2D MS/MS using Quadrupole Ion Trap Mass Spectrometry

Mr. Joseph Caruso - United States - Dept of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907

Mr. Thomas C. Sams - United States - Dept of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907

Dr. Edwin Gonzalez - United States - Teledyne FLIR Detection

Dr. Dalton Snyder - United States - Teledyne FLIR Detection

Prof. R. Graham Cooks - United States - Dept of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907

Abstract

The complexity of samples collected and analyzed outside of the laboratory is compounded by the lack of sophisticated sample clean up available in the field. One solution to this problem is use of a miniature fieldable mass spectrometer with ambient ionization. Such an instrument can provide chemically specific information for a wide range of sample types and matrix diversity with minimum to no sample clean up. 2D MS/MS is a scanning method implemented on ion traps which provides complete tandem mass spectrometric information on all ions generated from the sample. A spectrum is recorded in about a second while fragmenting each precursor ion using a supplementary ac frequency applied in the x-direction and then another much faster ac frequency scan for product ion ejection in the orthogonal y-direction. The additional dimension of information lends itself well to field-collected samples of a variety of types, including plant extracts, chemical reaction mixtures and drugs in biofluids. The 2D spectra are displayed so that for every precursor ion on the x-axis, the resultant product ions are displayed on the y-axis. 2D MS/MS can be used to identify classes of molecules through similar fragmentation patterns, especially by constant neutral loss signals which appear as diagonals, and precursor ion scans that occur as horizonal lines. Product ion scans (vertical lines on the plot) can be extracted from the 2D domain to characterize individual compounds. Ambient ionization methods like paper spray ionization lend themselves particularly well to combination with 2D MS/MS in complex sample field analysis. Figures of merit for 2D MS/MS data recorded on modified commercial ion trap instruments and on a miniature instrument are discussed. The identification of bacteria from their 2D lipid profiles is presented along with the measurements of drugs in biofluids.

Biography - Joseph Caruso

Joe is a chemistry graduate student in the Graham Cooks lab at Purdue University. His research interests center around applying miniature mass spectrometry for use in point-of-care analysis. Before grad school, Joe earned a bachelor's degree in environmental science from The University of Scranton. He then worked at a contract research organization in New Jersey, where he performed quality control testing on pharmaceutical products and medical devices using techniques such as LC-UV and GC-FID. The combination of industry and academic experience has shaped his interests in analytical chemistry and continues to guide his current research in mass spectrometry.

Keywords

Tandem mass spectrometry, Bioanalytical chemistry, Ion traps, Neutral loss scan