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Weeding Out the Methods to Enable Rapid Differentiation of Fiber-type and Drug-type Varieties of Cannabis sativa: A Combined Ambient Ionization Mass Spectrometric and Chemometric Approach

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Abstract: Fiber-type (hemp) and drug-type (marijuana) are the two major varieties of Cannabis sativa. Although both varieties contain Δ^9 -tetrahydrocannabinol (THC), which is responsible for the psychoactive properties of the plant, they differ in the amount of THC present. Current federal laws stipulate that C. sativa with greater than 0.3% THC is the drug-type, while material with less than or equal to 0.3% THC is the fiber-type. Distinguishing between these varieties by traditional approaches can be time-consuming and troublesome. Therefore, this project investigated the utilization of direct analysis in real time – high-resolution mass spectrometry (DART-HRMS) combined with chemometrics to rapidly differentiate them. C. sativa plant materials were obtained from several sources (e.g., commercial hemp flower, marijuana samples from DEA-registered suppliers, recreational marijuana flower). All plant materials were analyzed by DART-HRMS in positive-ion mode under soft ionization conditions with no sample pretreatment steps. After obtaining the DART-HRMS chemical profiles for all samples, advanced multivariate data analysis techniques (i.e., principal component analysis, random forest) were applied to differentiate the two C. sativa varieties. After a model was developed, external validation samples were used to assess the model's ability to classify unknowns. This assessment resulted in 100% accuracy for predicting the variety of the samples. In addition, several m/z values were classified as diagnostic for differentiating between the fiber-type and drug-type samples, the identities of which are under investigation. In summary, this combined mass spectrometric and chemometric method would aid significantly in the rapid identification of unknown material prior to launching confirmatory chromatography experiments.