A3 Trifluoroacetyl Derivatization of Amphetamine, Methamphetamine, 3,4-Methylenedioxymethamphetamine, and Other Controlled Substances With Similar Mass Spectra

Erin LaGrone, BS, Marshall University Forensic Science, 1401 Forensic Science Drive, Huntington, WV 25701; Christopher Kiyak, MS, and Gloria Rodriguez, BS, Austin Police Department, Forensic Chemistry Division, 812 Springdale Road, Austin, TX 78702; and J. Graham Rankin, PhD, Marshall University Forensic Science Program, 1401 Forensic Science Drive, Huntington, WV 25701*

The goal of this presentation is to provide attendees a look into a possible new way to analyze and identify controlled substances in a GC- MS with the use of chemical derivatization.

This presentation will impact the forensic science community by explaining how the use of TFA derivatives will enable drug analysts to utilize GC-MS to uniquely identify a number of amphetamine class compounds who have very similar mass spectra for the underivatized forms.

For the identification of a controlled substance, gas chromatography/mass spectrometry is the most commonly used method. However, there are some cases where the controlled substance shares a similar mass spectrum with a drug of a lower scheduling or a compound that is not even considered to be a controlled substance, such as methamphetamine and phentermine. Drug analysts then need to use chromatographic retention times to make a positive identification of the suspected compound. Here, it is proposed that the derivatization of these compounds will create mass spectra that are sufficiently different enough to make a positive identification without relying solely on retention time.

The major ion observed for amphetamine (AMP) was 44 m/z, sharing a similar mass spectra with 3,4-methylenedioxyamphetamine (MDA), 2,5-dimethoxy-4-bromoamphetamine (DOB), 2,5-dimethoxy-4-chloroamphetamine (DOC), and 2,5-dimethoxy-4-methylamphetamine (DOM). Methamphetamine (MA), with a major ion at 58 m/z, had a similar mass spectra to phentermine and 3,4- methylenedioxymethamphetamine (MDMA, ecstasy). 3,4- Methylenedioxyethylamphetamine (MDEA) and fenfluramine both had a major ion peak at 72 m/z.

Controlled substance standards, such as MA and AMP, were dissolved in chloroform and derivatized with trifluoroacetic anhydride (TFA), with pyridine acting as a catalyst and sodium hydroxide as a neutralizer, and analyzed by a GC-MS, resulting in unique, identifiable spectra for each standard. For example, after TFA derivatization it was observed that MA had major ions at 154, 110, and 118 m/z, while phentermine had major ions at 154, 91, and 59 m/z and MDMA at 154, 162, 135, and 110 m/z.

In most cases, a suspected controlled substance could be mixed with other drugs. Ecstasy tablets, for example, can be found containing MDA, MDEA, AMP, MA, and ketamine. When combining in a single GC vial equal amounts of these drug standards after TFA derivatization, the derivatized substances were shown to have adequate separation and could be uniquely identified by both their mass spectra and relative retention times through the gas chromatographic column.

 ** Presenting Author*