A182 Identification of Methamphetamine and Select Regioisomers

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After attending this presentation, attendees will be able to identify methamphetamine and select regioisomers unequivocally from one another by chromatography and mass spectrometry.

This presentation will impact the forensic science community by allowing the forensic scientist to identify methamphetamine from the similar regioisomers.

Regioisomers are positional isomers which vary only in the position of a functional group or other substituent. Positional changes will not only alter a compound's physical, chemical, and physiological properties, but in the case of methamphetamine, variations will also affect the legal status as a controlled substance. Methamphetamine has four regioisomers: N,α-dimethylphenethylamine, α,α-dimethylphenethylamine (phentermine), N,N-dimethylphenethylamine, N-ethylphenethylamine, and α-ethylphenethylamine.

Mass spectral data from these five compounds has been subjected to close scrutiny, since misidentification by using only a library search is a possibility. All four regioisomers have a molecular weight of 149 a.m.u. and have the same m/*z* 58 base peak seen in methamphetamine. The four regioisomers also display similar fragmentation patterns and ratios seen in methamphetamine. Despite these similarities, it has been shown that differentiation of methamphetamine from its various regioisomers is entirely possible, through the use of routine laboratory equipment. Various studies have been performed with methamphetamine and its regioisomers, and it has been shown that methamphetamine can be both chromatographically separated from its regioisomers and accurately characterized by confirmatory analysis.

The gas chromatography separation of the regioisomer mixture on both the non-polar HP-5 and mid-polar DB-17 columns will be discussed. Amphetamine and N,N-dimethylamphetamine was included with the methamphetamine regioisomer mixture as reference. Methamphetamine with a retention time of 1.575 minutes with the HP-5 column and 2.640 minutes with the DB-17 column did not co-elute with any of the four regioisomers.

The LC chromatography separation of the regioisomer mixture is comparable to other work. Methamphetamine had a retention time of 5.101 minutes and did not co-elute with any of the regioisomers. Complete baseline separation of all compounds in the regioisomer mixture was achieved.

The mass spectral data collected from the regioisomers closely match published spectral data. In the analysis of fragmentation patterns of similar compounds such as the regioisomers, it is necessary to expand the spectra in order to show the specific fragments and their abundance ratios. All four regioisomers and methamphetamine have the characteristic m/*z* 58 base peak. Furthermore, the fragmentation patterns are very similar except for a few distinguishing key ions. Sachs and Woo focus on the low mass region (m/*z* 39 – 56) as an area of distinction. In addition to the low mass region, a few unique/key ions are found in some of the compounds that allow for differentiation from methamphetamine and each other. For example, methamphetamine has a significant m/*z* 119:115 ratio not found in any of the regioisomers, which is a unique identifier for methamphetamine in addition to the low mass analysis. Both the nitrogen substituted compounds, N-ethylphenethylamine and N,N-dimethylphenethylamine have a significant m/*z* 105 fragment which would allow exclusion from methamphetamine. The regioisomer, α-ethylphenethylamine contains a uniquely identifying peak at m/*z* 120. Lastly, phentermine can be identified by its strong m/*z* 134 peak and lack of an m/*z* 148/ 149 (contains no alpha hydrogen's). In conclusion, methamphetamine can be distinguished from its regioisomers using chromatographic retention time *or* a thorough evaluation of the mass spectroscopy fragmentation pattern.

Methamphetamine Identification, Regioisomers, Mass Spectrometry

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