



B48 Deconvolution: An Automated Means of Unknown Identification in the Criminalistics Lab

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After attending this presentation, attendees will have a fundamental understanding of the benefits of using deconvolution.

This presentation will impact the forensic science community by allowing for more objective and efficient analysis of data. It will incorporate retention time, providing better matches to compounds in the target database.

Traditional means of identification in a forensic chemistry laboratory has been Gas Chromatography/Mass Spectrometry (GC/MS) using routine library search methods. The task of identifying drugs of abuse has become more challenging due to their increased diversity. There has been a proliferation of new psychoactive substances including the “bath-salts” and synthetic cannabinoids. In order to circumvent **Drug Enforcement Administration** (DEA) scheduling, illicit manufacturers of these compounds continually alter the molecules slightly, giving rise to a class of compounds with many structural similarities. The mass spectral similarity of these molecules can lead to misidentification using traditional library searching procedures. In addition to the growing list of drugs, many samples are complex mixtures containing active and inactive constituents (i.e., synthetic cannabinoid mixtures sprayed onto a botanical matrix). The chromatograms require additional manual manipulation to confirm the presence of these drugs, which can be subjective and time consuming. Trace amounts in these complex mixtures can be missed. Chemists must properly identify isomers and analogs of new compounds. In order to properly distinguish the closely related forms of these molecules, precise retention time measurements are required.

To maintain this precise control over retention time of the drugs, Retention Time Locking (RTL) is used. Deconvolution Reporting Software (DRS) is an automated and objective means of analyzing chromatographic data using the Automated Mass Spectral Deconvolution Identification System (AMDIS) -searching algorithm and Agilent® Chemstation®. The software analyzes extracted ion chromatograms for each mass throughout the entire chromatogram. Using the shape and apex of the chromatographic peak, masses are assigned to a specific component. This produces superior cleaned spectra compared to data processing using traditional searching algorithms. Coupled with retention time locking, DRS is able to generate match factors based not only on the cleaned mass spectrum, but also the expected retention time of analytes from the target compound library. Even with interferences and coelution, the process is capable of identifying trace components.

A database was built in-house under retention time locked conditions containing both traditional drugs of abuse and newer novel psychoactive substances. DRS was applied to multiple chromatographic situations encountered in real case work. Comparison data was generated for 550 drug identification cases, encompassing 1,757 findings and representing 131 individual drugs. These samples were processed using DRS and traditional data processing methods. These cases included five different scenarios: simple single component data, column overloads, trace amounts, samples with interferences/coelutions, and compounds with similar mass spectra. After the comparison study, DRS was implemented as the primary means of data analysis in the laboratory. Cases processed included samples that contain traces of fentanyl in heroin, coeluting peaks that share many of the same fragments (THC and hydrocodone), psilocin in mushroom samples, and specific isomeric determinations (2-Methylethcathinone (MEC), 3-MEC, and 4-MEC).

Because of retention time locking, the data generated from multiple instruments had virtually identical retention times, eliminating the need to run standards along with the case samples suspected to contain isomers and allowing the in-house library to be used on all instruments in the laboratory and at remote sites. DRS consistently identified components in multiple chromatographic scenarios. In the majority of cases, manual data processing yielded the same results as DRS; however, the time and level of experience necessary to make the identification via traditional data processing was far greater than that needed for DRS. In approximately 40 instances, traditional means failed to identify trace components in a sample whereas DRS properly identified these analytes. DRS is an automated, objective tool that was found to be more efficient and reliable for processing GC/MS data.

Deconvolution, GC/MS Data Processing, Retention Time Locking