K24 Benefits of Deconvolution Reporting Software in Forensic Toxicology

Cassandra L. Cavazos, BS, Department of Forensic Science, Sam Houston State University, 1003 Bowers Boulevard, Huntsville, TX 77341; Michael R. Manes, MS, Houston Police Department Crime Laboratory, 1200 Travis Street, Houston, TX 77002; and Monica Brady Mellon, MS, Houston Police Department Crime Laboratory, 1200 Travis Street, Houston, TX 77002*

After attending this presentation, attendees will understand how the use of Deconvolution Reporting Software (DRS) can improve efficiency in a busy toxicology laboratory.

This presentation will impact the forensic science community by decreasing the time an examiner spends performing routine data analysis and decreases the likelihood that substances are overlooked during labor-intensive manual searches.

Compounds of interest were added to the Agilent® Deconvolution Reporting Software (DRS). An existing validated procedure for the analysis of Basic, Acidic, and Neutral (BAN) drugs was used throughout the study. The method was retention-time locked for mepivacaine, one of three internal standards used in the procedure.

Deconvolution is a process by which ions are extracted from a complex Total Ion Chromatogram (TIC) and helps to identify compounds even when the target compound signal is at trace levels and/or hidden under co-eluting matrix compounds. The deconvolution reporting software for Gas Chromatography/Mass spectrometry (GC/MS) is designed to target compound analyses which combine data from the Agilent® Mass Selective Detector (MSD) Productivity ChemStation, the National Institute of Standards and Technology (NIST) Automated Mass Spectral Deconvolution and Identification Software (AMDIS), and the NIST 2008 Mass Spectral Search Program (NIST 08) into one simple report.

Over 100 of the most commonly reported drugs and metabolites were added to the DRS library. For the purpose of this evaluation, only drugs and drug metabolites were added that do not need special treatment, such as formation of a derivative. To evaluate the time taken to identify substances using the traditional (manual) and DRS approach, the same examiner evaluated a positive control blood sample containing 26 drugs. Manually, this identification process took 10-15 minutes. By comparison, the time to scan the TIC and produce the deconvolution report was less than a minute. The NIST library was searched for the components that were found in the AMDIS target library. Retention times, retention time differences, Chemical Abstracts Service (CAS) numbers, and percentage matches are also included in this report for each compound that was identified.

To determine the concordance of results between manual and automated approaches, a retrospective side-by-side comparison of 20 previously analyzed toxicology cases was performed. In three cases, the DRS identified additional substances that were not originally reported: fentanyl, diphenhydramine, temazepam, and a trace level of phenobarbital. In all three cases, these additional substances met the reporting criteria of the laboratory. In the 17 remaining cases, the DRS report was in agreement with the reported results or tentatively identified a substance that did not meet reporting criteria due to the quality of the library match. In addition to decreasing analysis time and improving efficiency, the DRS approach performs very well on complex biological matrices that may contain significant coextractives and interferences. These findings and the utility of DRS in routine forensic toxicology casework will be discussed.

DRS, GC/MS, AMDIS

 ** Presenting Author*