A187 Analysis of Thirteen Designer Drugs Using GCMS, UV-Vis, and FTIR

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After attending this presentation, attendees will learn how a combination of three techniques (Gas Chromatography/Mass Spectrometry (GC/MS), Ultraviolet-Visible Spectrometry (UV/Vis), and Fourier-Transform Infrared spectroscopy (FTIR)) were used to identify 13 different designer drugs.

This presentation will impact the forensic scientific community by demonstrating that a combination of techniques provides excellent discrimination potential for a challenging set of new designer street drugs. In particular, UV/Vis spectrometry, a technique that is often overlooked as a screening tool, is restored to prominence as a powerful, rapid screening tool that can differentiate between drugs that may not be resolvable by gas chromatography.

A variety of designer drugs, sold with labels such as “bath salts,” “research chemicals,” and “not for human consumption,” have been encountered recently in crime labs in Minnesota. The compounds chosen for this project were synthetic cathinones and analogs to Schedule I controlled substances that have been reported in the literature and mentioned in Erowid.org posts, including methcathinone, 3-fluoromethcathinone, 4-fluoromethcathinone, 4-methyl-methcatinone (mephedrone), butylone, ethylone, buphedrone, n-ethylcathinone, 2-fluoroamphetamine, 4-fluoroamphetamine, 2-fluoromethamphetamine, 4-fluoromethamphetamine, and methoxetamine.

One of the challenges with the new designer drugs is that they often show no color development with traditional color screening test reagents, such as the Marquis test. The 13 drugs analyzed demonstrated absorbance in the UV range, and in some cases the UV spectra provided sufficient discrimination to distinguish drugs with similar structures that were not resolvable by GC.

The UV-Vis sample preparation consisted of using 1mg/mL reference drug standards and diluting to maintain linear response. Each standard was diluted with methanol and sulfuric acid, with the amount varying.

The GC/MS sample preparation consisted of using 0.1µL of 1 mg/mL reference drug standard with a septum capped vial. Four methods of analysis were used, with three of the methods having parameters adapted from previous references for the available instrumentation.[1,2,3] The methods varied in the initial temperatures, temperature ramp rate, final temperature, and hold time, and all used a split injection with a split ration of 100:1.

The FTIR sample preparation consisted of allowing the 1mg/mL reference drug standards to evaporate overnight and placing the powder residue directly onto a diamond Attenuated Total Reflectance (ATR) stage crystal.

The 13 compounds were distinguishable using the combination of GC/MS, UV/Vis, and FTIR techniques. 3- and 4-fluoromethcathinone were distinguishable using UV-Vis, which showed variation in the number of maximum absorbance peaks. Ethylone and butylone showed distinct mass fragmentation patterns despite their similar structures and molecular weights. Buphedrone and n-ethylcathinone also demonstrated differences in their mass fragmentation patterns. The 2- and 4-fluoroamphetamines were resolvable by their gas chromatography retention times. For 2- and 4-fluoromethamphetamine, significant differences surfaced in the IR absorption wave numbers and the percent transmittance.

References:

[1]Archer RP. Fluoromethcathinone, a new substance of abuse. Forensic Science International. 185 (2009) 10-20.

1. Folker W, Junge T. Ring positional differentiation of isomeric N-alkylated fluorocathinone by gas chromatography/tandem mass spectrometry. Forensic Science International. (2012). Nov 30;223(1-3):97-105. http://dx/doi.org/10.1016/j.forsciint.2012.08.011 Epub 2012 Aug 30.
2. Maheux CR, Copeland CR. Chemical analysis of two new designer drugs: buphedrone and pentedrone. Drug Testing and Analysis. 4 (2012) 17-23.

Designer Drugs, Synthetic Cathinones, Spectroscopy

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