27th ASILOMAR CONFERENCE on
MASS SPECTROMETRY
Sponsored by
American Society for Mass Spectrometry

METABOLOMICS
Friday, September 30 - Tuesday, October 4, 2011
Asilomar Conference Center, Pacific Grove, CA

Program Chairs
Oliver Fiehn
University of California, Davis
A. Daniel Jones
Michigan State University

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ACMS Committee
Carolyn J. Cassady
University of Alabama
Gary Glish
UNC Chapel Hill
Glen Jackson
Ohio University
Rebecca A. Jockusch
University of Toronto
Internet Access. There is complimentary wi-fi access in the session room, sleeping rooms, and the temporary Social Hall (Woodside adjacent to Crocker Dining Hall.)

Meals at Asilomar. For attendees lodging at Asilomar you will receive a meal ticket for all meals beginning with dinner on Friday and ending with lunch on Tuesday. Vegetarian option is always available upon request at the meal line. For Tuesday a box lunch has been requested for you, please use your lunch ticket to pick up your box lunch on Tuesday morning at breakfast.

For attendees staying off-site you will receive lunch tickets for Saturday, Sunday and Monday. Off-site lodgers wishing to purchase breakfast or dinner meal tickets may purchase them at the Asilomar Conference Center registration area in the Administration Building.

To-Go Lunches on Saturday, Sunday or Monday: If you wish to take your lunch to the beach or elsewhere, please go to the regular lunch window and request a “To-Go Lunch”.

Conference Banquet and After-Dinner Talk. An upgraded meal served in Seascape (adjacent to Crocker Dining Hall). Ticket is required. For onsite loggers, please bring a regular dinner ticket and your special banquet ticket to the meal.

Following dinner we will reconvene in the session room for an after-dinner talk by Cheryl Kerfeld, DOE Joint Genomics Institute (JGI) and UC Berkeley, entitled Sequences and Consequences. All attendees are invited to attend this talk. Dessert will be served after Dr. Kerfeld's talk along with wine, beer and other beverages. This will also be the final viewing of the Session 2 posters.

Evening Wine & Beer Mixers and Poster Sessions. Each evening there is a Wine & Beer Mixer, many supported by the conference sponsors. These mixers are an opportunity to continue lively discussion and visit with poster presenters.

Presenter Guidelines.
Poster presenters in Session 1: Please mount your poster display on Friday before 6:00 pm. Remove your poster after the Saturday evening mixer. See pages 17-18 for listing of Session 1 posters.

Poster presenters in Session 2: Please mount your poster display on Sunday by 9:00 am. Remove your poster after the Monday evening mixer. See pages 19-20 for listing of Session 2 posters.

Speakers. Please arrive in the Chapel 15 minutes prior to the start of the session to set up your laptop computer or load your presentation onto the conference computer (PC). If you have a Mac, please bring your adapters.

Program Overview.
Friday Evening Session 7:15 – 10:00 pm
Saturday Morning Sessions 9:00 – 11:50 am
Afternoon Session 1:00 – 4:00 pm
Evening Session 7:15 – 10:00 pm
Sunday Morning Session 9:00 – 11:50 am
Free Afternoon
Evening Session 7:15 – 10:00 pm
Monday Morning Session 9:00 – 11:50 am
Afternoon Session 1:00 – 4:00 pm
Metabolomics Society 4:00 - 6:00 pm
Banquet 6:00 – 7:15 pm
After-Dinner Talk 7:15 – 8:00 pm

Survey. You will receive an email with a link to the online conference survey. Your feedback is appreciated.

Sunday Afternoon. There is a free afternoon scheduled for Sunday. Please see page 22 of this program for some suggested activities. Conference attendees are encouraged to join others for outings (rent bikes and ride on 17-Mile Drive, visit the Aquarium, etc.) A sign-up board available in the session room.

CONFERECE SPONSORS

Thank you to these companies for their generous support of the Wine & Beer Mixers. Look for their corporate poster and presentation on the day of their sponsorship.

Agilent Technologies, Friday Evening Mixer
Waters Corporation, Saturday Evening Mixer
Bruker Daltonics, Sunday Evening Mixer
METABOLOMICS

The 2011 ASMS Asilomar Metabolomics meeting will promote an in-depth discussion of current problems and perspectives of mass spectrometry-based metabolomics. This meeting is endorsed by the Metabolomics Society.

We will challenge ideas and concepts throughout the conference and have allocated ample time for discussions, e.g. during evening receptions. In addition to invited speakers, there will be poster sessions and oral contributions based on abstract submissions. We will focus on a range of hot topics, including: databases; metabolomic fluxes, compound identifications and separations; metabolite imaging; secondary metabolism; metabolomics in human diseases and quality control in metabolite quantifications.

FRIDAY, SEPTEMBER 30, 2011

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<td>3:00 pm</td>
<td>Guest Room Check-in, Asilomar Main Lobby</td>
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<tr>
<td>4:00 – 6:00 pm</td>
<td>Conference Registration, Asilomar Main Lobby</td>
</tr>
<tr>
<td>6:00 – 7:00 pm</td>
<td>Asilomar dinner for on-site lodgers, Crocker Dining Hall. Ticket required.</td>
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<tr>
<td>7:15 – 8:35 pm</td>
<td>Opening Session</td>
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<tr>
<td></td>
<td>Metabolomic Databases</td>
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<tr>
<td>7:15 – 7:20 pm</td>
<td>Opening Remarks from Conference Organizers</td>
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<tr>
<td></td>
<td>Oliver Fiehn and Dan Jones</td>
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<tr>
<td>7:20 – 7:55 pm</td>
<td>Sue Rhee, Carnegie Institution for Science</td>
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<tr>
<td></td>
<td>Reconstruction and Application of Plant Metabolic Networks</td>
</tr>
<tr>
<td>7:55 – 8:30 pm</td>
<td>Oliver Fiehn, UC Davis</td>
</tr>
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<td></td>
<td>Towards an International MassBank</td>
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<tr>
<td>8:30 - 8:35 pm</td>
<td>Steve Fischer, Agilent Technologies</td>
</tr>
<tr>
<td>8:30 – 10:00 pm</td>
<td>Wine &amp; Beer Mixer and Poster Session 1 (pages 17 - 18 for poster list)</td>
</tr>
<tr>
<td></td>
<td>Special thanks to Agilent Technologies for support of tonight's mixer!</td>
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</table>
Find the right solution for your metabolomics research

Metabolomics

Agilent’s metabolomics workflow solutions include software that can help you identify common metabolites. The new enhanced Agilent METLIN Personal Compound Database and Library contains more than 27,000 compounds with approximately 3,000 compounds having MS/MS spectra — you can identify metabolites with greater confidence.

With Agilent’s industry-leading separation technologies, high-performance MS systems, and integrated informatics software, Agilent offers comprehensive solutions for metabolomics studies.

www.metabolomics-lab.com
<table>
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<tr>
<th>Time</th>
<th>Event Description</th>
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<tbody>
<tr>
<td>7:30 – 9:00 am</td>
<td><strong>Asilomar Breakfast for on-site lodgers</strong>, <em>Crocker Dining Hall. Ticket required.</em></td>
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</table>
| 9:00 am – 12:10 pm | **Morning Session**, *Lloyd Sumner presiding*  
|                | **Quality Control in High-Throughput Metabolomics.**                               |
| 9:00 – 9:50 am | **Nicola Zamboni, ETH Zurich**  
|                | Deep Phenotyping of Genomes by High-Throughput Metabolomics                         |
| 9:50 – 10:10 am | **Mine Palazoglu, UC Davis**  
|                | Quality Control in a Metabolomics Laboratory - Back to Basics                        |
| 10:10 – 10:40 am | Coffee Break                                                                     |
| 10:40 – 11:15 am | **A. Daniel Jones, Michigan State University**  
|                | Large-scale Profiling of Plant Metabolites: How Should We Address Conflicts  
|                | Between Metabolome Depth and Analytical Throughput?                                |
| 11:15 – 11:50 am | **Chris Beecher, University of Michigan**  
|                | Lab Techniques to Minimize Technical Errors in Metabolomic Analyses                 |
| 12:10 – 1:00 pm | **Asilomar Lunch for all participants**, *Crocker Dining Hall. Ticket required.*    |
| 1:00 – 3:50 pm | **Afternoon Session**, *Bernd Markus Lange presiding*  
|                | **Separation/Identification of Complex Mixtures I**                                 |
| 1:00 – 1:35 pm | **Philip Britz-McKibbin, McMaster University**  
|                | New Advances in Capillary Electrophoresis-Mass Spectrometry for Metabolomics       |
| 1:35 – 2:10 pm | **Robert Synovec, University of Washington**  
|                | Application of GC-MS and GC x GC-TOFMS with Chemometrics to Address  
|                | Emerging Challenges in Metabolomics                                                |
| 2:10 – 2:40 pm | Coffee Break                                                                     |
| 1:00 – 3:50 pm | **Afternoon Session**, *Oliver Fiehn presiding*  
|                | **Separation/Identification of Complex Mixtures II**                                |
| 2:40 – 3:15 pm | **Robert Mistrik, HighChem**  
|                | Substructure Paths for Compound Identifications                                     |
| 3:15 – 3:50 pm | **John McLean, Vanderbilt University**  
|                | Structural Resolution of Carbohydrate Positional and Structural Isomers Based  
|                | on Gas-Phase Ion Mobility-Mass Spectrometry                                        |
| 6:00 – 7:00 pm | **Asilomar dinner for on-site lodgers**, *Crocker Dining Hall. Asilomar meal ticket required.* |
| 7:15 – 8:30 pm | **Evening Session**, *Nick Winograd presiding*  
|                | **Imaging**                                                                        |
| 7:15 – 7:50 pm | **Gary Siuzdak, The Scripps Research Institute**  
|                | Implications of Metabolite Imaging for Understanding Mechanisms of Disease           |
| 7:50 – 8:25 pm | **Jonathan Sweedler, University of Illinois**  
|                | Measuring Cell to Cell Differences in the Brain Metabolome                           |
| 8:25 – 8:30 pm | **Don Harris, Waters Corporation**                                                 |
| 8:30 – 10:00 pm | **Wine & Beer Mixer and Poster Session 1** (pages 17 - 18 for poster list)  
|                | Special thanks to **Waters Corporation** for support of tonight's mixer!            |
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Waters
THE SCIENCE OF WHAT’S POSSIBLE.
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</tbody>
</table>
| 9:00 – 11:50 am | Morning Session, *A. Daniel Jones presiding*  
**Secondary Metabolism** |
| 9:00 – 9:35 am | *William H. Gerwick, The Scripps Institute of Oceanography*  
Exploring the Secondary Metabolomes of Marine Cyanobacteria Using Mass Spectrometry |
| 9:35 – 10:10 am | *Lloyd W. Sumner, Noble Foundation*  
Integrated Metabolomics for Gene Discovery and Novel Insight Into *Medicago truncatula* Secondary Metabolism |
| 10:10 - 10:40 am | Coffee Break |
| 10:40 – 11:15 am | *Bernd Markus Lange, Washington State University*  
Regulation and Biotechnological Enhancement of terpenoid Essential Oil Biosynthesis |
| 11:15 - 11:50 am | *Joseph Noel, Salk Institute*  
Evolution of Terpene Synthases |
| 12:25 pm – 1:00 pm | Asilomar Lunch for all participants, *Crocker Dining Hall*.  *Asilomar meal ticket required.* |
| 1:00 – 6:00 pm | Free Time |
| 6:00 – 7:00 pm | Asilomar dinner for on-site lodgers, *Crocker Dining Hall. Ticket required.* |
| 7:15 – 8:25 pm | Evening Session, *Joseph Noel presiding*  
**Lipids** |
| 7:15 - 7:50 pm | *Gavin Reid, Michigan State University*  
High-Resolution Lipidomic Profiling and Chemical Labeling to Monitor the Metastatic Potential of Colon Adenocarcinoma Cell lines and their Secreted Exosomes |
| 7:50 - 8:25 pm | *Nick Winograd, Pennsylvania State University*  
TOF-SIMS Imaging of Lipid Membranes |
| 8:25 - 8:30 pm | *Sandy Yates, Bruker Daltonics* |
| 8:30 – 10:00 pm | *Wine & Beer Mixer* and *Poster Session 2* (pages 19 - 20 for poster list)  
Special thanks to *Bruker Daltonics* for support of tonight's mixer! |
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Innovation with Integrity
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<td><strong>Asilomar Breakfast for on-site lodgers,</strong> <em>Crocker Dining Hall. Ticket required.</em></td>
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<tr>
<td>9:00 – 11:50 am</td>
<td><strong>Morning Session, Chris Beecher presiding Human Diseases</strong></td>
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</table>
| 9:00 – 9:35 am | **Rima Kaddurah-Daouk, Duke University**  
Pharmacometabolomics |
| 9:35 – 10:10 am | **Andrew Patterson, Pennsylvania State University**  
Metabolomic Applications in Translational Medicine |
| 10:10 – 10:40 am | Coffee Break |
| 10:40 – 11:15 am | **Bill Wikoff, UC Davis**  
The Impact of Gut Microbes on Human Metabolism |
| 11:15 – 11:50 am | **Theresa Pedersen, USDA**  
Lessons from the Development of Targeted Quantitative Profiles of Low Abundance Endogenous Metabolites |
| 12:00 – 1:00 pm | **Asilomar lunch for all participants,** *Crocker Dining Hall. Asilomar meal ticket required.* |
| 1:00 – 2:10 pm | **Afternoon Session I, Rima Kaddurah-Daouk presiding Fluxes** |
| 1:00 – 1:35 pm | **Ana Alonso, Ohio State University**  
13C-Based Flux Analysis of Plant Metabolic Networks |
| 1:35 – 2:10 pm | **Christian Metallo, University of California, San Diego**  
Isotope-Based Flux Analysis in Cancer Cells Unravels Novel Pathways in Lipid Biosynthesis |
| 2:10 – 2:40 pm | Coffee Break |
| 2:40 – 4:00 pm | **Afternoon Session II, A. Daniel Jones presiding Short Talks from Selected Abstracts** |
| 2:40-2:50 pm | **Nichole Reisdorph, National Jewish Health and the University of Colorado**  
Metabolic and Genomic Profiles of Chronic Obstructive Pulmonary Disease (COPD) in Human Samples and Mouse Models: A Promising Role for Sphingolipids |
| 2:50-3:00 pm | **Peter Sander, Bruker Daltonik GmbH**  
Novel Approaches for Structure Elucidation and Confirmation for Plant Metabolomics |
| 3:00-3:10 pm | **Brandy Heath, Pacific Northwest National Laboratory**  
Identification of Metabolites Involved in Extracellular Respiration by Shewanella Oneidensis MR |
| 3:10-3:20 pm | **Leon Coulier, Netherlands Metabolomics Centre, TNO**  
Towards an Improved Automated Workflow for Metabolite Identification |
| 3:20-3:30 pm | **Jordan Aerts, University of Illinois at Urbana-Champaign**  
Capillary Electrophoresis Electrospray-Mass Spectrometry for Single-Neuron Metabolomic Profiling |
### MONDAY, OCTOBER 3, 2011, continued

<table>
<thead>
<tr>
<th>Time</th>
<th>Presenter(s)</th>
<th>Title</th>
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<tr>
<td>3:30 - 3:40 pm</td>
<td><strong>Grace (Xiaolu) Yang</strong>, Stanford University</td>
<td>A Systematic Investigation of Small Metabolite Interactions with Regulatory Proteins in Yeast</td>
</tr>
<tr>
<td>3:40 - 3:50 pm</td>
<td><strong>Bradley S. Evans</strong>, University of Illinois at Urbana-Champaign</td>
<td>Untargeted Metabolomics for Enzyme Functional Assignment: Rhodospirillum rubrum RubisCO-Like Protein Links S-methyl-thioadenosine Metabolism with Isoprenoid biosynthesis</td>
</tr>
<tr>
<td>3:50 - 4:00 pm</td>
<td><strong>Kyuil Cho</strong>, University of Illinois at Urbana-Champaign</td>
<td>Perturbation-Based Active Pathway Detection for <em>in vivo</em> Enzyme Function Annotation: Correlation Between Metabolite Profiles and metabolic Pathway Activities</td>
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</table>
| 4:00 – 6:00 pm | **Metabolomics Society: Forming a U.S. National Chapter**  
* Lloyd Sumner presiding  
Meet in conference session room, Chapel. All are welcome to stay for this meeting and participate in discussion. |
| 6:00 – 7:00 pm | **Banquet**, Seascape Room (left of Crocker Hall, main dining room). Banquet ticket required. |
| 7:15 – 9:30 pm | **After-Dinner Program: Genomics and Poster Session 2**  
* Oliver Fiehn, presiding  
  7:15 - 8:00 pm **Cheryl Kerfeld**, DOE Joint Genomics Institute (JGI) and UC Berkeley  
  Sequences and Consequences  
  8:00 - 9:30 pm **Dessert Reception** and **Poster Session 2** (pages 19 - 20 for poster list) |

### TUESDAY, OCTOBER 4, 2011

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<tr>
<th>Time</th>
<th>Event</th>
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| 7:30 – 9:00 am | **Asilomar Breakfast for on-site lodgers**, Crocker Dining Hall.  
Asilomar meal ticket required. |
| Morning    | **Departures**, Check-out is 11:00 am.                                                   |
POSTER SESSION 1 (Fri - Sat)

Session 1 posters are on display Friday evening through Saturday evening. Presenting authors will attend their posters during the Friday and Saturday evening mixers.

1. **Diagnosis of Inherited Metabolic Disorders Using a Targeted Metabolomics by Flow Injection Analysis-Tandem Mass Spectrometry**
   Tomas Adam, *Palacký University, Olomouc, Czech Republic*

2. **A Novel Global Lipid Biomarker Workflow from a Complex Biological Sample**
   Giuseppe Astarita, *Waters Corporation, Milford, MA*

3. **Changes in hydrophobic metabolites in Type II Diabetics**
   Jared N. Bowden, *Montana State University, Bozeman, MT*

4. **Molecular Imaging Studies of Drugs and Metabolites in Tissue Using Desorption Electrospray Ionization Coupled to Mass Spectrometer / Comparison to MALDI-MS**
   John Chakel, *Prosolia Inc, Indianapolis, IN*

5. **Perturbation-Based Active Pathway Detection for *in vivo* Enzyme Function Annotation: Correlation Between Metabolite Profiles and Metabolic Pathway Activities**
   Kyuil Cho, *University of Illinois at Urbana-Champaign, Champaign, IL*

6. **Towards an Improved Automated Workflow for Metabolite Identification**
   Leon Coulier, *Netherlands Metabolomics Centre, TNO, The Netherlands*

7. **Chemical Derivatization for Sub-Nanomolar Detection of Low Abundance Metabolites by ESI-MS for Expanded Coverage of the Metabolome**
   Alicia DiBattista, *McMaster University, Hamilton, ON, Canada*

8. **Chemical Diversity in the Glandular Trichome Metabolome of Wild Tomato Accessions**
   E. A. Prabodha Ekanayaka, *Michigan State University, East Lansing, MI*

9. **A UPLC-QTOF MS Method for Accurate Quantitation of Urinary 6β-Hydroxycortisol and Free Cortisol in a Cohort of Premenstrual Women**
   Jun Han, *University of Victoria-Genome BC Proteomics Centre, Victoria, BC, Canada*

10. **Identification of Metabolites Involved in Extracellular Respiration by *Shewanella Oneidensis* MR-1**
    Brandi Heath, *Pacific Northwest National Laboratory, Richland, WA*

11. **Metabolomic Approach on *Plumbago zeylanica* Using Gas chromatography Coupled with Quadrupole Mass Spectrometry and Data Integration**
    Malaiyandi Jayanthi, *Bharathiar University, Coimbatore, Tamilnadu, India*

12. **The MetaCyc Family of Metabolic Databases: Applications to Metabolomics**
    Peter D. Karp, *SRI International*

13. **Evaluating Complimentary UPLC/QTofMS Methodologies Applied to an *in vitro* Targeted Metabolomics Workflow**
    Richard J. Lawrence, *US Army ECBC, Aberdeen Proving Ground, MD*

14. **Development of LC-MS Methods for Profiling Protein-Interacting Metabolites**
    Xijan Li, *Stanford University, Stanford, CA*
15 Relative Quantitation and High Resolution Mass Spectrometry Imaging of Cholesterol and 7-Dehydrocholesterol Oxysterols in Smith-Lemli-Opitz Syndrome Mouse Model
John A. McLean, Vanderbilt University, Nashville, TN

16 Esophageal Cancer Metabolite Biomarkers Detected by LC-MS and NMR Methods
Daniel Raftery, Purdue University; West Lafayette, IN

17 On-Line Electrochemistry/MS - A Powerful Technique for Fast Prediction of Phase I and II Drug Metabolism
Jim Powers, Antec, Palm Bay, FL

18 Metabolic and Genomic Profiles of Chronic Obstructive Pulmonary Disease (COPD) in Human Samples and Mouse Models: A Promising role for Sphingolipids
Nichole Reisdorph, National Jewish Health and the University of Colorado, Denver, CO

19 Novel Approaches for Structure Elucidation and Confirmation for Plant Metabolomics
Peter Sander, Bruker Daltonik GmbH, Bremen, Germany

20 Coupling Multivariate Statistical Analysis with Static and Dynamic Lipidomic Flux Using High Resolution LC/MS
Vinit Shah, Merck & Co., Inc., Rahway, NJ

21 High Throughput Quantitative Analysis of Melamine and Triazines by MALDI-TOF MS
Ajeet Singh, National Chemical Laboratory, Pune, India

22 Mycobacteria on Steroids: Metabolite Profiling using Isotopically Labeled Cholesterol
Suzanne T. Thomas, Stony Brook University, Stony Brook, NY

23 In vivo Solid-Phase Microextraction: A New Sample Preparation Method for Untargeted LC-MS Metabolomics
Dajana Vuckovic, University of Waterloo, Waterloo, ON, Canada

24 Dansylated Dipeptide Retention Time Database
Manhong Wu, Stanford University, Stanford, CA

25 A Systematic Investigation of Small Metabolite Interactions with Regulatory Proteins in Yeast
Grace (Xiaolu) Yang, Stanford University, Stanford, CA

26 Targeted Metabolomics by LC- and FIA-MS/MS Delineates a Human Response to Ionizing Radiation
Shuchu Zhang, Fred Hutchinson Cancer Research Center, Seattle, WA
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<th>Title</th>
<th>Author and Institution</th>
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<td>Capillary Electrophoresis Electrospray-Mass Spectrometry for Single-Neuron Metabolomic Profiling</td>
<td>Jordan Aerts, University of Illinois at Urbana-Champaign; Champaign, IL</td>
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<tr>
<td>2</td>
<td>Dissecting Drug Mechanism by Metabolic Profiling of Yeast Sterols</td>
<td>Stephan Baumann, Agilent Technologies</td>
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<td>3</td>
<td>Targeted LC/MS Based Metabolomic Analysis Reveals Altered Metabolic Substrate Utilization in Renal Cortex in Diabetic Nephropathy</td>
<td>Carolyn L. Buller, University of Michigan; Ann Arbor, MI</td>
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<td>4</td>
<td>Structural Elucidation of <em>in vitro</em> and <em>in vivo</em> Metabolites of Lapatinib by DCE Platform and HPLC-UV-MSn</td>
<td>Changfu Cheng, CoNCERT Pharmaceuticals, Inc.; Lexington, MA</td>
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<td>5</td>
<td>Towards Metabolic Flux Analysis of <em>Lesquerella fendleri</em> Embryos</td>
<td>Jean-Christophe Cocuron, Ohio State University; Columbus, OH</td>
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<td>6</td>
<td>Laser Desorption/Ionization Mass Spectrometry Mediated by Inorganic Particles for Amino Acid Quantitation</td>
<td>Deepika Dhaware, National Chemical Laboratory; Pune, India</td>
</tr>
<tr>
<td>7</td>
<td>An Automated Data Analysis Pipeline for GC-TOF-MS Metabonomics Studies</td>
<td>Xiuxia Du, University of North Carolina at Charlotte; Charlotte, NC</td>
</tr>
<tr>
<td>8</td>
<td>Untargeted Metabolomics for Enzyme Functional Assignment: <em>Rhodospirillum rubrum</em> RubisCO-Like Protein Links S-methyl-thioadenosine Metabolism with Isoprenoid Biosynthesis</td>
<td>Bradley S. Evans, University of Illinois at Urbana-Champaign; Champaign, IL</td>
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<tr>
<td>9</td>
<td>Sensitive and Efficient Identification of Tissue Metabolites by Nano-Liquid Chromatography Coupled with LTQ 14.5 T Fourier Transform Ion Cyclotron Resonance Mass Spectrometry</td>
<td>Huan He, NHMFL; Tallahassee, FL</td>
</tr>
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<td>10</td>
<td>Searching for Metabolic Networks by Tracking Cellular Response to Perturbation Using Untargeted Profiles and Machine Learning Algorithms</td>
<td>Joshua Heinemann, Montana State University; Bozeman, MT</td>
</tr>
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<td>11</td>
<td>Identification of Novel Human and Mouse Vitamin E Metabolites by UPLC-ESIQTOFMS Metabolomics</td>
<td>Caroline H. Johnson, National Cancer Institute, National Institutes of Health; Bethesda MD</td>
</tr>
<tr>
<td>12</td>
<td>Metabolomic Profiling to Evaluate the Effects of Caloric Restriction on Aging</td>
<td>Indu Kheterpal, Pennington Biomedical Research Center, Louisiana State University System; Baton Rouge, LA</td>
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<td>13</td>
<td>Metabolomics at High Spatial Resolution: Mass Spectrometric Imaging of Plant Metabolites at Single Cell Level</td>
<td>Young-Jin Lee, Iowa State University; Ames, IA</td>
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Quantitative Determination of a Thiol Containing tri-Peptide L-α-aminoadipoyl-L-cysteinyl-D-valine in Cell Extracts of Penicillium chrysogenum Using IP-RP-UPLC-MS/MS
Reza Maleki Seifar, Delft University of Technology; Delft, The Netherlands

Capillary Electrophoresis Mass Spectrometry-Based Metabolomics Reveals Ethanolamine Phosphate as a Major Depression Biomarker
Yoshiaki Ohashi, Human Metabolome Technologies; Yamagata, Japan

High Speed and High Performance Precursor and Fragment Ion Analysis in Qualitative and Quantitative Metabolomics
Jeffrey S. Patrick, LECO Corporation

Quantitation of Bacterial Quorum Sensing Molecules Using Laser Desorption Ionization Mass Spectrometry
Venkateswarlu Panchagnula, National Chemical Laboratory, Pune, India

Combination of SPME as Non-Invasive Sample Preparation Technique and GCxGC-TOFMS for High Resolution Profiling of Metabolites in Apples: Method Development Considerations and Potential of New in vivo SPME Formats
Sanja Risticevic, University of Waterloo; Waterloo, ON, Canada

Quality Control of High-Throughput Metabolomics to Support Physiological Investigation of Saccharomyces cerevisiae in Industrial Synthetic Biology
Celeste Sandoval, Amyris Inc; Emeryville, CA

Tuber-Specific Gene Silencing to Lowering Acrylamide in Potatoes
Roshani Shakya, J R Simplot Company; Boise, ID

Ovarian Cancer Metabolomic Dynamics Using GCxGC-MS
Mark P. Styczynski, Georgia Institute of Technology; Atlanta, GA

Quantitative and Qualitative Profiling of Oxylipins and Phospholipins Using Novel State-of-the-Art Mass Spectrometry
Rob J. Vreeken, Leiden University; Leiden, The Netherlands

Comprehensive GC×GC-TOF MS Analysis in Human Metabolomic Studies
Petr Wojtowicz, Laboratory for Inherited Metabolic Disorders; Olomouc, Czech Republic

Simultaneous Identification and Quantification of Multiple Classes of Metabolites in Serum by LC-ESI-MS/MS
Jun Feng Xiao, Georgetown University; Washington, DC

Unknown Compounds Identified using GC-APCI-TOF Based Metabolic Profiling of a Corynebacterium Glutamicum ΔprpD2 Mutant Strain
Sandy Yates, Bruker Daltonics; Fremont, CA

Comprehensive Workflow for Metabolic Profiling of Secondary Metabolites from Myxobacteria
Gabriela Zurek, Bruker Daltonik GmbH; Bremen, Germany
MONTEREY BAY AREA ATTRACTIONS

Sunday afternoon is scheduled free time. You are encouraged to relax on your own or with your fellow attendees. Look for sign-ups in the session room for those interested in group activities. Do you have a car and wish to visit the aquarium, take a hike, or scenic drive? Do you want to rent bikes with others and tour around the area? Do you want to rent some clubs and play golf? Be an instigator and list your activity on the sign-up board for others to join you.

Some Ideas...
From historic adobes and landmarks to Fisherman's Wharf and the Monterey Bay Aquarium, Monterey has something for everyone. Visit Steinbeck's Cannery Row, Colton Hall and the Monterey Museum of Art. Stroll the recreational trail along the coast or see the wildlife close-up on a kayak adventure on the Bay.

When in Pacific Grove don't forget to check out the Monarch butterflies which make PG home for the winter, Asilomar State Beach, historic bed and breakfast inns, Lover's Point and the Pacific Grove Museum of Natural History.

Pebble Beach attractions include the 17-Mile Drive, Stillwater Cove, the Lone Cypress and an array of world-class golf courses. You can access 17-Mile Drive free-of-charge on foot or bike or enter by car for a fee.

Carmel Valley is home to many wineries, farms, ranches and the beautiful Garland Ranch Regional Park.

And don't miss Big Sur with its Esalen Institute, Henry Miller Memorial Library, Point Sur Lighthouse, camping, hiking, beautiful redwood groves and excellent whale-watching.

### Peninsula Attractions
Please visit www.monterey.com and click “Attractions” to view more details.

<table>
<thead>
<tr>
<th>Attraction</th>
<th>Address</th>
<th>Phone</th>
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<tbody>
<tr>
<td>Fishermans Wharf</td>
<td>140 W. Franklin St.</td>
<td>(831) 649-6544</td>
</tr>
<tr>
<td>Monterey Bay Aquarium</td>
<td>886 Cannery Row</td>
<td>(831) 648-4888</td>
</tr>
<tr>
<td>Monterey Bay National Marine Sanctuary</td>
<td>299 Foam St., Suite D</td>
<td>(831) 647-4201</td>
</tr>
<tr>
<td>Monterey Bay Scenic Tours</td>
<td>406 Calle Principal</td>
<td>(831) 372-6278</td>
</tr>
<tr>
<td>Monterey Bay Whale Watch</td>
<td>P.O. Box 52001</td>
<td>(831) 375-4658</td>
</tr>
<tr>
<td>National Steinbeck Center</td>
<td>One Main St.</td>
<td>(831) 775-4725</td>
</tr>
<tr>
<td>Pacific Yachting &amp; Sailing</td>
<td>790 Mariner Park Wy</td>
<td>(800) 374-2626</td>
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Additional information on local sights and the Asilomar State Beach may be found at the Asilomar temporary Front Desk or temporary Social Hall.