Y22 Gas Chromatography With Dual Cold Electron Ionization Mass Spectrometric and Vacuum Ultraviolet Detection (GC/MS-VUV) for the Analysis of Phenylethylamine Analogs

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Learning Overview: After attending this presentation, attendees will understand the advantage of GC/MS-VUV in improving confidence in the analysis of Phenylethylamine (PEA) analogs.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating a rapid method for the identification of PEA analogs involving no liquid-liquid extraction and/or derivatization. This study provides a novel set of tools for the reliable identification of emerging drugs.

PEAs belong to a class of psychoactive drugs that have become more prevalent during the past several years. Certain PEAs were popularized by Alexander Shulgin in his book PIHKAL.[1] Many of these drugs are currently being synthesized to circumnavigate drug laws. Online availability results in easy access to many emerging drugs. There have been several deaths attributed to 2C PEAs in both the United States and Europe. Several case studies have shown the adverse effects of PEAs in humans. Because of these reasons, drugs like synthetic PEAs are controlled substances scheduled by the Drug Enforcement Administration.

The majority of drug analyses are commonly performed by GC with Flame Ionization Detection (FID) or MS detection. MS detection is preferable due to its ability to identify compounds based on mass-to-charge ratios and fragmentation patterns, whereas identification by FID relies heavily on the retention time of analytes. The analysis of PEA analogs, including positional isomers, with classical detection methods such as MS poses a few challenges for the forensic chemist. Classical electron ionization of certain compounds, such as phenethylamine analogs results in mass spectra with little to no molecular ions. The mass spectra are also insufficient for discrimination of certain positional isomers. This study demonstrates that the use of GC/MS-VUV can improve the analysis of PEAs. Cold electron ionization can increase the relative intensity of the molecular ions in mass spectra, as well as providing major fragments, while VUV can discriminate between most positional isomers.

Excellent chromatographic performance was obtained for PEA analogs by adding sodium bicarbonate to methanolic solutions of standard compounds. From a mixture of 40 PEA compounds, 21 were resolved with a resolution greater than 1 using VUV detection. However, all solutes could be resolved using a combination of MS detection (single ion monitoring) and/or VUV detection (deconvolution). The relative intensity of the molecular ion was increased for all 2C compounds, while molecules in the NBOMe class showed lower or no increase in molecular ion relative intensity. VUV spectra can be added to a library database as an aid for the identification of PEAs, including positional isomers. The VUV software is also capable of deconvoluting coeluting analytes. PCA was performed on both VUV and MS data of 5 dimethoxymamphetamine positional isomers to demonstrate the improved capability for discrimination of VUV detection.

Reference(s):

1. A.O. Shulgin et al. 1991. *Pihkal: A Chemical Love Story.* Transform Press.

Substituted Phenylethylamines, Cold Electron Ionization, Vacuum Ultraviolet Detection

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