

## 20<sup>th</sup> ASILOMAR CONFERENCE ON MASS SPECTROMETRY

### *Metabolite Profiling: Biomarker Discovery, Drug Efficacy, and Fundamental Biochemistry*

Endogenous metabolites have gained increasing interest over the past five years largely for their implications in diagnostic and pharmaceutical biomarker discovery. Although numerous small molecules are routinely measured in biofluids as indicators of health, little is known about the vast majority of metabolites. For example, biofluids contain thousands of components, many of which remain structurally and functionally uncharacterized. For this reason, metabolite research and its potential in health and pharmaceutical development has become one of the most exciting areas of biological discovery. Three of the broad aims of this field are to identify new disease biomarkers, monitor physiological reactions to administered drugs and to understand the function of metabolites.

This Asilomar meeting will focus on the latest challenges in metabolite profiling, spanning a broad range of interests including research trends and instrument developments.

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### Friday Evening, October 15

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- 3:00 PM Check-in, *Asilomar Main Lobby*
- 6:00 - 7:00 PM **Asilomar dinner for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*
- 6:30 PM **Speakers**, please connect laptops to LCD projectors. *Chapel*
- 6:30 PM **Posters:** Please set up your poster on the board number corresponding to your poster in this program. *Chapel*
- 7:00 – 10:00 PM OPENING SESSION.** *Chapel*
- 7:00 - 7:10 PM Introductory Remarks, **Gary Siuzdak**, The Scripps Research Institute, La Jolla, CA
- 7:10 - 7:55 PM **Donald Chace**, Pediatrix, Bridgeville, PA  
*Newborn Screening for Metabolic Disease is One Model for the Practice of Clinical Mass Spectrometry*
- 8:00 - 8:40 PM **Xianlin Han**, Washington University School of Medicine, St. Louis, MO  
*Shotgun Lipidomics and Application for Biomarker Discovery in Alzheimer's Disease*
- 8:45 PM **POSTER PRESENTATIONS, 5 minutes each**
1. **Sarah Robinson**, University of York, York, UK
  2. **Thomas O. Metz**, Pacific NW National Lab, Richland, WA
  3. **Grace Tong**, The Scripps Research Institute, La Jolla, CA
  4. **Brian Frey**, University of Wisconsin, Madison, WI
- 9:15 - 10:00 PM **Poster Viewing and Reception.** *Chapel*

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**Saturday, October 16**

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7:30 - 9:00 AM **Asilomar breakfast for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*

8:30 - 9:00 AM **Speakers,** please connect laptops to LCD projectors. *Chapel*

**9:00 AM – 12:00 PM** ***ENDOGENOUS METABOLITES AND XENOBIOTICS***

9:00 - 9:30 AM **John Wagner,** Merck Research Laboratories, Rahway, NJ  
*Biomarkers in Rational Drug Development*

9:30 - 10:00 AM **John Vogel,** Lawrence Livermore Natl. Laboratory, Livermore, CA  
*AMS Quantitation of Metabolism: From Individual Humans to Individual Cells*

10:00 - 10:30 AM **Alan Saghatelian,** The Scripps Research Institute, La Jolla, CA  
*Assigning Endogenous Substrates of Enzymes by Global Metabolite Profiling*

10:30 - 10:45 AM **BREAK**

10:45 - 11:15 AM **William Griffiths,** University of London, London, UK  
*Targeted Metabolomics: Novel Cholesterol Metabolites in Brain*

11:15 - 11:45 AM **C. Logan Mackay,** Natl. High Magnetic Field Laboratory, Tallahassee, FL  
*Capillary Electrophoresis and Top Down ESI FT-ICR Mass Spectrometry for the Characterization of Renal Disease Biomarkers*

12:00 - 2:00 PM **Asilomar lunch.** *Crocker Dining Hall. Asilomar meal ticket required.*

1:30 - 2:00 PM **Speakers,** please connect laptops to LCD projector. *Chapel*

**2:00 – 6:00 PM** ***METABOLITE BIOINFORMATICS***

2:00 - 2:30 PM **Colin Smith,** Scripps Research Institute, La Jolla, CA  
*METLIN: A Metabolite Profiling Database*

2:30 - 3:00 PM **Robert Mistrik,** HighChem, Ltd., Bratislava, Slovakia  
*Mapping the Human Metabolome: A Software Problem?*

3:00 - 3:30 PM **Thomas Hankemeijer,** TNO/Leiden University, Leiden, Netherlands  
*Metabolomics: Quo Vadis?*

3:45 - 4:00 PM **BREAK. Poster presenters,** please connect laptops to LCD projector.

4:00 - PM **POSTER PRESENTATIONS, 5 minutes each**

5. **Paul E. Minkler,** Louis Stokes VA Medical Center, Cleveland, OH

6. **Emma Edwards,** University of York, York, UK

7. **Darren Dumlao,** University of California, Los Angeles, CA

8. **Zhihong O'Brien,** Ligand Pharmaceuticals, San Diego, CA

9. **Lekha Sleno,** National Research Council, Halifax, Canada

6:00 - 7:00 PM **Asilomar dinner for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*

7:00 - 10:00 PM **Taste of Monterey Wine Reception. Sponsored by Advion Biosciences.**  
*Scripps Conference Room*

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**Sunday, October 17**

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7:30 - 9:00 AM **Asilomar breakfast for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*

8:30 - 9:00 AM **Speakers,** please connect laptops to LCD projectors. *Chapel*

**9:00 AM – 12:00 PM** **SEPARATION TECHNOLOGY**

9:00 - 9:30 AM **Richard D. Smith,** Pacific Northwest National Laboratory, Richland, WA  
*Nanoflow Capillary Liquid Chromatographic-Mass Spectrometry for High Throughput Quantitative Metabolomic Analyses*

9:30 - 10:00 AM **Andrew Baker,** Waters Corporation, Beverly, MA  
*UPLC-MS for Increased Throughput, Sensitivity and Resolution*

10:00 - 10:30 AM **Ben Bolanos,** Pfizer, Inc., San Diego, CA  
*Leveraging SFC/MS to Broaden Plasma Biomarker Metabolite Profiling*

10:30 - 10:45 AM **BREAK**

10:45 - 11:15 AM **Elizabeth Want,** The Scripps Research Institute, La Jolla, CA  
*Metabolite Profiling in Disease*

11:15 - 11:45 AM **David Millington,** Duke University Medical Center, Durham, NC  
*Applications of Targeted Metabolic Profiling*

12:00 - 1:00 PM **Asilomar lunch.** *Crocker Dining Hall. Asilomar meal ticket required. If you wish to picnic, ask for a lunch “to go” when you go through the line!*

**AFTERNOON FREE**

**6:00 - 7:00 PM** **Asilomar dinner for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*

6:30 PM **Speakers,** please connect laptops to LCD projectors. *Chapel*

**7:00 – 8:30 PM** **GLOBAL SYSTEMS BIOLOGY AND THE HUMAN SUPERORGANISM**

7:00 - 7:40 PM **Jeremy Nicholson,** Imperial College, London, UK  
*Understanding Global Systems Biology and the Human Superorganism: The Greatest Challenge in Analytical Chemistry and the 21<sup>st</sup> Century Medicine?*

**7:45 - 8:30 PM** **POSTER PRESENTATIONS**

**10. Charles L. Hoppel,** Louis Stokes VA Medical Center, Cleveland, OH

**11. Qingfen Zhang,** University of Arizona, Tucson, AZ

**12. Ming Gu,** Cerno Bioscience, New Haven, CT

**13. Arman Yaghoubian,** University of California, Los Angeles, CA

**8:30 - 10:00 PM** **Informal Gathering.** *Scripps Conference Room*

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**Monday, October 18**

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**7:30 - 9:00 AM** **Asilomar breakfast for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required.*

8:30 - 9:00 AM **Speakers,** please connect laptops to LCD projectors. *Chapel*

**9:00 AM – 12:00 PM** **TECHNOLOGY DEVELOPMENTS**

9:00 - 9:30 AM **Jack Henion,** Cornell University/Advion Biosciences, Ithaca, NY  
*Chip-Based NanoElectrospray Screening of Biological Samples for Disease Biomarkers*

9:30 - 10:00 AM **James Kapron,** Ioalytics Corporation, Ottawa, Canada  
*Targeted Bioanalysis with LC-FAIMS-MS (and MS/MS)*

10:00 - 10:30 AM **Carsten Baessmann,** Bruker Daltonik, Bremen, Germany  
*Metabolic Profiling and Characterization of Potential Biomarkers in Biological Fluids using LC-MS-NMR*

**10:30 - 10:45 AM** **BREAK**

10:45 - 11:15 AM **Joseph Dalluge,** Cargill, Inc., Minneapolis, MN  
*Discovery of Novel Enzymatic Activity Using Stable Isotope Metabolite Labeling and LC/MS*

11:15 - 11:45 AM **Jennifer Granger,** Waters Corporation, Milford, MA  
*A Metabonomics Time Course Analysis of Zucker Rat Urine using UPLC-MS (TOF)*

**12:00 - 2:00 PM** **Asilomar lunch.** *Crocker Dining Hall. Meal ticket required.*

1:30 - 2:00 PM **Speakers,** please connect laptops to LCD projectors. *Chapel*

**2:00 – 3:30 PM** **TECHNOLOGY**

2:00 - 2:30 PM **Marlin Friesen,** International Agency for Research on Cancer, Lyon, France  
*Measurement of Metabolite Induced Ser-249 TP53 Mutation by Short Oligonucleotide Mass Analysis (SOMA): A Mass Spectrometric Approach to Mutation Analysis*

2:30 - 3:00 PM **Laszlo Boros,** SIBDMAP/UCLA Medical Center, Los Angeles, CA  
*Metabolic Profiling Using Stable Isotope Tracer Technology GC/MS*

3:00 - 3:30 PM **Mark O'Neil-Johnson,** Sequoia Sciences, San Diego, CA  
*Accelerated Structure Elucidation Using FT/MS and CapNMR Spectroscopy*

**3:30 - 6:00 PM** **POSTER VIEWING**

**6:30 PM** **BANQUET** for all registrants and registered guests, *Seascape in Crocker Dining Hall, ticket required. Please go directly to the Seascape entrance – to the right of the main dining hall entrance.*

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**Tuesday Morning, October 21**

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**7:30 - 9:00 AM** **Asilomar breakfast for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required. Box lunches will be available at the door as you depart breakfast.*

**12:00 - 1:00 PM** **Asilomar lunch for on-site lodgers.** *Crocker Dining Hall. Asilomar meal ticket required. Depart at leisure.*

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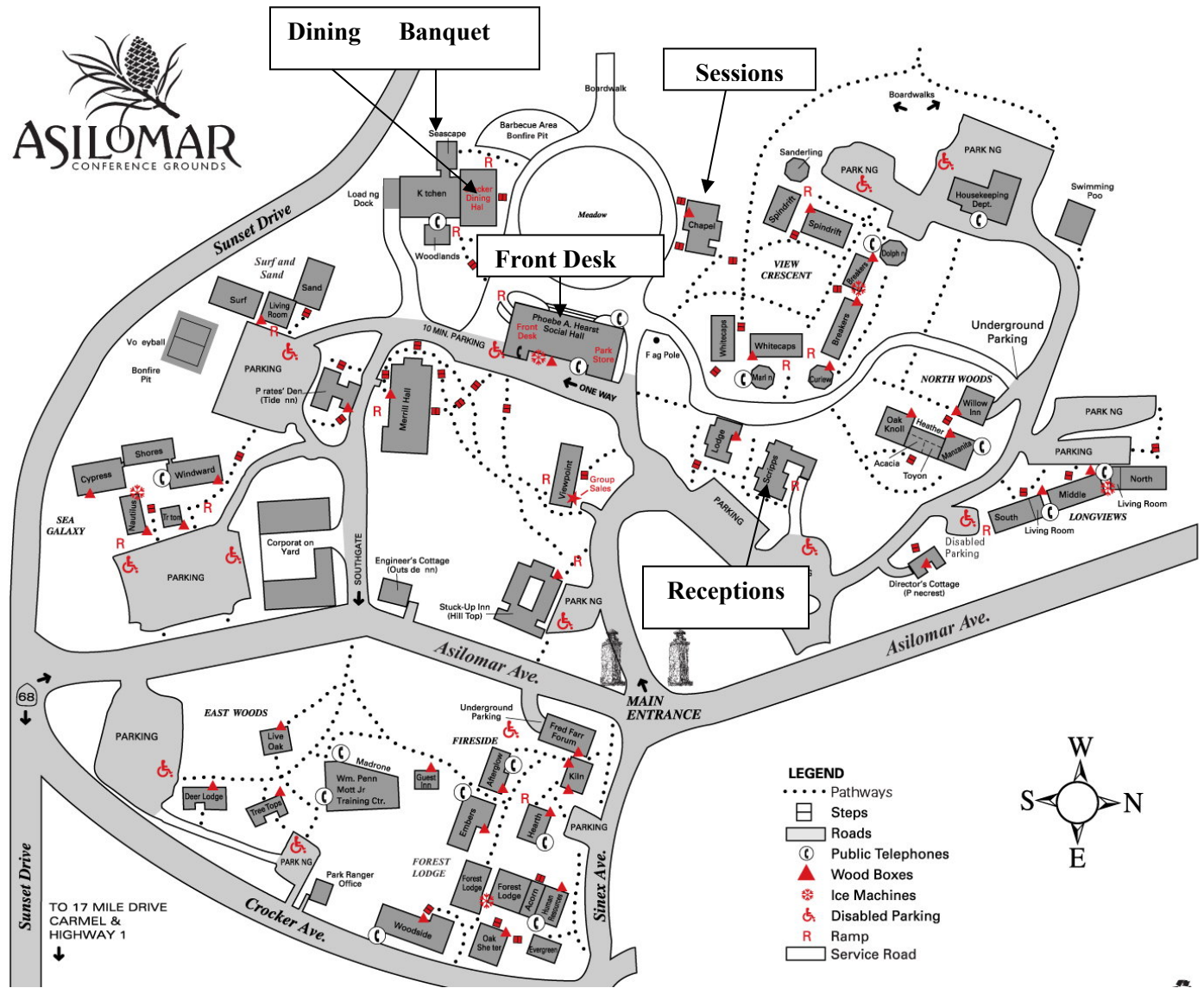
## POSTER PRESENTATIONS

Please set up Friday evening in the Chapel and remove at 5:30 PM on Monday

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**We wish to thank Taylor Technology and Eksigent Technologies for their support.**

- 1. Mass Spectrometric Approaches to Carbohydrate Metabolomics in Wheat;** S. J. Robinson<sup>a</sup>; M. Seymour<sup>b</sup>; J. E. Thomas-Oates<sup>a</sup>; *a Department of Chemistry, University of York, Heslington, York, England, Syngenta, Jealott's Hill, International Research Centre, Bracknell, England.*
- 2. Application of the Accurate Mass and Time (AMT) Tag Approach to Global Metabolomics Studies of Microbial Systems;** Thomas O. Metz; *Pacific NW National Laboratory, Richland, WA.*
- 3. Chemical Derivatization and Data Analysis Approaches to Metabolite Profiling;** Grace Tong; *The Scripps Research Institute, La Jolla, CA.*
- 4. Metabolic Profiling of Pancreatic Islets and a Novel Ionization Method for Mass Spectrometric Analysis of Metabolite Mixtures;** Brian Frey; *University of Wisconsin, Madison, WI.*
- 5. Determination of Carnitine and Acylcarnitines in Biological Matrices by HPLC/ESI/MS;** Paul E. Minkler; *Louis Stokes VA Medical Center, Cleveland, OH.*
- 6. LC-MS and CE-MS Approaches for the Analysis of Biologically Generated Pharmaceutical Metabolites;** Emma Edwards, Ed Bergstrom, Desmond O'Connor, David Goodall, Jane Thomas-Oates; *Department of Chemistry, University of York, Heslington, York, England, Merck Sharpe & Dohme Research Laboratories, Neuroscience Research Centre, Harlow, Essex, UK.*
- 7. Methyltransferome to Metabolites: The Use of Metabolomics in the Identification of the Major Substrate (3-isopropylmalate) for a Know *Saccharomyces Cerevisiae* Enzyme (Tras-Aconitate Methyltransferase);** Darren Dumlao; *University of California, Los Angeles, CA.*
- 8. Perillyl Alcohol, A Model Substrate for Multiple Phase I and Phase II Metabolic Profiling;** Zhihong O'Brien; *Ligand Pharmaceuticals, Inc, San Diego, CA.*
- 9. MALDI triple Quadrupole MS for Small Molecule Quantitation and Screening in Biological Samples;** Lekha Sleno and Dietrich A. Volmer; *National Research Council, Halifax, NS, Canada*
- 10. Isolation and Identification of Two Forms of Malonyl-CoA in Commercial Malonyl-CoA;** Charles L. Hoppel; *Louis Stokes VA Medical Center, Cleveland, OH.*
- 11. Ammonia Metabolism in Mosquitoes Examined by Mass Spectrometry in Multiple-reaction Monitoring Mode;** Qingfen Zhang, \*Patricia Y. Scaraffia Vicki H. Wysocki and \*Michael A. Wells; *Department of Chemistry. \*Department of Biochemistry & Molecular Biophysics, University of Arizona, Tucson, AZ.*
- 12. A Novel Approach to Achieve High Mass Accuracy for LC/MS Metabolite Identification;** Ming Gu; *Cerno Bioscience, New Haven, CT.*
- 13. Measurement of Urinary Psychosine using ESI-MS<sup>2</sup>;** Andrew J. Norris, Arman Yaghoubian, Apryl A. Chang, Julian P. Whitelegge, Claire Fluharty, Arvan Fluharty, Mai M Brooks, Kym F. Faull; *The Pasarow Mass Spectrometry Laboratory, The Johnson Comprehensive Cancer Center, The Developmental Disabilities Immersion Program, and The Department of Psychiatry and Biobehavioral Sciences, UCLA, Los Angeles, CA.*



- LEGEND**
- ..... Pathways
  - Steps
  - ▬ Roads
  - Ⓞ Public Telephones
  - ▲ Wood Boxes
  - ❄ Ice Machines
  - ♿ Disabled Parking
  - R Ramp
  - ▭ Service Road



## MONTEREY BAY ATTRACTIONS

**The Monterey Peninsula is a perfect place** for a romantic weekend or exciting adventure. There are so many year-round activities, that you're limited only by your time and sense of adventure.

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 and hotels.

Carmel Valley is home to many wineries, farms, ranches. 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			
<b>Carmel Walks</b> <i>Stroll Thru Secret Pathways, Courtyards, Gardens &amp; Enchanting Fairytale Cottages</i>	P.O. Box 975	Carmel	(831) 642-2700
<b>Chris' Whale Watching &amp; Fishing Trips</b>	48 Fisherman's Wharf	Monterey	(831) 375-5951
<b>Fishermans Wharf</b>	140 W. Franklin St.	Monterey	(831) 649-6544
<b>Monterey Bay Aquarium</b>	886 Cannery Row	Monterey	(831) 648-4888
<b>Monterey Bay National Marine Sanctuary</b>	299 Foam St., Suite D	Monterey	(831) 647-4201
<b>Monterey Bay Scenic Tours</b> <i>A new premier "Multimedia" bus tour of the Monterey Peninsula! Hear the narration in your language!</i>	406 Calle Principal	Monterey	(831) 372-MBST (6278)
<b>Monterey Bay Whale Watch</b>	P.O. Box 52001	Pacific Grove	(831) 375-4658
<b>National Steinbeck Center</b>	One Main St.	Salinas	(831) 775-4725
<b>Pacific Yachting &amp; Sailing</b>	790 Mariner Park Way	Santa Cruz	(800) 374-2626
<b>Santa Cruz Beach Boardwalk</b>	400 Beach St.	Santa Cruz	(831) 423-5590

## ACMS PARTICIPANT SURVEY

*Metabolite Profiling: Biomarker Discovery, Drug Efficacy, and Fundamental Biochemistry*

*Please give to registrar before you depart or send to:*

*ASMS, 2019 Galisteo St. Bldg. I, Santa Fe, NM 87505. Fax: 505 989 1073*

Circle 1 - 4 in each category

Poor

Fair

Good

Excellent

### CONFERENCE CONTENT

Topics covered.....1.....2.....3.....4

Discussion.....1.....2.....3.....4

Speakers.....1.....2.....3.....4

Posters.....1.....2.....3.....4

Comments:

### FORMAT

Talks.....1.....2.....3.....4

Discussion.....1.....2.....3.....4

Posters.....1.....2.....3.....4

Comments:

### ORGANIZATION

Value with respect to fee charged.....1.....2.....3.....4

Facilities.....1.....2.....3.....4

Comments:

Did the Conference content meet your needs on the topic?     Yes     No

Comments:

Suggested topic(s) for future conferences: