B167 Validation of a Portable Direct Analysis in Real-Time Mass Spectrometry (DART®-MS) System for Trace Explosives Detection in the Laboratory or in the Field

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The goal of this presentation is to provide performance characteristics of a portable DART®-MS system for the rapid analysis of trace explosives.

This presentation will impact the forensic science community by providing a validation framework for the use of a portable DART®-MS system in the detection of trace explosives and smokeless powders.

The detection and identification of trace explosives is critical to counterterrorism efforts as well as the forensic analysis of post-blast residues. While techniques such as Ion Mobility Spectrometry (IMS) are capable of rapidly screening for explosives with high sensitivity, benchtop instruments with a mass spectrometer detector are preferred due to their increased specificity. Forensic science practitioners are hopeful that the recent advances in the field of Ambient Ionization Mass Spectrometry (AIMS) will provide analysts with a robust analytical solution to meet the demands of both the laboratory and the field. AIMS techniques allow for the direct analysis of samples, or surfaces containing residues, without the need for sample preparation, extraction, and/or separation, thereby increasing sample throughput and reducing backlogs issues. The most popular and promising ambient MS technique for forensic applications is DART®-MS. Forensic laboratories around the country have already applied DART®-MS to the analysis of forensic evidence such as illicit drugs, pharmaceuticals, lotions and lubricants, and chemical warfare agents. Ionsense® (in collaboration with Waters Corporation) has recently released the DART® QDa, a mobile miniaturized mass spectrometer with a DART® source. This type of instrument has the potential to improve routine forensic analyses in the laboratory as well as be a reliable tool for first responders in the field by providing rapid and accurate detection.

Before a novel analytical technique can be fully adopted by forensic laboratories for casework, a thorough validation study must be completed to establish performance characteristics. This work was completed to address many of the components required for a thorough validation study. Initial studies utilized a Design Of Experiments (DOE) to identify the parameters most influential to method optimization for the analysis of mixtures, real-world samples, and unknowns. To accomplish this, two separate studies were completed, one examining source/desorption effects and one examining mass spectrometer effects. In both instances, a two-level full factorial DOE was implemented. Results identified the relative impact that instrument parameters, such as thermal desorber temperature, DART® ionization gas, and DART® grid voltage, have on explosive response.

After completion of the DOE studies, analytical figures of merit such as Limit Of Detection (LOD), linear dynamic range, repeatability, and reproducibility were determined. In order to accurately obtain these figures, inkjet printed standards were used. Inkjet printing technology allows for the precise deposition of traces of material on a surface with great reproducibility (<1% Relative Standard Deviation (RSD)).

Explosives studied included military explosives (RDX, TNT, PETN), peroxide-based (TATP, HMTD), inorganic explosives (AN, PC), and smokeless powder components (ethyl centralite, diphenylamine, dibutyl phthalate, nitroglycerin, and n-nitrosodiphenylamine). These compounds were analyzed both as pure compounds and in complex mixtures to better understand competitive ionization effects. For most explosives, performance was comparable to laboratory-based DART®-MS systems, with LODs in the sub-nanogram range, and minimal interferences from complex matrices.

Explosives, DART®-MS, Smokeless Powders

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