

# Chromatography free analysis of Cannabis on Terpene profiles, CBD and THC by CID on radical cations revealing EI-like spectra

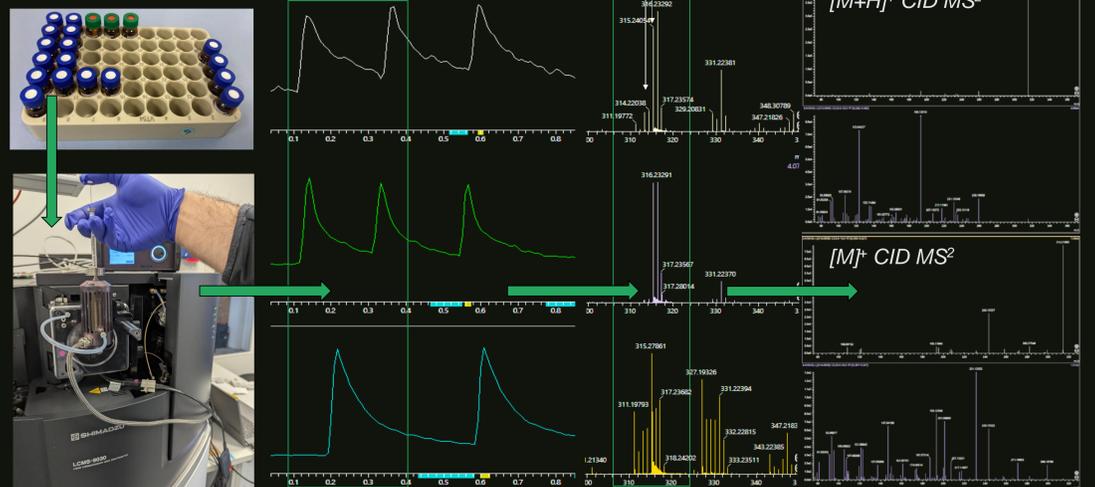
Sicrit  
technology

Ciara Conway<sup>1,2</sup>, Markus Weber<sup>1,2</sup>, Christoph Haisch<sup>1</sup>, Jan-Christoph Wolf<sup>2</sup>

## Introduction & Technology

Due to growing legalization of cannabis, the need for a rapid method to quantify CBD and THC in cannabis is apparent. While EI-MS provides unique structure elucidation for THC and CBD through odd-electron ionization, the resulting complex MS1 spectra cannot be deconvoluted without chromatography. ESI-MS softly ionizes THC and CBD with even-electron ionization, but the CID fragmentation is too similar to differentiate, thus also requiring chromatography (Fig A). Therefore, there needs to be a soft odd-electron ionization that produces EI-like fragmentation on an MS2 level. Soft ionization by Chemical reaction in transfer (SICRIT®), a dielectric barrier discharge-based ion source accomplishes this, allowing for soft ionization of these components as both the  $[M]^+$  and  $[M+H]^+$  allowing for chromatographic-free quantification of cannabis.

## Experimental



A GC-SPME Module was coupled, via the DBDI Source, to a Shimadzu 9030, where manual direct liquid injections were performed. These injections produce distinct chromatographic-like peaks, where the MS1 can be easily extracted to show the  $[M]^+$  and  $[M+H]^+$ . These species are fragmented to produce an MS<sup>2</sup> spectra.

## Results

### Even-Electron Ionization $[M+H]^+$ of CBD and THC

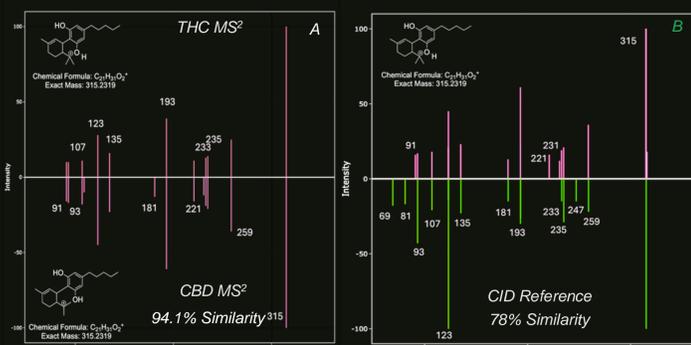


Figure D: Comparison of the MS<sup>2</sup> of the protonated forms (315 m/z) of THC - SICRIT (above) and CBD - SICRIT (below) with a CID spread of 5-35 eV.

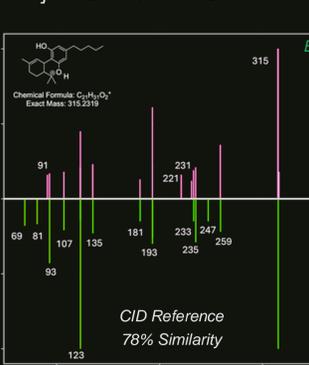
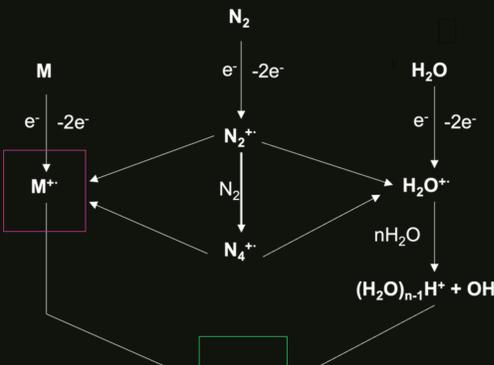


Figure C: MS<sup>2</sup> spectra of THC  $[M+H]^+$  precursor (315 m/z) compared to an HMDI orbitrap reference spectra (above) with a CID spread of 11-25 eV.



Ionization Mechanism Pathway of DBDI Source

### Odd-Electron Ionization $[M]^+$ of CBD and THC

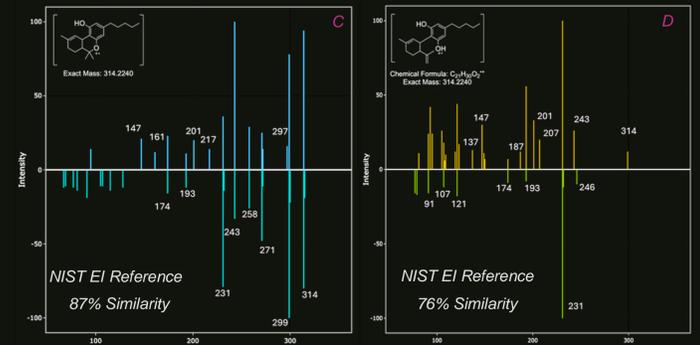
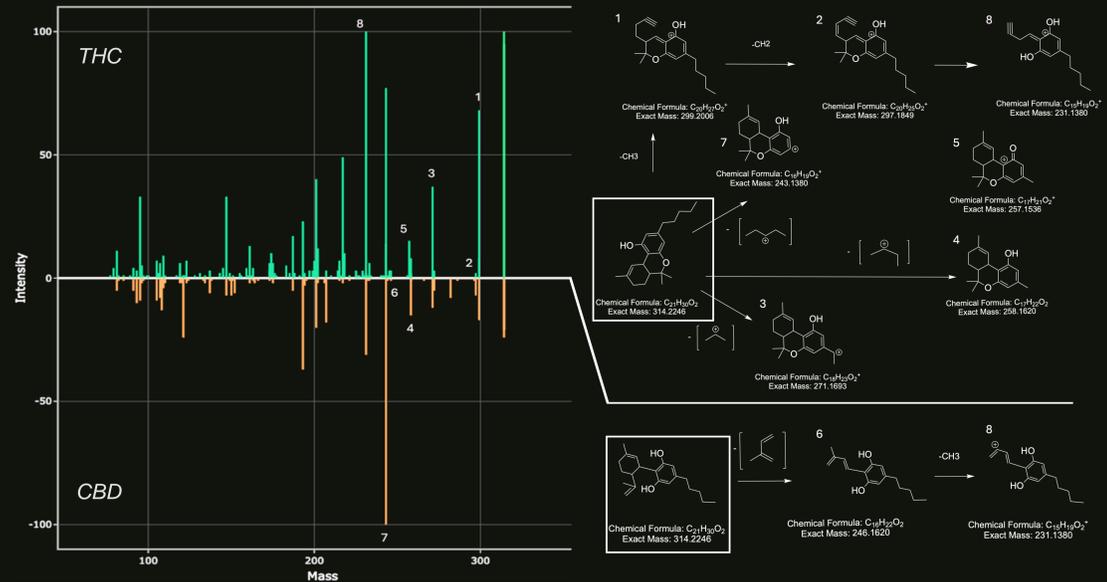


Figure A: MS<sup>2</sup> spectra of THC  $[M]^+$  (314 m/z) with a CID spread of 20-55 eV (above) compared to the GC-EI NIST spectra (below) Figure B: MS<sup>2</sup> spectra of CBD  $[M]^+$  precursor (314 m/z) with a CID spread of 25-35 eV (above) compared to a GC-EI NIST spectra (below).



MS<sup>2</sup> spectra with varying CID spreads of CBD (right) and THC (left), the labelled peaks correspond to reported EI fragments



Left: High resolution MS<sup>2</sup> spectra of  $[M]^+$  precursor THC (above) and CBD (below), with a CID spread of 5-35 eV. Right: EI-fragmentation pathway for THC (above) and CBD (below)

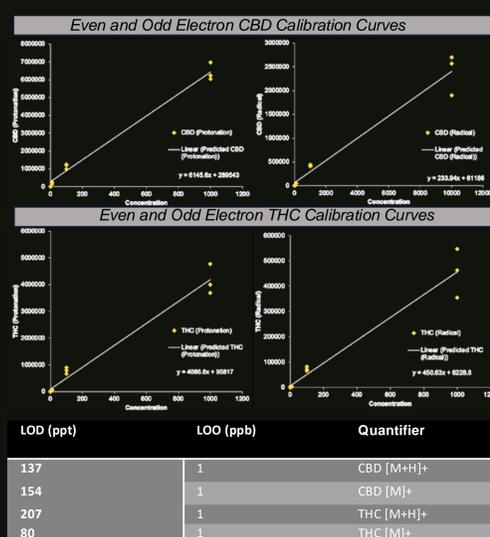
## Conclusion & Outlook

### 10 Second Quantification of Cannabinoids in Cannabis without Chromatography

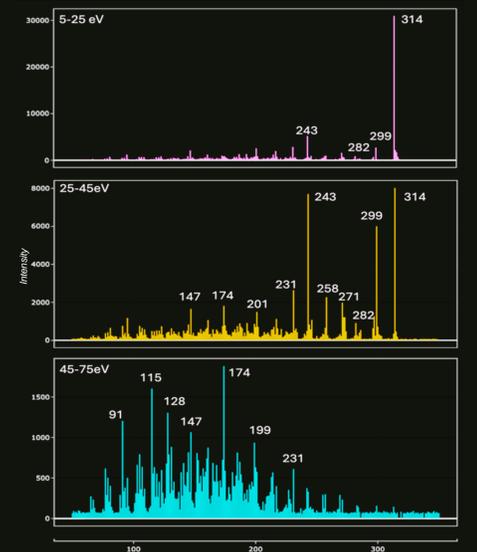
This study shows:

- Rapid quantification of THC and CBD without chromatography
- In a single ionization technique, it is possible to obtain both odd-electron and even-electron species, which leads to EI-like and CID fragmentation patterns, respectively.
- Identification through GC-MS and LC-MSMS libraries
- Analysis of extracted cannabis samples, with minimal sample prep.
- Sensitivity of identification within ppt range for both odd and even - electron ionizations

In the future, we plan to continue our study developing a direct injection MRM method, based on odd-electron precursors for routine analysis of cannabis.



LOD (ppt)	LOQ (ppb)	Quantifier
137	1	CBD $[M+H]^+$
154	1	CBD $[M]^+$
207	1	THC $[M+H]^+$
80	1	THC $[M]^+$



MS<sup>2</sup> of  $[M]^+$  Provided is the observed fragmentation of the radical species (m/z 314) within an extracted cannabis sample at three different CID fragmentation windows.