# Two-dimensional mass spectrometry on benchtop and portable ion trap mass spectrometers

Dalton Snyder, Lucas Szalwinski, Ryan Hilger, Robert Schrader, Valentina Pirro, R. Graham Cooks
Purdue University Department of Chemistry, West Lafayette, IN
Zachary St. John; The College of New Jersey, Ewing Township, NJ
Desmond Kaplan; KapScience LLC, Tewksbury, MA
Ryan Danell; Danell Consulting, Inc., Winterville, NC
Veronica Pinnick, Paul Mahaffy; NASA Goddard Space Flight Center, Greenbelt, MD
Mitch Wells; FLIR Systems, Inc., West Lafayette, IN

Although miniature mass spectrometers have been the subject of intense interest for nearly two decades, they have only recently become broadly available as commercialized products. Their recent availability can be attributed to important advances in atmospheric pressure sampling, vacuum system miniaturization, mass analyzer geometry optimization, miniaturization, and simplification, and the advent of highly accessible and broadly applicable ion sources. Even with these advances, the standard configuration for portable systems is still gas chromatography coupled to electron impact ionization (GC-EI) and either a quadrupole mass filter or a quadrupole ion trap for mass analysis. Portable ambient ionization systems (e.g. Mini 12, Purdue University) using ion trap mass analyzers are just beginning to emerge as the sampling, ionization, and MS/MS limitations of GC-EI are realized. Herein we argue that the paradigm shift from GC-EI to ambient ionization-ion trap should be coupled with new MS/MS scanning capabilities that we have recently demonstrated.

We describe the next generation of scan modes for portable ion trap mass spectrometers, including 1) a full set of MS/MS capabilities normally accessible only on triple quadrupole systems in addition to 2) analytically powerful two-dimensional MS/MS (2D MS/MS) scans. Firstly, we will show that all three main MS/MS scan types – namely precursor ion scans, neutral loss scans, and product ion scans – are possible on a single portable ion trap system using a combination of orthogonal double resonance excitation and ac frequency scanning. Precursor and neutral loss survey scans should be particularly valuable for detecting classes of compounds in the field; we demonstrate detection of chemical warfare agents, explosives, fentanyl analogues and other opioids, and amphetamines using a variety of ambient ionization sources. Highly multiplexed precursor and neutral loss scans – i.e. scans which traverse multiple scans lines simultaneously - are also possible in a quadrupole ion trap. Lastly, 2D MS/MS scans, in which all MS/MS data from a sample is acquired in a single scan (rather than from a *set* of scans), will also be demonstrated on these illicit samples.