Forensics and Homeland Security Interest Group
Workshop Report
Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence
Tuesday, June 6th, 5:45 pm-7:00 pm

Coordinators: **Ruth Smith**, Department of Chemistry and Forensic Science Program, Michigan State University
J. Tyler Davidson, Department of Forensic Science, Sam Houston State University

Panel: **Mr. Edward Erisman**, Research Chemist, Mass Spectrometry Data Center, National Institute of Standards and Technology
Dr. Edward Sisco, Research Chemist, National Institute of Standards and Technology
Mr. James T. Miller, Manager, Seized Drugs Section, Houston Forensic Science Center
Dr. Ryan Bain, Forensic Research Chemist, Forensic Science Laboratory, Bureau of Alcohol, Tobacco, Firearms and Explosives

Initial/Final Attendance: 76/64
Audience Composition: academia, industry, practitioner, federal agencies

Coordinator Ruth started the workshop with brief welcoming remarks, introduced the panelists, and explained the primary goal of the workshop, which was to inform the relevant forensic and homeland security mass spectrometry community about numerous mass spectral interpretation resources developed by the National Institute of Standards and Technology (NIST). Given participant comments from previous workshops that too much time was spent on panelist presentations, the coordinators emphasized the desire for audience interaction between each brief panelist presentation.

Mr. Edward Erisman was the first panelist and he spoke about the NIST electron-ionization (EI) mass spectral library, the automated mass spectral deconvolution and identification system (AMDIS), and MS Interpreter. Coordinator Tyler performed a straw poll of the audience regarding use of AMDIS and MS Interpreter to stimulate discussion. The overwhelming majority of the audience members do not use AMDIS or MS Interpreter. Questions about the cost associated with updated NIST libraries and third-party vendors were openly discussed. There was interest expressed in online or in-person training to learn about the resources developed by NIST, such as a short course at ASMS or an online training program.

Dr. Edward Sisco was the second panelist to speak, and he discussed the direct analysis in real time mass spectrometry (DART-MS) Forensics Database and Data Interpretation Tool (DIT), which were developed to address the challenges associated with seized drug mixture analysis using DART-MS. He also spoke about project REMEDY, which is a joint effort between NIST and the Drug Enforcement Administration Special Testing and Research Laboratory (DEA-STRL) to identify and characterize emerging seized drugs submitted by forensic laboratories.

Mr. James Miller was the third panelist to speak. Mr. Miller shared his perspective on the implementation challenges associated with the mass spectrometry tools developed by NIST. His primary concern was the training associated with implementing the developed tools within a functional forensic laboratory. Mr. Miller also expressed some of the challenges that he faces from a seized drug perspective including issues with the identification of compounds absent from his version of the NIST library, isomer identification, and challenges with co-elution. There was extensive discussion about the challenges faced by production laboratories that must balance case turnaround times with challenging samples, such as the identification of novel compounds.

To demonstrate how NIST tools can be used to address some of the identified issues, Mr. Edward Erisman demonstrated the application of AMDIS and MS Interpreter to identify the substance present in de-identified authentic casework data provided by Mr. Miller. This was presented in the form of a tutorial, with Mr. Erisman demonstrating the spectral deconvolution using AMDIS and compound identification using MS Interpreter in real time.

Unfortunately, due to extensive audience feedback and discussion about the previous topics, Dr. Ryan Bain was unable to discuss the challenges faced in identification of explosives. However, Dr. Bain has agreed to serve as the Co-Chair for the 2024 workshop, in which there will be a heavier emphasis on forensic analysis of explosives and ignitable liquids.

Respectfully Submitted,
Ruth Smith (Chair 2023) and J. Tyler Davidson (Chair 2024)