ANALYTICAL SEMINAR

PROF. JOHN MCLEAN

Vanderbilt University

"Structural Separations by Ion Mobility-Mass Spectrometry: New Prospects for Complex Biological Systems

Thursday

April 9, 2009

12:15 p.m.

Seminar Hall

Following the paradigm of the human genome project, much of 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). In support of high throughput systems biology research, 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 results for a variety of biomolecular classes including those of interest in metabolomics, proteomics, lipidomics, glycomics and genomics. The aim of this work is to define the conformation space in which different classes of biomolecules are observed. Furthermore, we report molecular dynamics simulations to elucidate structural differences within a given molecular class. 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 owing to differences in the degree of coordination that the anhydrous molecules can achieve with alkali metals in competition with intramolecular hydrogen bonding forces