

FROM SENSING TO MAKING SENSE

Two-dimensional Tandem Mass Spectrometry (2d Ms/ms) For Enhanced Target Detection And Identification On A Field-confirmatory Portable Mass Spec System

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Mass spectrometry (MS) is a gold-standard analytical technique for unknown chemical identification in the laboratory, and ruggedized portable versions have become available for field-confirmatory applications. MS is frequently hyphenated with gas chromatography (GC) in order to separate targets-of-interest from the complex environmental background present in real-world samples, to yield high-confidence confirmation of chemical identity. GC/MS has a number of advantages that have led to its widespread use both in and outside the lab, but it requires sample preparation, is time-consuming (several minutes to yield a response) and is not the ideal analyzer for low-volatility materials such as opioids and other non-traditional chemical agents. The work described here aims to develop a new field-confirmatory solution that can identify chemical agents in ad-hoc, highly cluttered environments with high probability of detection and low false/nuisance alarm rate, meeting or exceeding those of GC/MS, but with near-real time response.

The POrtable Environmental Monitoring System (POEMMS) is based on ambient ionization, or generation of ions in the ambient environment with little to no sample preparation, combined with a novel new method of performing tandem mass spectrometry (MS/MS) to generate more chemical identification information from the sample. MS/MS has been widely used for decades to detect and identify targets in complex mixtures, both with and without upfront separations. Typically, however, using MS/MS requires pre-knowledge of the target that is being monitored so that the instrument can be set up to collect the appropriate MS/MS data. Methods described in this presentation for performing two-dimensional tandem mass spectrometry (2D MS/MS) on a linear ion trap mass spectrometer allow the MS to perform complex mixture analysis without a separation step by collecting all the MS/MS data for all targets in the sample in approximately one second. This allows the method to provide detection and identification information very rapidly even for trace amounts of threats in the presence of much larger amounts of background interferences. Furthermore, by analyzing the 2D MS/MS data for indicators of certain chemical functionalities, variants of threats may be identified, even if that specific variant has not been previously programmed into the system's detection and identification algorithm. The capability for rapid (one second) complex mixture analysis offers a straightforward simplification of high fidelity field analyses supporting classification and identification of unknown threats packaged as a game-changing, easy to employ and sustain, capability for chemical and biological detection and identification and has a number of applications across DoD, DHS, and commercially.

The presentation will describe design, development, and testing of a small form-factor, fieldable MS system with ambient ionization and 2D MS/MS capability and show performance data for detection of trace levels of opioids and CWA simulants in complex matrices. Applications of the instrument for downrange chemical point detection, checkpoint screening, mobile and perimeter monitoring, and biological agent identification will be discussed.

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