K28 Development of a Web Accessible Cheminformatic Mass Spectral Database for Shared Utilization by Forensic Laboratories

Jeri D. Ropero-Miller, PhD, RTI International, 3040 Cornwallis Road, PO Box 12194, Building 3, Room 116, Research Triangle Park, NC 27709; Peter R. Stout, PhD, Center for Forensic Sciences, RTI International, 3040 Cornwallis Road, Research Triangle Park, NC 27709; Katherine N. Moore, BS, Virginia Commonwealth University, Richmond, 611 West Cary Street, #209, Richmond, VA 23220; Robert Steiner, BS, Virginia Division of Forensic Sciences, 700 North 5th Street, Richmond, VA 23219; and John M. Mitchell, PhD, and Michael R. Baylor, PhD, Center for Forensic Sciences, RTI International, 3040 Cornwallis Road, Building 3, Research Triangle Park, NC 27709-2194*

After attending this presentation, attendees will understand how to using a free web accessible library with multiple spectral methodologies will allow electronic searching and comparison of unknown spectra against verified reference spectra including nominal mass, accurate mass, NMR, and FTIR spectra which can be applied to forensic toxicology, drug chemistry, and trace evidence such as ink dyes and explosives.

This presentation will impact the forensic science community by providing a free, community driven web accessible mass spectral library cataloging a standardized collection of compounds of forensic interest analyzed by various spectral technologies, thus enabling a more definitive compound identification.

Introduction: Cheminformatic databases are used for searching unknown spectra against reference spectra and for retrieval of chemical data such as structural information. In addition to traditional mass spectra, NMR and FTIR are also included to improve compound identification in some databases. The forensic utility of these databases varied due to the existence of relevant compounds and spectral methods, data quality, accessibility, and ability to search against reference spectra. Forensic applications of these databases routinely contain spectra from traditional instrumentation, such as electron ionization (EI) mass spectrometers (MS) and do not allow for cross-searching of other spectral methods. Direct Analysis in Real Time (DART) is a novel ion source coupled to an accurate mass time-of-flight (AccuTOF™) mass analyzer DART has been primarily employed for controlled substances identification by forensic laboratories. Currently, there are no public databases that incorporate DART spectra, requiring laboratories to create in-house discipline specific library resulting in unnecessary duplicity. These in-house libraries are not readily accessible to the public.

Methods: Currently, RTI International in collaboration with Virginia Division of Forensic Sciences (VDFS) have begun the development and mass spectral population of a forensic cheminformatic database containing mass spectra, NMR and FTIR which will be Web- accessible and free for anyone with internet access. Users upload spectra through a Web portal to an editorial review board where selected, external "collaborator reviewers" evaluate the spectra based on established criteria. RTI staff, as the "database curator," also review the data and the reviewers' recommendations on whether the spectra should be accepted, rejected, or accepted with revisions. If all criteria are met the spectra is approved and moved into the cheminformatic database for

public accessibility. Otherwise, the spectra are either rejected or the contributing user may be contacted to determine if better spectra can be submitted. This multi-step, interactive forensic practitioner review process with established criteria of acceptance will help maintain the validity and reliability of the spectra. Duplicity of a compound within the cheminformatic databases can be limited or eliminated as appropriate. Inclusion of DART spectra into the database required spectral evaluation and comparison by RTI and VDFS laboratories. Several commonly altered DART parameters were investigated to determine whether enough spectral dissimilarity existed to cause a false identification in the developed database. Collection of reference drug standards at RTI using the same instrumental parameters as VDFS evaluated the inter-laboratory reproducibility. A form has been developed to systematically document and evaluate spectra under varying DART conditions and instrument parameters thus allowing the assessment of their affects on DART spectra and the matching quality within the database.

Results: The current public database consists of 2,400 EI mass spectra previously collected and maintained by the American Academy of Forensic Sciences Toxicology Section MS Database Committee and 224 compound records each with one to four DART spectra at different CID voltages collected simultaneously using function switching at VDFS. It appears that function switching sacrifices sensitivity for more spectral detail. All compounds have been analyzed and parameters documented for optimization and acceptable ranges by VDFS. Currently, the same procedures are being finalized for DART analysis at RTI.

Conclusion: Forensic laboratories that use mass spectral, NMR and FTIR technologies for forensic toxicology, drug chemistry, and trace evidence such as ink dyes and explosives may find this new Web-accessible Cheminformatic database to be a highly reliable and valid tool for identifying unknown compounds of interest.

 ** Presenting Author*

Cheminformatics, Mass Spectral Database, Collection Standardization

 ** Presenting Author*