A209 DART®-MS Collision Induced Dissociation (CID) for Structural Analysis of Synthetic Cannabinoids

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After attending this presentation, attendees will understand ambient ionization mass spectrometry, basics on synthetic cannabinoid detection, and how to use fragments for structural identification.

This presentation will impact the forensic science commmunity by demonstrating a cutting-edge technique applied to a current problem, and how chemical analysis can be performed without any sample preparation, extraction, or derivatization that are often required for GC/MS and LC/MS analyses.

The emergence of numerous cannabinoid designer drugs has been tied to large spikes in emergency room visits and overdoses. Identifying these substances is difficult due to: (1) the fact that the compounds are novel, structurally related, and do not usually test positive in drug screens; (2) the rapidity with which they appear on the market; (3) the absence of standard protocols for their identification; and, (4) the customized and extensive sample preparation/extraction and analysis procedures required to demonstrate their presence. Direct Analysis in Real Time Mass Spectrometry (DART®-MS) is a technique that utilizes an atmospheric pressure ion source that produces a heated stream of metastable helium species directed at sample surfaces to vaporize and ionize liquids or desorb and ionize molecules from solid surfaces in open air under ambient conditions. Semi-volatile substances, like the cannabinoids mixed on the plant material, desorb from the leaf surface and are ionized. The metastable helium atoms initiate a cascade of ion-molecule reactions in ambient air to provide protonated water clusters as a chemical ionization reagent to produce parent ions, $[M+H]^+$, from the cannabinoid drugs.

DART®-MS provided high mass accuracy, to 0.0001 Da, establishing the presence of the cannabinoids JWH-122, JWH-203, JWH-210, RCS-4, and AM-2201, alone and as mixtures of at least two cannabinoids. Mass spectra were acquired by simply suspending a small portion of sample between the ion source and the mass spectrometer. The ability to test minute amounts of sample is a major advantage when limited amounts of evidentiary material are available. This method circumvents time-consuming sample extraction, derivatization, chromatographic, and other sample preparative steps required for analysis by more traditional methods. The high throughput capabilities of DART®-MS enable the active components of designer drugs to be detected more quickly, reducing the time necessary to triage analytical evidence. Therefore, exploitation of this method has the potential to contribute to more timely criminal prosecution. In addition, DART®-MS employing CID conditions provided confirmatory structural information that was useful in characterizing the various isobaric cannabinoid analogs.

Specifically, DART®-MS CID induces fragmentation of the protonated parent ions when the electrode voltage at the inlet orifice to the mass spectrometer is increased, demonstrating the utility of fragmentation patterns for distinguishing among closely related structures. The researchers used in-source CID to produce product ions corresponding to the synthetic cannabinoid molecules desorbed from dried leaves. CID analysis illustrated that closely related compounds are likely to fragment in a similar fashion, but their inherent structural differences will result in unique fragments that vary enough between the singular cannabinoids that can serve as a means to better identify each substance. Closely related compounds fragmented with both consensus peaks and unique fragments, such that both their structural similarities and differences provided multiple diagnostic peaks that permitted additional confidence toward identification of each substance. DART®-MS spectra were acquired to rapidly differentiate among synthetic cannabinoids contained within “herbal” products purchased locally in New York (U.S.). The spectra exhibited the following parent ion peaks and product ion fragments unique to each cannabinoid that corresponded to major structural features: JWH-122 (*m/z* 356.1997, 298, 214, 169, 141), JWH-203 (*m/z* 340.1466, 342, 214, 127, 125), JWH-210 (*m/z* 370.2179, 312, 214, 183, 155), RCS-4 (*m/z* 322.1778, 164, 214, 186, 135), and AM-2201 (*m/z* 360.1757, 284, 232, 155, 127).

DART®-MS, Cannabinoids, Ambient Ionization

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