPF260  Automation of gel slice extraction and MALDI-TOF-MS sample preparation on a robotic platform; Tim Nadler; Ken Parker; Yulin Huang; Jon Degnore; Barbara Wolf; Leigh Anderson; Norman Anderson; John Lennon; Divya Bappanad; Andy McGrath; PE Biosystems, Framingham, MA; Large Scale Proteomics, Rockville, MD

WPF261  Characterization of Blood Proteins Using Mass Spectrometric Immunoassay in Combination with Enzymatically-Active MALDI-TOF Targets; Nelson W. Randall; Kemmons A. Tubbs; Dobrin Nedelkov; Intrinsic Biobprobes Inc., Tempe, AZ

WPF262  Mass Spectrometric Characterization of the Photoreaction Products of Benzophenone and Diazirine Photocleavable Probes Coupled to Corticotropin-Releasing Factor; Klaus Eckart; Olaf Jahn; Olaf Brauns; Bernhard Hofmann; Joachim Spiess; MPI Experimental Medicine, Goettingen, Germany

WPF263  Strategic Use of Affinity Techniques in the Drug Discovery Process; Philip J. Rosner; Kristin Kelly; Frank Menniti; Michele A. Kelly; Nora Charn; Darren Lewis; David Schreier; Pfizer Central Research, Groton, CT; INH Technologies, Calgary, Canada

WPF264  Rapid Protein Identification from Non-Specific Enzyme Digests with a TOF-TOF Analyzer; Arnold M. Falick; Peter Juhase; Jennifer M. Campbell; Marvin L. Vestal; PE Biosystems, Foster City, CA

WPF265  Simultaneous Monitoring of Multiple Enzyme Reactions in Crude Biological Mixtures by Electrospray Ionization Mass Spectrometry; Scott A. Gerber; C. Ronald Scott; Michael H. Glei; Frantisek Turecek; University of Washington, Seattle, WA

WPF265b  Protein Epitope Mapping by a Combination of Liquid-Phase Isoelectric Focusing and MALDI-
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**PEPTIDES, 266 – 294**

| WPG 266 | Clustering of Amino Acids in the Gas Phase by Electrospray Ionization Mass Spectrometry; Daxi Zhang1; Kim J. Koch1; W. Andy Tao1; R. Graham Cooks1; Purdue University, West Lafayette, IN |
| WPG 267 | Molecular Radical Cations of Oligopeptides from the Fragmentation of Metal Complexes of Peptides; Ivan K. Chu1; Christopher F. Rodriguez; Alan C. Hopkinson1; K.W. Michael Siu1; Tai-Chu Lau1; City University of Hong Kong, Hong Kong; York University, Toronto, Canada |
| WPG 268 | Sequencing of Sulfonic Acid-Derivatized Peptides by Electrospray Mass Spectrometry; Yiping Sun1; Mark D. Bauer1; Martin P. Lacey1; Thomas W. Keough1; The Procter & Gamble Company, Cincinnati, OH |
| WPG 269 | Multipole Storage Assisted Dissociation for Enhancing Sequence and Structural Studies in LC-TOF-MS; Craig M. Whitehouse1; Bruce A. Andrien1; Analytica of Branford, Inc., Branford, CTA |
| WPG 270 | Sequencing the Cyclic Peptide Inhibitors of Mammalian Ribonuclease (mRR) by ESI/MS/MS; Shanhuo Lin1; Sebastian Liehr1; Barry S. Coopermann1; Robert J. Cotter1; School of Medicine, Johns Hopkins University, Baltimore, MD; University of Pennsylvania, Philadelphia, PA |
| WPG 271 | Characterization of S-Glutathionyl-Benzoxiquinone Peptide Adducts by Electrospray Mass Spectrometry; Daniel E. Mason1; Serrine S. Lau1; Daniel C. Liebler1; University of Arizona, Tucson, AZ; University of Texas, Austin, TX |
| WPG 272 | Electron capture dissociation of phosphopeptides; Allan Stensballe1; Ole N. Jensen1; Peter Koeppe1; Roman Zubarev1; University of Southern Denmark, Odense University, Odense, Denmark |
| WPG 273 | Differentiation of Diastereomer Tertiarybutyloxycarbonylprolylproline Derivatives by ESI MS/MS; Hideaki Tsunematsu1; Hiroshi Hanazono1; Magoichi Yamamoto1; Ryuchi Isohe1; Masanori Inagaki1; Yumiko Sode1; Ryuchi Higuchi1; Fukui University, Japan; Towa University, Japan; Kyushu University, Japan |
| WPG 274 | Microbore LC/MS Determination of an ACE Inhibitor, Lisinopril, Angiotensins I - III and their Peptide Based Agonists and Antagonists; Arthur J. Boyer1; Shimadzu Scientific Instruments, Inc., Columbia, MD |
| WPG 275 | Microwave Enhanced Rapid Peptide Analysis; Birendra N. Premamani1; Yao Hain Ing1; Petia A. Shipkova1; Peter L. Bartner1; Ajay K. Bose2; Chaitanya Sareen2; Nova Lavinskaia2; Schering-Plough Research Institute, Kenilworth, NJ; Stevens Institute of Technology, Hoboken, NJ |
| WPG 276 | Accurate Determination of the Isotopic State of Single Amide Hydrogen Interstitial Peptides; Jos Buiks1; Kristina Hakansson1; Charlotte Hagman1; Per Hakansson1; Sven Oscarsson1; Uppsala University, Uppsala, Sweden; Mälardalen University, Eskilstuna, Sweden |
| WPG 277 | Migration of Peptide Amide Hydrogens in the Gas Phase; Kristina Hakansson1; Jos Buiks1; Youyi Tsibin1; Jan Hinmmer Richter1; Per Hakansson1; Uppsala University, Uppsala, Sweden |
| WPG 278 | Mobility Labeling for Parallel CID of Ion Mixtures; Cherokee S. Hoaglund-Hyzer1; David E. Clemmer1; Indiana University, Bloomington, IN |
| WPG 279 | Ultrarurate Analysis of Neuropeptides; William E. Haskins1; Steven R. Witowski1; Robert T. Kennedy1; University of Florida, Gainesville, FL |
| WPG 280 | Fast peptide mapping by MALDI using a harmonic field reflectron mass spectrometer; Steve P. Thompson1; Vic P. Cass1; Jonas Astrom1; Scientific Analysis Instr., Manchester, UK; Amersham Pharmacia Biotech, Uppsala, Sweden |
| WPG 281 | De Novo Sequencing of Novel Peptides Using a Hybrid Quadrupole TOF Using Dynamic Ion Bunching and MS3; Tina A. Settiener1; David Hawke1; PE Biosystems, Foster City, CA |
| WPG 282 | A MS/MS Analysis Strategy to Confirm the Sequence of Large Synthetic Peptides Using Nanospray IT-MS; Denise A. Keen1; Curtis Croker1; John Pearcy1; Terry Lee1; Helen Ge1; Mary K. Young1; Beckman Research Institute of the City of Hope, Duarte, CA |
| WPG 283 | Can ABO be Incorporated into Peptide Maps Post-Digestion?; David H. Hawke1; ($.2 M. Wuaysir1; Tina Settiener1; PE Biosystems, Foster City, CA |
| WPG 284 | Low energy fragmentation pathways of protonated oligopeptides containing basic and acidic amino acid residues Arpad Somogyi1; Balazs Hargittai1; Bela Paizs1; Sandor Suzai1; Gyorgy Lendval1; University of Arizona, Tucson, AZ; German Cancer Research Center, Heidelberg, Germany; Hungarian Academy of Sci., Budapest, Hungary |
| WPG 285 | ESI-MS of Non-Covalent Complexes: Application to Molecular Recognition and the Stabilization of Zwitiererions in the Gas Phase Via Salt-Bridge Interactions and Specific Hydrogen Bonding; Ryan R. Julian1; Jesse L. Beauchamp1; California Institute of Technology, Pasadena, CA |
| WPG 286 | The Structure of Glycine-M+ (M = Be, Mg, Ca, Sr, Ba); Effects of Cation Size on Zwitieron Stability; Andrew S. Lemoff1; Eric F. Strittmatter1; Evan R. Williams1; University of California, Berkeley, CA |
| WPG 287 | Characterization of brain in vivo microdialysis content using ES Q-TOF MS; Per E. Andresen1; Ingela Lindstrom1; Mikael Hedeland1; Ulf Bondesson1; Uppsala University, Uppsala, Sweden; National Veterinary Institute, Uppsala, Sweden |
WEDNESDAY POSTERS

7:30 – 8:00 am SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
6:00 – 6:30 pm REMOVE POSTERS. Please leave posters for the full day.

WPG 288 Characterization of Retrovirally Delivered Intracellular Peptide Libraries by MALDI-TOF Mass Spectrometry; Beau Peelle1; Weiqun Li1; Dave Anderson1; Rigel, Inc., South San Francisco, CA

WPG 289 Charge Location on Gas Phase Peptide Ions; G. Reid Ashby1; Chandelier H. Hill1; Herbert H. Hill, Jr.1; Washington State University, Pullman, WA

WPG 290 Mass Spectrometric Analysis of Variably Protected Peptide from Solid Phase Synthesis Following Cleavage from the Resin Support through the Use of Cyanogen Bromide; Mark W. Ruszewczyk1; Thomas H. Morton1; University of California, Riverside, CA

WPG 291 Binding site locations of peptides and proteins covalently linked to surfaces; James P. Reilly1; Laura S. Baker1; Indiana University, Bloomington, IN

WPG 292 Rapid Sequencing of the N-Terminal Peptide from Blocked Proteins by Mass Spectrometry; Toshiyuki Mikami1; Kazunori Yana1; Hiroshi Nakazawa1; Sumitomo Chemical Co., Ltd., Japan

WPG 293 Isotope labeling enhances the interpretation of MS-spectra of "de novo" peptide sequencing; Guido Spermann1; Axel Romer2; Dietmar Schomburg3; University of Cologne, Germany; A&M Labor für Analytik und Metabolismusforschung, Bergheim, Germany

WPG 294 Factors affecting amino acid sequence information in collision-induced dissociation spectra of triply charged tryptic peptides with an internal histidine; Belinda B Willard1; Michael Kent1; Cleveland Clinic Foundation, Cleveland, OH

HIGH-THROUGHPUT, 295 - 325

WPH 295 Application of Liquid Chromatography-Mass Spectrometry-NMR Spectrometry (LC-MS-NMR); Tetsuichiro Morita1; Yukata Takahashi1; Takao Fujimoto1; Hiroaki Uemura1; Naoyuki Fujii1; Tetsuo Higuchi1; JEOL, Ltd., Tokyo, Japan

WPH 296 High Throughput LC-MS/MS Analysis of Ritonavir and ABT-378 Using an Automated Liquid/Liquid Extraction Sample Preparation Method; Anita T. Shen1; Hoppe T. Skriba1; Huong Mai1; Ray Wieboldt1; Min S. Chang2; Qin C. Ji2; Tawakol El-Shourbagy1; Abbott Laboratories,Abbott Park, IL

WPH 297 Technology for sensitive, high throughput protein identification from 2-DE; Johan Gobom1; Holger Eickhoff1; Martin Horn1; Thomas Przewieszlik1; Christine Luebbe1; Hans Lebrach1; Eckhard Nordhoff1; Max-Planck Institute for Molecular Genetics, Berlin, Germany

WPH 298 Comparison of on-line extraction with semi-automated protein precipitation in 96-well format for drug discovery bioanalysis; Jian Wang1; Shu-Ying Chang2; Celia D'Arienzo3; David Wang-Ivron1; Bristol-Myers Squibb, New Brunswick, NJ

WPH 299 384-Well Solid-Phase Extraction for the Analysis of Methotrexate and its 7-Hydroxy Metabolite from Human Urine; Geoffrey Rule1; Matthew Chappell1; Stephen Lowes1; Jack Henion1; Advanced BioAnalytical Services, Ithaca, NY

WPH 300 Automated LC/MS/MS Method Development to Support in vitro/in vivo High Throughput Screening; Euphachai Freiwald1; Hua-Fen Liu1; Gary Hudson1; Steven Michael1; Parke-Davis, Ann Arbor, MI

WPH 301 Coordinated Selection of Stationary and Mobile Phases for Fast LC/MS Used in Parallel Synthesis and Open Access Applications; Mark J. Hayward1; Mary S. Martin1; Leonard O. Hargiss1; James L. Munson1; Novartis Pharmaceuticals, Summit, NJ

WPH 302 Surface Treatment of MALDI Targets for Automation of Synthetic Polymer Analysis; Patricia M. Peacock1; Charles N. McEwen1; Dupont Company, Wilmington, DE

WPH 303 Pin-tools for high throughput MALDI-MS sample preparation; Klaus-Dieter Kleoppel1; Holger Eickhoff1; Martin Horn1; Hans Lebrach1; Eckhard Nordhoff1; Max-Planck-Institute for Molecular Genetics, Berlin, Germany

WPH 304 Automated Accurate Mass Measurement of Small Organic Molecules on a Magnetic Sector Mass Spectrometer; James E. Carlson1; W. Rodney Mathews1; Olga V. Nemirowsky1; Pharmacia & Upjohn, Kalanazoza, MI

WPH 305 Combining Autoinjector and Nebulizer Hardware for Enhanced Automation in FIA-MS; Bruce A. Andrien, Jr.1; James G. Boyle1; Analytica of Branford, Inc., Branford, CT

WPH 306 High Throughput Flow Injection Mass-Spectrometry Using a Custom Built Rapid Wash Station on a Gilson 215 AutoSampler; Kurt Edinger1; Thomas Swann1; Harold N. Wellner1; James Mongillo1

WPH 307 Comparison of Plasma Sample Preparation by Manual Protein Precipitation and Automated 96-Well Filtration for LC-MS-MS Analysis of Protease Inhibitors; Sahale L. King1; David J. Foltz1; Timothy R. Baker1; Sean X. Peng3; Procter & Gamble Pharmaceuticals, Mason, OH

WPH 308 Quantitative and comprehensive one step proteome analysis by the molecular scanner coupled with ICA technologies; Manfred Heller1; Willy V. Bienvenut1; Salvo G. Paesano1; Jean-Charles Sanchez1; Pierre-Alien Binz1; Markus Muller1; Steven P. Gyg11; Beate Rist1; Ruedi Aebersold1; Denis F. Hochstrasser1; Geneva University Hospital, Geneva, Switzerland; Swiss Institute of Bioinformatics, Geneva, Switzerland; University of Washington, Seattle, WA

WPH 309 A LC-MS High Throughput IAM Chromatography Method to Evaluate Permeability; Hua-fen Liu1; David T. Ross1; Keith L. Hoffman1; Linda A. Stilgenbauer1; Narayan Surendran1; Barbra H. Stewart1; O. Helen Chan1; Parke-Davis, Ann Arbor, MI

WPH 310 Automated Peptide Analysis of Body Fluids with MALDI TOF and Hybrid Tandem Mass Spectrometry; Helmut Muenster1; Reinhold Pesch1; Markus Kellmann1; Finnigan MAT GmbH, Bremen, Germany; BioVisioN GmbH & Co KG, Hanover, Germany

WPH 311 Conversion of Existing Shimadzu HPLC Autosamplers to an LC-MS Assay Friendly Format, Dual-Microlitre Plates-196 Samples Total Capacity; Rich DeMuro1; Min S. Chang1; Anita T. Shen1; Jack Conrad1; Craig Schiller1; Richard N. Koeritz1; Greg Mason1; Tawakol El-Shourbagy1; Shimadzu, Wood Dale, Abbott Laboratories, Abbott Park, IL

WPH 312 Determination of Concentration and Purity of High Throughput Screening Samples Using Liquid
WEDNESDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
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6:00 – 6:30 pm  REMOVE POSTERS. Please leave posters for the full day.

Chromatography-Chemoluminescence Nitrogen Detection-Tandem Mass Spectrometry; Nata S. Bass¹; Luke A. Miller¹; Glaxo Welcome Inc, RTP, NC

WPH 313 Direct Recognition of Unchained Micro-Droplet-Events (DRUM) for Fast Arraying of Microscale MALDI-MS Samples; Martin Müller¹; Holger Eickhoff²; Eckhard Nordhofer²; Hans Lehbrach³; Markus Kalkum³; Max-Planck-Institute Molekulare Genetik, Berlin, Germany; The Rockefeller University, New York, NY

WPH 314 Pep-O-Matic: An Expert Virtual Instrument for the Automated Data Dependent MS/MS Analysis of Synthetic Peptides; Curtis G. Croker¹; John O. Pearcy¹; Denise A. Keen¹; Terry Lee¹; Beckman Research Institute of the City of Hope, Duarte, CA

WPH 315 Automated MALDI Sample Preparations of Proteome Samples on Anchor Targets; Peter Hunagel¹; Martin Schüüenberg¹; Barbara Ehrhard¹; Anja Resemann¹; Detlev Suckau¹; Bruker Daltonik GmbH, Bremen, Germany

WPH 316 Rapid and automated method development and sample analysis for assessment of metabolic stability and Caco-2 cell permeability of new compounds: A tool combined with the application of α: φ Automaton; Helen Gu¹; Phi Tran¹; Elina Dunn¹; Kelly Masonıc; Hequn Yin¹; James Mangold¹; Eva Duchoslov³; Novartis Pharmaceuticals, East Hanover, NJ; MDS Scieix, Canada

WPH 317 Lab Automation Strategy to Increase the Throughput of LC-MS in Drug Discovery; Jeffrey L. Dage¹; Aventis Pharmaceuticals Inc., Bridgewater, NJ

WPH 318 A Simple Open Access Interface for Finnigan Unis-Based Mass Spectrometers; Mark Sanders¹; Harry L. Burdette¹; Bristol-Myers Squibb PRL, Princeton, NJ

WPH 319 High Throughput Compound Integrity Checking Using Data-Dependent SMARTLCMS; Mark E Hal¹; Mark Sanders¹; Novartis Corporation, Yardley, PA; Bristol-Myers Squibb, Princeton, NJ

WPH 320 Software Package for the Analysis of High-throughput: Hui Tong¹; Franklin Moy¹; Marshall Siegel¹; Keiko Tabei¹; Robert Powers¹; Wyeth-Ayerst Research, Pearl River, NY

WPH 321 AutoScan: An Automated Workstation for Rapid Determination of MS and MS/MS Conditions for High-Throughput Quantitation of New Chemical Entities; John S. Janiszewski¹; Kevin M. Whalen¹; Katrina J. Rogers¹; Mark J. Cole¹; Pfizer Inc, Groton, CT

WPH 322 High Throughput Parallel LC/MS Analysis of Combinatorial Libraries; David A. Tolson¹; Andrew J. Organ¹; Daniel L Brooke¹; Roger Martin¹; SmithKline Beecham, Harlow, UK

WPH 323 Characterization and Optimization of Direct Plasma Injection for Bioanalysis Using Cohesive Technologies' HTLC System; Surendra Bansal¹; Paul Weigl¹; Mei Liu¹; Zhenmin Liang¹; Hoffmann-La Roche, Nutley, NJ

WPH 324 An automated method that enhances the analytical throughput of Pharmacokinetic drugs in plasma using LC-MS/MS; Marilyn Lam¹; Jih-Lie Tseng¹; Jun
THURSDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
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3:30 – 3:30 pm  REMOVE POSTERS. Please leave posters until 3:00 pm.

THURSDAY POSTERS

ThPA001  Historical Highlights of the Early Days of SIMS; Bryan L. Bentz; Saranoff Corporation, Princeton, NJ
ThPA002  Mass Spectrometry in an Adversarial Context: A Proposal for Demonstrating Method Fitness; Robert Bingham, Joe Boison, John Chakel, Jane Gale, David Heller, Steven Musser, Phil Price, Stephen Stein

GENOMIC ANALYSIS, 004 - 019

ThPA004  Linking Genetic Variants to Disease by ESI/MS: Risk Profiles for Combined Heterozygosity; Lesa M. Nelson; Kenneth Ward; Chad C. Nelson; University of Utah, Salt Lake City, UT
ThPA005  ESI Quadrupole, or Quadrupole Ion Trap MS for Identification of SNPs in PCR Products and ESI Quadrupole Ion Trap MS/MS for Discrimination of PCR Products with the Same Nucleotide Composition but Different Sequence; Mark T. Kraemer; James J. Walters; Karen F. Fox; Alvin Fox; Kim E. Creek; Lucia Pirisi-Creek; David S. Wunsche; Richard D. Smith; David L. Tabb; John R. Yates, III; University of South Carolina, Columbia, SC; Pacific Northwestern National Laboratory, Richland, WA; University of Washington, Seattle, WA
ThPA006  One-Vial Sanger Cycle Sequencing Optimized for MALDI-TOF-MS; Christine Luebbecke; Hans Lehrach; Eckhard Nordhoff; Max-Planck-Institute for Molecular Genetics, Berlin, Germany
ThPA007  The Application of MALDI-TOF Mass Spectrometry in the Validation of Single Nucleotide Polymorphisms; Justin G. Stroh; Stephanie K. Hall; Linda H. Pezzullo; Jason P. Affourtit; Albert B. Seymour; Pfizer Central Research, Groton, CT
ThPA008  Optimization of Parameters for the Validation of Single Nucleotide Polymorphisms (SNP) via MALDI-TOF MS; Linda H. Pezzullo; Stephanie K. Hall; Jason P. Affourtit; Albert B. Seymour; Patrice M. Milos; Jodi L. Richmond; Justin G. Stroh; Pfizer Central Research, Groton, CT
ThPA009  A New Vset Assay for Genotyping of SNPs; Baochuan Gu; X. Sun; H. Ding; K. Hung; Cleveland State University, Cleveland, OH
ThPA010  Studies towards multiplexed oligonucleotide fingerprinting by the use of MALDI-TOF-MS; Anna Guerasmova; Christine Luebbecke; Ivo Gut; John O'Brien; Matthias Steinfähn; Eckhard Nordhoff; Hans Lehrach; Uwe Radelof; Max-Planck-Institute for Molecular Genetics, Berlin, Germany; Centre National de Genotypage, Evry, France
ThPA011  Genotyping of five coagulation factors by the GOOD assay; Thomas Fröhlich; Thomas Wenzel; Constanze Franke; Markus Kostrewa; Doris Lechner; Ivo G. Gut; Bruker Saxonia Analytik GmbH, Leipzig, Germany; Centre National de Genotypage, Evry, France
ThPA012  Application of MALDI-TOF MS for Quantitation of Jeryl Lynn Viral Strain in Mumps Vaccine; Charlotte C. Jp; Hui Wang; Gwo-Hwa Lee; Deepa Patel; Paul Keller; Merck Research Laboratory, West Point, PA
ThPA013  Application of MALDI-TOF/MS for the Multiplex Detection of Hereditary Hemochromatosis; Jack Simpson; Qi Liang; Barry Thompson; Joseph Nelson; James Girard; Center for Medical and Molecular Genetics, AFIP, Rockville, MD; American University, Washington, DC
ThPA014  Detection of Point Mutations of Forensic Importance by Peptide Nucleic Acid Probes and MALDI-TOF Mass Spectrometry; Brian Wendelburg; James Girard; Jack Simpson; American University, Washington, DC; Center for Medical and Molecular Genetics, AFIP, Rockville, MD
ThPA015  The Efficiency of Incorporation of Four Different Stable-isotope Labeled Precursors into DNA in Cell Culture; Gavin F. Black; Yoon C. Boller; Katherine A. Kennedy; Paolo Leech; Fred P. Abramson; George Washington University, Washington, DC
ThPA016  Characterization of Enzymatic Digestion of Labeled Oligonucleotides for Sequence Determination by Mass Spectrometry; Huiqiong Wu; Xiaoxing Xu; Hoda Abolenne; Abbott Laboratories, Abbott Park, IL
ThPA017  Sample Preparation Techniques for Improved MALDI-TOFMS of High Molecular Weight Oligonucleotides; Tracey A. Simmons; Phoebe Balthrop; Jessica A. Ragas; Rama Tummala; Patrick A. Limbach; Louisiana State University, Baton Rouge, LA
ThPA018  A novel magnetic bead DNA purification system for SNP genotyping by MALDI-TOF MS; Markus Kostrewa; Jacqueline Bimmel; Isabelle Thomas; Thomas Wenzel; Eckhard Nordhoff; Holger Rauth; Thomas Froehlich; Bruker Saxonia Analytik GmbH, Leipzig, Germany; Max-Planck-Institute for Molecular Genetics, Berlin, Germany
ThPA019  New magnetic purification chemistry for the use of MALDI-MS in genomics; Holger Rauth; Hans Lehrach; Markus Kostrewa; Thomas Froehlich; Eckhard Nordhoff; Max-Planck-Institute for Molecular Genetics, Berlin, Germany; Bruker Saxonia Analytik GmbH, Leipzig, Germany

PROTEINS: STRUCTURE/FUNCTION, MICROORGANISMS, AND PLANTS, 020 - 097

ThPB020  Biochemical Mapping of Functional Domains of HIV-1 Integrase Involved in Viral and Target DNA Binding; Kai Zhu; Julian P. Whitelegge; Kym F. Faulk; Samson A. Chow; University of California, Los Angeles, CA
ThPB021  Using Mass Spectrometry, Chemical Crosslinking and Computation Methods to Determine Domain-Domain Interactions in Full-Length HIV-1 Integrase; Ning Tang; Malin Young; Ken Bruneld; Ann Tang; Gavin Dollinger; Irwin D Kuntz; Andrew Leavitt; Bradford G Gibson; University of California, San Francisco, CA; Sandia National Laboratories, Albuquerque, NM; Chiron Corporation, Emeryville, CA
ThPB022  Copper insertion pathway in human copper/zinc superoxide dismutase; Hongbin Liu; Haining Zhu; Aram Neressian; Kym F. Faulk; Joan S. Valentine; UCLA, Los Angeles, CA
ThPB023  Application of New MS/MS Methodologies to the Characterization of Enzymes Involved in Thiamin Biosynthesis; Ying Ge; David M. Horn; Tadhg P. Begley; Fred W. McLaflerty; Cornell University, Ithaca, NY
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<th>Session</th>
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<td>3:00-3:30 pm</td>
<td>REMOVE POSTERS. Please leave posters until 3:00 pm.</td>
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**ThPB024** Caspase Mediated Prothymosin alpha Fragmentation in Apoptosis: Time Resolved Mapping of Cleavage Sites; Markus Kalkum; Alexandra G. Evtuafieva; Andrey B. Vartapetian; The Rockefeller University, New York, NY; Moscow State University, Moscow, Russia

**ThPB025** A new variant of the gamma subunit of renal Na,K-ATPase. Identification by Mass Spectrometry, Antibody binding and Expression in Cultured Cells; Alla Shamskaya; Berndhard; Bernhard Kubier; Matthias Mann; Helen X. Pu; Rhoda Blostein; Rivka Goldshlager; Steven Karlsh; Weizmann Institute of Science, Israel; University of Southern Denmark, Odense M, Denmark; McGill University, Montreal, Canada

**ThPB026** Novel Protein Recoding: Translational Shift and Bypass Events; Chadi C. Nelson; Alan J. Herr; Norma Wills; John F. Atkins; Ray F. Gesteland; University of Utah, Salt Lake City, UT

**ThPB027** Conformational Changes in Beta-Endorphin as Studied by ESI-MS; Hui Lin; Chhabil Dass; The University of Memphis, Memphis, TN

**ThPB028** Differences in I/D Exchange of Modified Insulins; Michael A. Greaves; Charles Gloeckner; Stephen Bayne; Michael L. Gross; Washington University, St Louis, MO; NOVO Nordisk S/A, Denmark

**ThPB029** Application of a New Immobilization I/D Exchange Protocol: Calmodulin; Jiang Zhao; Mei Zhu; Daryl E. Gibin; Michael L. Gross; Washington University, St Louis, MO

**ThPB030** Electrospray Ionisation Fourier Transform Ion Cyclotron Resonance: Calmodulin - The Archetypal Calcium Binding Protein - How Well Does It Bind Calcium?; Peter J. Derrick; Helen J. Cooper; Xiaodong Feng; Tessa J. Hill; Jennifer K. Mitchell; Marjana Noustiain; Daniel Lafitte; University of Warwick, Coventry, UK; Universite de la Mediterranee, Marseilles, France

**ThPB031** Withdrawn

**ThPB032** Investigation of structure and metal binding properties of transferrins by electrospray ionization mass spectrometry; Dmitry R Gumenov; Anne B Mason; Igor A Kaltashov; Univ. of Massachusetts, Amherst, MA; Univ. of Vermont, Burlington, VT

**ThPB033** Tagging techniques in the mass spectrometric characterization of protein complexes: Mueller Dieter; Schindler Patrick; Wirth Urs; Steinmetz Michel; Tovbin Harry; Voshol Hans; Novartis Pharma AG, Basel, Switzerland

**ThPB034** Hydrogen / Deuterium Exchange Monitored by Electrospray Mass Spectrometry: Application to Recombinant Human Macrophage Colony Stimulating Factor beta; Xuqiang Yan; Y. Heidi Zhang; Mark E. Harder; Michael L. Schimerlik; Max L. Deinzer; Oregon State University, Corvallis, OR

**ThPB035** A Study of Intermediates Involved in the Unfolding Pathway of Recombinant Human Macrophage Colony-Stimulating Factor (rh-CSF) by Hydrogen / Deuterium Exchange; Y. Heidi Zhang; Xuqiang Yan; Michael L. Schimerlik; Max L. Deinzer; Oregon State University, Corvallis, OR

**ThPB036** Influence of calcium and zinc binding on the conformation of the human protein S100b; Jean-Philippe Pichon; Jean-Christophe Deloulme; Jacques Baudier; Eric Frest; Jean Armonnag; Institut de Biologie Structurale, Grenoble, France; DBMS; Institut de Biologie Structurale, France

**ThPB037** Protein Folding Mechanisms Elucidated by Hydrogen-Deuterium Exchange Monitored by Electrospray Mass Spectrometry; Alison E. Ashcroft; Victoria J. McParland; Joseph E. Coyle; Sunita K. Kulkarni; Sheena E. Radford; University of Leeds, UK

**ThPB038** Myoglobin refolding kinetics monitored by time-resolved ESI-MS with online H/D exchange; Douglas A. Simmons; Lars Konermann; The University of Western Ontario, London, Canada

**ThPB039** Identifying Unfolding Domains in Alpha-1A Barrel Proteins Using Hydrogen Exchange and Mass Spectrometry; Ashraf S. Razal; Yuzhong Deng; David L. Smith; University of Nebraska-Lincoln, Lincoln, NE

**ThPB040** Stability of Apomyoglobin Helices by Synchrotron Radiolysis and Mass Spectrometry; Mark R. Chance; Kevin M. Downard; Simin D. Maleknia; Albert Einstein College of Medicine, Bronx, NY

**ThPB041** Refolding of Aldolase Denatured in Acid: Hydrogen Exchange-Mass Spectrometry; Hai Pan; David L. Smith; University of Nebraska, Lincoln, NE

**ThPB042** Mass Spectrometric Characterization of the Nuclear Envelope; Mathias Deger; Henning Otto; Ferdinand Hucho; Institute for Biochemistry, Free University Berlin, Berlin, Germany

**ThPB043** Characterization of the Coordination between Copper and Prions by Chemical Modification of Histidine and Mass Spectrometry; Ying Yang; Kefeng Qin; Lingjie Meng; David Westaway; University of Toronto, Toronto, Canada

**ThPB044** Using MALDI mass spectrometry to locate the coagule binding site of the dopamine transporter protein; Suchitra. S. Bhattacharyya; Kermit. K. Murray; Joseph B. Justice; Brian Reed; Emory University, Atlanta, GA

**ThPB045** Profiling Protein Interfaces by Chemical Cross-Linking: The Application of a Fluorogenic Cross-Linker and Mass Spectrometry; Andrea Singh; Kuan Wang; NIH/NIMAS, Bethesda, MD

**ThPB046** Rapid Identification and Analysis of a Conserved Protein Complex Using Stable-Isotope Assisted Mass Spectroscopy (SIAMS); Thomas C. Hunter; John J. Kelley; III; E. Morton Bradbury; Vahid Majidi; Xian Chen; Los Alamos National Laboratory, Los Alamos, NM; Dartmouth College, Hanover, NH; University of California, Davis, CA

**ThPB047** Hydrogen-Deuterium Exchange/ Proteolytic Digestion/ ESIMS for Determining Conformation of Large Protein Aggregates; Jiong Yu; Azeem S. Hasan; Jean B. Smith; David L. Smith; University of Nebraska, Lincoln, NE

**ThPB048** Rapid Determination of Inhibitor Effects on Quaternary Protein Structure Using On-line Size Exclusion Chromatography-Micro Electrospray Ionization Mass Spectrometry; Maryann L. Shen;
THURSDAY POSTERS

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ThPB049

**Mass Spectrometric Studies of the Covalent Intermediate of CD38 Inhibition**
By Haifeng Deng, Linda Siconolfi-Baez, Edward Nieves, Ruth Hogue-Andreletti, Anthony A. Sause, Vern L. Schramm - Albert Einstein College of Medicine, Bronx, NY

**Abstract**
This poster presents a study on the covalent intermediate of CD38 inhibition, using mass spectrometry techniques. The research aims to elucidate the mechanism of action of CD38 inhibitors and their potential therapeutic applications.

ThPB050

**Identification and Sequencing of O-phosphorylated Peptides**
By J. Lipsky, S. Naylor - Mayo Foundation, Rochester, MN

**Abstract**
This poster focuses on the identification and sequencing of O-phosphorylated peptides, using MALDI-PSD-TOFMS conditions. The research involves the use of a novel approach to analyze phosphopeptides, providing insights into post-translational modifications.

ThPB051

**Evaluation of CID Spectra**
By A. Jones, D. Mason, D. Liebler - University of Arizona, Tucson, AZ

**Abstract**
This poster discusses the evaluation of CID spectra for peptide analysis, highlighting the importance of accurate fragmentation patterns in peptide identification.

ThPB052

**Collision Induced Dissociation of Argininated Phosphopeptides**
By Xi Guo, C. Rodriguez, A. Hopkinson - York University, Toronto, Canada

**Abstract**
This poster presents research on the collision induced dissociation of argininated phosphopeptides, aiming to improve the understanding of protein phosphorylation sites.

ThPB053

**The Fragmentation of Alkali Metallated Phosphopeptides**
By W. Feng, S. Groenert, C. Lebrilla - University of California, Davis, CA

**Abstract**
This poster focuses on the fragmentation of alkali metallated phosphopeptides, exploring the impact of metal ions on peptide fragmentation patterns.

ThPB054

**Determination of ESI/MS/MS Fragmentation Patterns of Carboxymethylated and S-(2-Chlorosulfonylethyl)glutathione Modified Peptides**
By J. A. Jones, D. C. Liebler - University of Arizona, Tucson, AZ

**Abstract**
This poster discusses the determination of fragmentation patterns for carboxymethylated and S-(2-chlorosulfonylethyl)glutathione modified peptides, providing insights into the chemical properties of these modifications.

ThPB055

**Electrospray Ionization Mass Spectrometry of Peptides Terminally Derivatized with Sulfonic Acid**
By Tse-Fang Chen, Philip R. Gaeken, Sung-hwan Kim, Douglass F. Barofsky - Oregon State University, Corvallis, OR

**Abstract**
This poster presents research on the electrospray ionization mass spectrometry of peptides derivatized with sulfonic acid, highlighting the utility of this method in peptide analysis.

ThPB056

**Peptide Sequencing Using Seamless PSD from a High Reflection Reflectron TOF Mass Spectrometer**

**Abstract**
This poster discusses peptide sequencing using seamless PSD from a high reflection reflectron TOF mass spectrometer, showcasing advancements in mass spectrometry techniques.

ThPB057

**Automated Detection of Metastable Losses in Reflectron MALDI MS**
By Urs Wirth, D. Dieter Mueller, Patrick Schindler, J. Lange - Novartis Pharma AG, Basel, Switzerland

**Abstract**
This poster presents research on automated detection of metastable losses in reflectron MALDI MS, highlighting the importance of loss detection in peptide analysis.

ThPB058

**A Model of the Random Matching of Mass Spectrometric Proteolytic Peptide Maps and Proteins in a Genome Database**
By Jan Eriksson, David Fenyo, J. C. Eriksson - Swedish Agricultural University, Uppsala, Sweden

**Abstract**
This poster discusses a model for random matching of mass spectrometric proteolytic peptide maps and proteins in a genome database, providing insights into proteome analysis.

ThPB059

**Searching Raw Prokaryotic Genome Data with Peptide CID Spectra**
By K. E. Laidig, W. Weinben, J. R. Yates, R. J. Lamont, M. Hackett - University of Washington, Seattle, WA

**Abstract**
This poster presents research on searching raw prokaryotic genome data with peptide CID spectra, highlighting the potential of this approach in bacterial genome analysis.

ThPB060

**Identification of unknown proteins through Mining Distant Protein Homology with Mass Spectral Information**
By L. Huang, J. Jacob, P. R. Baker, M. A. Baldwin, P. Babbitt, A. L. Burlingame - UCSD, San Francisco, CA

**Abstract**
This poster discusses the identification of unknown proteins through mining distant protein homology with mass spectral information, providing insights into protein identification methods.

ThPB061

**Enhanced Detection of Modified Peptide Motifs Using a Data Reduction Algorithm to Automate the**

**Abstract**
This poster presents research on enhanced detection of modified peptide motifs using a data reduction algorithm to automate the detection process, highlighting the importance of automated data reduction in proteomics.

ThPB062

**Improvements in protein identification by MALDI-TOF peptide mapping**
By Volker Egelhofer, Konrad Buesow, Christine Luebber, Hans Lehrach, Eckhard Nordhoff - Max-Planck-Institute for Molecular Genetics, Berlin, Germany

**Abstract**
This poster discusses improvements in protein identification by MALDI-TOF peptide mapping, highlighting advancements in peptide mapping techniques.

ThPB063

**Automated Peak Detection Algorithms For Mass Spectrometry Based on Pattern Recognition Techniques**

**Abstract**
This poster presents research on automated peak detection algorithms for mass spectrometry based on pattern recognition techniques, providing insights into automated data analysis.

ThPB064

**Objective and Rapid Data Analysis in Comparing Proteome Gel Images**
By Edward S. Umeto, Dominic M. Desiderio - University of Tennessee, Memphis TN

**Abstract**
This poster discusses objective and rapid data analysis in comparing proteome gel images, highlighting the importance of efficient data analysis in proteomics.

ThPB065

**Characterization of Novel Peptides from \textit{Vicia sativa} (Vetch) by Electrospray Ion Trap and Electrospray Time-of-Flight Mass Spectrometry**
By Yan Zhang, James L. McMannan, Mark W. Duncan - University of Colorado Health Sciences Center, Denver, CO

**Abstract**
This poster presents research on the characterization of novel peptides from \textit{Vicia sativa} (Vetch) by electrospray ion trap and electrospray time-of-flight mass spectrometry, providing insights into the analysis of plant peptides.

ThPB066

**Direct Identification of a yeast protein complex by automated nanoscale LC-MS/MS**
By Adele Rowley, Martina Marziochi, Walter Blackstock, Jytõ Choudhary, GlaxoWellcome, Medicines Research Centre, England

**Abstract**
This poster discusses direct identification of a yeast protein complex by automated nanoscale LC-MS/MS, highlighting the potential of automated techniques in protein complex analysis.

ThPB067

**Archaeal Proteome Identification by MALDI Peptide Mass Mapping and Micro-LC-ESI Tandem Mass Spectrometry**

**Abstract**
This poster presents research on archaeal proteome identification by MALDI peptide mass mapping and micro-LC-ESI tandem mass spectrometry, providing insights into archael proteomics.

ThPB068

**Profilin Identification and Viral and Host Proteins in Tobacco Mosaic Virus RNA Replicase Complexes by 2D PAGE and MALDI-TOF-MS**
By Lloyd W. Summer, Svetlana Foliemonova, Richard S. Nelson - The Noble Foundation, Ardmore, OK

**Abstract**
This poster discusses the identification of profilin and viral and host proteins in Tobacco Mosaic Virus RNA replicase complexes using 2D PAGE and MALDI-TOF-MS, highlighting the potential of these techniques in viral research.

ThPB069

**Utilization of MALDI-TOF/MS Mass Spectrometry to Obtain Topological Information about Cytomegalovirus**
By Suzanne M. Ramirez, Robert J. Cotter, D. Wade Gibson, John Hopkins University School of Medicine, Baltimore, MD

**Abstract**
This poster presents research on the utilization of MALDI-TOF/MS mass spectrometry to obtain topological information about Cytomegalovirus, providing insights into viral protein analysis.

ThPB070

**Identification of Proteins in the Photosystem II Complex of \textit{Synechocystis} sp. PCC 6803**
By James A. Carroll, Wendy M. Lauer, Yafuhiro Kasaho, Himadri B. Pakrasi, Monsanto Co., St. Louis, MO, Washington University, St. Louis, MO

**Abstract**
This poster discusses the identification of proteins in the Photosystem II complex of \textit{Synechocystis} sp. PCC 6803, highlighting the importance of protein identification in photosystem analyses.

ThPB071

**Development of a Maize Mitochondrial 2-D Gel Database**
By Ronald L. Cerry, Adam J. Liska, Thomas E. Elthon - University of Nebraska, Lincoln, NE

**Abstract**
This poster presents research on the development of a maize mitochondrial 2-D gel database, providing insights into mitochondrial protein analysis.
THURSDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
3:00 – 3:30 pm  REMOVE POSTERS. Please leave posters until 3:00 pm.

ThPB 073  Bacterial Protein Identification by HPLC Fractionation, Nanoliter Digestion and Microspot MALDI Analysis; Zhengping Wang⁴; Bernd O. Keller¹; Liang Li¹; S. Randolph Long²; University of Alberta, Edmonton, Canada; Edgewood RDE Center, SCBRD-RT, Aberdeen Proving Grnd, MD

ThPB 074  Characterization of Lentil Lectin Non-covalent Complex Isomers by on-line CIEF-FTICR Mass Spectrometry; Suzana Martinovic¹; Scott J. Berger²; Richard D. Smith³; Pacific Northwest National Laboratory, Richland, WA

ThPB 075  Characterization of In Situ Thermal Hydrolysis Methylation (THM) Produced Biomarker Proteins by High Resolution Mass Spectrometry; Mohammed A. Meemani¹; Franco Basile¹; Kent J. Voorhees¹; Colorado School of Mines, Golden, CO

ThPB 076  Mass Spectral Characterization of Generic Variants and Glycoforms in Several Lectins from the Erythrina Family; Eric Bonnel³; Pierre Thibault¹; N. Martin Young¹; Halina Lis²; Nathan Sharon²; National Research Council of Canada, Ottawa, Canada; Weizmann Institute of Science, Rehovot, Israel

ThPB 077  Rapid analysis of bacterial proteins by automated capillary LC/MS; Hari Nair¹; K.C. Van Horn²; Laurie F. Carey¹; Dennis Roser¹; Ravi Lall¹; Peter Snyder¹; U.S. Army (Geo-centers, Inc.), APG, MD; Jones Chromatography, Lakewood, CO

ThPB 078  Profiling Proteins in Phytoplankton Using HPLC/Electrospray Ionization Mass Spectrometry; A. Daniel Jones¹; Janice L. Hironaka¹; The Pennsylvania State University, University Park, PA; Oklahoma State University, Stillwater, OK

ThPB 079  The use of electrospray ionisation Fourier transform ion cyclotron resonance tandem mass spectrometry for the analysis and characterization of disulphide-rich & disulphide-reduced anti-fungal proteins; Philip S. Green¹; Anastassios E. Giannakopoulos¹; Peter J. Derrick¹; Susan Crosland¹; University of Warwick, Coventry, UK; Zeneca Agricultural Chemicals, Bracknell, UK

ThPB 080  Detection and Identification of Bacterial Proteins by ESI LC/MS and Non-spray MS; Kevin Y. Dunlop⁴; Liang Li¹; University of Alberta, Edmonton, Canada; University of Saskatchewan, Saskatoon, SK

ThPB 081  Characterization of Post-translational Modifications of Recombinant Pectate Lyase; Jeremi D. Johnson¹; Jennifer L. Colangelo¹; Ron Orlando¹; Carl Bergmann¹; Jacques Benen²; Jaap Visser³; University of Georgia, Athens, GA; Wageningen Ag. Univ., The Netherlands

ThPB 082  Characterization of sorting reaction in Staphylococcus aureus by mass spectrometry; Hung Ton-That¹; Kym F. Faul¹; Olaf Schneewind¹; UCLA Los Angeles, CA

ThPB 083  LC/MS/MS as a Potential Method for Characterizing Bacterial Contamination during Spacecraft Assembly; Leticia Cornett¹; Cecilia Basic²; Terry D. Lee¹; Beckman Research Institute, City of Hope, Duarte, CA; Jet Propulsion Laboratory, Pasadena, CA

ThPB 084  Definitive Identification of Proteins from Bacteria Having Unsequenced Genomes; Martin P. Lacey¹; Thomas W. Keough¹; Angela M. Fieno¹; Raymond A. Grant¹; David W. Bauer¹; The Procter and Gamble Company, Cincinnati, OH

ThPB 085  Fragment-specific unfolding dynamics of E. coli thioredoxin by continuous denaturant labeling experiment and ESI-MS; Mop-yoon Kim¹; Max L. Deinzer¹; Oregon State University, Corvallis, OR

ThPB 086  Photoaffinity Labeling Investigation of the Allosteric Site of E. coli Citrate Synthase by ESI-TOFMS, MALDI-TOFMS and CE/ESI-TOFMS; Mark E. McComb¹; Gillian Sadler¹; Lynda J. Donald¹; Colin H. Lee¹; Werner Ens¹; Kenneth G. Standing¹; Harry W. Duckworth¹; Helene Perreault¹; University of Manitoba, Winnipeg, Canada

ThPB 087  In vivo Bacterial Enzyme Activity Profiling with Simultaneous Substrate Tag Detection with ESI-Ion Trap MS; Franco Basile¹; Imma Ferrer²; Edward T. Furlong²; Colorado School of Mines, Golden, Colorado; USGS, Denver, CO

ThPB 088  In Vivo Assay of Peptide Deformylation Inhibition Based on MALDI-MS of Whole Cellular Cells; Rachel R. Ogrzyalez Loo¹; Ruth VanBogelen¹; Erin Schiller¹; Tod Holler¹; Parke-Davis Pharmaceutical Research, Ann Arbor, MI

ThPB 089  Microbiological applications of high resolution MALDI peptide mass mapping; Jee-Hong Park¹; David H. Russell¹; Texas A&M University, College Station, TX

ThPB 090  Carbohydrate Affinity Capture Surfaces for Mass Spectrometric Analysis of Microorganisms; Jonathan L. Bundy¹; Catherine Fenselau¹; University of Maryland, College Park, MD

ThPB 091  Identification of New In Vivo Phosphorylation Site in the G Protein-Binding Phosphoprotein, Phosducin; Rehwa H. Lee¹; Fuyu Chen¹; Robert Simon¹; Stephon La¹; Hoon Yu¹; Kym F. Faul¹; UCLA and VAGLAHS at Sepulveda, Sepulveda, CA; UCLA, Los Angeles, CA

ThPB 092  Rapid and ultra-sensitive analysis of global protein expression in Sheawalella putrefaciens using Fourier transform ion cyclotron resonance mass spectrometry; Pamela K. Jensen¹; Kim K. Pedden¹; Mary S. Lippton¹; Gordon A. Anderson¹; Yuri A. Gorby¹; Margaret F. Romine¹; Richard D. Smith¹; Timothy D. Venstra¹; Pacific Northwest National Laboratory, Richland, WA

ThPB 093  Identification of Escherichia coli virulence proteins by LC-MS; Sonja Hess¹; Frederick J. Cassels¹; Lewis K. Pannell¹; NIDDK, National Institutes of Health, Bethesda, MD; Walter Reed Army Institute of Research, Washington, DC

ThPB 094  Unusual degradation characteristics in the in-source decay of peptides in MALDI/TOFMS compared to CID, PSD and S1D; Mitsuo Takayama¹; Akira Tsugita¹; Toho University, Funabashi, Chiba, Japan; Proteomics Laboratory, Tsukuba, Ibaraki, Japan

ThPB 095  How Much Mass Accuracy Is Enough to Identify a Protein Using MALDI-TOF MS Peptide Mapping?; Ron Orlando¹; J. Shaun McLeod¹; Scott R. Weinberger¹; CCRRC, UGA, Athens, GA; Ciphergen Biosystems, Inc., Palo Alto, CA

ThPB 096  A New Method to Evaluate the Quality of Database Search Results; Wenzhu Zhang¹; Chao Tang¹; David Fenyö¹; Brian T. Chart¹; ProteomeMetrics, LLC, New York, NY
<table>
<thead>
<tr>
<th>Time</th>
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<tbody>
<tr>
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<td>3:00 – 3:30 pm</td>
<td>REMOVE POSTERS. Please leave posters until 3:00 pm.</td>
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**TOXICOLOGY, 098 - 124**

**ThPB 097**
Assessing the performance of different protein identification algorithms; Chao Tang; Wenzhu Zhang; David Fenyo; Brian T. Chait; ProteoMetrix, LLC, New York, NY

**ThPC 098**
Quantitative Analysis of Mutagenic Heterocyclic Aromatic Amines (HAAs) in Cooked Meat by LC-APCIMS/MS: Screening of Unknown HAAs; Philippe A. Gay; Eric Gremaud; Janique Richoz; Robert J. Turesky; Nestec Ltd., Lausanne, Switzerland

**ThPC 099**
Following in vitro Microsomal Metabolism Reactions of Tetrahydrofuran in Rats, Mice and Humans by Solid Phase Micro-extraction Mass Spectrometry; Timothy A. Snow; Shawn A. Gannon; Diane L. Nabb; DuPont - Haskell Laboratories, Newark, DE

**ThPC 100**
The Quantification of Leucine Isonomers for the Determination of Maple Syrup Urine Disease; Mike Morris; Don Cooper; Sook Za Kim; Micromass UK Ltd, Manchester, UK; Korea Genetics Research Centre, Chung Buk, Korea

**ThPC 101**
Detection and Confirmation of Quaternary Ammonium Drugs in Horse Urine by Capillary Electrophoresis/MS/MS Spectrometry; Terence S. M. Wan; Francis P. W. Tang; Gary N. W. Leung; Racing Laboratory, Hong Kong Jockey Club, Sha Tin, Hong Kong

**ThPC 102**
Analysis of Quaternary Ammonium Neuroumescular Blocking Agents in Forensic Tissue and Fluid Specimens by LC-MS/MS; Francis X. Diamond; Kevin D. Ballard; William E. Vickers; Fredrick R. Rieders; Anders Lund; National Medical Services, Inc., Willow Grove, PA; Micromass, Inc., Beverly, MA

**ThPC 103**
Detecting Tainted Blood Evidence in Criminal Cases: EDTA, Oxalic Acid, Citric Acid, and a Case in Point; Kevin D. Ballard; National Medical Services, Inc., Willow Grove, PA

**ThPC 104**
Determination of PCB in blood with GC/MS in NCI mode; Petra Gerhards; Joerg Seeig; Shimadzu Deutschland GmbH, Duisburg, Germany; Labor Dr. Lempfrid, Köln, Germany

**ThPC 105**
Oxidative Damage and Carcogenesis in Living Organisms: Oxidative Stress in Oxazepam-treated Mice as Measured by MS-based Isoprostan Analysis; LeRae B. Graham; Carol E. Parker; Theodora R. Devereux; Maria Kadiiska; Michael L. Cunningham; J. Carl Barrett; Kenneth B. Tomer; NIEHS/NIH, RTP, NC

**ThPC 106**
Use of Mass Spectrometry to Investigate the Role of Glycated Hemoglobin in Formation of N-(carboxymethyl)valine Adduct in Hemoglobin; Jian Cai; Harrell E. Hurst; University of Louisville, Louisville, KY

**ThPC 107**
Solution Reactivity of Brevetoxins as Monitored by ESI-MS; Richard B. Cole; Yousheng Hua; University of New Orleans, New Orleans, LA

**ThPC 108**
Simultaneous Determination of the Amide LY397584, Its Primary Amine, and Its Acetylamine Metabolites in Plasma by LC/MS/MS Using Tacrine as an Amidase Inhibitor; Jean-Marie A.M.G. Defly; J. Dubsky; Dominique Ingels; Marc Lastelle; Eli Lilly Development Center, Mont-St-Guibert, Belgium

**ThPC 109**
Rapid Confirmation of 11-Nor-Tetrahydrocannabinol-9-Carboxylic Acid in Urine by LC/MS/MS Using Negative APCI; Wolfgang Weinnmann; Mylene Goerner; Rolf Goerner; Susanne Vogt; Michal Svorba; Andre Schreiber; Institute of Legal Medicine, Freiburg, Germany; PE Biosystems, Langen, Germany; MDS Scieix, Toronto, Canada

**ThPC 110**
GC/ECNCl/MS/MS Analysis of N,N-diethyl-2,4-dihydroxybutyrate in Tobacco: Analysis of Tobacco Using Negative APCI; Asoka Pangasinghe; Nadia I. Christova-Georgieva; Ramiah Sangaiath; Hasan Koc; James A. Swenberg; University of North Carolina, Chapel Hill, NC

**ThPC 111**
Structural Characterization of a Contaminant in L-Tryptophan Associated With Eosinophilia-Myalgia Syndrome; Klaus Klarkov; Kenneth L. Johnson; Gerald J. Gleich; Stephen Naylor; Mayo Clinic/Foundation, Rochester, MN

**ThPC 112**
Characterization of in vivo Metabolites of N-(3,3-dichlorophenyl)succinimide (NDPS) in Rats by HPLC-ESI/MS/MS: DONGKUI (Dan) Cui; Xing Hu; Pete Harvisen; Merck & Co., Inc., West Point, PA; Phila. College of Pharm, USIP, Philadelphia, PA

**ThPC 113**
Determination of Tobacco Specific Nitrosamines in Tobacco Filter by LC/MS/MS: Richard B. Luchei; Nadia Moore; R. Bruce Westerberg; Scott Harvey; Battelle Toxicology Northwest, Richland, WA; Pacific Northwest National Laboratory, Richland, WA

**ThPC 114**
Rapid Screening and Confirmation of Diuretics in Human Urine By Electrolyospray Tandem Mass Spectrometry; Hayati Muhamad Noh; Aishah Abdul Latiff; Doping Control Centre, USM, Penang, Malaysia

**ThPC 115**
Analytical Protocol of Urinary Hcg - Confirmation Methodology for Athletics Doping; Lay Harn Giam; Aishah Abdul Latiff; Doping Control Centre, USM, Penang, Malaysia

**ThPC 116**
A Rapid and Sensitive LC/ACPI/MS/MS Method for the Determination of 9-Tetrahydrocannabinol and its Metabolites in Human Matrices; Pierre Picotte; Pascal Mireault; Laboratoire de Sciences Juridiques et de Medicine, Montreal, Canada

**ThPC 117**
A GC/MS/MS Method for the Determination of Diacyl Phosphates Pesticides Traces in Urine; Roberto Bravo; William J. Driskell; Ralph D. Whitehead; Samuel E. Baker; Dana B. Barry; Centers for Disease Control and Prevention, Atlanta, GA

**ThPC 118**
Rapid Confirmation of Benzodiazepines in Human Matrices by LC/APCI/MS/MS: Pascal Mireault; Pierre Picotte; Laboratoire de Sciences Juridiques et de Medicine, Montreal, Canada

**ThPC 119**
Quantitation of Kinetin, Nfurfuryladenine, in DNA by Liquid Chromatography/Electrospray Ionization/Tandem Mass Spectrometry; Hasan Koc; James A. Swenberg; University of North Carolina, Chapel Hill, NC

**ThPC 120**
2-D Mass Spectral Analysis of Aflatoxin B1 in Peanuts Using Positive APCI; William F. Hadden; Leslie A. Harden; Thomas F. Schatzki; Western Regional Research Center, ARS, USDA, Albany, CA

**ThPC 121**
Validation of a GC-MS/MS Method for Quantitative Analysis of delta-9-tetrahydrocannabinol (THC) in Whole Blood; Henning Willads Petersen; Charlotte
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<th>Time</th>
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**DRUGS & METABOLISM: NEW METHODS, 125 - 165**

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<tr>
<th>Session ID</th>
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<th>Authors/Institutes ____________________________</th>
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<tbody>
<tr>
<td>ThPD125</td>
<td>Application of column-switching to the high-speed separation of drugs and isobaric metabolites for HPLC/MS/MS quantitation</td>
<td>Mark Cole¹, Shane Needham², Emily Fiese³, Patrick Jeanville¹, Pfizer Inc, Groton, CT</td>
</tr>
<tr>
<td>ThPD126</td>
<td>Biomonitoring of Tamoxifen and its Metabolites from Breast Cancer Patients using Nonaqueous Capillary Electrophoresis with Electrospray Mass Spectrometry</td>
<td>Spencer J. Carter¹, Xing-Fang Li¹, John Mackey¹, Shunyini², John Hanson³, Norman J. Savich³, University of Alberta, Canada</td>
</tr>
<tr>
<td>ThPD127</td>
<td>A fast, selective and robust on-line HPLC-MS/MS assay for the determination of seven human CYP isom-selective substrates (probes) in cytochrome P450 inhibition studies</td>
<td>Richard K. Lam¹, Faye Hsieh², Agen Inc, Thousand Oaks, CA</td>
</tr>
<tr>
<td>ThPD128</td>
<td>Investigation of the Derivatization of Amino Acids and Organic Amines with S-PhenylureaPhenyl Tris(trimethoxysilyl)Phosphonium Aceate Bromide and Analysis by Electrospray Ionization Mass Spectrometry</td>
<td>William J. Leavens¹, Stephen J. Lane¹, Richard M. Carr¹, Glaxo Wellcome R&amp;D, UK</td>
</tr>
<tr>
<td>ThPD129</td>
<td>N-in-One Dosing Combined with Stable-Isotope Coadministration to Simultaneously Study Pharmacokinetics and Metabolism of Two Benzimidazol-based Compounds in Primates</td>
<td>Mike Quijano¹, Thomas A. Neubecker¹, Sara J. Juenger¹, Roy L. M. Dobson¹, George R. Tonn³, Procter &amp; Gamble Pharmaceuticals, Mason, OH, DuPont Pharmaceuticals Company, Wilmington, DE</td>
</tr>
<tr>
<td>ThPD130</td>
<td>Structure Elucidation of Drug Metabolites in a Complex Matrix using a Hybrid Quadrupole Orthogonal Time of Flight Mass Spectrometer and Automated Data Processing</td>
<td>Claire Beaumont¹, Paul J. Kelly¹, Jose Castro-Perez², SmithKline Beecham Pharmaceuticals, Welwyn, Herts., UK; Micromass UK Limited, Wythenshawe, UK</td>
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<tr>
<td>ThPD131</td>
<td>Using MALDI Mass Spectrometry in Conjunction with On-line SPE-ESI/MS/MS to Increase the Throughput and Usable Dynamic Range in the</td>
<td>Analysis of Plasma Samples for Pharmacokinetic Studies: Jianmei Ding¹, Sarah Chol¹, Susan Hill¹, James Vath¹, Praxies Pharmaceuticals, Inc., Cambridge, MA</td>
</tr>
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</table>

**ThPD132** A highly sensitive method for the analysis of isoflavones in microliter samples of physiological fluids by nanoelectrospray mass spectrometry (nanoES-MS): Chao-Cheng (Sam) Wang¹, Marion Kirk¹, Michelle Smith¹, Stephen Barnes¹, University of Alabama, Birmingham, AL

**ThPD133** An Integrated Approach to Metabolite Identification for the Drug Discovery Compound SCH 123 using the Triple Quadrupole, Ion Trap and Q-TOF Instruments: Diane Rindgen¹, Kathleen A. Cox¹, Nigel J. Clarke¹, Walter A. Kornfein², Schering-Plough Research Institute, Kenilworth, NJ

**ThPD134** Generic SPE-LC-MS/MS assay protocol for the fast determination of drugs in biological fluids: Gerard Haak¹, Annick Schellen², Bert Ooms², Dick van de Lagemaat², William van Dongen², Robin Vreken², Elwin Verheij², Spark Holland, The Netherlands; TNO Pharma, The Netherlands

**ThPD135** Discovery of Sulfotransferase Inhibitors Using Immobilized Enzyme FT-ICR Mass Spectrometry (IEMS): Mark T. Cancilla¹, Dawn Verdugo¹, Joshua I. Armstrong¹, Carolyn R. Bertozzi¹, Julie A. Leary¹, University of California, Berkeley, CA

**ThPD136** Comparison of Triple Quadrupole, Ion Trap and Quadrupole/Orthogonal-Acceleration-Time-of-Flight Mass Spectrometers for Characterizing Metabolites of an Anticoagulant Agent, CI-1031, using Doubly Charged Precursor Ions: Ragu Ramathan¹, Rasmy Talat¹, Jasminder Sahi², Parke-Davis Pharmaceutical Research, Ann Arbor, MI

**ThPD137** LC-MS Methods For Exploratory Pharmacokinetics and Brain Distribution Study of a Neuropeptide FF Antagonist: Laslo Prokai¹, Alevtina D. Zharkov¹, Katolin Prokai-Tatari¹, University of Florida, Gainesville, FL

**ThPD138** Fast metabolite profiling by LC/Q-TOF using simultaneous on-line accurate mass measurement and data-dependent tandem mass spectrometry: H.K. Lim¹, K.W. Chan¹, Pyth-Ayers Research, Monmouth Junction, NJ

**ThPD139** A Novel Approach to the Analysis of Basic Drugs by LC/MS/MS: Mark L. L. Reimer¹, Mathieu Lautie¹, Patricia Ryan², Themis Flarakos³, Edward J. Daly¹, Jie Zhang³, Phoenix International Life Sciences, Saint-Laurent, Montreal, Canada

**ThPD140** Profiling and Identification of Memantine Metabolites by a LC-MS/MS System Equipped with Online Extraction HTLC, Beta-RAM Radiometric Detector, and API-365 Mass Spectrometer: Dahai Dong¹, Jiang Ying¹, John Ling¹, Andrew Acheson³, Diane Tang-Liu¹, Allergan, Inc., Irvine, CA

**ThPD141** Quantitation of Urine 17-Ketosteroid Sulfates and Glaucuronides by Sonic Spray Ionization LC/MS; Qi Jia¹, Mei-Feng Hong¹, Steve Orndoff¹, Ruidan Chen¹, Uiviera Pharmaceuticals, Inc., Broomfield, CO; Hitachi Instruments, Inc., San Jose, CA
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**THURSDAY POSTERS**

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<tbody>
<tr>
<td>ThPD142</td>
<td>In vitro Mimicry of Metabolic Oxidation Reactions by Electrochemistry/mass Spectrometry</td>
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<td>Ujik Jurjev 1; Hakan V. Wikstrom 2; Andries P. Bruins 3; University of Groningen, The Netherlands</td>
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<tr>
<td>ThPD143</td>
<td>Cocktail Analysis for Accelerating Pharmacokinetic (PK) Screening</td>
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<td>Hsiao-Yen J. Chang 1; Erik L. Nimz 1; Pfizer Central Research, Groton, CT</td>
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<tr>
<td>ThPD144</td>
<td>An Alternative Method for the Analysis of Drug Metabolites in Biological Matrices, Using</td>
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<td>Microspray ESI-MS: Chungying Yu 1; Feng Li 1; Neil Spooner 2; Smithkline Beecham Pharmaceuticals, King of Prussia, PA</td>
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<tr>
<td>ThPD145</td>
<td>Small Molecule Quantitation Using Automated Single Shot Averaging MALDI TOF Mass Spectrometry</td>
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<td>Steven C. Hall 1; Sally U 1; H. Ewa Witkowska 1; Melanie Lin 1; Arnold M. Falick 1; PE Biosystems, Foster City, CA</td>
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<td>ThPD146</td>
<td>A New Method for Improving the Accuracy and Reproducibility of Caco-2 Permeability Assay</td>
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<td>Mark G. Qian 1; James P. Bulgarie 1; Joseph A. Tweed 1; Kristi Oates-Lenz 1; Jacquelyn McClain 1; Bruce J. Augst 1; Maria D. Ribadeneira 1; The DuPont Pharmaceuticals Company, Wilmington, DE</td>
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<td>Fast-gradient microbeare column-switching LCM/MS/MS for the quantitative analysis of drugs in plasma</td>
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<td>ThPD148</td>
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<td>Applications to Natural Products and Metabolites</td>
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<td>Brian J. Boucher 1; Brian Williamson 1; Robert Deutschemann 1; Liening Chen 1; John Peltier 1; PE Biosystems, Framingham, MA</td>
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<td>Chiral Amino Acid Assay for Leuprolide Analysis</td>
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<td>for Bioanalytical Assays: Joseph W. Pav 1; Richard T. Frey 1; Lois S. Rowland 1; Boehringer Ingelheim, Ridgefield, CT</td>
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<td>Jean-Louis Dasseaux 1; J. Paul Spire 1; Clay Cramer 1; Tom J. Rea 1; Micahael E. Pepe 1; Gary H. Kruppa 1; Esperion Therapeutics, Ann Arbor, MI; Bruker Daltonics, Inc, Billerica, MA</td>
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<td>ThPD153</td>
<td>Tandem Turbulent Flow Chromatography Mass Spectrometric Analysis of Ciprofloxacin in Human Serum at Low ppm Levels</td>
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<td>Charles Grandmaison 1; Danielle Lachance 1; Yves G. Leblanc 1; Lorella Di Donato 1; Phoenix International Life Sciences, Montreal, Canada</td>
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<td>ThPD155</td>
<td>A Clinical Trial on a Plate: The potential of 384 format SPE for high throughput bioanalysis using LC-MS-MS: Stephen Pleasance 1; Bob Biddlecombe 1; Christopher Benevides 1; GlaxoWellcome, Ware, Herts, UK; Waters Corporation, Milford, MA</td>
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<td>ThPD156</td>
<td>Comparison of Triple Quadrupole and Ion Trap for a Neutral Loss Experiment</td>
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<td>Optimization of CE-ESI-MS for the Analysis of Tropone Alkaloid Enantiomers: K. Minoura 1; W. Eberhardt 2; A. Namura 1; S. Yamaji 2; T. Tadato 2; Yokogawa Analytical Systems Inc., Tokyo, Japan; Agilent Technologies, Waldbronn, Germany; Toyama Medical and Pharmaceutical Univ., Toyama, Japan</td>
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<td>Biomedical Applications for AMS at PRIME Lab: George S. Jackson 1; Frank Rickey 1; Darren Hilligons 1; Sharif Musameh 1; Mary A. Rounds 1; David Elmore 1; Louis Court 1; Pete Kissinger 1; Purdue University, W. Lafayette, IN; Bioanalytical Systems, Inc., W. Lafayette, IN</td>
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<td>Reduction of Ion Suppression Effects in Electrospray Ionization Mass Spectrometry: Eric T. Gang 1; Paul Vouros 1; Meg Annan 1; Neil Spooner 1; Northeastern University and Barnett Institute, Boston MA; SmithKline Beecham Pharmaceuticals, King of Prussia, PA</td>
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<td>Determining the Best MS Methodology to Analyze in vivo Drug Metabolism Data: Darlene Murphy 1; Sara J. Kamboursis 1; Iain Mylchreest 1; Eric Hemenway 2; Adolor Corporation, Malvern, PA; ThermoQuest Corporation, San Jose, CA</td>
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<td>New Strategies for the Analysis of Synthetic Vaccines by Mass Spectrometry: Paolo Lechi 1; Fred P. Abruamson 1; Kelly Sloan 1; Rachel Schneerson 1; Alfred L. Yergey 1; George Washington University-Washington, DC; NICHD, National Institutes of Health, Bethesda, MD</td>
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<td>ThPD163</td>
<td>High Throughput Analysis of Multiple Pharmaceuticals in Rat Plasma Using Turbulent Chromatography with Tandem Mass Spectrometry: Gao Vince 1; Elliott Jones 1; PE Biosystems, Foster City, CA</td>
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<td>ThPD164</td>
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<td>Atmospheric Pressure Photoionization (APPI) and APCI Compared for Metabolic Profiling using Testosterone and Related Steroids: Peter L. Jacobs 1; Harriss A. Peters 1; Chris H. Swaen 1; NV Organon</td>
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<td><strong>ThPE167</strong> A High Performance, Field-Portable, Ion Trap TOFMS; Jack A. Suyce³; Karl A. Hanold¹; Mark A. Hanning-Lee³; Syagen Technology, Inc., Tustin, CA</td>
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<td><strong>ThPE168</strong> Concept for a Miniaturized Confocal Plane Mass Spectrometer using an Inhomogeneous Magnet in Combination with a Faraday Cup Detector Array; Adi A. Scheidemann¹; R.B. Darling³; Frank J Schumacher IV¹; University of Washington, Seattle, WA</td>
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<td><strong>ThPE169</strong> Quantification of Aldehydes in Car Exhaust Samples by HPLC/MS using the DNPH method; Gabriela Zurek¹; Uwe Karst³; UC Davis, Davis, CA; University of Münster, Münster, Germany</td>
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<td><strong>ThPE170</strong> Comparison of PAHs and Nitro-PAHs Emissions among Standard Diesel Fuel, Biodiesel Fuel, and their Blend on Diesel Engines; Joseph C. Pan¹; Shraddha Quaraderi¹; Tina M. Smeal¹; Christopher A. Sharp³; Southwest Research Institute, San Antonio, TX</td>
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<td><strong>ThPE171</strong> Trends and Comparisons of Sealed ATOMFS Data Measured During August in Atlanta, GA; Ryan J. Wenzel¹; Don-Yuan Liu¹; Kimberly A. Prather¹; University of California, Riverside, CA</td>
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<td><strong>ThPE172</strong> Aerosol Compositions Measured by Bipolar On-line Laser Mass Spectrometry in the Field Experiment LACE; Achim Trimborn¹; Klaus-Peter Hinz¹; Bernhard Spengler³; Univ. of Würzburg, Würzburg, Germany</td>
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<td><strong>ThPE173</strong> Determination of PACs in Aerosol from an Indoor Smoking Environment by Two Step Laser Desorption/Ionization Mass Spectrometry (L2MS); Bradley D. Morrical¹; Renato Zenobi³; Swiss Federal Institute of Technology, Zurich, Switzerland; ETH Swiss Federal Institute of Technology, Zürich, Switzerland</td>
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<td><strong>ThPE175</strong> Laser Ablation Efficiencies at 193nm of Ultrafine particles; David B. Kane¹; Murray R. Johnston¹; University of Delaware, Newark, DE</td>
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<td><strong>ThPE177</strong> Using Electrostatic Focusing of Charged Nanoparticles in an Aerosol Mass Spectrometer; Berk Oktem¹; David B. Kane¹; Murray R. Johnston¹; University of Delaware, Newark, DE</td>
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<td><strong>ThPE178</strong> Application of Quadrupole Mass Spectrometer in Analysis of PCDDs/PCDFs by using large volume injection and a new sampling system; Junko Iida¹; Yutaka Nagayama¹; Yoshihiro Saito¹; Akira Aono¹; Mika Kato¹; Kojiro Urano¹; Shimadzu Corporation, Tokyo, Japan; Yokohama National University, Yokohama, Japan</td>
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<td><strong>ThPE179</strong> Controlling Laboratory Air Contamination from Rotary Vacuum Pumps by using a Two-Stage Vacuum Pump Exhaust Filter System; John J. Manura¹; Scientific Instrument Services, Ringoes, NJ</td>
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<td><strong>ThPE180</strong> Method Development for Evaluation of Asphalt Fume Components by Mass Spectrometry; Jin Wang¹; Janet Simpson¹; Daniel M. Lewis¹; Paul D. Siegel¹; HELD/NIOSH, Morgantown, WV</td>
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<td><strong>ThPE181</strong> Analysis of PAHs in Tobacco Smoke Using SPME Isotope Dilution GC/MS; Michelle D. Beeson¹; Cliff H. Watson¹; David L. Ashley¹; Centers for Disease Control and Prevention, Atlanta, GA</td>
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<td><strong>ThPE182</strong> Infrared MALDI of Polycyclic Aromatic Hydrocarbons; Shelley N. Jackson¹; Kermit K. Murray¹; P. Barry Ryan¹; Emory University, Atlanta, GA</td>
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<td><strong>ThPE183</strong> Selective Detection of Nitro-PAHs using ESI-MS and Constant Neutral Loss; Tamika T. J. Williams¹; Helene Perreault¹; University of Manitoba, Winnipeg, MB, Canada</td>
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<td><strong>ThPE184</strong> Identification of Organic Nitrogen Containing Species in Ambient Particulate Matter by Aerosol Time-of-Flight Mass Spectrometry; Stefania Angelino¹; Kimberly A. Prather¹; University of California, Riverside, CA</td>
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<td><strong>ThPE185</strong> The Efficiency of After-Burners in Reducing Semi-Volatile Combustion Emissions; Joel Carlson¹; Jun Wang¹; Yiannis Leventis¹; U.S. Army SBCOM, Natick Soldier Center, College of Engineering, Northeastern University, Boston MA</td>
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<td><strong>ThPE186</strong> Analysis of Hydroxymethanesulphonate in Single Particles by ATOMFS; Jeffrey R. Whiteaker¹; Kimberly A. Prather¹; University of California, Riverside, CA</td>
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<td><strong>ThPE187</strong> Highly sensitive analysis of volatile compounds in water by gas chromatograph/mass spectrometer combined with deactivated headspace sampler; Norihito Sakui¹; Misuzu Kaise¹; Shigeaki Daishima¹; Yokogawa Analytical Systems Inc, Musashino-shi, Tokyo; Kaise Giken Inc., Shibuya-ku, Tokyo</td>
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<td><strong>ThPE189</strong> Improvements to the Determination of Ambient Volatile Organic Compounds (VOCs) Using Thermal Desorption/Gas Chromatography-Mass Spectrometry (TD/GC-MS); Michael A. Sage¹; Vince Taguchi¹; Ministry of the Environment, Toronto, Canada</td>
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<td><strong>ThPE190</strong> Hydrocarbon analysis in petroleum tainted salmon by the use of electronic nose and dynamic headspace gas chromatography mass spectrometry; E. Aladar Bencsath¹; Terrani Reilly¹; Michael DiLiberti¹; Lawrence C. Hufnagel¹; James D. Barnett¹; US Food and Drug Administration, Dauphin Island, AL; National Oceanic and Atmospheric Administration, Gloucester, MA; NOAA, Seattle, WA; US FDA, Bothell, WA</td>
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<td><strong>ThPE191</strong> A mass spectrometric approach in odor impact assessment; Enrico Davoli¹; Michele Giavini¹; Emilio Benfenati¹; Roberto Fanelli¹; Mario Negrì Institute, Milano, Italy</td>
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ThPE 192  Possibilities and Limitations of Using Mass Spectra Libraries for HPLC/MSD-MS in Environmental Analysis;  Andre Schreiber;  Juergen Eger;  Wolfgang Weinmann;  Werner Engewald;  PF Biosystems GmbH, Langenhagen, Germany; University of Leipzig, Leipzig, Germany; University of Freiburg, Freiburg, Germany

ThPE 193  A New Approach in LC/MS Library Search Using Combined MS and MS^n ESI Ion Trap Spectra;  Catherine Stacey;  Miriam Ritter;  Bernd Jastorff;  Peter Sander;  Arnd Engeloh;  Bruker Daltonics, Billerica, MA; Center of Environmental Research and Technology, Bremen, Germany; Bruker Daltonics, Bremen, Germany

ThPE 194  Determination of Elemental Compositions of Ions from Trace Levels of Pharmaceuticals and Disinfection Byproducts in Water Supplies Using Mass Peak Profiling from Selected Ion Recording Data (MPPSIRD);  Andrew H. Grange;  G. Wayne Sowaco, US EPA, Environmental Chemistry Branch, Las Vegas, NV; U. S. EPA, Environmental Chemistry Branch, Las Vegas, NV

ThPE 195  Application of Quantitative Chemometric Analysis Techniques to Direct Sampling Mass Spectrometry;  William P. Gardner;  Ronald E. Shafer;  John H. Callahan;  James E. Girard;  American Univ. & GeoCenters Inc., Washington DC; Naval Research Lab, Washington DC

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ThPF 197  On-Chip Sheathless Electrospray Emitters;  Stefan Nilsson;  Leif Nyholm;  Karin Markides;  Malin Svedberg;  Fredrik Nikolajeff;  Dept. of Analytical Chemistry, Uppsala, Sweden; Dept. of Materials Science, Uppsala, Sweden

ThPF 198  Microfluidic System for Automated Electrophoresis-Electrospray Mass Spectrometry;  Bailin Zhang;  Barry L. Karger;  Frantisek Foret;  Northeastern University, Boston, MA

ThPF 199  SFC-MS: A Tool for Structural Characterisation;  Curtiona Thorn;  Susan Davidson;  Frank Pullen;  Adrian Wright;  Pfizer Central Research, UK

ThPF 200  A Novel Electrospray Interface for Capillary Electrophoresis-Mass Spectrometry;  Norman J. Dovichi;  Chun-Sheng Liu;  Jianzhong Zhang;  Bob Polakowski;  University of Alberta, Edmonton, Canada

ThPF 201  Development of on-line sheathless capillary electrophoresis/MS with an orthogonal acceleration Time-of-Flight mass spectrometer as mass analyzer;  Xiaoying Jin;  Peiqing Huang;  David M. Lubman;  Stephen J. Kurzyniec;  Nanayan Zhang;  David T. Rossi;  University of Michigan, Ann Arbor, MI; Parke-Davis Pharmaceutical Research, Ann Arbor, MI

ThPF 202  Enhancing CE-MALDI-MS Through the Incorporation of Complementary Detection Methods;  Jason S. Page;  Stanislav S. Rubakhin;  Jonathan V. Sweedler;  University of Illinois, Urbana-Champaign, Urbana, IL

ThPF 203  Development and Application of Thin Layer Chromatography (TLC) - Matrix Assisted Laser Desorption Ionization - Time-of-Flight Mass Spectrometry (MALDI-TOF/MS);  Tetsuji Asa;  Toshiharu Muto;  Kazuki Taira;  Tomio Nagan;  Taiho Pharmaceutical Co., Ltd., Hanno, Japan; Nikkkyo Technos, Tokyo, Japan

ThPF 204  Off-line Vacuum Deposition Interface for Coupling Liquid Phase Separation Techniques to Commercial MALDI/TOF MS Instrument;  Tomas Rejata;  Ping Hu;  Jan Preisler;  Frantisek Foret;  Barry L. Karger;  Barnette Institute, Northeastern University, Boston, MA

ThPF 205  ICP-MS as a Novel Element Specific LC-Detector for Generic Detection of Pharmaceutical Drugs;  Magnus Karlsson;  Bengt-Olof Axelsson;  Peter Michelsen;  AstraZeneca R&D, Lund, Sweden; Nycomed Innovation AB, Malmo, Sweden

ThPF 206  Improved Sample Analysis for Affinity Selection Mass Spectrometry;  Houjun Yang;  James Lord;  Hua Tang;  Lan Gao;  Xueheng Cheng;  Mark Schurak;  David Bums;  Bruce Beutel;  Abbott Laboratories, Abbott Park, IL

ThPF 207  Construction of a 9.4 Tesla FTMS for High Resolution MS/MS;  Steven M. Patrie;  FanYun Menge;  David Whipple;  Christopher L. Hendrickson;  John P. Quinn;  Neil L. Keller;  University of Illinois, Urbana, IL; National High Magnetic Field Lab, Florida State University, Tallahassee, FL

ThPF 208  Development and Application of a System to Evaluate Compound Identity, Purity, and Concentration in One Experiment Using HPLC-ECL-ESL-TOF/MS;  David A. Yusuk;  Ming-Shang T. Kuo;  Phamcacia Corporation, Kalamaam, MI

ThPF 209  Recent advances in the development of hyphenated techniques for the solution of problems in agrochemical metabolism;  Nigel J. C. Bailey;  John C. Lindon;  Jeremy K. Nicholson;  Steve T. Hadfield;  Paul D. Stanley;  Ian J. Wilson;  Fadi Abou-Shakra;  Jose Castro-Perez;  Ashley B. Sage;  Imperial College, London, UK; Zeneca Agrochemicals, Braintree, UK; AstraZeneca, Macclesfield, UK; Micromass UK, Manchester, UK

ThPF 210  Simultaneous IRMPD Dissociation and Detection for LC/ESI/FTICR/MS/MS;  Jared J. Drader;  Hans J. Gaus;  Steven A. Hofstadler;  Ibis Therapeutics, Carlsbad, CA

ThPF 211  Application of Particle Beam LC/MS to the commercially available Agilent 5973 benchtop mass spectrometer;  Curtis Weiler;  Scott Niemann;  CSS Analytical Co., Inc., Shrewsbury, NES

ThPF 212  Improved LC/MS Throughout with On-line Sample Cleanup, Peak Focusing, and Composition and Flow Gradient;  Jeanne B. Li;  Eric H. Block;  Michael P. Balogh;  Waters Corporation, Milford, MA

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ThPF 215  NanoFlow LCMS and LC/MSMS on a Quadrupole-OA-TOF-ESI Instrument; David A Malby1; Michael A Balwin1; Kati Medzhiradska1; Lan Huang1; A.L. Burlingame1; UCSF, San Francisco, CA

ThPF 216  Evaluation of Micro-HPLC/Ion Mobility Spectrometry (IMS)/Mass Spectrometry (MS); Laura E. Markowsky1; G. Reid Asbury1; Herbert H. Hill, Jr.1; Washington State University, Pullman, WA

ThPF 217  Enhanced Sensitivity Using a Direct Flow Capillary HPLC/MS System with NanoFlow Capability; Cozette M Cuppett1; Jeffrey Holyoke2; Steven A Cohen1; Waters Corporation, Milford, MA; Micromass Inc., Beverly, MA

ThPF 218  Drug Discovery Applications of 'Fast' Chromatography in High-Throughput LC-MS/MS Quantitation; Tony Pereira1; Leslie A. Romanishyn1; Philip R. Tiller1; Cornelis E.C.A. Hop1; Merck Research Laboratories, Rahway, NJ

ThPF 219  Rapid Polarity Switching for the Quantitation of Beclomethasone and its Metabolites in Human Lung Tissue Using On-line Column Switching and ESI LC/MS/MS; Mathieu Lahaye1; Art Grittas1; Donald Chun1; Thienis Plarakos1; Mark L. J. Reimer1; Phoenix International Life Sciences, Saint-Laurent, Canada

ThPF 220  Ramifications of Pump-Switching Step Gradients for Bioanalytical LC/MS/MS Assays; Brian D. Beatt1; Donald D. Gray1; Philip S.H. Wong1; Bioanalytical Systems, Inc., West Lafayette, IN

ThPF 221  A Dual Column Application in LC/MS/MS Bioanalysis; Xinpang Fang1; Kevin Cook1; Danlin Wu1; Purdue Pharma L.P., Ardsley, NY

ThPF 222  The Investigation and the Use of Turbulent Flow Column-Switching LC/MS/MS as a High-Throughput Approach for Direct Plasma Sample Analysis of Pharmaceutical Compounds N-in-1 Pharmacokinetic Studies; Hang Zeng1; Jing-Tao Wu1; Steve E. Unger1; DuPont Pharmaceuticals Company, Newark, DE

ThPF 223  Isolation and Analysis of Complex Mixture Components Using Column Switching LC/MS; Jon D. Williams1; John R. Allen1; David J. Burinsky1; Steve Cole1; Glaxo Welcome, Inc., RTP, NC

ThPF 224  Optimization of LC-MS Conditions for the Analysis of Acidic Compounds Using Design of Experiments; Carmia Seoi1; Kevin P. Bateman1; Berton Gunter1; Merck Frosst Canada, Inc., Kirkland, Canada; Merck & Co., Inc., Rahway, NJ

ThPF 225  Generating Structure-Informative Ion-Trap Mass Spectra in LC/MS of Pharmaceutical Drugs Using Filtered Noise Fields (FNF) Techniques; Dietrich A. Volmer1; Stefan Niedziella1; Martin Lehmann1; Merck Analytical Research, Darmstadt, Germany

ThPF 226  Preparative LC/MS as an Efficient Method of Purification for Automated Synthesis; Marian G. Young1; Harold N. Welter1; Michael C. Nyman1; Bristol-Myers Squibb, Princeton, NJ

ThPF 227  Chemiluminescent Nitrogen Quantitation Used with Prep. LC/MS to Quantify Yield in Large Numbers of Purifications; Dean P. Phelps1; Ken C. Lewis1; Anthony J. Parker1; Glaxo Welcome, RTP, NC

ThPF 228  On-Line Flow Injection Analysis of Purification Fractions – New Ways to Link Prep-HPLC and MS; Jeffrey P. Kiplinger1; Paul M. Lefebvre1; Gilson CIFT, Lincoln, RI

ThPF 229  Fundamentals of Assay Design: Carryover in Direct-Injection Bioanalytical Assays; Joseph J. Takarewski1; Matthew M. Pegram1; Jeffrey P. Kiplinger1; Michael J. Dameron2; Paul M. Lefebvre3; Cohesive Technologies Inc., Franklin, MA; Gilson Inc., Lincoln, RI

ThPF 230  A Strategy for Expanding the Operating Linear Range in Quantitative API LC/MS/MS Bioanalysis: Let the Mass Spec Do the Work; Luca C. Matussil1; Roger Demers1; Tung Chau1; Michael A. Curtis3; MAXXAM Analytics Inc., Ontario, Canada; Alcon Research Limited, Fort Worth, TX

ThPF 231  Practical Aspects of Using Phosphate Buffers for CE/MS Analyses; Christine A. Miller1; Steven M. Fischer1; Agilent Technologies, Palo Alto, CA

ThPF 232  Investigation of Signal Suppression Effects in Quantitative LC-MS Analysis: Arkady I. Gusev1; Bernard K. Cho1; David M. Hercules1; The Rohm and Haas Company, Spring House, PA; Vanderbilt University, Nashville, TN

ThPF 233  LC/MS/MS Library Searching for Rapid Confirmation of Analogues in Clinical, Environmental and Food Chemistry; John M. Hacker1; Matthias Eichler1; Maria A. Cintora1; Elisabet Lifante1; Michael Cooke1; Anna Przyborowska1; Stephen Down1; Raj K. Patel1; Royal Holloway University of London, Egham, UK; JD Science Limited, Nottingham, UK; Veterinary Laboratories Agency, Addlestone, UK

ThPF 234  Mass Spectrometer- and UV-Triggered High Throughput Purification, Fractionation, and Identification of Chemical Libraries; Ruidan Chen1; Peter B. Grosshans1; Kiasuburo Deguchi1; Steve Fannin1; Hitachi Instruments, Inc., San Jose, CA

ThPF 235  Ballistic Gradient HPLC Coupled with ESI-TOF/MS for High Throughput, High Resolution Analysis of Combinatorial Chemistry Libraries; Lori Ann Upton1; Wayne Scott1; Kerry Nugent1; David Hawke1; Kerry Spear1; Micromon BioResources, Auburn, CA; PB Biosystems, Foster City, CA; ICAGEN, Research Triangle Park, NC

ThPF 236  A Comparison of Fast GC/MS with LC/MS for the Detection of Compounds in Biological Screening Libraries; Paul R. West1; Jeff Wang1; Houjun Yang1; Xueheng Cheng1; Kenneth P. Matuszak1; Abbott Laboratories, Abbott Park, IL

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ThPG 238  Improving Background and Sensitivity in LC-MS: Analysis of Reagent Water Sources; Byron M. Stewart1; Brian L. Williamson1; Millipore, Bedford, MA; PE Biosystems, Framingham, MA

ThPG 239  Structural Elucidation Studies of 6-Deoxyerythronolide B Analogues by Accurate Mass
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ESI-FT-ICR-MS; Paul Gates¹; Marc Roddis²; Ylva Roddis¹; Peter Leadlay¹; James Staunton¹; Cambridge University, Cambridge, UK

ThPG240 Coulombically-Mediated Conformations of the Fourth Generation Poly (propylene imine) Dendrimer in the Gas Phase; Gina A. Zientara¹; Anne E. Counterman¹; David E. Clemen³; Indiana University, Bloomington, IN

ThPG241 Identification of taxoids in extracts from Taxus wallichiana by ESI-MS and MS/MS; P. Stefanowic³; J. Prasain¹; Y. Konishi¹; Biotechnology Research Institute, Montreal, Canada

ThPG242 Analysis of anabolic steroids with liquid chromatography/tandem mass spectrometry; Pieter E. Joos¹; Marc Van Ryckeghem⁴; Rene E. Van Grieken⁴; Jos Vanckx²; University of Antwerp, Antwerp, Belgium; SGS De Paauw & Stokoe, Mechelen, Belgium

ThPG243 Amino Acid Analysis by CE-ESI-MS; Werner Eberhardt¹; Tomoyoshi Soga²; Agilent Technologies, Waldbronn, Germany; Yokogawa Analytical Systems Inc., Tokyo, Japan

ThPG244 The analysis of boronic acids by ESI and APCI positive and negative ionization; John A. Castor³; DuPont Pharmaceuticals Co., Chemical Process R&D, Deepwater, NJ, USA

ThPG245 LC/ESI/MS/MS and GC/MS Analyses of Oxidized Amino Acids from Tissue Proteins: Analytical Tools for Exploring the Role of Oxidative Stress and Protein Damage in vivo; Joseph P. Gaunt¹; Jaeman Byun¹; Jay W. Heinecke¹; Washington University, St. Louis, MO.

ThPG246 Identification of an Unknown Impurity: An Investigation of the Physical Property of 4-Trifluoromethylnilinone; Narasimhan Kasthurikrishnan¹; Derek Tiekert¹; Tamim Braish¹; Pfizer, Inc, Groton, CT

ThPG247 Identification of a Potential Anti-Bacterial Basic Lipid; W. J. Griffiths¹; M. Ibrahim¹; B. Agerberth¹; Karolinska Institutet, Stockholm, Sweden

ThPG248 HPLC-MS-MS analysis of bitter acids in hops and beer; Peter Kovalak¹; Yves Mouget¹; Takeo Sakuma¹; Pe Sci, Toronto, Canada

ThPG249 Negative Ion Exact Mass MS/MS of Orselinic Acid; Gordon C. Kearney¹; Neil J. Johnson²; Micromass UK LTD, Manchester, UK; University of Southampton, Southampton, UK

ThPG250 Α- Laetam Antibiotics in Milk: a Multi-Residue Method using Liquid Chromatography Coupled with Electrospray Ionization Tandem Mass Spectrometry; Sonia Riediker¹; Jean-Marc Dierrens¹; Richard H. Stadler¹; Nestlé Research Center, Nestec Ltd., CH-1000 Lausanne 26, France

ThPG251 DIMP-T-R-MIMS: Its Use for the Analysis of Vitamin C, of Metabolites in Urine, and of Aminoacids in Blood Plasma; Maria A. Mendes¹; Marcos N. Eberlin¹; Lilian L. Rocha¹; Renato Haddad¹; Nelci F. Höehr¹; State University of Campinas – UNICAMP, Brazil

ThPG252 Cycokallycarbonyl Derivatives for the Determination of Amino acid Methyl Esters by GC/MS; Vladimir G. Zakin¹; Vladislav V. Sook²; Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

ThPG253 Alkyl chain structure determination of zinc diethophosphates in lubricating oils by GC/EI/MS and GC/ECNCl/MS; Michel Becchi¹; Frederic Perret¹; Bernadette Carraze²; Jean-François Bezard²; Jean-Pierre Michel³; CNRS, SCA, BP22, Vernaon, France; PSA, S.C.A. Physico-chemiques, Velizy, France; Service Lubrifiants, PSA, Bechamp, France

ThPG254 GC/MS Analysis of Intact Synondine Ring; Jongsam Lee¹; Song Ja Park¹; Hesoo Pyo¹; Dong Seok Lho¹; Korea Institute of Science and Technology, Seoul, Korea

ThPG255 Mass Spectrometric Analysis of Dinuclear Lewis Acid Complexes with Aluminum; Lidia Matveeva¹; Andrew Cottone¹; Michael J. Scott¹; Oleg Matveev¹; David H. Powell¹; University of Florida, Gainesville, FL

ThPG256 Fluorour amine scavenger compounds as a new calibration standard for the EI-MS in the mass range of 100-300 amu; Kasi V. Somayajula¹; Vyacheslav N. Fishman¹; Bruno Linclau¹; Dennis P. Curran¹; University of Pittsburgh, Pittsburgh, PA

ThPG257 The synthesized chromatography separation for non-hydrocarbon fraction in heavy oils; Li Yunn¹; Ren-hua Kang; Rong-sheng Lio; Li Ren-wei; Institute of geology and geophysics, CAS, Beijing, China; Hekou petroleum factory, Shengli Oil Field, Dongying, Shandong, China; Institute of Petroleum Geology Exploration, Dongying, Shandong, China

ThPG258 Automated Identification of Trace Contaminants in Natural Essential Oils by Rapid Exact Mass GC-MS Analysis Using a GC Mass Spectrometer; Peter M. Hancock¹; Anthony Newton¹; Martin R. Green²; Micromass UK Limited, UK

ThPG259 A mass spectrometrical study of doubly-charged porphyrins; Mathias Schäfer¹; Herbert Budzikiewicz¹; University Köln, Cologne, Germany

ThPG260 Analysis of Freeze Dried Planar Supported Phospholipid Bilayers by Secondary Ion Mass Spectrometry; Chris W. Diehnelt¹; Hanbin Mao¹; Paul S. Cramer¹; Emile A. Schweikert¹; Texas A&M University, College Station, TX

ThPG261 C2H2 /N2 Microwave Discharge Plasma: Production of C3N4; Mikhail Katsyev¹; Toshihiro Fujii¹; Junichi Muraki¹; Sundaram Arulmozhiraja¹; National Institute for Environmental Studies, Tsukuba, Japan

ThPG262 Electron Impact Induced Fragmentation of Fused Sila-oxa-norbornenes; Sasa Kazazic¹; Dunja Srlza¹; Srecko Kirin¹; Snjezana Peur¹; Leo Klasnic¹; Institute Rudjer Boskovic, Zagreb, Croatia

ION ACTIVATION, 263 - 309

ThPH263 Alkali Metal Ion Affinities of Alkali Metal Hydroxides Measured by Threshold Collisionally Activated Dissociation; Da Ren¹; Chrys Wesdemiotis¹; The University of Akron, Akron, OH

ThPH264 Rule Governing Hydrogen Transfer during Low-Energy CID of Small Molecules; Paul W. Brown¹; Adeboye Adejare²; Jason Morrill³; Quintiles, Kansas City, MO; Idaho State University, Pocatello, ID; University of Missouri, Kansas City, MO
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>7:30 - 8:00 am</td>
<td>SET UP POSTERS, Exhibit Hall B</td>
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<td>8:45 - 10:15 am</td>
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<tr>
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<td>REMOVE POSTERS. Please leave posters until 3:00 pm.</td>
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| ThPH265 Energy Deposition in SN2 Reaction Products; Jianhua Ren; John I. Brauman; Stanford University, Palo Alto, CA |
| ThPH266 Thermochemistry and Potential Energy Surfaces of Hypohalite Anions; John W. Torchia; Lee S. Sunderlin; Cynthia A. Pomerening; Northern Illinois University, DeKalb, IL |
| ThPH267 Surface-Induced Dissociation of Ions: Energy Transfer and Scattering of Fragment Ions; Atish D. Sen; Anil K. Shukla; Jean H. Futrell; University of Delaware, Newark, DE; Pacific Northwest National Laboratory, Richland, WA |
| ThPH268 SID and CID: A Comparative Study of Small Alanine-Containing Peptides Using FTMS; Eduard V. Denisov; Julia Laskin; V. Sergey Rakov; Jean H. Futrell; Pacific Northwest National Laboratory, Richland, WA |
| ThPH269 Parameters influencing the performance of a TOF-SID-TOF instrument; Jonathan R. Beck; Andrew R. Hilgenbrink; Donald E. Riederer; University of Missouri, Columbia, MO |
| ThPH270 Velocity Measurements of CNa+ Ion-Surface Reaction Products; Nathan D. Leight; Donald E. Riederer; University of Missouri, Columbia, MO |
| ThPH271 Low Energy Ion-Surface Reactions at Labeled Self-Assembled Monolayers: Effects of Film and Substrate Topography; Darrin Smith; Vicki H. Wysoczki; Vincent J. Angelico; University of Arizona, Tucson, AZ |
| ThPH272 Time Development of Ion Internal Energy in Multiple Collisions; Karoly Vekey; Laszlo Drahos; Hung. Acad. Sci., Budapest, Hungary |
| ThPH273 Internal energy of ions produced in a heated capillary electrospray ion source; Edwin De Pouw; Francoise Renoule; Valerie Gabi; University of Liege, Belgium |
| ThPH274 IRMPD as an efficient method for fragmentation of singly charged biopolymer ions generated by MALDI using FTMS; Christian B. Berg; J. Paul Speir; Bruker Daltonics Inc., Billerica, MA |
| ThPH275 FT-MS Characterization of HPTH Analogs Using SORI-CID, IRMPD, and ECD Methods; Scott W. Robinson; Runshi Zhao; Robert McKean; Stephen M. Condon; Gary H. Kruppa; Douglas P. Ridge; University of Delaware, Newark, DE; Rhode-Poulenc Rorer, Collegeville, PA; Bruker Daltonics, Billerica, MA |
| ThPH276 Structural Elucidation of Bioactive Fungal Metabolites by HPLC-FTMS Using IRMPD and SORI-CAD; Paul D. Schnier; Leonard A. McDonald; Marshall M. Siegel; Wyeth-Ayerst Research, Pearl River, NY |
| ThPH277 Analysis of a Microisolated Host-Guest System Using Blackbody Infrared Radiative Dissociation; Sarah N. Ward; David V. Dearden; Brigham Young University, Provo, UT |
| ThPH278 Advances in Infrared Photodissociation for Structural Characterization in the Quadrupole Ion Trap; Karin M. Keller; Brian J. Goosby; Jennifer S. Brodbelt; The University of Texas at Austin, Austin, TX |
| ThPH279 Investigation of the kinetic method for the determination of proton affinity (PA) through amines; Jie Cao; John Holmes; University of Ottawa, Ottawa, Canada |
| ThPH280 An experimental dissection of alkali cation glycine interactions; Peter B. Armentrout; Bob Moision; University of Utah, Salt Lake City, UT |
| ThPH281 Gas-phase dissociation of glyceraldehyde with silver and copper cations: Collisional activation and theoretical studies; Emmanuelle Leon; Jeanne Tortajada; Pierre Touilhoat; Badia Amekraz; Christophe Moulin; Lawrence Boureau; LAE, Institut des Sciences, Evry, France; CEA SACLY, DPE/PSEA/SAIS, GIF-sur-Yvette, France; CEA SACLY, DCC/DESD/SESd, GIF-sur-Yvette, France |
| ThPH282 Energy Dependent Collision-Induced Dissociation of CS2 to S2; Anil K. Shukla; Jean H. Futrell; Xuedong Zhou; PNNL, Richland, WA; University of Delaware, Newark, DE |
| ThPH283 The Bond Dissociation Energy of trifluoride ion; Alexander Artua; Paul G. Wenthold; Katrina E. Nizzii; Lee S. Sunderlin; Purdue University, West Lafayette, IN; Northern Illinois University, DeKalb, IL |
| ThPH284 Heats of Formation for the Ethanol and Propenol Cations by Photoionization Mass Spectrometry; John C. Traeger; La Trobe University, Melbourne, Australia |
| ThPH285 The Proton Affinity of beta-Alanine, the Simplest beta-Amino Acid; In-Su Hahn; Chrys Wesdemiotis; The University of Akron, Akron, OH |
| ThPH286 First Solvation Shell Energies of Organometallic Cluster Ions; Stanley Stevens; Linda Nichols; David Richardson; John Eyler; Marcelo Sena; Jose Riveros; University of Florida, Gainesville, FL; Universidade de Sao Paulo, Sao Paulo, Brazil |
| ThPH287 The generation of neutral chromium complexes with bridged ligands by neutralization-reionization mass spectrometry; Dimitri Zagorsky; Dietmar Kuck; John L. Holmes; University of Missouri, Columbia, MO; University of Bielefeld, Bielefeld, Germany; University of Ottawa, Ottawa, Canada |
| ThPH288 Cluster Formation and Fragmentation of Typical MALDI Matrix Compounds with Different Analyses in a Supersonic Jet Investigated by Multi Photon Ionization; Juergen Grotemeyer; Anja Meffert; University Kiel, Kiel, Germany |
| ThPH289 FT-ICR Study of the Radiatively Induced Dissociation of Gas-Phase Cluster Ions; Eugene M. Marlin; Terrance B. McMahon; University of Waterloo, Waterloo, Canada |
| ThPH290 Chemical Reactivity of [(NO)_n (ROH)_m] Cluster Ions; Jay P. Charlebois; Robert L. DeLeon; James F. Garvey; University of Buffalo, Buffalo, NY |
| ThPH291 Electron Capture Dissociation of Multiply Charged Polymers; Blas A. Cerda; David M. Horn; Kathrin Breuker; Fred W. McLafferty; Cornell University, Ithaca, NY |
| ThPH292 Mechanisms of Electron Capture Dissociation; Kathrin Breuker; David M. Horn; Blas Cerda; Fred W. McLafferty; Cornell University, Ithaca, NY |
| ThPH293 Theoretical Study on Reactions of Multiply Charged Peptide Cations Followed by Electron Capture; Hideyuki Konishi; Shingo Sasaki; Aichi Kyoiku University, Kariya, Aichi, Japan |
THURSDAY POSTERS

7:30 – 8:00 am  SET UP POSTERS, Exhibit Hall B
8:45 – 10:15 am  POSTER SESSION: Authors of ODD numbered posters (i.e. 001, 003) present.
1:30 – 3:00 pm  POSTER SESSION: Authors of EVEN numbered posters (i.e. 002, 004) present.
3:00 – 3:30 pm  REMOVE POSTERS. Please leave posters until 3:00 pm.

ThPH294  Substituent Effects in the Binding of Alkalai Metal Ions to Pyridines Determine by Threshold Collision-Induced Dissociation and Ab initio Theory: Mary T. Rodgers, Ravi Amunugama, Wayne State University, Detroit, MI

ThPH295  The Fragmentation of PAH-Purine Adducts, a Theoretical Modeling Study: Daryl E. Giblin, Michael L. Gross, Washington University, St. Louis, MO

ThPH296  NRMS and Computational Study of [C, H, N, O] Cations, Anions and Radicals: Miroslav Polasek, Frantisek Turecek, University of Washington, Seattle, WA

ThPH297  Tandem Mass Spectrometric Studies of a Farnesyl Transferase Inhibitor and its Bromo-Analog: Henry Y. Wu, Xue-Zhi Qin, Michael H. Wang, Merck & Co., Inc., West Point, PA

ThPH298  Electrospray Mass Spectrometric Studies of the Fragmentation Mechanism for Simvastatin and Lovastatin: Michael H. Wang, Henry Wu, Merck & Co., Inc., West Point, PA


ThPH300  Fragmentation mechanism of amphetamine, methamphetamine, and N-alkyl substituted norephedrines: David A. Herold, Jeffery D. Rivera, Robert L. Fitzgerald, VA Med Center/University of California, San Diego, CA

ThPH301  Structural and Kinetic study of Peptide Ions Using a New Method of Ion Rotating Excitation in a Gas Filled RFQ Coupled to High Resolution ortho-TOF MS: Alexandre Dodonov, Valeri Razinkov; Viatcheslav Kozlovski, Ilia Soulimenko, Zhen Zhou, Alexander Kholomeev, Thomas Horvath; Hermann Wollnik, Institute of Energy Problems of Chemistry, Chernogolovka, Russia; II Physikalisches Institut Universität, Giessen, Germany; Justus-Liebig Universität, Giessen, Germany

ThPH302  Collisional Activation of Small Peptides: Fragmentation Energies and Energy Transfer: Julia Laskin, Eduard Denisov, Jean H. Futrell, Pacific Northwest National Laboratory, Richland, WA

ThPH303  Why are Larger Fragments Lost in Preference to Smaller Ones with Lower Thresholds?: David J. McAdoo, Charles E. Hudson, John C. Traeger, Larry L. Griffin, University of Texas Medical Branch, Galveston, Texas; LaTrobe University, Victoria, Australia; Texas A&M University, Galveston, Texas

ThPH304  Collision-Induced Dissociation of Protonated Peptides Containing Aspartic Acid and Glutamic Acid Residues: Carolyn Cassidy, Talat Yalcin, Michael Peterson, University of Alabama, Tuscaloosa, AL


ThPH306  Boundary Activated Dissociation in a Flow-Through Linear Quadrupole: James W. Hager, Lisa M. Cousins, PE-SCIDEX, Canada

ThPH307  Effects of Using Only Pulsed Heavy Gases in a Quadrupole Ion Trap: Allison S. Daniel, Gary L. Glish, University of North Carolina, Chapel Hill, NC

ThPH308  Structure and Reactivity of a1 Ions in the Low-energy CID Spectra of Protonated Peptides: Tomas Vaisar, Jan Urban, Molecotechnics Ltd., Bellevue, WA

ThPH309  Investigation of a Number of Structural Isomers by Translational Energy Spectroscopy (TES): Mathew A. Kennedy, Gareth Brenton, MRSU, University of Wales, Swansea, UK

ISOTOPE RATIO MS, 310 - 316

ThPI 310  Reduction of amino acids to amino alcohols to enhance volatality for high precision C isotope analysis: J. Thomas Brenna, Bassem I. Zaidel, Nabil M. Saad, Betty A. Lewis, Cornell University, Ithaca, NY

ThPI 311  Silyl Derivatives In Gas Chromatography-Combustion (GC-C) Isotope Ratio Mass Spectrometry (IRMS) Retains Carbon and Alters Expected 13C/12C Measurements: Steven B. Shiner, Michael Haish, Michael J. MacCoss, Dwight E. Matthews, University of Vermont, Burlington, VT

ThPI 312  High Precision Position-Specific Isotope Analysis of the Carboxyl Carbon of Short Chain Organic Acids: Nabil M. Saad, J. Thomas Brenna, Cornell University, Ithaca, NY

ThPI 313  Quantitative Comparison of GCMS and GC-C-IRMS Instrumentation for the Measurement of Stable Isotope Tracer Enrichments: Michael J. MacCoss, Dwight E. Matthews, University of Vermont, Burlington, VT


ThPI 315  A Computer-Based Control System for High Precision Position Specific Isotope Analysis (PSIA): Jason Sepp, J. Thomas Brenna, Cornell University, Ithaca, NY
