

**Automated Characterization and Detection of Unknown Chemical Agents in
Battlefield Environments Using a Ruggedized Ion Trap Mass Spectrometer**

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Novel Aspect: Instrumentation and Algorithms for Automated Unknown Agent Detection

Introduction:

A new, ruggedized and integrated detection system for volatile chemical agents, liquid chemical agents and bioaerosols has been developed for use in military reconnaissance vehicles. The primary focus of the method development work for this project has been the creation of highly specific and reliable detection schemes for the most likely threat agents. Also of concern are agents that have not been prioritized and may include new designer agents. Additionally, toxic industrial chemicals that may be released during the course of a battle represent a potential chemical threat to soldiers in the field. This presentation focuses on the liquid and vapor chemical agent detection modes and the potential application of this technology to homeland defense / anti-terrorism needs.

Methods and Instrumentation:

The chemical detection scheme for this instrument employs a sequence of EI, CI, EI-MS/MS and CI-MS/MS scans to detect and identify targeted chemical agents. The full EI and CI scans are used to detect and identify interferences and so-called unknown agents. Algorithms have been developed that first determine whether any targeted agent is present based on the spectra generated from the sequence of scans. If no targeted agent is found, the EI spectrum is checked to determine if any of the known interferences are present. If no interferences are present but peaks are detected above a specified detection threshold, an unknown agent is declared and a detection method

is automatically generated based on the EI and CI spectra to allow for subsequent detection and identification of that unknown agent.

Preliminary Data:

The algorithm to identify 23 targeted agents including nerve, blister and riot control agents has been evaluated using dilute agents in a RDTE laboratory. Common battlefield interferences such as diesel fuel, jet fuel and fog oil have also been analyzed using this instrument. An algorithm to identify common hydrocarbon interferences was created to allow the system to notify the user that interferences were detected.

An additional algorithm was required to allow the system to automatically detect and characterize non-targeted agents (i.e. unknown agents). The algorithm developed to provide this capability has been tested with three simulants: perchloroethylene, diisopropyl phosphonate (DIMP) and dimethyl methyl phosphonate (DMMP). Detection criteria for all individual m/z channels in the EI scan are established by collection of a background buffer of 30 scans, calculation of mean abundance values for each channel, calculation of the standard deviation of the abundance for each channel and specification of the number of standard deviations that must be exceeded to trigger an unknown agent alarm. Once an alarm is triggered, peak selection criteria have been established to provide a list of peaks to be added to the monitoring algorithm for subsequent detection and identification of the unknown agent. The detection criteria and spectra associated with an unknown agent alarm are transmitted for offline expert evaluation. It is also standard procedure to collect a physical sample for more detailed chemical analysis. Results of testing of this algorithm will be discussed.

Keywords: Instrumentation; Ionization, Chemical; Ionization, Electron; Mass Spectrometry, Ion Trap Quadrupole; MS/MS;