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### **B26 High-Resolution MS/MS Spectral Library for Synthetic Cannabinoids by Direct Analysis in Real-Time Quadrupole Time-of-Flight Mass Spectrometry**

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After attending this presentation, attendees will learn how Direct Analysis in Real-Time Quadrupole Time-of-Flight Mass Spectrometry (DART<sup>®</sup>-Q-TOF/MS) can be applied for the identification of synthetic cannabinoids and the usefulness of a spectral library for these compounds. This presentation will highlight the advantages and limitations of DART<sup>®</sup>-Q-TOF/MS over traditional Gas Chromatography/Mass Spectrometry (GC/MS) and Liquid Chromatography/Mass Spectrometry (LC/MS) drug analysis as well as show the development of a spectral library for synthetic cannabinoids using this technique.

This presentation will impact the forensic science community by demonstrating how DART<sup>®</sup>-Q-TOF/MS can be used to rapidly produce high-resolution data for synthetic cannabinoids that can then be compiled into a spectral library to allow for faster identification of these compounds in seized products.

Abuse of synthetic cannabinoids has increased dramatically since the first report in Europe in 2004 and first detection in the United States in 2008. Typically sprayed on plant leaves, flowers, or stems, and packaged as herbal incense mixtures under the names “Spice” and “K2” among others, these compounds are marketed as “legal highs.” Although legislation has been passed such as the Synthetic Drug Abuse Prevention Act in 2012, the number of synthetic cannabinoids has continued to increase, many of which are analogs of other compounds developed to circumvent this legislation. This complicates identification of synthetic cannabinoids due to the high level of similarities in structure. DART<sup>®</sup> is an ambient ionization technique that requires little-to-no sample preparation and utilizes lower energy ionization than electron ionization, typically used with GC/MS, meaning less fragmentation and the observance of molecular ions. The DART<sup>®</sup> and Q-TOF/MS parameters were optimized and are reported. When paired with a mass spectrometer, DART<sup>®</sup> allows for rapid analysis and identification as the sample only needs to be introduced into the gas stream for a few seconds in order to produce spectra. Over 100 synthetic cannabinoid standards were analyzed by DART<sup>®</sup>-Q-TOF using the optimized method to generate molecular ions and fragmented spectra and searched on an existing database of Electrospray Ionization (ESI) -generated spectral database with excellent results. The DART<sup>®</sup>-Q-TOF method is a fast and effective tool that provides rapid analysis and identification of seized synthetic cannabinoid products.

This presentation will describe the capabilities of DART<sup>®</sup>-Q-TOF to quickly and accurately identify synthetic cannabinoids and their analogs while also describing the spectral library development. DART<sup>®</sup>-Q-TOF provides an alternative technique for the more commonly used GC/MS and LC/MS which are slower, increasing the amount of analysis time required in drug seizure cases.

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#### **Direct Analysis in Real Time, Synthetic Cannabinoids, Spectral Library**