B80 **The Differentiation of Synthetic Cathinone Isomers by Gas Chromatography/Electron Ionization/Mass Spectrometry (GC/EI/MS) and Multivariate Analysis**

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Learning Overview: After attending this presentation, attendees will have learned about the differentiation of synthetic cathinone isomers using GC/EI/MS and multivariate analysis. Attendees will learn about the concepts of multivariate discriminant analysis, characteristic ion ratios, and methodologies to reduce the required number of replicate sample injections for multivariate classification.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing practitioners with a multivariate analysis approach for the differentiation of synthetic cathinone isomers using GC/EI/MS. Specifically, the development of methodologies to decrease the required number of replicate sample injections for multivariate classification will enhance the applicability of this approach to forensic practitioners.

The central hypothesis of this study is that each synthetic cathinone isomer has a unique EI fragmentation pattern that allows for the identification of characteristic ion ratios and, ultimately, the successful identification of each isomer using multivariate classification. Additionally, it is hypothesized that the characteristic ion ratios used for synthetic cathinone isomer differentiation will remain conserved across various sample concentrations.

An Agilent® GC/EI/MS was used for the analysis of synthetic cathinone constitutional and positional isomer drug standards. The synthetic cathinone constitutional isomer drug standards included dibutylone, eutylone, and pentylone, whereas the synthetic cathinone positional isomer drug standards were comprised of 2-, 3-, 4-chloroethcathinone, and 2-, 3-, 4-methoxymethcathinone. Each synthetic cathinone drug standard was analyzed at concentrations of 10ppm, 100ppm, and 1,000ppm to assess the influence of concentration on the observed characteristic ion ratios. For each synthetic cathinone drug standard, the relative ion abundances were extracted for further data analysis.

Statistical Package for the Social Sciences (SPSS) software from the IBM® Corporation was used to perform Canonical Discriminant Analysis (CDA) for each set of constitutional and positional isomers. CDA is a supervised multivariate discriminant analysis technique capable of discriminating between two or more groups by maximizing the between-group variance and minimizing the within-group variance. In addition, structure matrix correlation data was used to identify characteristic ion ratios that allowed for the differentiation of constitutional or positional isomers. Finally, the use of multiple mass spectral scans across the chromatographic peak and reducing the number of extracted ions used to create the CDA models were evaluated as methodologies to reduce the required number of replicate sample injections for multivariate classification.

The results indicate that CDA models can be used to differentiate between synthetic cathinone constitutional and positional isomers based on characteristic ion ratios derived from subtle differences in EI fragmentation patterns. Likewise, the use of multiple scans across the chromatographic peak and the development of CDA models based on a reduced number of extracted ions show promise as methodologies to reduce the number of required replicate sample injections for multivariate classification.

Seized Drugs, EI Fragmentation, Multivariate Analysis

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