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Supplementary Material

Identification of Δ^9-tetrahydrocannabinol (Δ^9-THC) in *Cannabis* seeds by Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI(-)FT-ICR MS)

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Table S1. Molecular formula, theoretical *m/z*, DBE, proposed compound and mass error identified in the *Cannabis* seeds by ESI(-)FT-ICR MS.

Nº	molecular formula	Theoretical *m/z*	DBE	Proposed compound	Error (ppm)			Reference
					Whole Seed	Seed shell	Internal Part	
1	$[C_6H_{12}O_6+Cl]^-$	215.03279	1	Glucose, galactose, fructose or mannose	-0.32	-0.43	-	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; L. Boutegrabet, et al.Chem Eur J. 18(41) (2012) 13059-13067; H. Li, et al. J mass spectrum. 43(11) (2008) 1545-1552;
2	$[C_{16}H_{30}O_2–H]^-$	253.21730	2	Palmitoleic acid	-0.33	-0.45	-1.43	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487;
3	$[C_{16}H_{32}O_2 – H]^-$	255.23295	1	Palmitic acid	-0.31	-0.63	-1.42	R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502;
4	$[C_{18}H_{30}O_2 – H]^-$	277.21730	4	α-Linolenic acid	-0.26	-0.58	-1.1	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487;
5	$[C_{18}H_{32}O_2 – H]^-$	279.23295	3	Linoleic acid	-0.16	-0.50	-0.68	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502; M.O. Salazar, et al. Phytochem analysis. 25(2) (2014) 155-160;
6	$[C_{18}H_{34}O_2 – H]^-$	281.2486	2	Oleic acid	-0.44	-0.78	-1.66	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502; M.O. Salazar, et al. Phytochem analysis. 25(2) (2014) 155-160;
7	$[C_{18}H_{36}O_2 – H]^-$	283.26425	1	Stearic acid	-0.36	-0.64	-1.62	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502;
8	$[C_{16}H_{32}O_2+Cl]^-$	291.20963	1	Palmitic acid	-0.30	-0.55	-1.25	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; C. da Porto, et al. J food sci tech. 52(3) (2015) 1748-1753;
9	$[C_{18}H_{32}O_3–H]^-$	295.22787	3	Vernolic acid	-0.51	-0.76	-	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487;
10	$[C_{11}H_{19}NO_9–H]^-$	308.09870	3	Sialic Acid	-0.46	-0.44	-1.79	
11	$[C_{21}H_{26}O_2 – H]^-$	309.18600	9	Cannabinol, Cannabinodiol or Cannabifuran	-0.23	-0.43	-1.46	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9

								(2017) 4070-4081;
12	$[C_{18}H_{30}O_2+Cl]^-$	313.19398	4	α Linolenic acid	-0.48	-0.91	-1.86	
13	$[C_{21}H_{30}O_2-H]^-$	313.21730	7	Δ^9- THC, Cannabichromene, Cannabidiol, Δ^8 – THC, Δ^6 – THC, Cannabicyclol or Cannabicitran	-0.51	-0.69	0.13	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
14	$[C_{18}H_{34}O_4-H]^-$	313.23843	2	Octadecanedioic acid	-0.38	-0.64	-1.58	
15	$[C_{18}H_{32}O_2+Cl]^-$	315.20963	3	Linoleic acid	-0.27	-	-1.17	C.D. Porto, et al. J diet suppl. 12(1) (2015) 1-10.
16	$[C_{18}H_{34}O_2+Cl]^-$	317.22528	2	Oleic acid	-0.34	-0.62	-1.27	R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502;
17	$[C_{18}H_{36}O_2+Cl]^-$	319.24093	1	Stearic acid	-0.32	-0.61	-1.38	R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502;
18	$[C_{21}H_{26}O_3-H]^-$	325.18092	9	Hydroxycannabinol	-0.67	-0.82	-2.30	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
19	$[C_{21}H_{28}O_3-H]^-$	327.19657	8	10-Oxo-Δ6a(10a)-Tetrahydrocannabinol (OTHC), 8-*Oxo*-Δ9-Tetrahydrocannabinol (8-*Oxo*-Δ9-THC) or Cannabicoumaronone	-0.38	-0.69	-2.14	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
20	$[C_{20}H_{26}O_4-H]^-$	329.17583	8	Cannabidivarinic acid or Δ^9-Tetrahydrocannabivarinic acid A	-0.23	-0.59	-0.18	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
21	$[C_{21}H_{30}O_3-H]^-$	329.21222	7	11-hydroxy-Δ9-tetrahydrocannabinol or Cannabiesoin	-0.46	-0.62	0.05	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
22	$[C_{18}H_{34}O_5-H]^-$	329.23335	2	Tiansic acid	-0.32	-0.63	-	
23	$[C_{20}H_{28}O_4-H]^-$	331.19148	7	Cannabigerovarinic acid A (trans-CBGVA-C3 A) or Cannabichromanone (CBCN)	-0.50	-0.53	-0.07	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
24	$[C_{18}H_{32}O_3+Cl]^-$	331.20455	3	Vernolic Acid	-0.51	-0.89	-	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487;
25	$[C_{21}H_{32}O_3-H]^-$	331.22787	6	9α-Hydroxyhexahydrocannabinol, 10α-Hydroxyhexahydrocannabinol or Hydroxycannabichromane	-0.74	-1.03	-0.05	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
26	$[C_{17}H_{17}NO_4+Cl]^-$	334.08516	10	N-trans-Caffeoyltyramine	-0.51	-0.79	-	I. Sakakibara, et al. Phytochemistry. 30(9) (1991) 3013-3016; T. Chen, et al. Food chem. 134(2) (2012) 1030-1037;
27	$[C_{22}H_{44}O_2-H]^-$	339.32685	1	Behenic acid	-0.53	-0.81	-1.98	R. Garrett, et al. Food Sci Technol-

								LEB. 50(2) (2013). 496-502;
28	$[C_{12}H_{22}O_{11} - H]^-$	341.10894	2	Saccharose	-0.56	-0.57	-1.86	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; H. Li, et al. J mass spectrum. 43(11) (2008) 1545-1552;
29	$[C_{21}H_{28}O_4 - H]^-$	343.19148	8	Δ^9-Tetrahydrocannabinolic acid-C4 A and B (Δ^9-THCA-C4 A and B), 10aα-Hydroxy-10-*oxo*-Δ8-Tetrahydrocannabinol (10aα-OH-10-*oxo*-Δ8-THC) or 9α-Hydroxy-10-*oxo*-Δ6a,10a-Tetrahydrocannabinol (9α-OH-10-*oxo*-Δ6a,10a-THC)	-0.51	-0.78	-2.04	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
30	$[C_{21}H_{26}O_2 + Cl]^-$	345.16268	9	Cannabinol, Cannabinodiol or Cannabifuran	-0.60	-0.49	-1.71	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
31	$[C_{21}H_{30}O_4 - H]^-$	345.20713	7	Cannabitriol	-0.48	-0.72	-1.79	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
32	$[C_{18}H_{19}NO_4 + Cl]^-$	348.10081	10	N-trans-Feruloyltyramine	-0.54	-0.81	-	I. Sakakibara, et al. Phytochemistry. 30(9) (1991) 3013-3016;
33	$[C_{21}H_{30}O_2 + Cl]^-$	349.19398	7	Δ^9- THC, Cannabichromene, Cannabidiol, Δ^8 – THC, Δ^6 – THC, Cannabicyclol or Cannabicitran	-0.36	-0.64	-1.42	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
34	$[C_{16}H_{18}O_9 - H]^-$	353.08781	8	Chlorogenic Acid	-0.33	-0.71	-	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487; R. Garrett, et al. Food Sci Technol-LEB. 50(2) (2013). 496-502;
35	$[C_{22}H_{26}O_4 - H]^-$	353.17583	10	Cannabinolic acid A	-0.68	-0.94	-2.33	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
36	$[C_{22}H_{28}O_4 - H]^-$	355.19148	9	Estradiol	-0.96	-0.96	-0.30	
37	$[C_{22}H_{30}O_4 - H]^-$	357.20713	8	Δ^9-Tetrahydrocannabinolic acid, Cannabichromenic acid, Cannabicyclolic acid, Cannabidiolic acid or Δ^8-Tetrahydrocannabinolic acid	-0.62	-0.92	-2.23	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
38	$[C_{22}H_{32}O_4 - H]^-$	359.22278	7	Cannabigerolic acid	-0.47	-0.82	-0.17	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
39	$[C_{21}H_{28}O_3 + Cl]^-$	363.17325	8	10-Oxo-Δ6a(10a)-Tetrahydrocannabinol (OTHC)	-0.55	-0.73	-0.73	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
40	$[C_{21}H_{30}O_3 + Cl]^-$	365.18890	7	Cannabicoumaronone or Cannabielsoin	-0.50	-0.69	-1.64	M.M. Eiras, et al.Anal Methods. 6(5) (2014) 1350-1352;
41	$[C_{18}H_{34}O_5 + Cl]^-$	365.21003	2	Thianshic acid	-0.50	-0.79	-1.94	
42	$[C_{19}H_{38}O_4 + Cl]^-$	365.24641	1	Palmitoylglycerol	-0.61	-0.89	-2.11	
43	$[C_{20}H_{28}O_4 + Cl]^-$	367.16816	7	Cannabigerovarinic acid or Cannabichromanone	-	-	-0.72	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
44	$[C_{21}H_{32}O_3 + Cl]^-$	367.20455	6	9α-Hydroxyhexahydrocannabinol	-0.61	-0.82	-1.90	K. Watanabe, et al. Forensic Toxicol. 25(1) (2007) 16-21; B.T.

								Borille, et al. Anal Methods. 9 (2017) 4070-4081;
45	$[C_{24}H_{48}O_2 - H]^-$	367.35815	1	Lignoceric acid	-0.49	-0.73	-1.83	J.B. Kill, et al. Forensic sci int. 266 (2016) 474-487;
46	$[C_{22}H_{28}O_5 - H]^-$	371.18640	9	Cannabicoumaric acid	-0.49	-0.95	-2.33	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081; O. Aizpurua-Olaizola, et al. Anal bioanal chem. 406(29) (2014) 7549-7560;
47	$[C_{23}H_{32}O_4 - H]^-$	371.22278	8	(±)-Cannabichromenic acid A	-0.36	-0.92	-1.32	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
48	$[C_{22}H_{30}O_5 - H]^-$	373.20205	8	11-Hydroxy-Δ^9-Tetrahydrocannabinolic acid	-0.77	-0.90	-2.33	J. Jung, et al. J mass spectrom. 44(10) (2009) 1423-1433;
49	$[C_{23}H_{34}O_4 - H]^-$	373.23843	7	Cannabigerolic Acid Monomethylether (CBGAM)	-0.61	-0.97	-	O. Aizpurua-Olaizola, et al. Anal bioanal chem. 406(29) (2014) 7549-7560;
50	$[C_{12}H_{22}O_{11} + Cl]^-$	377.08561	2	Saccharose, melibiose or gentiobiose	-0.52	-0.81	-1.08	Boutegrabet, et al.Chem Eur J. 18(41) (2012) 13059-13067;
51	$[C_{21}H_{28}O_4 + Cl]^-$	379.16816	8	(±)-Cannabichromevarinic acid	-0.80	-1.07	-2.41	M.M. Eiras, et al.Anal Methods. 6(5) (2014) 1350-1352;
52	$[C_{21}H_{30}O_4 + Cl]^-$	381.18381	7	Cannabitriol	-0.71	-0.88	-2.26	I.R. Nascimento, et al. Anal Methods. 7(4) (2015) 1415-1424; B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081; W.R. Chan, et al. Cell Mol Life Sci. 32(3) (1976) 283-284;
53	$[C_{22}H_{28}O_6 - H]^-$	387.18131	9	11-nor-9-COOH-Δ^9-Tetrahydrocannabinolic acid	-0.49	-0.86	-	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
54	$[C_{22}H_{30}O_6 - H]^-$	389.19696	8	8β,11-Dihydroxy-Δ^9-Tetrahydrocannabinolic acid (8β,11-Di-OH-Δ^9-THCA)	-0.60	-1.19	-	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
55	$[C_{21}H_{42}O_4 + Cl]^-$	393.27771	1	Glyceryl Monostearate	-0.38	-0.67	-1.63	
56	$[C_{21}H_{30}O_5 + Cl]^-$	397.17873	7	Cortisol	-0.51	-0.85	-1.79	U. Thieme, et al. Drug test anal. 6(1-2), (2014) 17-23;
57	$[C_{24}H_{32}O_5 - H]^-$	399.21770	9	Δ^9-Tetrahydrocannabinolic acid + Ethynol (C_2H_2O)	-0.59	-0.86	-2.23	B.T. Borille, et al. Anal Methods. 9 (2017) 4070-4081;
58	$[C_{22}H_{28}O_5 + Cl]^-$	407.16308	9	Cannabicoumaric acid	-0.28	-0.69	-1.86	O. Aizpurua-Olaizola, et al. Anal bioanal chem. 406(29) (2014) 7549-7560;

-not detected