



AMERICAN CHEMICAL SOCIETY KENTUCKY LAKE SECTION

February 2011 Kentucky Lake Section Meeting

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Fresh Market

Paris, TN

Thursday, February 17, 2011

Social @ 5:30, Dinner @ 6:00, Presentation @ 7:00

*The Fresh Market is located at
2255 East Wood Street
Paris, TN 38242-9611*

The price is \$10 (Students \$5)

Menu – Choice of:

Grilled chicken w/ veggie & potato or fries or rice, & salad
Grilled pork chop w/ veggie & potato or fries or rice, & salad
Pasta primavera w/ salad

Presentation:

**Advanced Structural Mass Spectrometry for Systems Biology
Pulling the Needles from Haystacks**

By

John A. McLean

Vanderbilt University

See Reverse Side for Abstract & Biographical Sketch

Comments from the Chair

Thank you to everyone that attended the January meeting in Martin. It was a huge success with one of the largest turnouts we have had in awhile. Please continue to come and support your local section. As a reminder please sign up to Go Green and receive this newsletter via email by emailing me or Brent. Remember that you can get information about the section on our website and please befriend us on Facebook. Lastly, we still need volunteers to serve on committees. If you are willing please email a KLS officer.

Robbie Montgomery

KLS-ACS 2011 Officers

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KLS-ACS Web Page

<http://kentuckylake.sites.acs.org/>

Abstract

Current systems biology research entails characterizing, quantifying, and cataloging the biomolecular inventory of a sample at specific dimensions of space (*e.g.* cellular, tissue, or organism level) and time (*e.g.* point in the life cycle, healthy vs. diseased state). New measurement strategies are necessary that incorporate simultaneous omics data. Rapid (μs - ms) two-dimensional separations based-on ion mobility-mass spectrometry (IM-MS) techniques have demonstrated great utility in characterizing complex biological samples, primarily because different biomolecular classes (*e.g.* peptides, carbohydrates, oligonucleotides, lipids, etc.) adopt structures in conformation space (correlation of structures vs. m/z), which are predictable based on prevailing intramolecular folding forces. This report describes recent structural biology results for a variety of biomolecular classes including those of interest in metabolomics, proteomics, lipidomics, glycomics and genomics. These results are interpreted using molecular dynamics simulations to elucidate structural differences within a given molecular class that are consistent with the IM-MS results. For example, structural differences for carbohydrates and glycans are observed in a predictable manner for different isobaric (same mass) positional and structural isomers. Analogously, isobaric lipids of different classes (*e.g.* sphingolipids and glycerophospholipids) adopt distinct structures characteristic of the lipid class. Using these structural separations, we demonstrate spatial and temporal “omics” resolution by imaging MALDI-IM-MS and microfluidic cell trapping nESI-IM-MS, respectively, for numerous applications in life sciences and cancer biology research.

Brief Biographical Sketch

John A. McLean is presently an Assistant Professor in the Department of Chemistry at Vanderbilt University and a faculty fellow in the Institute of Chemical Biology and Institute of Integrative Biosystems Research and Education. His recent awards include an Excellence in Teaching Award from the student members of the American Chemical Society, a Defense Threat Reduction Agency Research Award, an American Society for Mass Spectrometry Research Award, a Spectroscopy Society of Pittsburgh Award, an R&D 100 Award, and the Bunsen–Kirchhoff Prize from the GDCh. He has published over 50 manuscripts in the peer-reviewed literature, 8 book chapters, and 15 patents. He and colleagues have also disseminated their research in over 250 presentations at national and international meetings. His research interests focus on the design, conceptualization, construction, and application of technologies for structural mass spectrometry, in particular for studies in structural proteomics, systems biology, biophysics, and bionanotechnology.

