DIRECT SAMPLE ANALYSIS

Detecting THC/Cannabinoids in Contraband by Compact Mass Spectrometry



INTRODUCTION

Direct sample analysis is possible via an Atmospheric Solids Analysis Probe (ASAP[®]) combined with atmospheric pressure chemical ionization (APCI) on a compact mass spectrometer (CMS) (Figure 1 and 2). This technique allows for the rapid investigation (<30 sec) of material suspected of containing THC/cannabinoids (example chemical structures and molecular weights shown in Figure 3).

METHOD

Touch the closed end of the glass melting point capillary to the sample material, and then insert the direct analysis probe into the mass spectrometer for analysis. Obtain results in seconds.



Figure 3: Chemical structures, elemental composition and molecular masses of select cannabinoids detected in this study.



Figures 1 and 2: Direct analysis probe and compact mass spectrometer (Figure 1 Insert) Probe with extended glass capillary sampling in a 10 mg suspect cannabis sample. Red arrow shows the glass capillary touching the test material.

RESULTS

ASAP/APCI/CMS analysis shows that the majority of the sample is desorbed and ionized within 20 sec (Figure 6) giving strong m/z signals at 311.2/309.1; 315.2/313.2 and 357.2 corresponding to the (M+H)⁺ and (M-H)⁻ for cannabinol (CBN) and THC/CBD as well as the deprotonated molecule of THC-acid/CBD-acid at m/z 357.2.



Figure 4: TIC profile of the collected MS data in alternating positive (top trace) and negative ion mode (bottom trace). After a short baseline acquisition period, the CMS detects a signal within <20 sec. when analytes are volatilized from the ASAP glass capillary probe surface and ionized in the APCI source region.



Figure 5: Mass spectral data for both positive (top trace) as well as negative ion mode (bottom trace) ASAP analysis. The intense m/z signals at 311.2/309.1; 315.2/313.2 and 357.2 correspond to the $(M+H)^+$ and $(M-H)^-$ for cannabinol (CBN) and THC/ CBD as well as the deprotonated molecule of THC-acid/CBD-acid at m/z 357.2.



As further sample, a pinch of the known cannabis material was rolled between the thumb and forefinger and the latter swiped with the ASAP probe for analysis (Figure 6). Compared to a control skin sample, abundant signal is visible at m/z 311.2/309.1 and 315.2/313.2, consistant with the respective (M+H)⁺ and (M-H)⁻ of THC/CBD and Cannabinol (Figure 7). It is noteworthy that only the combined positive and negative ion mode data provides a reliable confirmation for the presence of cannabinoids since for example skin sample shows a variety of signals across the mass range (data not shown).



Figure 6: To simulate skin contact with Cannabis material as it would occur when e.g. rolling a cigarette or handling raw material, a pinch of the sample was rolled between the thumb and forefinger and the latter sampled with the ASAP glass capillary probe prior to analysis.



Figure 7: MS data showing both positive ionization (top trace) and negative ionization (bottom trace) of the ASAP finger skin analysis before and after cannabis exposure (control left side, exposed skin right side). The typical m/z signals at 311.2/309.1 and 315.2/313.2 are indicative of the respective (M+H)⁺ and (M-H)⁻ for Cannabinol and THC/CBD respectively.

CONCLUSIONS

- ASAP-APCI-CMS is a rapid mass spectral analysis approach that can screen a variety of samples and surfaces for presence of cannabinoids
- Dried plant material can readily be screened for the presence of cannabinoids such as Cannabinol, THC/CBD or THC/CBD-acid
- Alternating acquisition of positive and negative ion mass spectra improves prediction certainty when sampling from complex samples such as skin contaminated with small quantities of plant material
- Alternating acquisition of positive and negative mass spectra improves prediction certainty when sampling from complex samples such as skin

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Advion is a leader in mass spectrometry & synthesis solutions. The expression CMS is a high performance, compact, affordable single quad mass spectrometer. Its compact size allows it to fit into space-limited labs for direct access and immediate results for chemists requiring mass confirmation, reaction monitoring, quality control and purity analysis.