## B194 The Utility of Ultra High-Performance Liquid Chromatography with Time-of-Flight Detection for the Identification of Synthetic Cannabinoids: Part II — The Role of the Detection Technique

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After attending the presentation, attendees will understand the advantages and disadvantages of using a Time-Of-Flight (TOF) high resolution mass spectrometer as detector following separation by Ultra High-Performance Liquid Chromatography (UHPLC) as compared to the traditional capillary Gas Chromatography-Quadrupole Mass Spectrometry (GC/MS). Attendees will also be exposed to the differences between classical electron-impact mass spectra and those of electrospray ionization mass spectra with and without in-source fragmentation.

The presentation will impact the forensic science community by further exploring the role of high resolution mass spectrometry in the identification of forensic drugs. Examples will include analyses of emerging drugs such as synthetic cannabinoids and some of their isomers.

The Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) classified mass spectrometry in the category A (highest discriminating power), with the exception of techniques that only produce molecular weight information. The SWGDRUG recommendations do not specifically address the issue of high-resolution mass spectrometry, as it is addressed by other similar groups (e.g., the recommendations of Scientific Working Group for Forensic Toxicology (SWGTOX)). This research tackles the role of high-resolution mass spectrometry in the context of the analysis of synthetic cannabinoids.

Currently, there are 25 synthetic cannabinoids on the list of controlled substances by the Drug Enforcement Administration and more synthetic cannabinoids are likely to become controlled in the future. A mixture of 23 controlled synthetic cannabinoids was subjected to analyses by GC/MS using a 0.25µm 0.25mm x 30m Elite-5MS capillary column (equivalent to DB-5, HP-5) and UHPLC-TOF/MS with three 2.1 x 150mm columns packed with 2.7µm superficially porous stationary phases (C18, Phenyl-Hexyl, and pentafluorophenylpropyl (PFP)). The analyses were also performed on a mixture of ten positional isomers of JWH018 to assess their identification in potentially complex mixtures.

The mass spectra resulted from the GC/MS experiments showed a high degree of specificity with the exception of diastereoisomers (CP47, 497and epi CP47, 497; CP47, 497-C8 and epi CP47, 497-C8); however, all chromatographic systems were able to separate these diastereoisomers. The ten positional isomers of JWH018 were also easily distinguishable based on their mass spectra.

The masses measured by UHPLC-TOF/MS experiments were generally within a few ppm of the accurate mass of the synthetic cannabinoids. Measurement of the accurate mass can bring an increased level of confidence to a forensic analysis. Mass spectra using in-source fragmentation brought additional information regarding the analytes; however, the fragmentation pattern did not have the degree of specificity observed in GC/MS experiments. Especially in the case of JWH018 isomers, where the difference between compounds was mostly limited to a side alkyl chain, the mass spectra did not include specific peaks allowing differentiation between compounds. Although all solutes could be uniquely identified by GC/MS, UHPLC-TOF/MS provides a highly orthogonal technique that greatly enhances the confidence in the analysis.

**Synthetic Cannabinoids, High Resolution MS, Forensic Drugs**