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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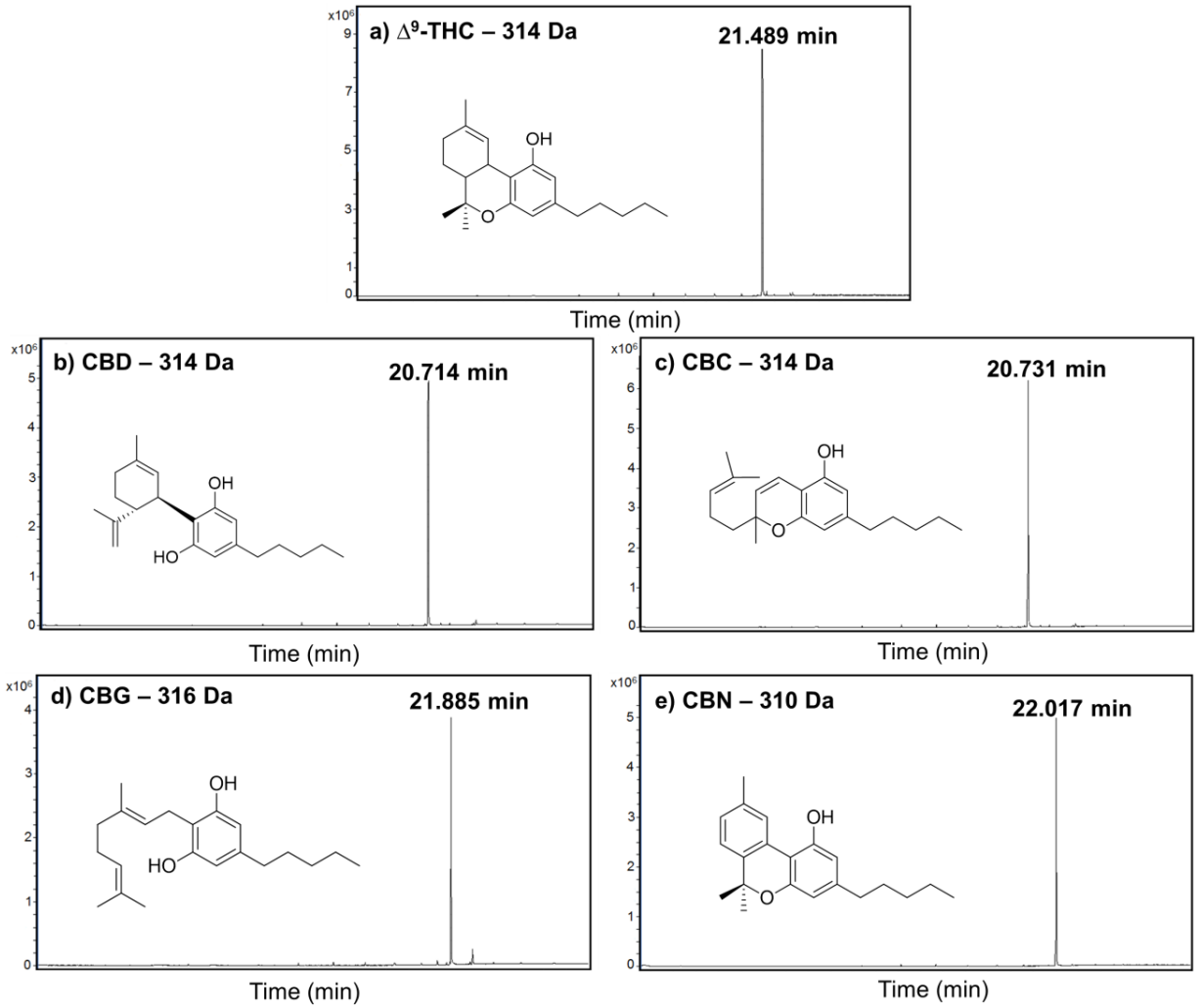

Figure S1. The chromatographic profile for the (a) Δ^9-THC; (b) CBD; (c) CBC; (d) CBG; and (e) CBN standards.

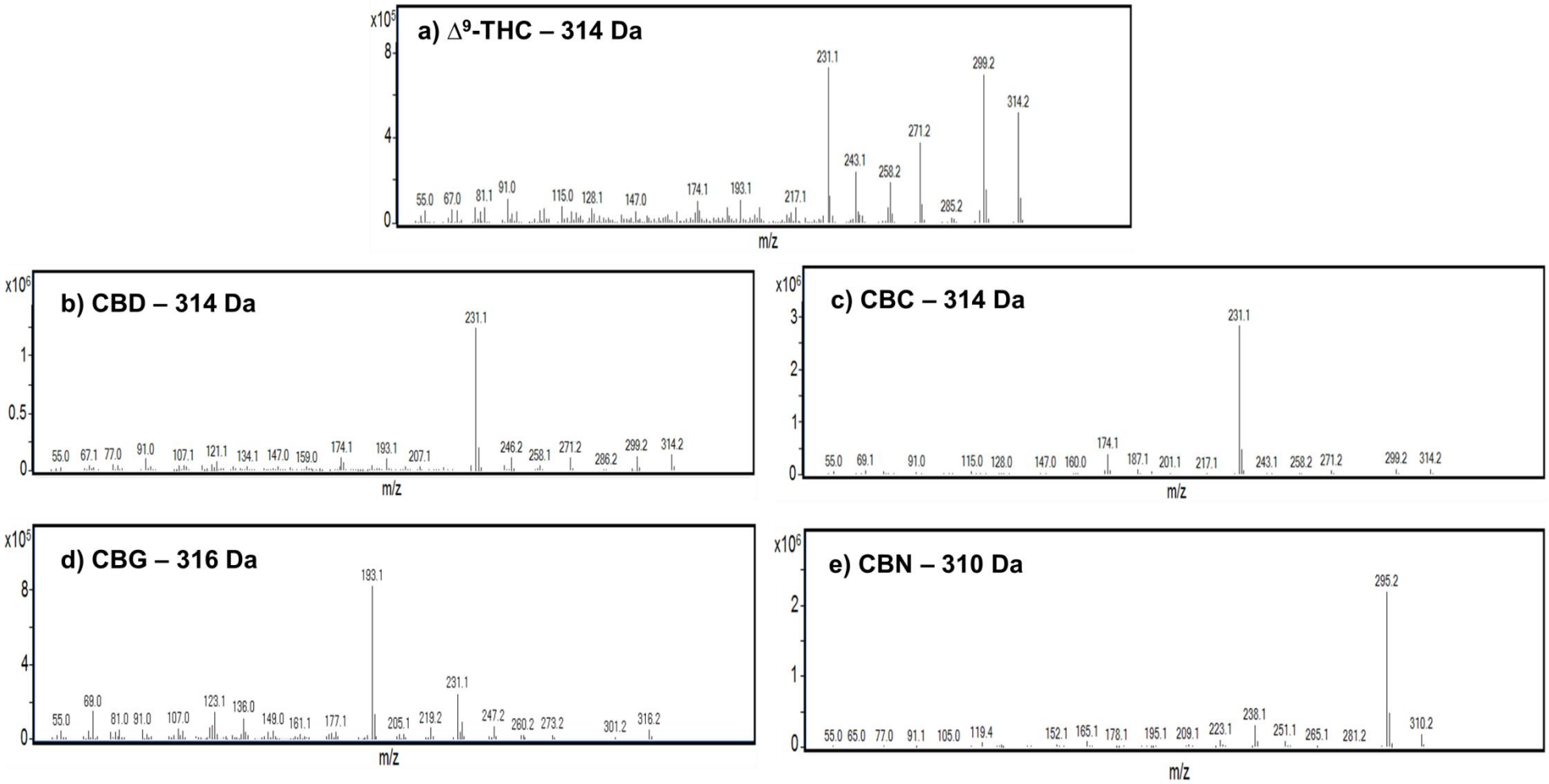

Figure S2. EI mass spectra of the five neutral cannabinoids standards: (a) Δ^9-THC; (b) CBD; (c) CBC; (d) CBG; and (e) CBN.

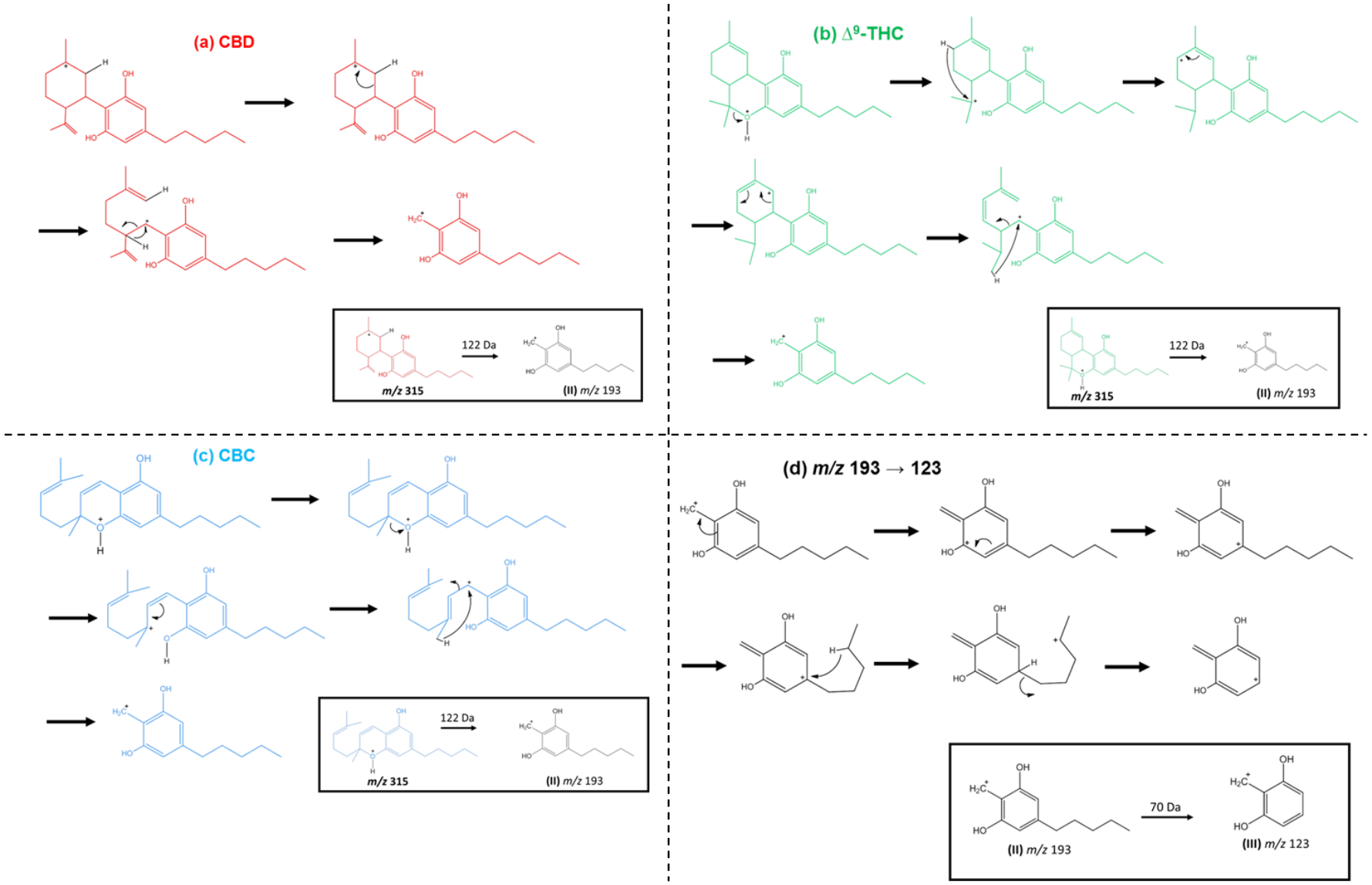

Figure S3. Proposed mechanism from main fragments produced via CID experiments for the *m/z* 315 → 193 transitions ((a) CBD; (b) Δ^9-THC; and (c) CBC) and (d) *m/z* 193 → 123 transitions.

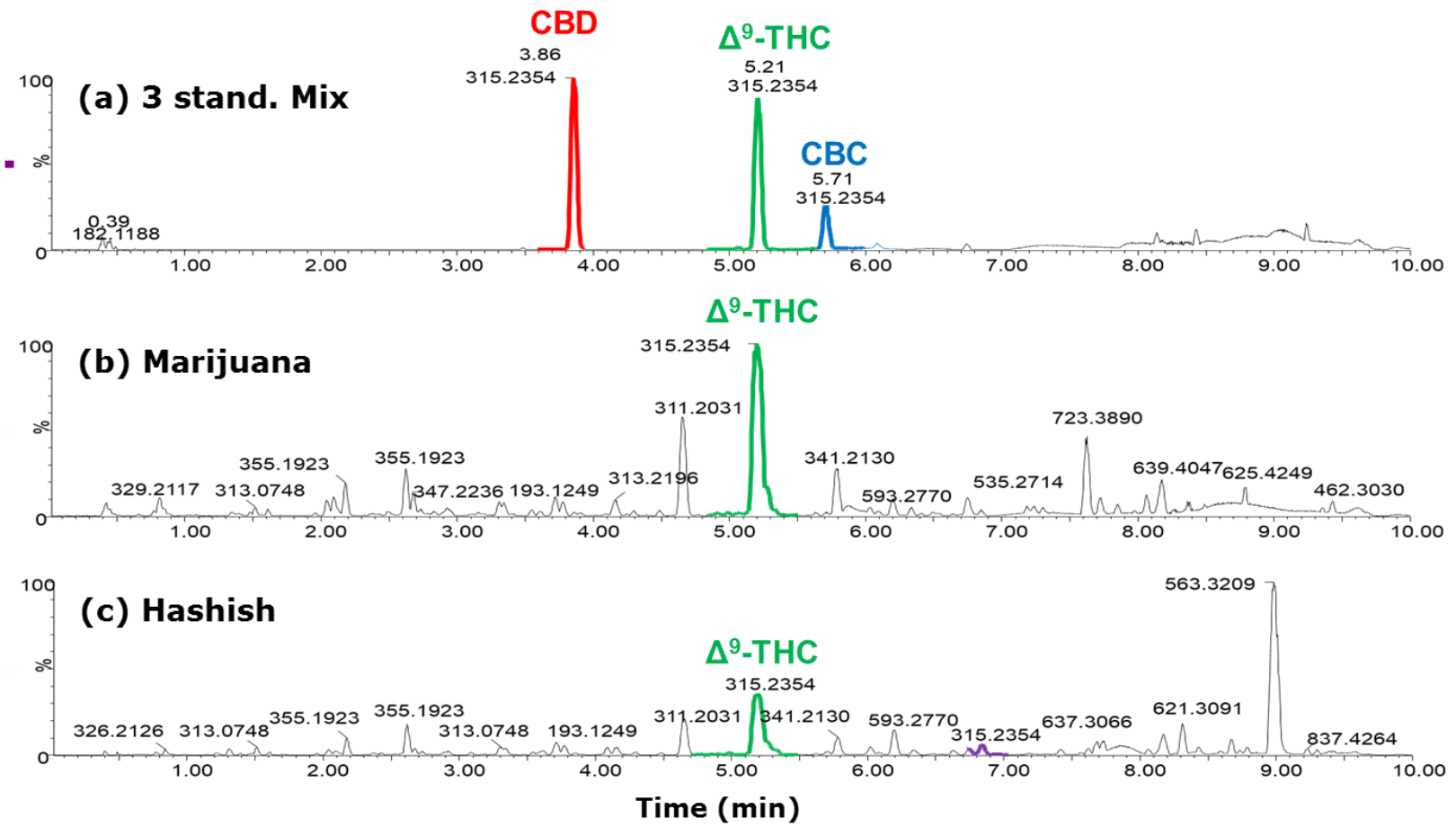

Figure S4. Chromatograms obtained from the UPLC-ESI(+)-QTOF-MS analysis of (a) standards isomeric mixture of Δ^9-THC, CBD and CBC; (b) marijuana; and (c) hashish samples. In all cases, the mass spectra were acquired in the full scan mode.

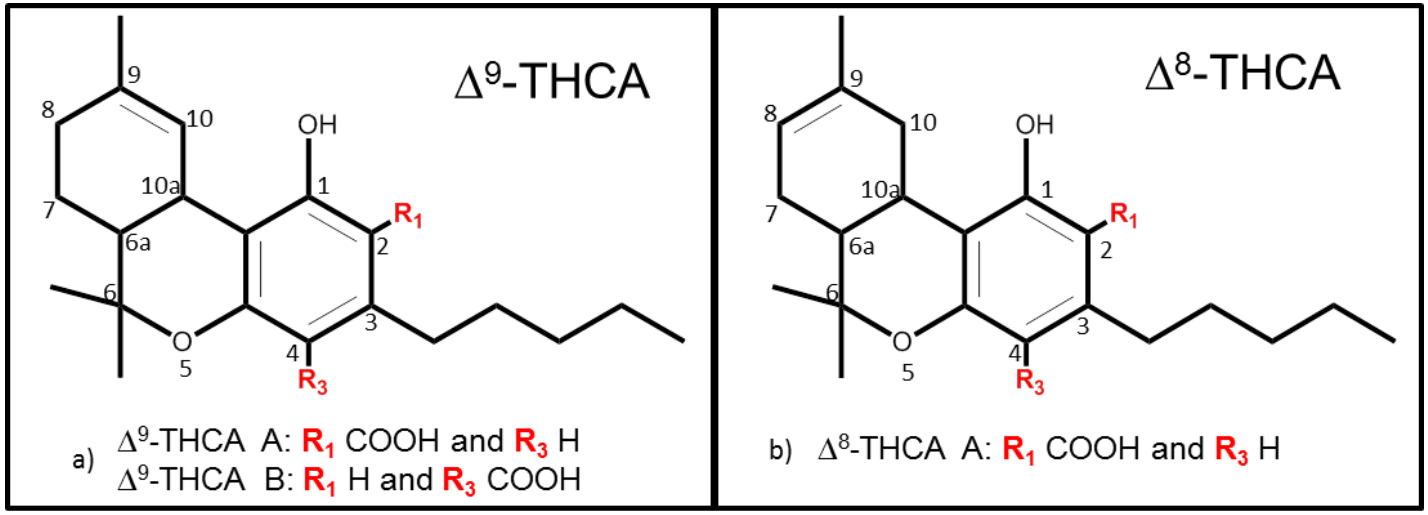

Figure S5. Molecular structure of (a) Δ^9-THCA A or B and (b) Δ^8-THCA A.

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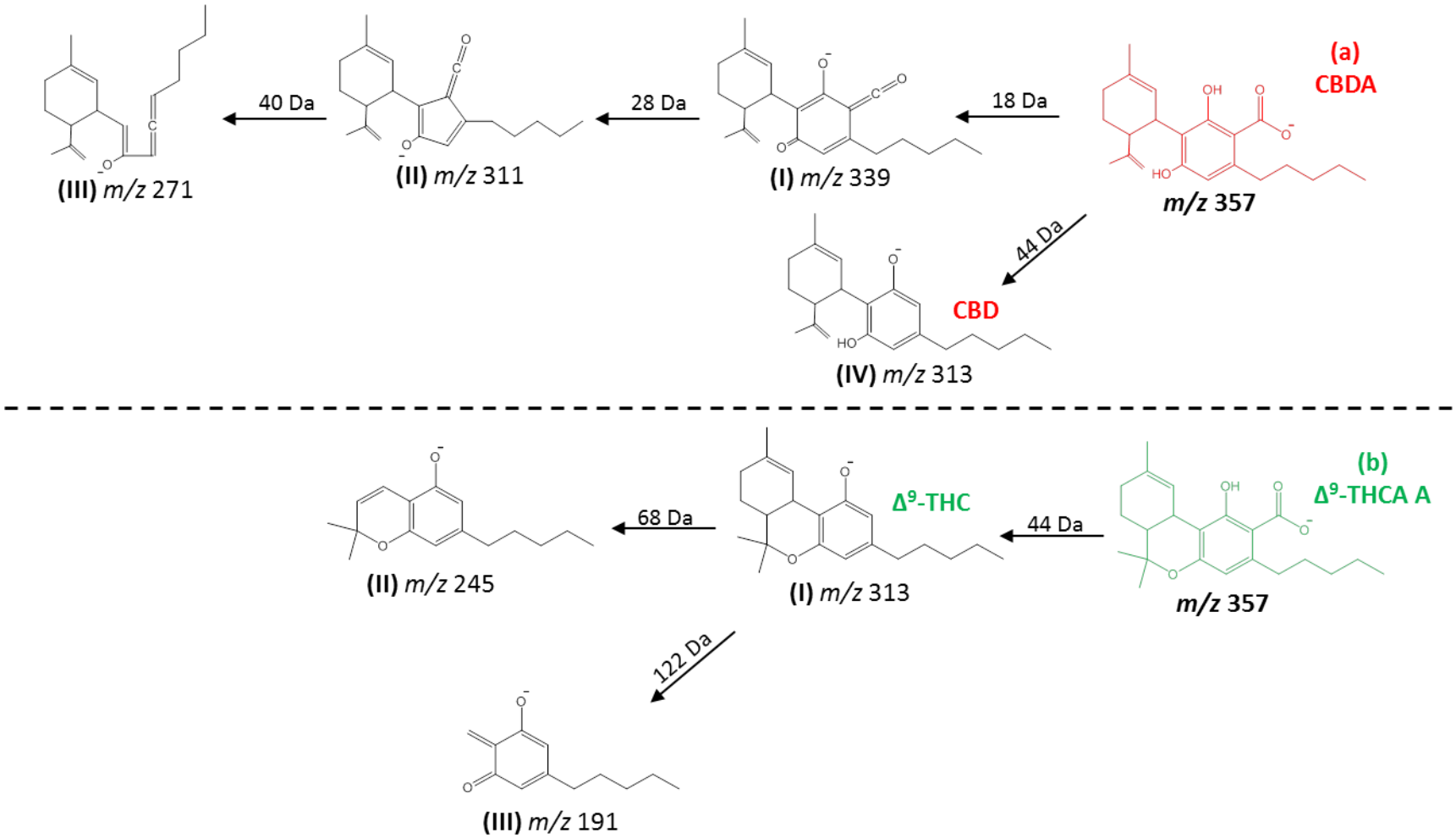

Figure S6. Proposed mechanism for the CID experiments for *m/z* 357 corresponding to two acid cannabinoid standards: (a) CBDA and (b) Δ^9-THCA A.

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

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

–: non-detected.

References

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