

24th ASILOMAR CONFERENCE on MASS SPECTROMETRY

Sponsored by
American Society for Mass Spectrometry

NEW METHODS, INSTRUMENTATION, AND APPLICATIONS OF ION TRAPS

Friday, October 10 - Tuesday, October 14, 2008
Asilomar Conference Center, Pacific Grove, CA

Program Chairs

Jennifer Brodbelt

University of Texas, Austin

Alan Marshall

NHMFL, Florida State University

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ACMS Committee

Veronica Bierbaum

University of Colorado

Robert B. Cody

JEOL USA, Inc.

Facundo Fernandez

Georgia Institute of Technology

Barbara Larsen

DuPont

GENERAL INFORMATION

Internet Access. There is complimentary wi-fi access in the Administration Building.

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. 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 at Asilomar. Should you wish to take your lunch to the beach, please go to the regular lunch window and request a “To-Go Lunch”. Special box lunches (for pick-up at breakfast) are available, if reserved 48 hours in advance.

Program Overview.

Friday	Evening Session	7:00 – 10:00 pm
Saturday	Morning Session	9:00 – 11:50 am
	Afternoon Session	1:00 – 3:15 pm
	Evening Session	7:00 – 10:00 pm
Sunday	Morning Session	9:00 – 11:50 am
	Evening Session	7:00 – 10:00 pm
Monday	Morning Session	9:00 – 11:50 am
	Afternoon Session	1:00 – 3:15 pm

Poster Presenters. Please set up your poster display on Friday during the evening reception, 8:20 – 10:00 pm. Boards are numbered. See poster list on pages 12-13 to learn your assigned board space.

Speakers. Please arrive in the Chapel, session room, 15-30 minutes prior to the start of the session to set up your laptop computer.

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 pages 12-13 of this program for suggested activities or visit the Front Desk/Administration Hall building where many maps and brochures are available.

CONFERENCE SPONSORS

Evening Reception Sponsors

Applied Biosystems/MDS Analytical Technologies

Shimadzu

Waters Corporation

Banquet Wine Sponsor

Thermo Scientific

CONFERENCE INTRODUCTION

New Methods, Instrumentation, and Applications of Ion Traps

Ion trap technology and its applications remain at the peak of an unsurpassed period of development. The emergence of an array of new ion trapping instruments, including linear ion traps, multipole traps, Orbitrap, miniature traps, and hybrid devices, as well as the increasing mass accuracy of FT-ICR instruments due to advances in high-field magnets, trap designs and innovative application of trapping potentials, have propelled ion trap methods to the forefront. Ion trap mass spectrometers have also had enormous impact on proteomics, glycomics, metabolomics, drug discovery, biomarker discovery, and numerous other emerging fields. The Asilomar Conference 2008 will bring together leaders in the development of ion trap instrumentation, methods, and applications, to share recent findings and stimulate future discoveries.

FRIDAY, OCTOBER 10, 2008

3:00 pm **Guest Room Check-in**, *Asilomar Main Lobby*

4:00 – 6:00 pm **Conference Registration**, *Asilomar Main Lobby*

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

Evening presenters should arrive in the Chapel (session room) by 6:45 pm to set up laptops.

7:00 – 10:00 pm **OPENING SESSION**, *Chapel*
Session Chair: Jennifer Brodbelt, *University of Texas, Austin*

7:00 – 7:05 pm Opening Remarks

7:05 – 7:40 pm **Alan G. Marshall**, *NHMFL, Florida State University*
Ions in Jail: Capture, Control, Transformation, and Release

7:40 – 8:15 pm **Eugene Nikolaev**, *The Institute for Energy Problems*
Computer Simulations of Ion Cloud Motion in Ion Traps: Current Status and Perspective

8:15 – 8:20 pm Remarks from **Waters Corporation**
Sponsor of tonight's reception

8:20 – 10:00 pm **Evening Reception** *sponsored by Waters Corporation*

Posters should be mounted during reception, thank you.

[REACTION]

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SATURDAY, OCTOBER 11, 2008

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) at 8:30 am to set up laptops.

9:00 – 11:50 am **Ion Activation**, *Chapel*
Session Chair: Mary Rodgers, *Wayne State University*

- 9:00 – 9:35 am **Jennifer Brodbelt**, *University of Texas at Austin*
Novel Photodissociation Strategies for Ion Traps
- 9:35 – 10:10 am **James P. Reilly**, *Indiana University*
Vacuum Ultraviolet Photofragmentation of Peptide and Glycan Ions in Ion Trap and Hybrid Instruments
- 10:10 – 10:40 am Coffee Break **and** Group Photo
- 10:40 – 11:15 am **Scott A. McLuckey**, *Purdue University*
Ion/Ion Reactions: New Methodologies and New Chemistries in Linear Ion Traps and Hybrid Ion Trap/Beam-type Tandem Mass Spectrometers
- 11:15 – 11:50 am **Ryan Julian**, *University of California, Riverside*
Hitting the Nail on the Head: Photoinitiated Radical Directed Dissociation in a Linear Ion Trap
- 12:00 pm – 1:00 pm** **Asilomar Lunch for all participants**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Afternoon presenters should arrive in the Chapel (session room) by 1:45 pm to set up laptops.

1:00 – 3:15 pm **Biological Applications**, *Chapel*
Session Chair: Julie Leary, *University of California, Davis*

- 1:00 – 1:35 pm **Carlito Lebrilla**, *University of California, Davis*
Clinical Glycomics with FT ICR Methods: Implications to Maintaining Health and Disease Marker Discovery
- 1:35 – 2:10 pm **Carol Nilsson**, *Pfizer, Inc.*
Quantitative Cancer Stem Cell Phosphoprotein Profiling by Use of Tandem Mass Tags and LC-MS/MS in an LTQ-Orbitrap
- 2:10 – 2:40 pm Coffee Break
- 2:40 – 3:15 pm **Ljiljana Pasa-Tolic**, *Pacific Northwest National Laboratory*
FTICR MS Optimization for the Analysis of Intact Proteins
- 6:00 – 7:00 pm** **Asilomar dinner for on site lodgers**, *Crocker Dining Hall.*
Asilomar meal ticket required.

SATURDAY EVENING, OCTOBER 11, 2008

Evening presenters should arrive in *Chapel* by 6:45 pm to set up laptops.

7:00 – 10:00 pm	Spectroscopy, Chapel Session Chair: John Eyler, <i>University of Florida</i>
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7:00 – 7:35 pm	Rebecca Jockusch , <i>University of Toronto</i> Optical Spectroscopy of Gas Phase Ions Isolated in a QIT
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7:35 – 8:10 pm	Valerie Gabelica , <i>Université de Liège</i> IR and UV Spectroscopy of DNA Ions Stored in Trap Instruments
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8:10 – 8:15 pm	Remarks from Shimadzu <i>Sponsor of tonight's reception</i>
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8:15 – 10:00 pm	Evening Reception <i>sponsored by Shimadzu</i>
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Poster Session. Presenting authors will be attending posters.
Please see list of posters on pages 12-13.



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SUNDAY, OCTOBER 12, 2008

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers, Crocker Dining Hall.**
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) at 8:30 am to set up laptops.

9:00 – 11:50 am **Instrumentation I**
Session Chair: Gary Kruppa, *Bruker Daltonics*

9:00 – 9:35 am **Chris Hendrickson, NHMFL, Florida State University**
SIMION Modeling of Ion Image Charge for FT-ICR Trap Optimization

9:35 – 10:10 am **Alexander Makarov, Thermo Fisher Scientific**
Recent Developments of the Orbitrap Technology

10:10 – 10:40 am Coffee Break

10:40 – 11:15 am **James Hager, MDS Analytical Technologies**
Recent Advances in QTRAP Technology

11:15 – 11:50 am **James E. Bruce, University of Washington**
Trap Design: Control and Correction of Ion Kinetic Energy

12:00 pm – 1:00 pm **Asilomar Lunch for all participants, Crocker Dining Hall.**
Asilomar meal ticket required.

1:00 – 6:00 pm **Free Time, please see page 14 for sightseeing activities.**

6:00 – 7:00 pm **Asilomar dinner for on site lodgers, Crocker Dining Hall**
Asilomar meal ticket required.

SUNDAY EVENING, OCTOBER 12, 2008

Evening presenters should arrive in the Chapel (session room) at 6:45 pm to set up laptops.

7:00 – 10:00 pm Emerging Methods
Session Chair: David Russell, *Texas A&M University*

7:00 – 7:35 pm **Evan Williams**, *University of California, Berkeley*
Nanodrops in Ion Storage Devices: A Route to Understanding Ion Chemistry in Aqueous Solution

7:35 – 8:10 pm **Hilkka Kenttamaa**, *Purdue University*
Petroleum Characterization by Laser-induced Acoustic Desorption/Chemical Ionization/FT-ICR Mass Spectrometry

8:10 – 8:45 pm **David Muddiman**, *North Carolina State Univ*
New Ionization Sources for Biological Mass Spectrometry

8:45 – 8:50 pm Remarks from **Applied Biosystems/MDS Analytical Technologies**.
Sponsor of tonight's reception.

8:50 – 10:00 pm Evening Reception sponsored by *Applied Biosystems/MDS Analytical Technologies*.

Poster Session. Presenting authors will be attending posters.
Please see list of posters on pages 12-13.

SPONSOR OF SUNDAY EVENING RECEPTION



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MONDAY, OCTOBER 13, 2008

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) at 8:30 am to set up laptops.

9:00 am – 11:50 am **Instrumentation II**
Session Chair: Daniel Austin, *Brigham Young University*

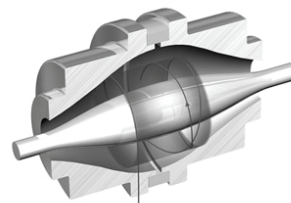
- 9:00 – 9:35 am **Donald J. Douglas**, *University of British Columbia*
Linear Quadrupole Ion Traps with Added Multipole Fields
- 9:35 – 10:10 am **Jae C. Schwartz**, *Thermo Fisher Scientific*
Design and Performance Aspects of a Dual Cell Linear Ion Trap
- 10:10 – 10:40 am Coffee Break
- 10:40 – 11:15 am **Li Ding**, *Shimadzu Research Laboratory*
Coupling Between Digital Ion Traps for Multi-Channel / Dimensional Tandem Mass Analysis
- 11:15 – 11:50 am **Zheng Ouyang**, *Purdue University*
Special Modes of Trapping, Isolating and Mass-analyzing Ions using Rectilinear Ion Traps
- 12:00 – 1:00 pm** **Asilomar lunch for all participants**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Afternoon presenters should arrive in the Chapel (session room) at 8:30 am to set up laptops.

1:00 – 3:15 pm **Ion Activation II**
Session Chair: Richard Vachet, *University of Massachusetts*

- 1:00 – 1:35 pm **Gary L. Glish**, *University of North Carolina*,
Ion Activation with Photons and Electrons in rf-Ion Traps
- 1:35 – 2:10 pm **Joshua Coon**, *University of Wisconsin*
Why Hybrids with Multiple Ion Traps and Multiple Dissociation Methods Will Transform Protein Sequence Analysis
- 2:10 – 2:40 pm Coffee Break
- 2:40 – 3:15 pm **Yury Tsybin**, *Ecole Polytechnique Fédérale de Lausanne*
Amino Acid Nature Effect on Intramolecular Energy Relaxation upon Ion Activation and Dissociation
- 6:30 pm – The End** **Banquet**, *Seascape Room (to the **RIGHT** of Crocker Dining Hall).*
Banquet ticket required.
Wine served at the Banquet is sponsored by Thermo Scientific.

Come learn about our latest, exciting developments in ion trap technology!



Sunday, October 12

9:35 - 10:10 am

Alexander Makarov, "Recent Developments of the Orbitrap Technology"

Monday, October 13

9:35 - 10:10 am

Jae C. Schwartz, "Design and Performance Aspects of a Dual Cell Linear Ion Trap"

Visit www.thermo.com/ms to learn about our newest technologies

Be sure to join us at the closing banquet! We'll see you there.

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POSTERS

Board Space *Posters should be mounted Friday evening during the reception. Thank you.*

1. Identification of Phosphorylated Sites on Proteins with High Mass Accuracy Using the LTQ-Orbitrap; Armann Andaya, William Jewell, Weitao Jia, John W. B. Hershey, Julie A. Leary; *University of California, Davis*.
2. Planar Electrode Ion Traps; Daniel E. Austin¹, Brett J. Hansen¹, Aaron R. Hawkins¹, Ivan Miller¹, Ying Peng¹, Zhiping Zhang¹, and Samuel Tolley²; ¹*Brigham Young University*, ²*Torion Technologies, Inc.*
3. Detection of Oligonucleotide Gas-Phase Conformers: H/D Exchange and Ion Mobility as Complementary Techniques; Dorothee Balbeur¹, Joëlle Widart¹, Bernard Leyh¹, Laetitia Cravello³ and Edwin De Pauw¹; ¹*University of Liège, Belgium*; ²*Waters Corporation, Manchester, UK*.
4. Imaging Single Particles & Biomolecules with Xray Lasers: Opportunities for Ion Trap Technology; Michael J. Bogan; *Stanford PULSE Institute, Menlo Park, CA*.
5. Development of a Broadband Cryo-Detection System for FT-ICR MS; Myoung Choul Choi¹, Seung Yong Kim¹, Stefan Stahl², Jong Shin Yoo¹, and Hyun Sik Kim¹; ¹*Korea Basic Science Institute, Republic of Korea*; ²*Stahl Electronics Co., Germany*.
6. Using a Pulsed Gas to Increase the Fragmentation Efficiency of Ions in the MS³ Mode of Operation in a Low Pressure Linear Ion Trap; Bruce Collings; *MDS Analytical Technologies; Concord, ON, Canada*.
7. Measurement of Momentum Transfer Collision Cross Sections by Analysis of Fourier Transform Ion Cyclotron Resonance Linewidths as a Function of Damping Gas Pressure; David V. Dearden; *Brigham Young University, Provo, UT*.
8. Selective Photodissociation of Chemically Cross-linked Peptides in Quadrupole Ion Traps; Myles W. Gardner, Jennifer S. Brodbelt; *The University of Texas at Austin, TX*.
9. Methods to improve the Extraction Efficiency and Resolution of the Mass Selective Axial Ejection from a Linear Quadrupole Ion Trap; Mircea-Michael Guna, Tom Biesenthal, James. W. Hager; *MDS Analytical Technologies*.
10. Quantitation of iTRAQ-labeled IκB-α Protein in the Quadrupole Ion Trap on a Chromatographic Time-Scale; Unige A. Laskay, Shannon L. Cook, Csaba F. Laszlo, Shiyong Wu, Glen P. Jackson; *Ohio University*.
11. Data-dependent Supplemental Activation to Enhance ETD Efficiency for High m/z Precursors Regardless of Charge; Aaron R. Ledvina; Graeme C. McAlister; and Joshua J. Coon; *University of Wisconsin at Madison, WI*.
12. Investigating Hydrogen Atom Migration in Peptide Radicals Generated by Photodissociation in a Linear Ion Trap; Tony Ly, Ryan R. Julian; *University of California, Riverside, CA*.

POSTERS

Board Space

Posters should be mounted Friday evening during the reception. Thank you.

13. A Multi Reaction Cell, ETD-enabled Orbitrap Mass Spectrometer; Graeme C. McAlister and Joshua J. Coon; *University of Wisconsin at Madison, WI.*
14. QIT Glycan Sequencing: Simplicity from Perceived Complexity; Vernon Reinhold; *University of New Hampshire, Durham, NH.*
15. The Development of a New Approach to Tandem Mass Spectrometry Based Upon the Emerging Technology of Electrostatic Ion Traps; Vasiliy Goncharov, Yu Chen, Mary T. Rodgers, and A. G. Suits; *Wayne State University, Detroit, MI.*
16. A Mechanistic Study of the H/D Exchange Reactions of Protonated Arginine and Arginine-containing di- and tri-peptides; Yiqun Huang, Joe A. Marini, John A. McLean*, Shane E. Tichy, David H. Russell; *Texas A&M University, College Station, TX;*
*Current address: *Vanderbilt University, Nashville, TN.*
17. Current Perspectives on Fourier Transform Imaging Mass Spectrometry; Donald F. Smith¹, Ioana M. Barbu², Marc C. Duursma¹, Ron M.A. Heeren¹; ¹*FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands;* ²*LUMC, Leiden, The Netherlands*
18. ETD of Positively Charged DNA in a Linear Ion Trap; Suncerae Smith, Jennifer S. Brodbelt; *University of Texas at Austin, TX.*
19. Mass-based Classification (MBC) of Phosphorylated and Nonphosphorylated Peptides using an Open-access Table of Accurate Precursor Ion Mass Values; Bernhard Spengler, Alfons Hester; *Justus Liebig University Giessen, Germany.*
20. Investigation of Transferrin Structure via Novel Electron Capture Dissociation Techniques using a Hybrid Linear Ion Trap Time-of-Flight Mass Spectrometer; M. Alexander Shaw¹, Makoto Hashimoto², Masaki Watanabe², Akira Tsuboyama¹, Chad Ostrander¹; ¹*Hitachi High-Technologies America, Inc., Dallas, TX;* ²*Naka Applications Center, Hitachi High-Technologies, Ibaraki, Japan.*
21. Micro-fabrication and Testing of Cylindrical Ion Trap Mass Spectrometer Arrays; Friso H.W. van Amerom, Ashish Chaudhary, John Bumgarner, and R. Timothy Short; *SRI International, St. Petersburg, FL*
22. Excite-coupled Trapping Ring Electrode Cell: A Novel Approach for Linearization of Radio Frequency Excitation and DC Trapping Electric Fields; Chad R. Weisbrod, Gunnar E. Skulason, Nathan K. Kaiser, James E. Bruce; *Washington State University, Pullman, WA.*
23. N-linked Glycosylation Profiling of Pancreatic Cancer Serum Using Capillary LC-MS (MS) and MALDI QIT TOF MS; Fan Xiang², Jia Zhao¹, Scott A. Kuzdzal³, David M. Lubman¹; ¹*University of Michigan, Ann Arbor, MI,* ²*Shimadzu Biotech, Pleasanton, CA,* ³*Shimadzu Scientific Instruments, Columbia, MD.*
24. Ion Trap Operation at High Pressures; Wei Xu, Qingyu Song, William Chappell, Graham Cooks, Zheng Ouyang; *Purdue University, West Lafayette, IN.*



MONTEREY BAY AREA 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 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.

Carmel Walks	P.O. Box 975	Carmel, CA	(831) 642-2700
Chris' Whale Watching & Fishing Trips	48 Fisherman's Wharf	Monterey, CA	(831) 375-5951
Fishermans Wharf	140 W. Franklin St.	Monterey, CA	(831) 649-6544
Monterey Bay Aquarium	886 Cannery Row	Monterey, CA	(831) 648-4888
Monterey Bay National Marine Sanctuary	299 Foam St., Suite D	Monterey, CA	(831) 647-4201
Monterey Bay Scenic Tours	406 Calle Principal	Monterey, CA	(831) 372-6278
Monterey Bay Whale Watch	P.O. Box 52001	Pacific Grove, CA	(831) 375-4658
Monterey Wine Festival	140 W. Franklin St.	Monterey, CA	(831) 649-6544
National Steinbeck Center	One Main St.	Salinas, CA	(831) 775-4725
Pacific Yachting & Sailing	790 Mariner Park Wy	Santa Cruz, CA	(800) 374-2626
Santa Cruz Beach Boardwalk	400 Beach St.	Santa Cruz, CA	(831) 423-5590

Additional information on local sights and the Asilomar State Beach may be found in the Administration Building of the Asilomar Conference Center.