B18 National Institute of Standards and Technology (NIST) Direct Analysis in Real Time Mass Spectrometry (DART®-MS) Tools for Seized Drug Analysis

Arun S. Moorthy, PhD, National Institute of Standards and Technology, Gaithersburg, MD 20899; Edward Sisco, PhD, NIST, Gaithersburg, MD 20899*

Learning Overview: After attending this presentation, attendees will have an understanding of how DART®-MS can be employed for screening seized drug evidence using updated NIST databases and software tools.

Impact on the Forensic Science Community: By leveraging the increased information content available through multiple in-source collisionally induced dissociation fragmentation spectra, drug screening using DART®-MS analysis has the potential to greatly reduce false positive presumptive identifications. This can prevent unnecessary subsequent analysis or better inform subsequent analysis, impacting resource and time management for seized drug evidence casework.

Over the past decade, forensic drug chemists have been faced with increasing case backlogs. This is in part due to the influx of synthetic opioids and other novel psychoactive substances, the complexity of which often lead to increased time required to confidently detect and identify these compounds. In an effort to speed up analyses, some laboratories have begun to implement Direct Analysis in Real Time Mass Spectrometry (DART®-MS). This technology is capable of detecting a number of forensically relevant compounds including drugs of abuse, explosives, chemical warfare agents, lotions and lubricants, and Toxic Industrial Chemicals (TICs) in seconds. While the technology shows promise, especially for forensic analysis of seized drugs, the data analysis necessary for confident presumptive identifications is currently cumbersome and impractical and often only incorporates a single, low-fragmentation spectrum.

NIST scientists have developed new tools to support the analysis of DART®-MS data, in particular, an updated NIST DART®-MS Forensics Database containing reference mass spectra measured at multiple orifice energies for several hundred compounds of interest, a software script for building custom DART®-MS databases with automated quality control measures, and an interactive software program designed specifically for interacting and searching DART®-MS databases. The updated reference DART®-MS database is freely available and is expected to be continually updated as mass spectra of drugs and other compounds of interests are acquired. The software tools are open-source and freely available. By using some or all of these tools, drug chemists can greatly improve their ability to provide presumptive identifications of seized drugs using DART®-MS, with subsequent impact on downstream confirmatory analyses.

DART®-MS, Screening, Seized Drugs

*Presenting Author