

B14 Candies and Cannabinoids—The Rapid Identification of Cannabinoids in Plant Material and Edible Complex Matrices by Ambient Mass Spectrometry

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Learning Overview: After attending this presentation, attendees will better understand how ambient ionization mass spectrometric techniques can assist with the identification and differentiation of cannabinoids in complex plant and edible matrices.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing a protocol that will enable law enforcement and forensic crime laboratories to rapidly identify plant material and food products that contain cannabinoids, while circumventing problems often encountered using conventional methods.

As cited in the National Institute of Justice (NIJ) 2019 *Report to Congress: Needs Assessment of Forensic Laboratories and Medical Examiner/Coroner Offices*, some of the greatest challenges to emerge in recent years are consequences of the “legalization and decriminalization of marijuana.”¹ Furthermore, the report indicates that the issues require the “implementation of new testing strategies,” and that “testing methods must be developed to test THC (tetrahydrocannabinol),” in a variety of plant-based substances, edibles, and extracts. Current protocols utilized by law enforcement and crime laboratories, among which there is little uniformity, can be cumbersome and often require extensive sample preparation, time-consuming samples runs, and complex data processing. This study focuses on the unique capabilities of Direct Analysis In Real Time-High-Resolution Mass Spectrometry (DART®-HRMS) for the rapid detection of cannabinoids in *Cannabis sativa* plant material and cannabinoid-infused complex edible matrices. This ambient, high-resolution technique permits direct analysis of samples in their native forms, as well as rapid interrogation of samples following their chemical alteration through exposure to derivatizing agents.

A wide variety of samples were investigated, including commercial Cannabidiol (CBD) products, edible Certified Reference Materials (CRMs) infused with cannabinoids, hemp plant material (which is a variety of *C. sativa*), and edible samples prepared in-house, such as candies, baked goods, and other food products. DART®-HRMS analysis rapidly reveals the presence of cannabinoids in the plant and edible products without sample preparation. While several cannabinoid molecules were detected, including Cannabigerol (CBG) and Cannabinol (CBN), each DART®-HRMS-derived spectrum exhibited a peak at m/z 315.232, which is consistent with protonated THC and CBD. Because these two molecules share the same molecular formula of $C_{21}H_{30}O_2$ and therefore the same protonated mass, they are indistinguishable by DART®-HRMS under soft ionization conditions without sample pretreatment. Furthermore, they remain indistinguishable even under Collision-Induced Dissociation (CID) conditions that induce fragmentation of the molecules. As such, an alternative approach must be taken to differentiate and identify these two cannabinoids. It was found that THC and CBD are readily distinguishable under both soft ionization and CID conditions when the derivatizing agent *N*-Methyl-*N*-(Trimethylsilyl)Trifluoroacetamide (MSTFA) was used. Engagement by the derivatizing agent of the single –OH group in THC and the two –OH groups in CBD converts the two compounds to molecules with protonated $[M+H]^+$ masses of 387.272 and 459.312, respectively. This results in THC and CBD chemical standards producing distinguishable mass spectra through DART®-HRMS analysis. Furthermore, chemical signatures with additional cannabinoid-related information are provided when plant materials, commercial products, and edibles are analyzed by DART®-HRMS after derivatization. In summary, the data demonstrate that DART®-HRMS can detect and differentiate cannabinoids in complex matrices and provide a method to triage edible marijuana evidence in crime laboratories while circumventing problems often encountered using conventional methods.

Reference(s):

1. National Institute of Justice (NIJ) 2019 *Report to Congress: Needs Assessment of Forensic Laboratories and Medical Examiner/Coroner Offices*. <https://www.justice.gov/olp/page/file/1228306/download>.

Mass Spectrometry, Cannabinoids, Edibles