A151 Rapid Determination of Adulterants in Aqueous Mixtures by DART®-MS

Edward Sisco, MS, 6819 Old Waterloo Road, Apt 1035, Elkridge, MD 21075; Jeffrey H. Dake, MSFS, 4930 N 31st Street, Forest Park, GA 30297; and Candice Bridge, PhD, US Army Crime Lab, 4930 N 31st Street, Forest Park, GA 30297*

After attending this presentation, attendees will understand how Direct Analysis in Real Time Mass Spectrometry (DART®-MS) can be used to screen for the presence of common adulterants in aqueous mixtures. Additionally, attendees will understand how the inclusion of a dopant can aid in obtaining better specificity in the identification of these compounds.

This presentation will impact the forensic science community by providing a method for the rapid screening of liquids to determine the presence or absence of common adulterants without the need for sample preparation.

DART®-MS is a rapidly growing technique in forensic science. In comparison to traditional mass spectrometry-based techniques, such as Gas Chromatography Mass Spectrometry (GC/MS), DART®-MS provides the benefits of analysis under ambient conditions without the need for sample preparation. Additionally, sample analysis can be completed in a number of seconds, unlike GC/MS which typically takes several to tens of minutes. However, the pitfall of DART®-MS is the potential lack of specificity in chemical identification due to a lack of chromatography or other separation technique. In complex mixtures, where a number of chemicals and their fragments are present, complex and ambiguous spectra are obtained, making it difficult to ascertain whether low weight peaks are individual chemicals or merely the fragments of larger molecules. This lack of specificity can, in part, be mitigated through the use of a dopant compound, which can provide characteristic adduct ions.

The application of DART®-MS discussed here deals with the detection of adulterants in aqueous mixtures, namely beverages. Detection of adulterants in beverages is necessary in a number of different cases including: homicide; attempted homicide; sexual assault; suicide; and domestic violence. Common adulterants in beverages include alcohols (such as methanol and isopropanol), acetone, ammonium, hypochlorite-based bleach, and radiator fluid (ethylene glycol). Detection of these compounds in beverages can be difficult due to their low molecular weight — which can make detection against background difficult — and high volatility.

In this study, a number of adulterants, including those listed above, were analyzed by DART®-MS, both in aqueous solutions and in complex mixtures. An optimized method for the detection of the compounds was determined, and it was found that this method provided limits of detection at 0.1% by volume or lower. The limits of detection exceeded that of headspace GC/MS, which is the traditional technique commonly used to analyze these samples. Furthermore, it has been found that these chemicals can be detected in a number of different beverages, including sports drinks, sodas, and energy drinks. The use of dopants is also employed to allow for the determination of specific compounds which have similar fragmentation and dimerization products. The use of these dopants has been shown to differentiate the structural isomers propanol and isopropanol in both pure aqueous solutions and in beverages. Current work is being completed for the evaluation of a mixture of adulterants in solution as well as the detection of adulterants in ethanol-containing beverages.

The opinions or assertions contained herein are the private views of the author and are not to be construed as official or as reflecting the views of the Department of the Army or the Department of Defense. Names of commercial manufacturers or products included are incidental only and inclusion does not imply endorsement by the authors, the Department of the Army, or the Department of Defense.

DART®-MS, Adulterants, Chemical Analysis

 ** Presenting Author*