B33 Application of Gas Chromatography-Vacuum Ultraviolet (GC-VUV) Spectroscopy in the Analysis of Synthetic Cathinones

Angelica D. Szewczak, BS, 8105 Leon Street, Philadelphia, PA 19136; Cory A. Vaught, BSc, The George Washington University, 3905 Davis Place, NW, Apt 102, Washington, DC 20007; Jonathan P. Smuts, PhD, VUV Analytics Inc, 715 Discovery Boulevard, Ste 502, Cedar Park, TX 78613; Walter F. Rowe, PhD, George Washington University, Dept of Forensic Science, 2100 Foxhall Road, NW, Washington, DC 20007; and Ira S. Lurie, PhD, George Washington University, Dept of Forensic Science, 2100 Foxhall Road, NW, Somers Hall, Lower Level, Washington, DC 20007*

After attending this presentation, attendees will understand characteristics of synthetic cathinones, problems surrounding current methods of analysis for these compounds, principles of VUV spectroscopy, and the application of this instrumental analysis to synthetic cathinones.

This presentation will impact the forensic science community by providing an additional and complementary method of analysis for emerging drugs, such as synthetic cathinones. VUV methodology will be particularly valuable for previously problematic analysis of positional isomers of synthetic cathinones.

Gas Chromatography/Mass Spectrometry (GC/MS) is a standard method of analysis for synthetic cathinones; however, GC/MS, as well as alternative Liquid Chromatography/Mass Spectrometry (LC/MS), often show limitations in the differentiation between isomers with the same molecular weight (positional isomers and diastereomers) that may co-elute and/or have identical mass spectra.

In order to address this limitation, new detectors have begun to emerge, including the introduction of VUV. This instrument rapidly measures absorption in the range of 115nm to 240nm. One distinct advantage to VUV is the unique ability to probe the excitation energy associated with electrons forming most single bonds (σ à σ^*) as well as monitor some π à π^* bond transitions. VUV also has the ability to deconvolute multiple co-eluting compounds when the spectra are different and properly added to the working library. This is extremely valuable for screening and confirmation purposes and could lead to faster separations where resolution is sacrificed. GC-VUV, which combines the high resolving power of GC with a detector that can provide a unique spectrum for a given compound, appears well suited for the analysis of emerging drugs, such as synthetic cathinones.

Comparisons of 35 spectra taken from multiple classes of synthetic cathinones were examined, including spectra from ten sets of positional isomers. Synthetic cathinones provide a unique UV spectrum. This was particularly valuable for the identification of positional isomers. For solutes differentiated by MS, VUV provides useful complementary information. VUV also allows for unique overall VUV patterns for different classes of synthetic cathinones, proving to be very useful in the analysis and identification of unknown compounds. In some instances, VUV can also tell substitution in the aromatic position. The potential for quantitative analysis, the repeatability of VUV detection, and the effect of concentration on spectral identification will be described.

GC-VUV, which provides excellent peak shapes and high specificity of detection, is well suited for the analysis of synthetic cathinones. In order to accomplish good chromatographic performance, de-salting of the analytes is required, which is easily accomplished by the addition of sodium bicarbonate to the methanolic sample solution.

GC-VUV, Synthetic Cathinones, Positional Isomers