K21 Analysis of Synthetic Cannabinoids by Mass Spectrometric Methods Coupled With Accurate Mass Determination

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After attending this presentation, attendees will learn about the role of accurate mass determination in gas chromatography-mass spectrometry (GC/MS) and liquid chromatography-mass spectrometry (LC/MS) methods for analyzing synthetic cannabinoid products. The synthetic cannabinoid compounds of herbal products along with the full range of organic compounds present in the gas and particulate phases of smoke samples of the herbal products will be discussed. The findings and methodologies will contribute to future development of a protocol for analyzing banned synthetic cannabinoid substances and assessing their toxicological effects.

This presentation will impact the forensic science community by emphasizing the advantages of accurate mass determination in mass spectrometric analysis of illegal drugs and how it will be beneficial to the drug enforcement and forensic communities by providing rapid and reliable analysis of synthetic cannabinoid substances. Sound analytical methods based on mass spectrometry for characterizing products seized in police raids and assessing the levels of the related drug compounds in the urine and smoke samples will contribute to effectiveness in drug enforcement and toxicological studies of the synthetic cannabinoid products, respectively.

The use of illegal synthetic cannabinoids has become increasingly popular over the past several years. These drugs have been successful in providing a "high" just like marijuana and yet these drugs and their metabolites can circumvent detection by most standard drug testing methods for natural cannabinoids. As a result, herbal products containing the synthetic cannabinoids such as JWH-018 and JWH-073 have become more appealing to drug users. These synthetic cannabinoids have shown harmful health effects in the human body and may even cause death from high concentrations of toxic compounds accumulated via extended drug abuse or accidental overdoses through haphazard manufacturing practices involved in these illegal products. It is therefore critical for these drugs and their metabolites to be identified and quantitatively determined by law enforcement and clinical laboratories. The study aims to develop an efficient and reliable method that will identify the synthetic cannabinoids in a forensic testing laboratory.

Forensic analysis of illegal compounds usually involves methods that could provide unequivocal evidence in a court of law. Most current methods involve GC/MS and LC/MS for analyzing commonly abused drugs like cocaine, heroine, and methamphetamine. Although both GC/MS and LC/MS have been reported for determining synthetic cannabinoids in the herbal products and urine samples,[1-3] there has not been any study of cannabinoid distribution in the gas and particulate phases of the smoke inhaled by the users. In this study, the smoke of the herbal products containing synthetic cannabinoids is studied in order to estimate the range of doses of the active ingredients in commonly available products. The GC/MS method developed in this project also relies on accurate mass determination to provide greater confidence in MS analysis based on quadrupole mass analyzers. The goal of developing such a method is that the analytical chemist can either bypass the GC analysis or use a short GC column to achieve rapid analysis to cope with the sample throughput issue in most forensic laboratories. Furthermore, the possibility of a portable mass spectrometer with accurate mass analysis can be conducive toward the development of mobile laboratory testing of illegal drugs for the law enforcement community. GC/MS instrumentation is fairly bulky and is too cumbersome for crime scene analysis. Therefore, it is beneficial to develop "GC-less" MS methods for onsite analysis in order to exclude possible contamination when crime scene samples are collected and brought back to the laboratory for GC/MS analysis. Also, accurate mass analysis is more efficient in unequivocal identification of target compounds relative to GC that is prone to chromatographic co-elution. Preliminary analysis of this study has shown that software-based accurate mass determination using quadrupole mass data allow highly specific and accurate mass-to-charge analysis to the third decimal places for the parent and fragment ions of commonly abused drugs, thus allowing reliable determination these banned substances.

There is great variability in the drug concentrations found in different herbal blends of synthetic cannabinoids. The amount of JWH-018 ranged from 4.09±0.04 mg/g herbal blend in K2 Blond to the highest concentration in Ultra Cloud 10 of 41.80±0.62 mg/g of herbal blend. The amount of JWH-073 ranged from 6.11±0.27 mg/g of herbal blend in K2 Blond to the highest concentration in Ultra Cloud 10 of 13.20±0.24 mg/g of herbal blend. Low concentrations of JWH-018 in K2 Blonde are likely compensated by the presence of JWH-250, a compound not found in the other 4 herbal blends studied. When the smoke samples were analyzed, it was found that the synthetic cannabinoids were not detectable in the gas phase but were detected in the particulate phase collected using a cascade impactor. This indicates that JWH-018, JWH-073, and other synthetic cannabinoids are inhaled in the particulate phase with a particle size fraction of less than 0.25 μm. The analysis also revealed that most of the flavor or scent additives for the herbal products were detected in the particulate phase. Further analysis using LC/MS with a time-of-flight mass spectrometer and ion mobility instrumentation allows the complete characterization of the synthetic cannabinoids and their related metabolites and by-products in the mainstream smoke samples.

References:

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Illegal Synthetic Cannabinoids, Accurate Mass Determination, Mass Spectrometric Analysis

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