DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2018

DATE: THURSDAY, FEBRUARY 1, 2018

WHERE: TIERNAN HALL 373
TIME: 10:00AM

GUEST SPEAKER

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TOPIC

Advancing mass spectrometry analysis of proteins, lipids, and carbohydrates: CF-EDESI and boronic acid shift reagents

ABSTRACT

I will present two recent advances in mass spectrometry techniques for analyzing biomolecules. First, I will discuss our continuous flow-extractive desorption electrospray ionization (CF-EDESI) technique for ambient ionization. Mass spectrometry separates ions by their mass-to-charge ratio. Mass spectrometry of large proteins requires "soft" ionization techniques that won't destroy the tertiary structure of the molecules. Mass spectrometry of lipids is difficult, as it is challenging to find a solvent that holds both ions and nonpolar lipids. In CF-EDESI, a continuous flow of analyte in nonpolar solvents is delivered via hypodermic needle into the mass spectrometer, orthogonal to an electrospray source that gives ions in polar solvent B. CF-EDESI lets us control the charge state distribution of proteins by dopant super charging reagent separated from protein solution.

Second, I will discuss a new boronic acid shift reagent for mass spectrometry of carbohydrates. Mass spectrometry of carbohydrates is challenging for two reasons: carbohydrates can be difficult to ionize, and their many structural isomers can't be distinguished by mass spectra alone. Ion mobility measurements can separate isomers, but small sugar isomers are difficult due to their small collision cross section differences. Commercially available 3-carboxy-5-nitrophenylboronic acid (3C5NBA) readily derivatizes carbohydrates' 1,2-diols in aqueous solution. This bulky, charged derivative ionizes the carbohydrates, and increases the differences between carbohydrate isomers' shape and ion mobility, with up to 3-fold gain in resolution when compared to previous literature reports. Moreover, the specific MS/MS fragmentation information gathered from these sugar derivatives provided further validation of the isomers' structure.

Committee members:
Dr. Som Mitra, Dr. Nancy Jackson, Dr. Mengyan Li