

NEWS AND VIEWS



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Announcements

For more information and online registration for any of the conferences listed below, please visit www.asms.org/conferences.

ASMS Asilomar Conference Impact of Metabolomics in Translational and Clinical Research

September 29 - October 3, 2017

Asilomar Conference Center
Pacific Grove, California

www.asms.org/conferences/asilomar-conference



Organizers

Timothy J. Garrett, *University of Florida and Southeast Center for Integrated Metabolomics*

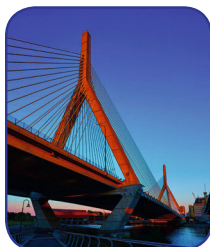
Christopher Petucci, *Sanford Burnham Prebys Medical Discovery Institute*

ASMS Fall Workshop Top-Down Proteomics

November 2 - 3, 2017

Hyatt Regency Boston Harbor
Boston, MA

<http://www.asms.org/conferences/fall-workshop>



Organizers

Ying Ge, *University of Wisconsin-Madison*

Ljiljana Paša-Tolić, *Pacific Northwest National Laboratory*

ASMS Sanibel Conference Computational Methods: Modelling Structure and Reactivity in Mass Spectrometry and Ion Mobility Experiments

January 25 - 28, 2018

Hilton St. Petersburg Bayfront Hotel
St. Petersburg, Florida

<http://www.asms.org/conferences/sanibel-conference>



Organizers

Iain Campuzano, *Amgen*

Frank Sobott, *University of Antwerp*

Michael van Stipdonk, *Duquesne University*

ASMS Diversity and Outreach Working Group

At the 2016 ASMS Conference, the ASMS Board led by Susan Weintraub, invited several members to a meeting to discuss forming a Diversity and Outreach Working Group. Several ideas on enhancing diversity across many areas of the society were discussed, and it was decided that the working group should submit a Workshop proposal for the 2017 ASMS Conference, organized by Ben Garcia and Renā Robinson. At this inaugural workshop, short talks were given by Renā Robinson, Livia Eberlin and Hilda Hernandez-Barry that crossed between their personal journeys into science and their cutting-edge research. Additionally, a Panel Discussion that also included Lisa Jones, led an open forum of the planned initiatives of the Diversity and Outreach Working Group to solicit feedback from the ASMS community. There were a number of suggestions provided by the ASMS community regarding mentorship for students, scholarship programs for undergraduates, website and social media presence for diverse groups, training for postdoctoral associates, sharing of best practices across institutions, and K-12 outreach activities. Importantly, several workshop attendees agreed to be a part of the committees necessary to help implement the programs. Currently, the primary initiatives underway by the Working Group include a summer undergraduate research fellowship program, a “Faces of MS” interview website feature, a postdoctoral speaker program, and a 2018 ASMS Conference tutorial lecture to be given by a diversity-oriented speaker. Proposals on these initiatives are being submitted to the ASMS board this summer. The ASMS Diversity and Outreach Working Group includes Jenny Brodbelt, Livia Eberlin, Facundo Fernandez, Francisco Fernandez-Lima, Ben Garcia, Hilda Hernandez-Barry, Lisa Jones, Jessica Prenni and Renā Robinson.

The Working Group is interested in your feedback and suggestions, and also your commitment in helping to carry forth the initiatives. Feel free to contact Ben Garcia (bgarci@mail.med.upenn.edu) or Renā Robinson (rena@pitt.edu) to get connected.

Contributed by Prof. Ben Garcia (University of Pennsylvania) and Assoc. Prof. Renā Robinson (University of Pittsburgh)

JASMS Editors at ASMS



JASMS Editors (from left to right): Gavin Reid, Joyce Neff, Lingjun Li, David Russell, Veronica Bierbaum, Jennifer Brodbelt, Richard O’Hair and Joe Loo.

The *JASMS* Editors held their annual meeting on Sunday, June 4, 2017, prior to the ASMS conference in Indianapolis. *JASMS* also hosted a booth in the poster/exhibition hall during the conference, where delegates had the opportunity to meet several of the Editors to informally discuss or provide feedback on the Aims and Scope and possible future directions of the journal, and to learn about submission of manuscripts for publication in the journal. Editor-in-Chief Joe Loo also presided over an evening workshop, “*JASMS* - Present Status and Future,” which discussed the “nuts and bolts” of the operation of *JASMS*, and the process of how manuscripts are handled – from the time a manuscript is first submitted to the time the paper is published in the print journal. The important role of the manuscript reviewers in this process was particularly emphasized. Feedback on potential changes to the journal, including a new journal cover design, was provided by the audience.

Meet the *JASMS* Editorial Board

Editorial Board Members are invited by the ASMS Board of Directors based on several criteria, including being a frequent contributor and reviewer for the journal. Duties of Editorial Board members include active support of the journal’s editorial functions, i.e., reviewing manuscripts, encouraging submissions to *JASMS*, creative input, and participation in the annual Editorial Board meetings that are held during the ASMS Conference. A brief biographical sketch of one of the recently appointed members of the Editorial Board is highlighted below.

Brandon T. Ruotolo is an Associate Professor in the



Department of Chemistry, University of Michigan. He earned his B.S. in Chemistry from Saint Louis University in 1999, and then received his Ph.D. from Texas A&M University in 2004 under the direction of David H. Russell. He then did postdoctoral work at the University of Cambridge with Dame Carol V. Robinson, and was awarded the first ever Waters Research Fellowship in 2008. Brandon moved to the University of Michigan in 2009, where he began his independent career.

The Ruotolo research group seeks to enable breakthroughs in structural biology and drug discovery by leveraging the potential of ion mobility-mass spectrometry (IM-MS) for the comprehensive 3D structural analysis of the proteome. To this end, Ruotolo and his team have studied the role of solvation on biomolecular structure, introduced collision induced unfolding (CIU) - a new fingerprinting technology capable of detecting the structural state of protein-ligand complexes and biotherapeutics, developed software packages for the enhanced interpretation and throughput of IM-MS and CIU data, and investigated the structural consequences of small molecule drug-like compounds on amyloid peptides. Ruotolo’s work has resulted in over 83 peer-reviewed publications, and several awards (including the ASMS Research Award in 2011).

Brandon has been a continuous ASMS member since 2000, serving as a member of several ASMS committees, including the program committee for the annual conference (one year) and the publications committee (three years). In addition, he coordinated the ASMS IM-MS interest group for three years, organizing workshops at the annual conference. He also co-organized the 2012 Sanibel Conference, which covered mass spectrometry technologies for structural biology. Brandon is currently on the board of the new Advancing Mass Spectrometry (AMS) for Biophysics and Structural Biology meeting, and is Chair of the inaugural meeting in 2017. He is an active and avid peer reviewer, having received the *Journal of the American Society for Mass Spectrometry* award for an Outstanding Reviewer in 2016, and is also a member of the editorial boards for *Analytical Chemistry* and *International Journal of Mass Spectrometry*.

Celebration of Mass Spectrometry at Purdue

A celebration of mass spectrometry at Purdue University was held June 1-3, 2017, prior to the ASMS conference in Indianapolis. Involving a mixture of presentations from prominent members of the mass spectrometry community, discussion of the future of the technology, laboratory tours, and demonstrations, the program highlighted the rich history and continuing advancements at Purdue in the development of mass spectrometry. The meeting also celebrated the recent selection of Professor R. Graham Cooks to the US National Academy of Sciences. A special Focus Section of *JASMS*, containing 20 articles contributed by his former coworkers, students and postdoctoral researchers, was presented to Prof. Cooks, a long-time member of the ASMS and a former President of the society.

(See photo on next page)



Former *JASMS* Editor-in-Chief, Prof. Michael Gross (Washington University in St. Louis) presenting Prof. R. Graham Cooks (right) the June 2017 issue of *JASMS* containing the Focus Section honoring Cooks' election to the National Academy of Sciences.

John Fenn Centennial Celebration at Yale University

A celebration of the 100th anniversary of the birth of the late Nobel Laureate, John B. Fenn, took place at Yale University on Saturday June 10, 2017. The one-day event brought to New Haven, CT an outstanding group of invited speakers, including engineers and chemists actively working in areas pioneered by Fenn (for the full program see <http://seas.yale.edu/sites/default/files/imce/other/Poster-Fenn%20Centennial-rev1.pdf>).

The first talk by Dan Neumark (UC Berkeley) described a high resolution, spectroscopic technique relating to free jet beam techniques pioneered by Fenn in his "pre-electrospray (ES)" career. Subsequent contributions focused on various aspects of ES. Mike Bowers (UC Santa Barbara) combined gas phase and atomic force microscopy to capture the essence of amyloid protein fiber formation. David Clemmer (Indiana University) dwelt on the strong dependence of the gas phase structure of peptides and proteins on their prior conformation in solution. Scott McLuckey (Purdue University) reviewed his masterful manipulations of the charge states of multiply charged ions, a truly new state of matter bequeathed to us by Fenn. The subject of secondary electrospray ionization (SESI), pioneered by Fenn's and Herb Hill's (Washington State University) groups, relies on atmospheric pressure ionization of neutral vapors, presumably by charge exchange with selected ions electrosprayed from a clean solution including volatile salts. This alternative use of the same MS type common in ESI-MS of liquid samples has developed slowly, even though it could be much faster and sensitive than conventional GC-MS. Real-time SESI was represented by two contributions focusing on sensing low concentration vapors in the atmosphere. Roderick Kunz (MIT Lincoln lab) showed how to improve the training of dogs for explosive detection. He provided insightful examples of erroneous feedback by the trainer to the dog, and showed how to overcome this difficulty by on-line monitoring of the sample

presented to the dog. Pablo Martinez-Lozano Sinués (ETH and U. Basel) described the use of on-line SESI to monitor the breath of respiratory disease patients. The initial diagnostic success of this technique was impressive, and was greatly strengthened by identification of classes of molecular markers observed as well as as expected from concrete metabolic pathways.

Fenn's position at Yale's Chemical Engineering Department deeply influenced many of his engineering colleagues. This centennial celebration included a sample of technologies dear to Fenn and born from the electrospray revolution. Presentations by Manuel Gamero (UC Irvine), Paulo Lozano (MIT), and Brad King (Michigan Tech) described electrospray sources of low-volatility liquids placed directly in vacuum. The applications were to space propulsion as well as to materials modification with nano-drops moving at many km/s. Also covered were King's studies combining electric and magnetic fields in conducting ferrofluids. These contributions connect to the interesting subject of electrohydrodynamic (EHD) mass spectrometry (K.D. Cook, *Mass Spectrometry Reviews*, 1986, 5, 467-519). Interestingly, the substitution of glycerol by far better solvents, such as room temperature molten salts, renews the potential interest of EHD MS. The fact that a considerable fraction of the ES emission *in vacuo* is often dominated by monoenergetic ions is of analytical interest, and offers a new way to directly observe the much-debated phenomenon of ion evaporation from a liquid-vacuum interface.



Partial image of the audience during the Fenn centennial held at Yale. First row: M. Johnson and D. Neumark. Second Row: M. Gamero, P. M-L Sinues, M. Bowers, D. Clemmer. Third row: A. Gomez, R. Kunz, B. King.

The final talk by Michael Zachariah (University of Maryland) connected with the field of aerosols and nanoparticles in liquids, where ion masses are typically too large to be characterized by mass spectrometry, and ion mobility of singly charged species is preferable. Of particular interest was Zachariah's use of strong pulsed electric fields to orient large ions, enabling the inference of mobility information along two different axes.

The conference was followed by a dinner where many anecdotes were shared about John Fenn that complemented the formal remarks previously made by his Yale faculty colleagues Dan Rosner and Mark Johnson (co-organizers of the centennial with Alessandro Gomez, Gary Haller, and Juan Fernandez de la Mora). Fenn's generosity with his ideas was a widely reported

trait, including his often insistent push of others to see these ideas developed elsewhere, his keen interest in people's intellectual and personal development, his Spartan frugality, his phenomenal memory, and his outstanding physical intuition, often beating his colleagues' mathematical skills. The perceived initial failure of some of Fenn's ideas (the inertia of heavy molecules mixed with light gases; ESI-MS from 1968 to 1984, SESI, etc) did not stop them from being eventually vindicated.

Among the attendants were younger collaborators of Fenn in the ESI-MS revolution, including Mike Labowsky (early development of the heated counter-flow drying scheme), Masamichi Yamashita (ESI-MS of inorganic salts), Takashi Nohmi (first high-mass industrial polymer studies), and Craig Whitehouse. Other illustrious participants from the free-jet community were Giacinto Scoles and Nobel Laureate Dudley Herschbach (via Skype).

Related Events

ASMS is pleased to offer announcements for other non-profit organizations. Please email details including website to info@asms.org.

September 4 – 7, 2017

38th British Mass Spectrometry Society Annual Meeting
Manchester, UK
www.bmss.org.uk/meetings.shtml

September 10 – 14, 2017

Mass Spectrometry Applications to the Clinical Laboratory 2017 EU
Salzburg, Austria
www.msac1.org/

September 17 – 21, 2017

HUPO 2017 Annual World Congress
Dublin, Ireland
<http://hupo2017.ie>

September 25 – 28, 2017

OurCon: Accelerating Potential for Mass Spectrometry Imaging
Doorn, The Netherlands
<https://ourcon.org/ourconV>

October 8 – 13, 2017

SciX presented by FACSS
Reno, NV
www.scixconference.org/

November 29 – December 2, 2017

30th Annual Tandem Mass Spectrometry Workshop
Lake Louise, Alberta, Canada
<http://lakelouisemsms.org/>

December 11 – 13, 2017

Seventh Asia Oceania Mass Spectrometry Conference (AOMSC2017)
Singapore
www.aomsc2017.org

January 21 – 25, 2018

Mass Spectrometry: Applications to the Clinical Laboratory
Palm Spings, CA
www.msac1.org/

March 11 - 14, 2018

US HUPO: 14th Annual Precision Proteomics Conference
Minneapolis, MN
www.ushupo.org