B128 Identification of Regioisomers Via Gas Chromatography Coupled With Vapor-Phase Infrared Detection (GC-IRD)

Janice L. Aleman, BS, 510 Deerview Drive, Fredericksburg, TX 78624; Jesse M. Zavala, MS, Harris County Institute of Forensic Sciences, 1885 Old Spanish Trail, Houston, TX 77054; Kyle E. Vircks, MS, Harris County Institute of Forensic Sciences, 1885 Old Spanish Trail, Houston, TX 77054; and Warren C. Samms, PhD, 1885 Old Spanish Trail, Houston, TX 77054*

After attending this presentation, attendees will be informed about the utility of using GC-IRD to differentiate regioisomers of abused substances.

This presentation will impact the forensic science community by providing information about how to utilize GC-IRD to distinguish regioisomers that are often difficult to differentiate using common methodologies. Due to identical mass spectra and similar retention times, laboratories are often unable to distinguish regioisomeric groups. The ability to differentiate these isomers allows the forensic science community to unambiguously identify newly designed substances. This is especially important when one isomer is controlled but another is not.

Designer drugs are appearing at an alarming rate across the world, requiring forensic chemists to develop new techniques for analysis. In many jurisdictions, designer drugs circumvent existing laws and are sold online or in smoke shops. In a previous validation study, various isomer sets of designer phenethylamines and cathinones were investigated. During the validation process, a few compounds presented potential data quality issues, such as low reproducibility of IR spectra resulting in incorrect library matches. Four of these compounds were 2,3-dimethylmethcathinone (2,3-DMMC), 3,4-dimethylethcathinone (3,4-DMEC), 2-methylmethcathinone (2-MMC), and 3-methylmethcathinone (3-MMC). Interestingly, the standards 2,4-dimethylmethcathinone (2,4-DMMC) and 2,4-dimethylethcathinone (2,4-DMEC) did not present these issues during the initial study and data was satisfactorily acquired. In the present study, analytical standards of 2,3-DMMC, 3,4-DMEC, 2-MMC, and 3-MMC were studied along with 5-(2-aminopropyl) indole (5-IT), alpha-methyltryptamine (AMT), as well as others. Prior to this investigation, this drug chemistry laboratory was unable to confirm these substances because they could not be separately and unambiguously identified. This is problematic in Texas, and presumably other states, as AMT is a controlled substance, while 5-IT is not. The additional compounds studied included controlled and non-controlled substances under Texas law.

To determine if the spectral details were stable and reproducible over time with the goal of capturing the optimal spectrum for library entry, standards for each substance were analyzed via GC-IRD twice daily for five days. Visual as well as library match analysis of each standard's chromatography and vapor phase IR spectra was conducted. Spectra were examined for their reproducibility over time, as well as any visually distinguishing features between closely related isomer sets.

A significant difference was noted between 5-IT and AMT vapor phase IR spectra and chromatography. IR spectra for both standards were found to be highly reproducible over the course of this study. Differences observed in the IR spectra were the sharpness and general peak shape primarily within the fingerprint region. AMT reproducibly suffered poor chromatography whereas 5-IT chromatography was consistently ideal.

The four cathinone controls, 2,3-DMMC, 3,4-DMEC, 3-MMC, and 2-MMC constituted in methanol, initially presented issues with chromatography. Therefore, a basic (0.45 N sodium hydroxide)/hexane extraction was performed and resulted in improved chromatography. It was noted that two of the four cathinone controls (2,3-DMMC and 2-MMC) began to degrade at a faster rate when compared to others during the validation process, resulting in low reproducibility for their IR spectra and lower likelihood of identification via library search. Frequent manipulation of averaged peak areas and background reference areas was required to compensate for decomposition products. Degradation of the injected samples could possibly be due to the instability of the compound itself, method parameters, or interaction of the sample with the reflective coating of the light pipe. Method optimization was attempted by changing a variety of parameters such as split ratios, flow rates, oven programming, and inlet temperatures. Overall, differentiation of these compounds was successful using obtained IR spectra.

Following this study, the analysis of forensic casework containing these substances resulted in unambiguous identification, allowing the laboratory to confirm which isomer was present in a given sample. These cases, along with other factors relating to positive identification via GC-IRD, will be discussed.

Drug Analysis, Regioisomers, GC-IRD

*Presenting Author