A212 Identification of Cannabimimetrics and Cathinones by GC/EI-MS and LC/ESI/QTOF-MS

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After attending this presentation, attendees will learn how Liquid Chromatography Electrospray Ionization Quadrupole Time-Of-Flight Mass Spectrometry (LC/ESI/QTOF-MS) and Gas Chromatography Electron Impact Ionization Mass Spectrometry (GC/EI-MS) can be applied to the analysis of cannabimimetrics and cathinones that are currently found in "legal high" products.

This presentation will impact the forensic science community by emphasizing an analytical approach for identifying synthetic designer drugs using accurate mass determination along with EI fragmentation elucidation. The findings and methodology will provide forensic laboratories the ability to identify alternative means for detecting and identifying designer drug substances.

The use of illegal synthetic cannabinoids and cathinone derivatives has become popular in recent years. Many of these products are often marketed using labels such as "bath salts" and "herbal blends" and are packaged with a disclaimer that they are not for human consumption. Labels on the packaging do not often reflect the actual contents, misleading the consumers that the products are safe and legitimate. Consequently, these substances are increasingly popular as legal alternatives to illicit psychoactive substances for recreational drug users. The demand is further enhanced by their widespread and easy availability on the Internet and head shops across America.

The majority of cases encountered by forensic chemists are analyzed utilizing traditional methodologies such as GC/MS, GC/FID, FTIR-ATR, and LC/MS. Identification of unknowns has been largely dependent on mass spectral libraries from SWGDRUG, Cayman Chemical, and scientific discussion forums such as Forendex. Moreover, due to the vast variety of synthetic drugs, authenticated reference standards may not be easily available, thereby increasing analysis time and cost of unusual cases. The introduction for newer and efficient methodologies into the classical workflow is essential. The objective of this study is to demonstrate how synthetic substances (target or unknown) can be identified using accurate mass spectrometry analysis alongside with EI fragmentation elucidation.

Preliminary results of this study demonstrated that ESI/QTOF-MS software-based accurate mass determination provided highly specific mass-to-charge spectral data with accuracies spanning in the milli-Dalton range for parent and fragment ions. The method employs chromatographic separation using Zorbax Extend C18, 2.1mm x 50mm, 1.8um particle size stationary phase. TOF-MS full-scan spectra were acquired in positive mode over 50-1000 m/z scan range using reference masses m/z 121.0509 and 922.0098. Additional TOF-MS parameters were set as follows: fragmentor voltage at 150 V; capillary voltage at 4000 V; skimmer voltage at 65 V; nebulizer pressure at 50 psi; gas temperature at 350 C; and gas flow rate at 13 L/min. Collision-induced-dissociation (CID) of precursor ions were obtained in targeted MS/MS mode using a collision cell with nitrogen as a collision gas.

Applications presented will include the analysis of some of the emerging cannabimimetrics such as AM-1220, AM-2233, UR-144, and XLR-11. In addition, cathinone derivatives such as butylone, ethylone, pyrrolidinopropiophenones, and 4-methylbuphedrone will be discussed. The results showed that ESI/QTOF-MS can be used in complement with GC/MS to provide principal means of identification of designer cathinones and synthetic additives in herbal mixtures. By applying these techniques, forensic laboratories will have the ability to characterize designer synthetic drugs.

Cannabinoids, Cathinones, QTOF/MS

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