B25 The Classification of Synthetic Phenethylamines According to Structural Subclass Using Multivariate Statistical Procedures

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The goal of this presentation is to demonstrate the application of multivariate statistical procedures for the classification of synthetic phenethylamines according to structural subclass.

This presentation will impact the forensic science community by increasing familiarity with the use of Principal Components Analysis (PCA) to identify ions characteristic of the phenethylamine subclasses and the subsequent use of Discriminant Analysis (DA) to develop classification models based on mass spectral data.

Recently, synthetic designer drugs have become a major concern in the United States. These drugs are synthesized with a slightly different molecular structure than already scheduled compounds to mimic the effects while avoiding legal ramifications; however, definitive identification of these rapidly emerging analogs is often challenging as no reference standard is immediately available to aid in identification.

The study presented describes the development of statistical models that can be used to classify a new analog to a known designer drug class or subclass. The initial work focused on three phenethylamine subclasses: Aminopropylbenzofuran (APB); 2,5-dimethoxy- (2C); and 2,5-dimethoxy-N-2-methoxybenzyl- (NBOMe) phenethylamines. A number of compounds from each subclass were selected to represent the variety of substitutions on the core structure.

Each phenethylamine was analyzed by Gas Chromatography/Mass Spectrometry (GC/MS) and the resulting mass spectra were first subjected to PCA to identify ions that were most characteristic of each subclass. In the PCA scores plot, members of each subclass were grouped together, with clear distinction among the three phenethylamine subclasses. The loadings plot for each PC was then assessed to identify the ions contributing most to the variance described in the scores plot. For example, *m/z* 91, 121, and 150, which are dominant ions in the NBOMe-phenethylamines, were weighted positively on PC1 whereas, *m/z* 44, which is the base peak in the APB-phenethylamines, was weighted negatively. As a result, the NBOMe- and APB-phenethylamines were distinguished on the first PC. The same *m/z* values were weighted positively on PC2 while *m/z* 165, 180, and 197 were weighted negatively. These latter ions are present in many of the 2C-phenethylamines with the result that this subclass was distinguished from the other two subclasses on PC2. Additional PCs were investigated in a similar manner to identify additional characteristic ions.

The ions identified in the PC loadings were used as the variables to develop classification models using DA. To do this, a training set was defined that included phenethylamines representative of the three subclasses. Models were tested using an external test set that consisted of phenethylamines representative of the three subclasses that were analyzed on a different day.

The first model included the nine characteristic ions identified in the first two PCs, which accounted for 46% of the variance in the data set. With this model, the classification success was 79%, with two of the 2C-phenethylamines and two of the NBOMe-phenethylamines misclassified. The second model included 14 characteristic ions that were identified in the first three PCs, which accounted for 56% of the variance in the data set. With this model, classification success increased to 89%, although two of the NBOMe-phenethylamines were still incorrectly classified as 2C-phenethylamines. A third model was developed that included the 18 characteristic ions identified in the first four PCs, which accounted for 64.6% of the total variance; however, despite the increased number of variables, there was no improvement in the rate of successful classification.

This presentation will demonstrate the utility of multivariate statistical procedures for the classification of synthetic phenethylamines. While this research focuses on phenethylamines, the statistical methods can be applied to develop classification models for different classes of drugs to combat the growing problem of new emerging designer drugs.

Synthetic Phenethylamines, Classification, GC/MS

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