

Supplementary Information

Analysis of Isomeric Cannabinoid Standards and *Cannabis* Products by UPLC-ESI-TWIM-MS: a Comparison with GC-MS and GC × GC-QMS

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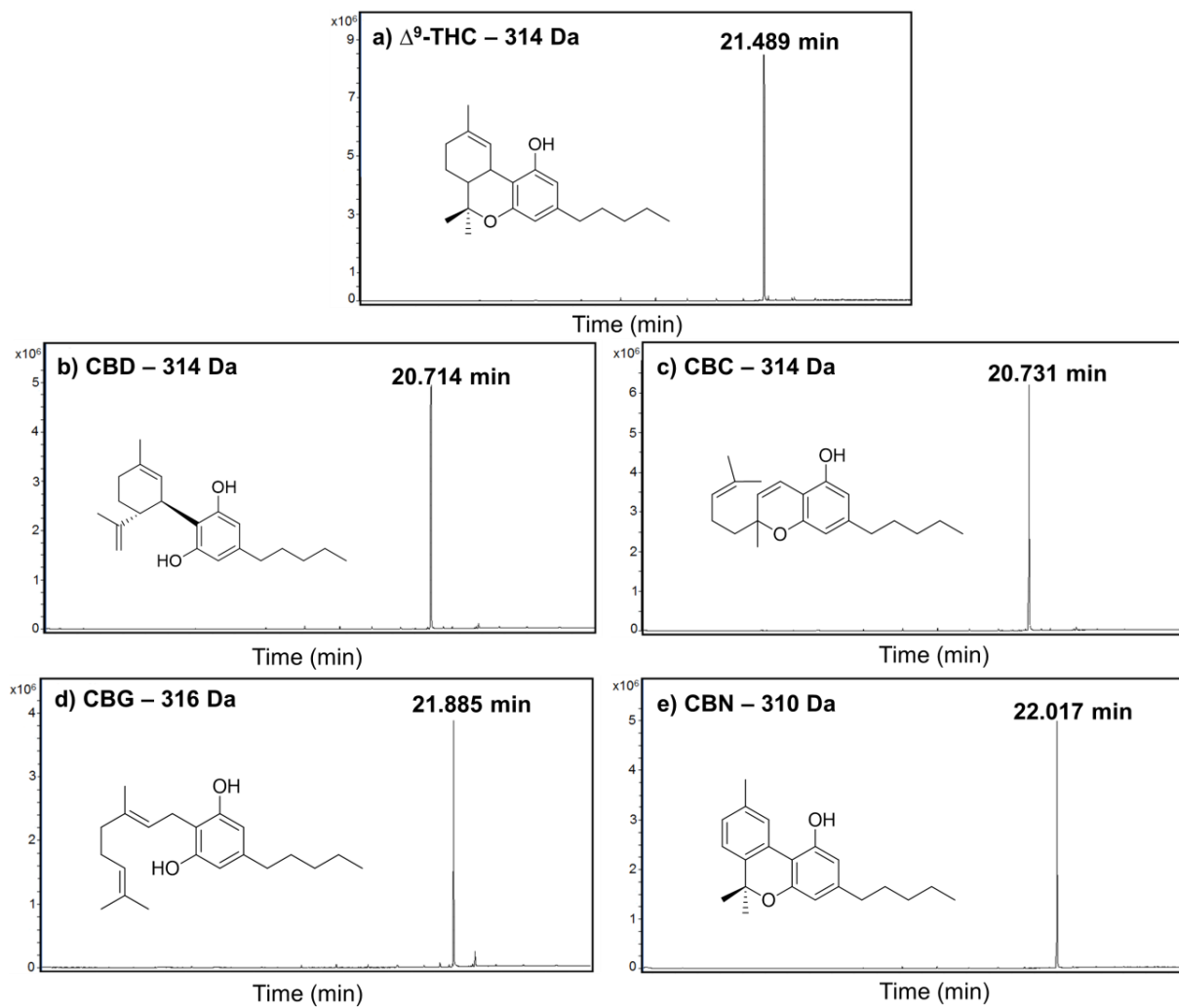


Figure S1. The chromatographic profile for the (a) Δ^9 -THC; (b) CBD; (c) CBC; (d) CBG; and (e) CBN standards.

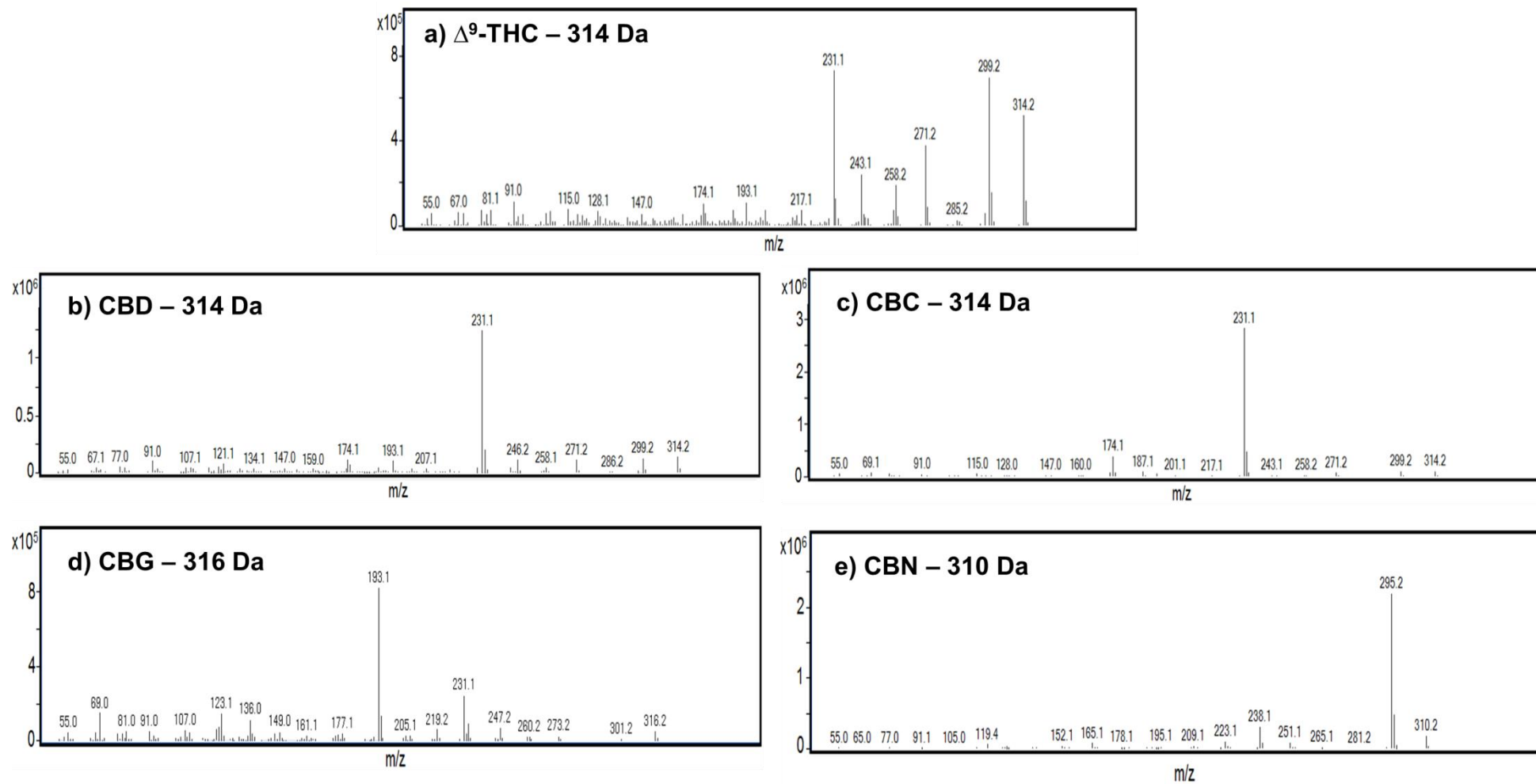


Figure S2. EI mass spectra of the five neutral cannabinoids standards: (a) Δ^9 -THC; (b) CBD; (c) CBC; (d) CBG; and (e) CBN.

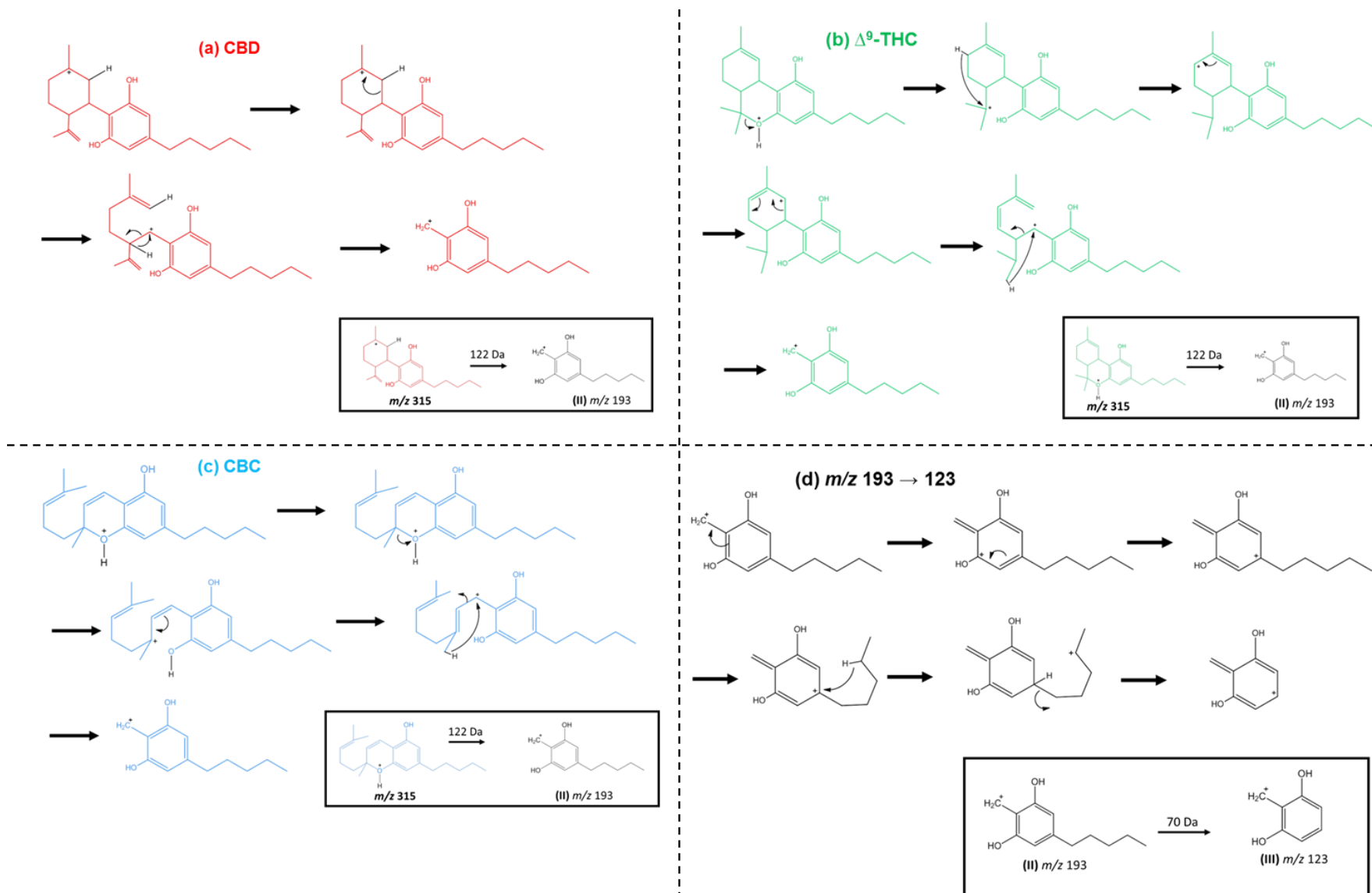


Figure S3. Proposed mechanism from main fragments produced via CID experiments for the m/z 315 \rightarrow 193 transitions ((a) CBD; (b) Δ^9 -THC; and (c) CBC) and (d) m/z 193 \rightarrow 123 transitions.

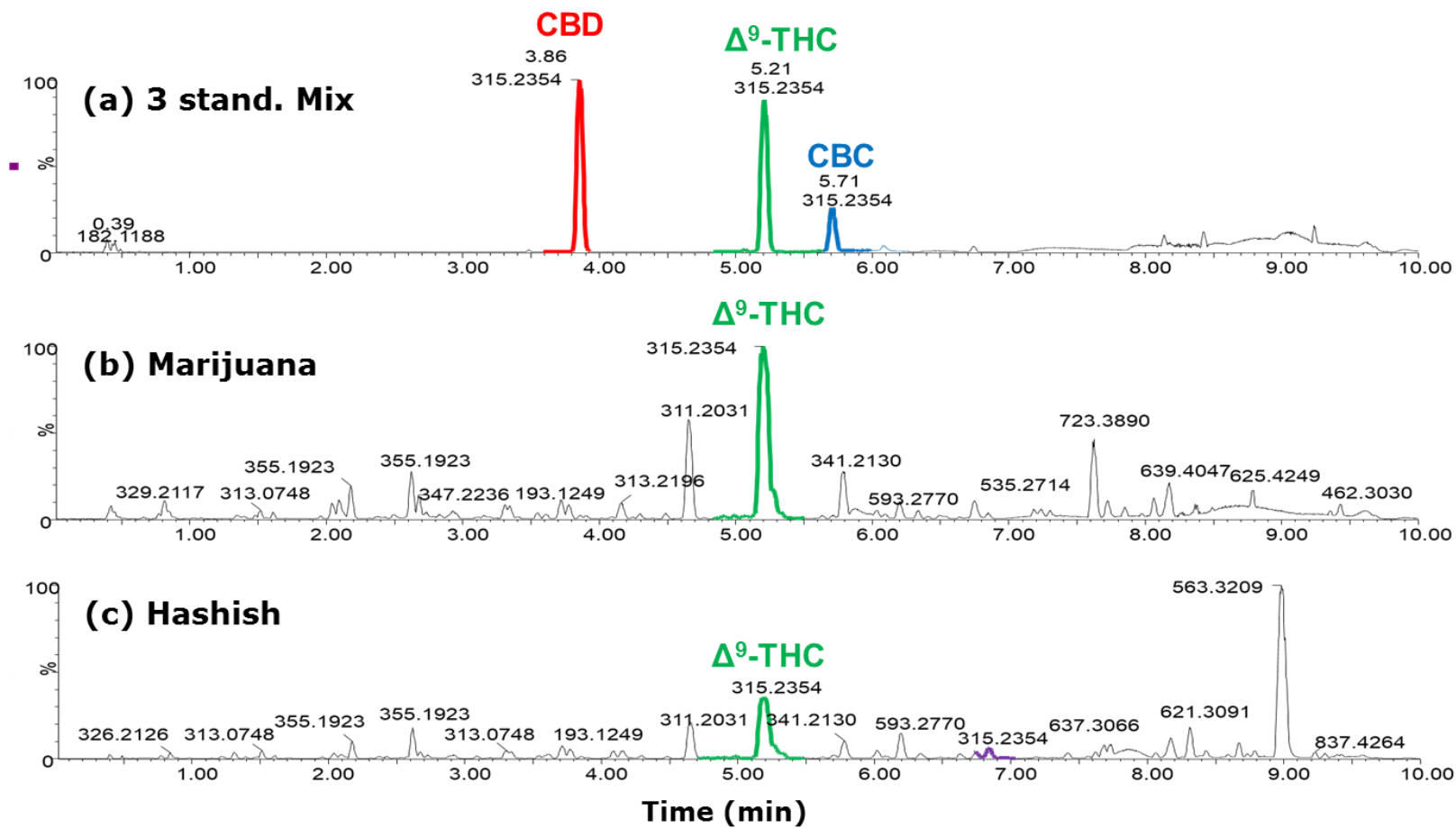


Figure S4. Chromatograms obtained from the UPLC-ESI(+)-QTOF-MS analysis of (a) standards isomeric mixture of Δ^9 -THC, CBD and CBC; (b) marijuana; and (c) hashish samples. In all cases, the mass spectra were acquired in the full scan mode.

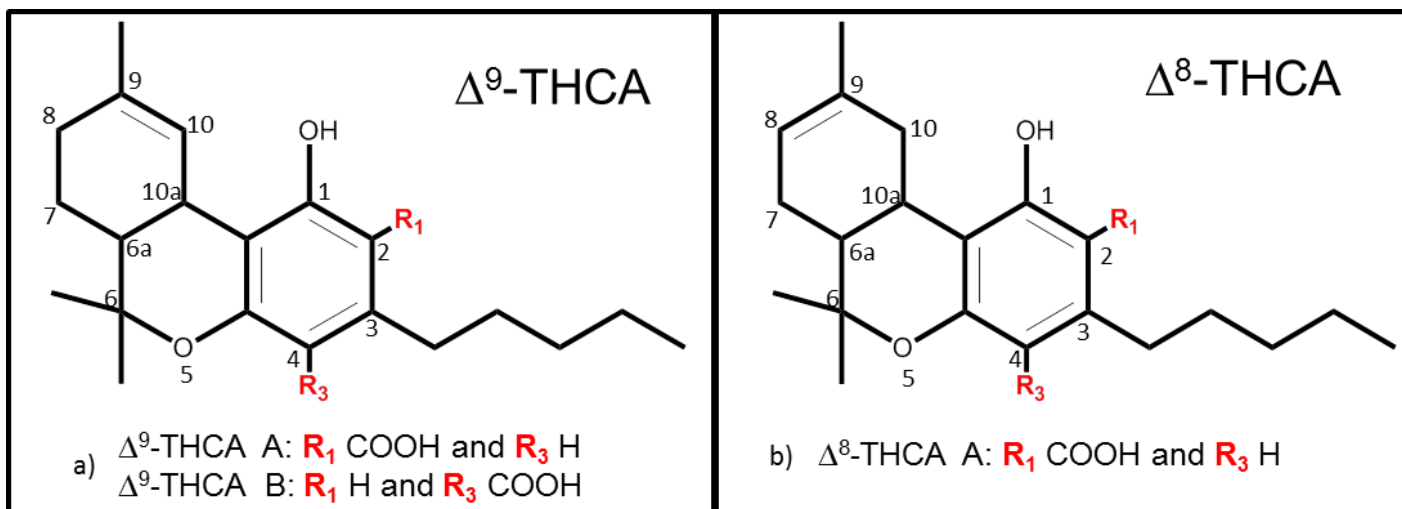


Figure S5. Molecular structure of (a) Δ^9 -THCA A or B and (b) Δ^8 -THCA A.

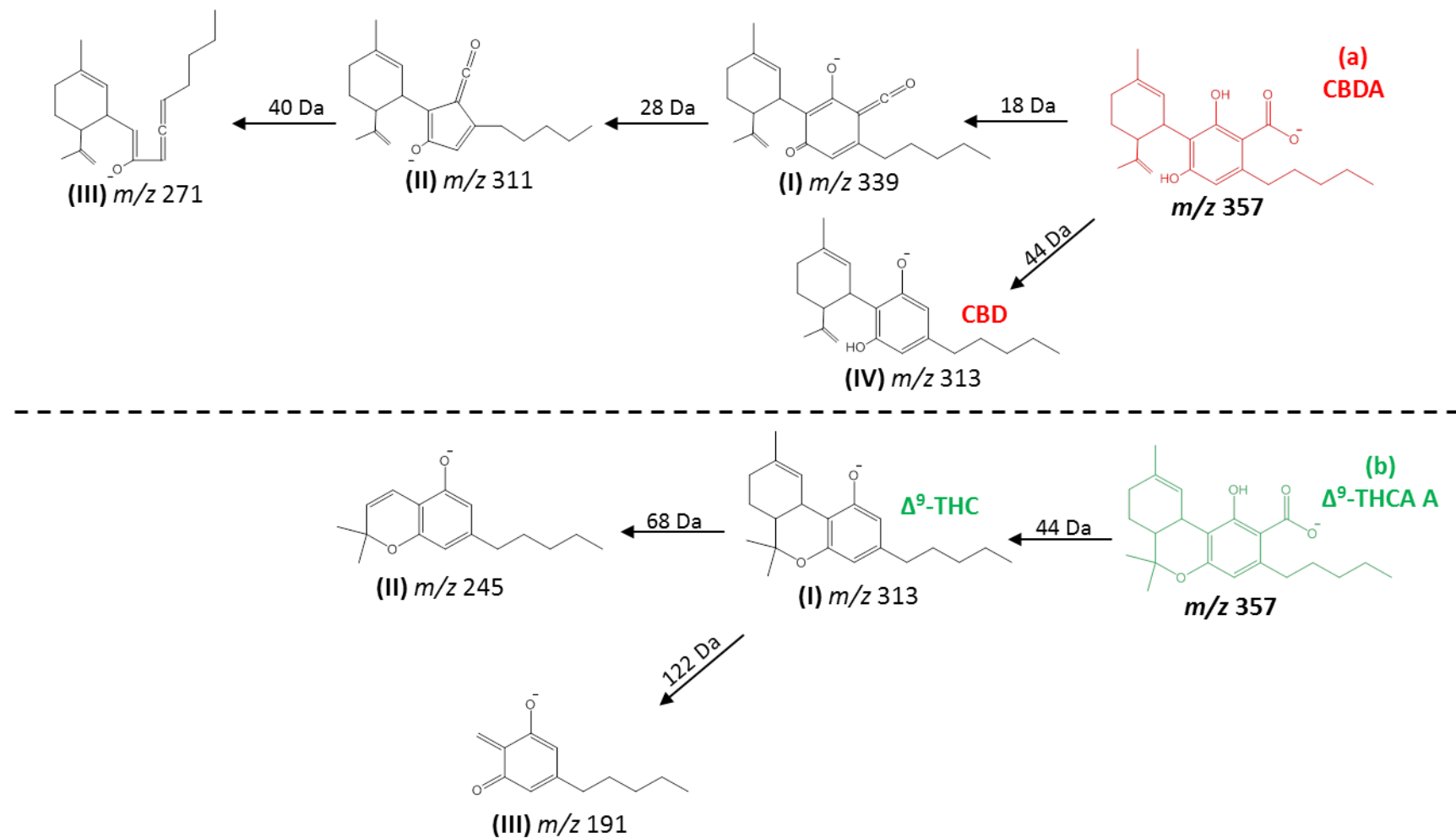


Figure S6. Proposed mechanism for the CID experiments for m/z 357 corresponding to two acid cannabinoid standards: (a) CBDA and (b) Δ^9 -THCA A.

Table S1. Measured *m/z* values, and assigned and detected species in leaf, flower and hashish samples using a UPLC-ESI(-)TWIM-MS

No.	<i>m/z</i> measured	Proposed compound	Leaf	Flower	Hashish	Reference
1	309.1869	cannabinol, cannabinodiol or cannabifuran	–	1	1	Nascimento <i>et al.</i> ¹ and Borille <i>et al.</i> ²
2	345.2080	cannabitrinol, cannabielsoic acid A or B	3	2	3	Borille <i>et al.</i> ²
3	353.1774	cannabinolic acid A	1	1	1	Tose <i>et al.</i> , ³ Elsohly and Slade ⁴ and Borille <i>et al.</i> ²
4	357.2086	Δ^9 -tetrahydrocannabinolic acid A or B, cannabichromenic acid, cannabicyclolic acid, cannabidiolic acid or Δ^8 -tetrahydrocannabinolic acid A or B	1	3	3	Borille <i>et al.</i> ²
5	359.2265	cannabigerolic acid	–	1	1	Nascimento <i>et al.</i> ¹ and Borille <i>et al.</i> ²
6	367.1207	8-hydroxycannabinolic acid A	–	1	1	Borille <i>et al.</i> ² and Watanabe <i>et al.</i> ⁵
7	373.2411	11-hydroxy- Δ^9 -tetrahydrocannabinolic acid, cannabigerolic acid monomethylether	1	2	1	Jung <i>et al.</i> ⁶ and Aizpurua-Olaizola <i>et al.</i> ⁷

–: non-detected.

References

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