A145 Differentiation and Thermal Degradation of Synthetic Cathinone Regioisomers During Gas Chromatography/Mass Spectrometry Analysis

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After attending this presentation, attendees will learn about the thermal degradation of cathinones that occurs during Gas Chromatography/Mass Spectrometry (GC/MS) analysis and various methods to differentiate between regioisomeric compounds.

This presentation will impact the forensic science community by providing Electron Ionization (EI) mass spectral data for the regioisomeric compounds and the presumed thermal degradation products of several synthetic cathinones, as well as some preventative and reductive measures related to this decomposition.

Synthetic cathinones, often referred to as "bath salts," are central nervous system stimulants and have been implicated in numerous fatalities.[1] Modifications to the aromatic ring, the alkyl side chain, and the amino group have all been observed for the synthetic cathinones. These compounds may be synthesized with ring substitutions at the *ortho*, *meta*, or *para* position to create new regioisomers for the controlled substance. This presents an analytical challenge in differentiating between some of the regioisomers, because the EI spectra and the retention times are often very similar using routine GC/MS analyses. Several methods with detailed mass spectral data will be presented to demonstrate methods for differentiation of 14 groups of regioisomeric synthetic cathinones, 35 total compounds. Adjustment of the method and chemical derivatization are the techniques used to achieve unambiguous identification of the regioisomeric compounds.

Thermal decomposition has been reported for some of these cathinones which was confirmed by data from this study.[2-6] Stability of the regioisomers and their subsequent propensity for thermal decomposition were influenced by the positioning of the functional group on the aromatic ring for each group of regioisomers. The decomposition occurred in the injector port and/or the column, but the location varied between the groups of regioisomers. 2-Fluoromethcathinone exhibited unique decomposition products, supporting a previous study.[2,6] Mass spectral data for the presumed degradation products will also be presented and the patterns observed regarding the decomposition location and functional group positioning will be discussed.

There is one major difference between data from this study and data reported previously by others. Others have found the use of splitless injection mode dramatically reduced the occurrence of thermal decomposition. In the present study, only split mode was used; however, increasing the split ratio actually increased the level of decomposition. This contrasted with the results observed in another study, but the change between ratios was greater in the present study and probably accounts for the difference.[5,6] Other means for the prevention of thermal decomposition of these compounds have been determined by others and confirmed by the data from this study. Cleanliness of the liner and the use of a deactivated liner will substantially decrease thermal decomposition. Adjusting the GC/MS method may also decrease the thermal decomposition, as data indicate that some of the decomposition is occurring on the column; however, decreasing the temperature would also decrease the resolution and may prohibit the differentiation between the regioisomers of that compound.

The material included in this presentation is expected to be of interest to other forensic chemists, forensic toxicologists, and laboratory personnel involved in the analysis and evaluation of synthetic cathinone regioisomers.

References:

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Thermal Decomposition, Cathinones, Regioisomers

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