

Supporting Information for Publication

A new ESI-LC/MS approach for comprehensive metabolic profiling of phytocannabinoids in *Cannabis*

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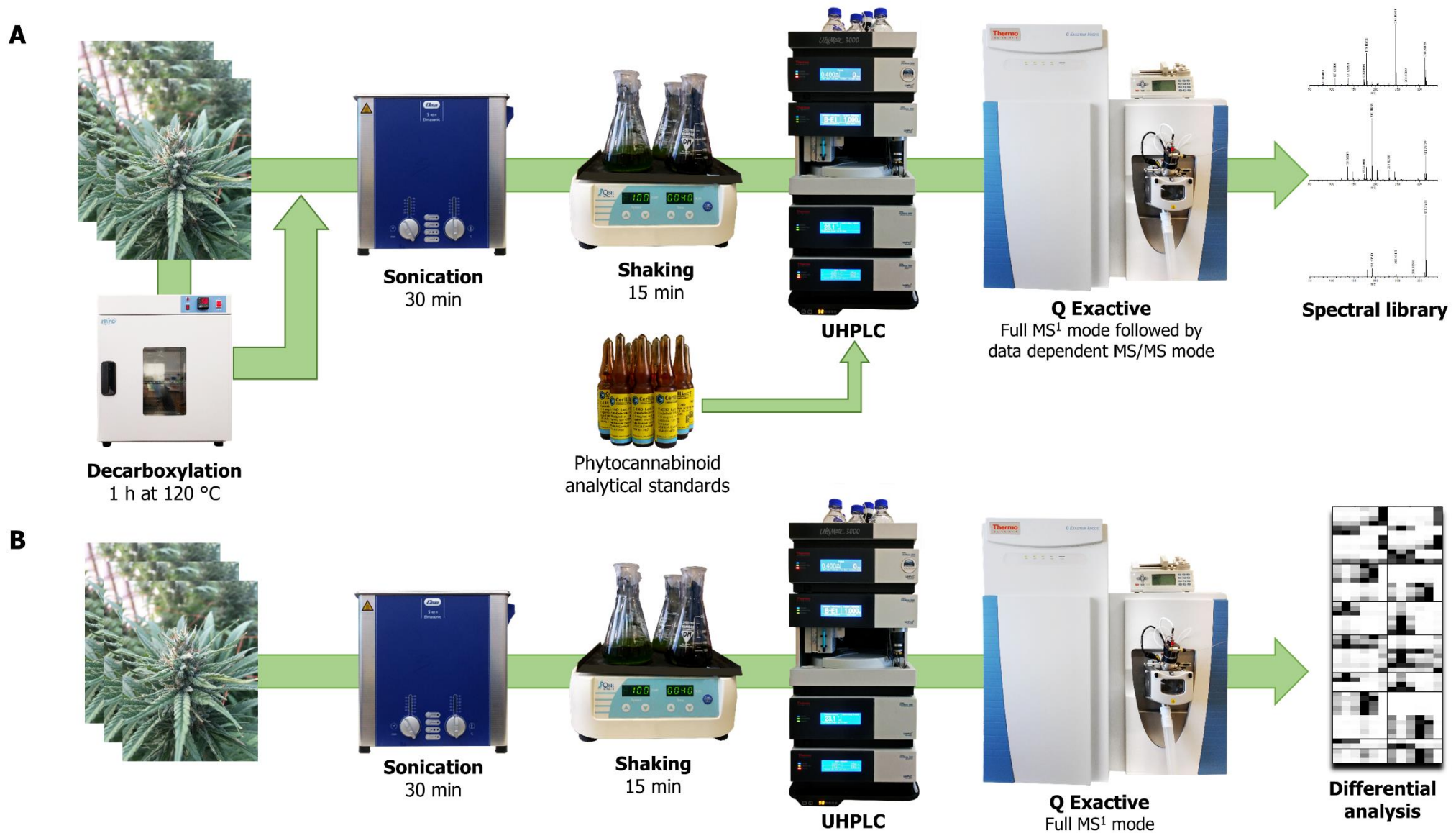


Figure S1. General overview of work methodology. (A) In the identification process, phytocannabinoids were chromatographically separated by reversed phase ultra HPLC (RP-UHPLC) and detected via MS/MS analysis. (B) Differential profiling of numerous medical *Cannabis* strains was performed by LC/MS according to the retention times and accurate masses of the identified phytocannabinoids in the spectral MS/MS library.

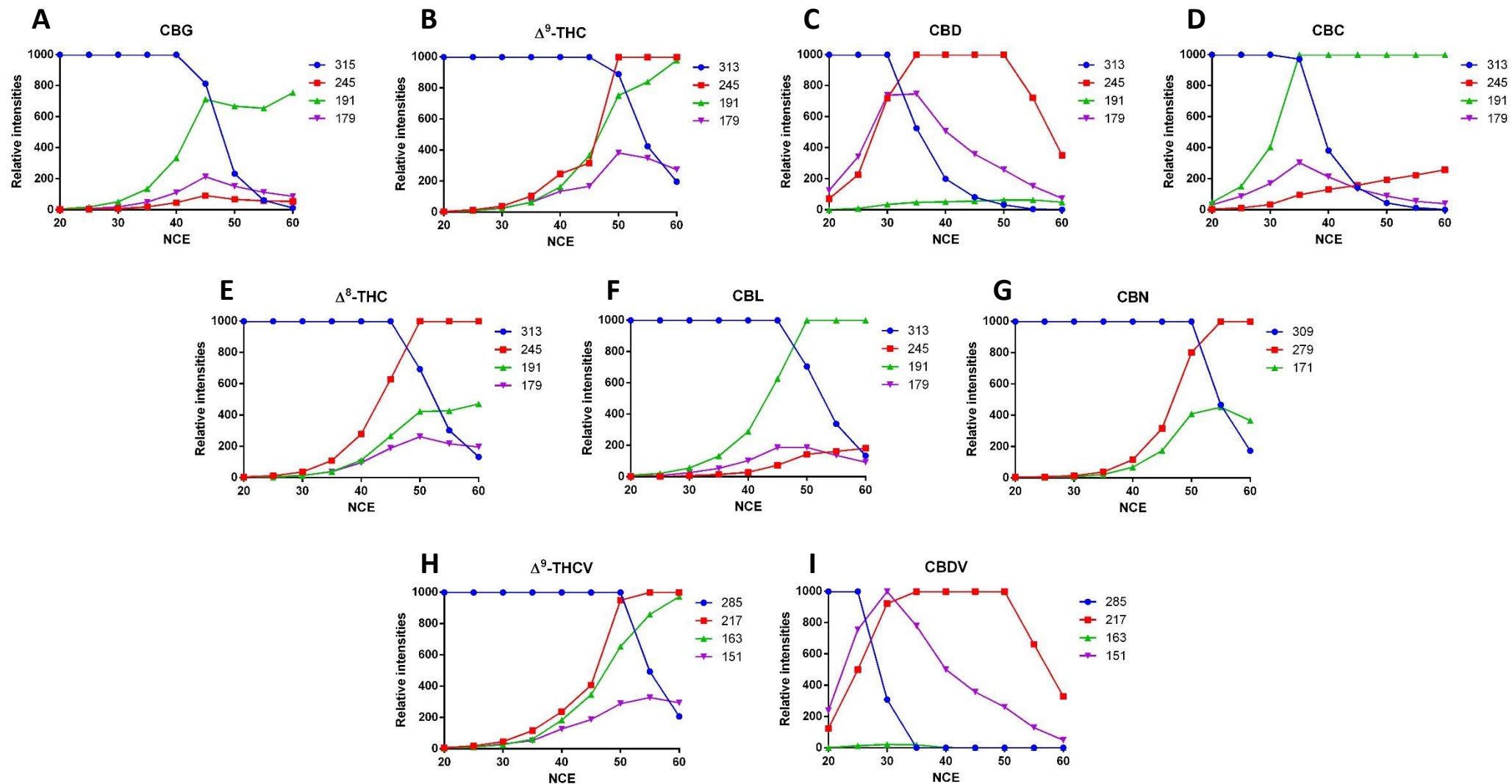


Figure S2. Plots of the LC/MS/MS ion abundance of the deprotonated precursor and product ions as a function of NCE energy for the available neutral pentyl and propyl phytocannabinoid standards. (A) CBG, (B) Δ^9 -THC, (C) CBD, (D) CBC, (E) Δ^8 -THC, (F) CBL, (G) CBN, (H) Δ^9 -THCV, and (I) CBDV. Accurate masses according to high-resolution LC/MS in descending order are as follows: 315.2329, 313.2173, 309.1860, 285.1860, 279.1391, 245.1547, 217.1234, 191.1078, 179.1078, 171.0815, 163.0765 and 151.0765.

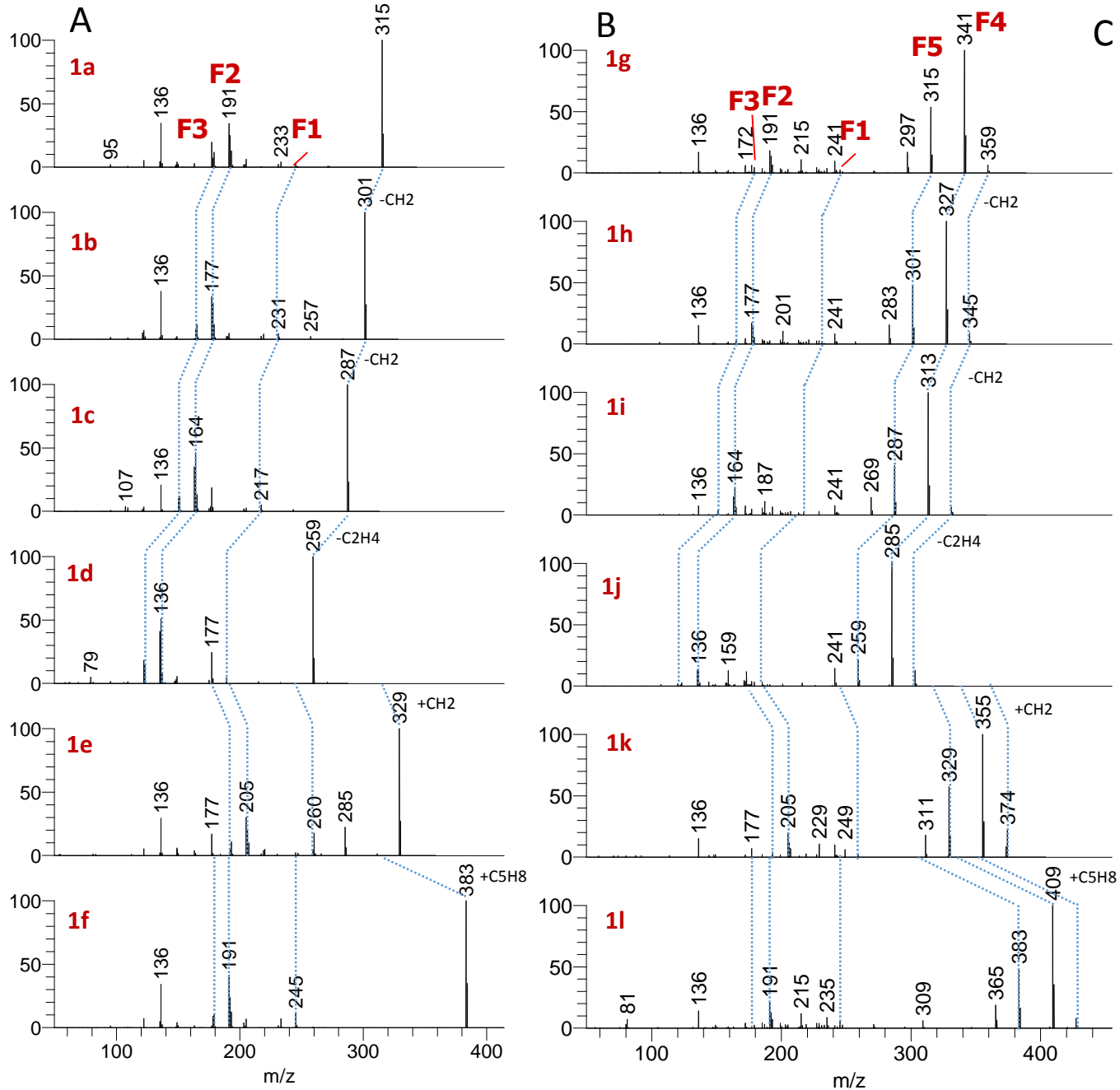


Figure S3. MS/MS spectral library of CBG-type phytocannabinoids. MS/MS spectra of the identified CBG type (A) neutral and (B) acid phytocannabinoids, (C) names, retention times and accurate masses, and (D) their fragmentation structures. Values of m/z in (A) and (B) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (C).

C

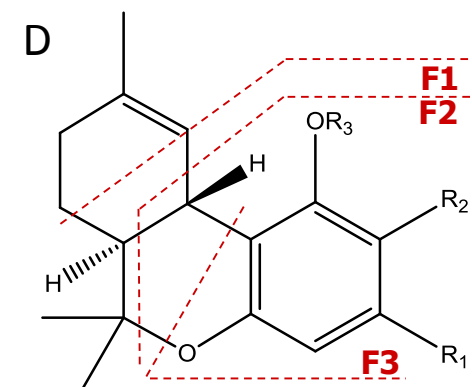
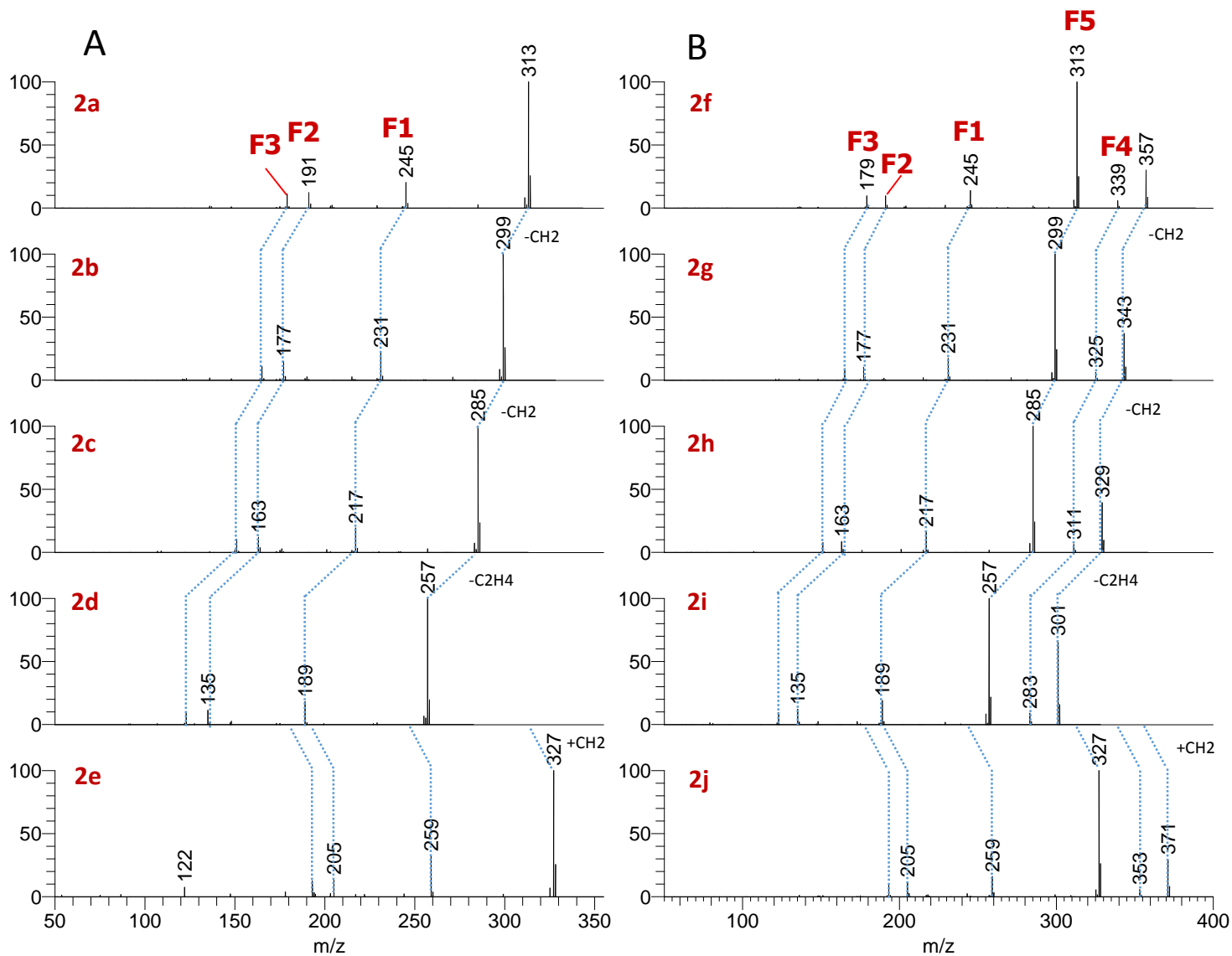
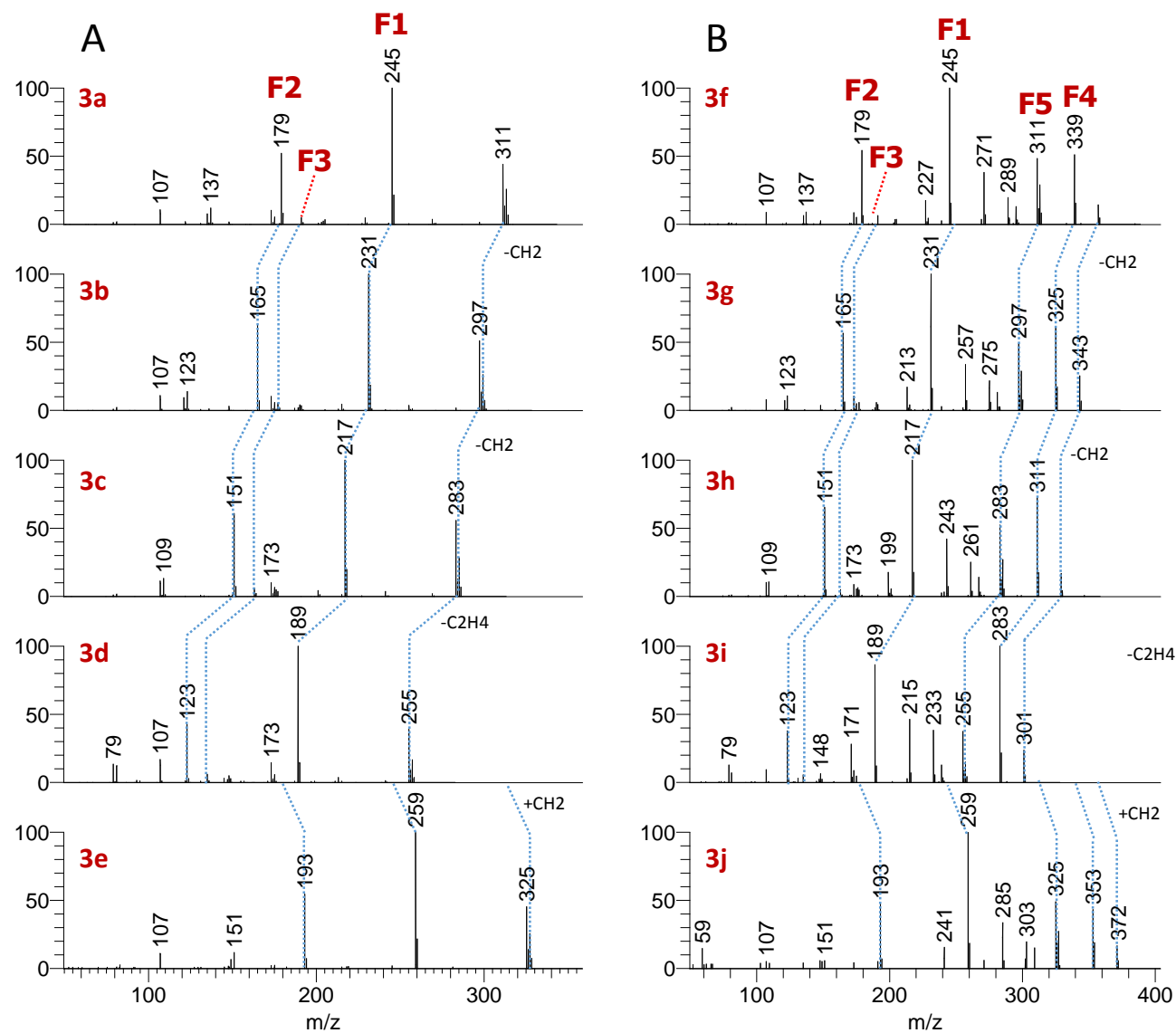


Figure S4. MS/MS spectral library of Δ^9 -THC-type phytocannabinoids. MS/MS spectra of the identified Δ^9 -THC type (**A**) neutral and (**B**) acid phytocannabinoids, (**C**) names, retention times and accurate masses, and (**D**) their fragmentation structures. Values of m/z in (**A**) and (**B**) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (**C**).



C

	Name	R1	R2	R3	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-	[MF4-H]-	[MF5-H]-
3a	CBD ^a	C5H11	H	H	7.96	313.2173	245.1547	191.1078	179.1067	-	-
						C21H29O2	C16H21O2	C12H15O2	C11H15O2		
3b	CBD-C4	C4H9	H	H	6.74	299.2017	231.1391	177.0921	165.0921	-	-
						C20H27O2	C15H19O2	C11H13O2	C10H13O2		
3c	CBDV ^a	C3H7	H	H	5.86	285.1860	217.1234	163.0765	151.0765	-	-
						C19H25O2	C14H17O2	C10H11O2	C9H11O2		
3d	CBDO	CH3	H	H	4.61	257.1547	189.0921	135.0452	123.0452	-	-
3e	CBDM	C5H11	H	CH3	10.7	327.2329	259.1704	205.1234	193.1234	-	-
						C22H31O2	C17H23O2	C13H17O2	C12H17O2		
3f	CBDA ^a	C5H11	COOH	H	7.67	357.2071	245.1547	191.1078	179.1067	339.1966	313.2173
						C22H29O4	C16H21O2	C12H15O2	C11H15O2	C22H27O3	C21H29O2
3g	CBDA-C4 ^b	C4H9	COOH	H	6.64	343.1915	231.1391	177.0921	165.0921	325.1809	299.2017
						C21H27O4	C15H19O2	C11H13O2	C10H13O2	C21H25O3	C20H27O2
3h	CBDVA ^a	C3H7	COOH	H	5.90	329.1758	217.1234	163.0765	151.0765	311.1653	285.1860
						C20H25O4	C14H17O2	C10H11O2	C9H11O2	C20H23O3	C19H25O2
3i	CBDOA ^b	CH3	COOH	H	4.92	301.1445	189.0921	135.0452	123.0452	283.1340	257.1547
						C18H21O4	C12H13O2	C8H7O2	C7H7O2	C18H19O3	C17H21O2
3j	CBDMA ^b	C5H11	COOH	CH3	9.16	371.2228	259.1704	205.1234	193.1234	353.2122	327.2329
						C23H31O4	C17H23O2	C13H17O2	C12H17O2	C23H29O3	C22H31O2

^aAnalytical standard

^bNon-isolated and identified phytocannabinoid in the literature

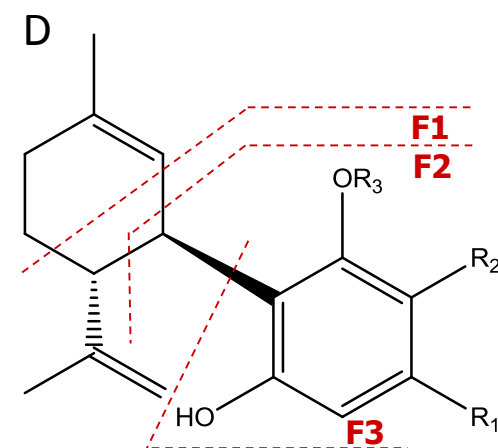
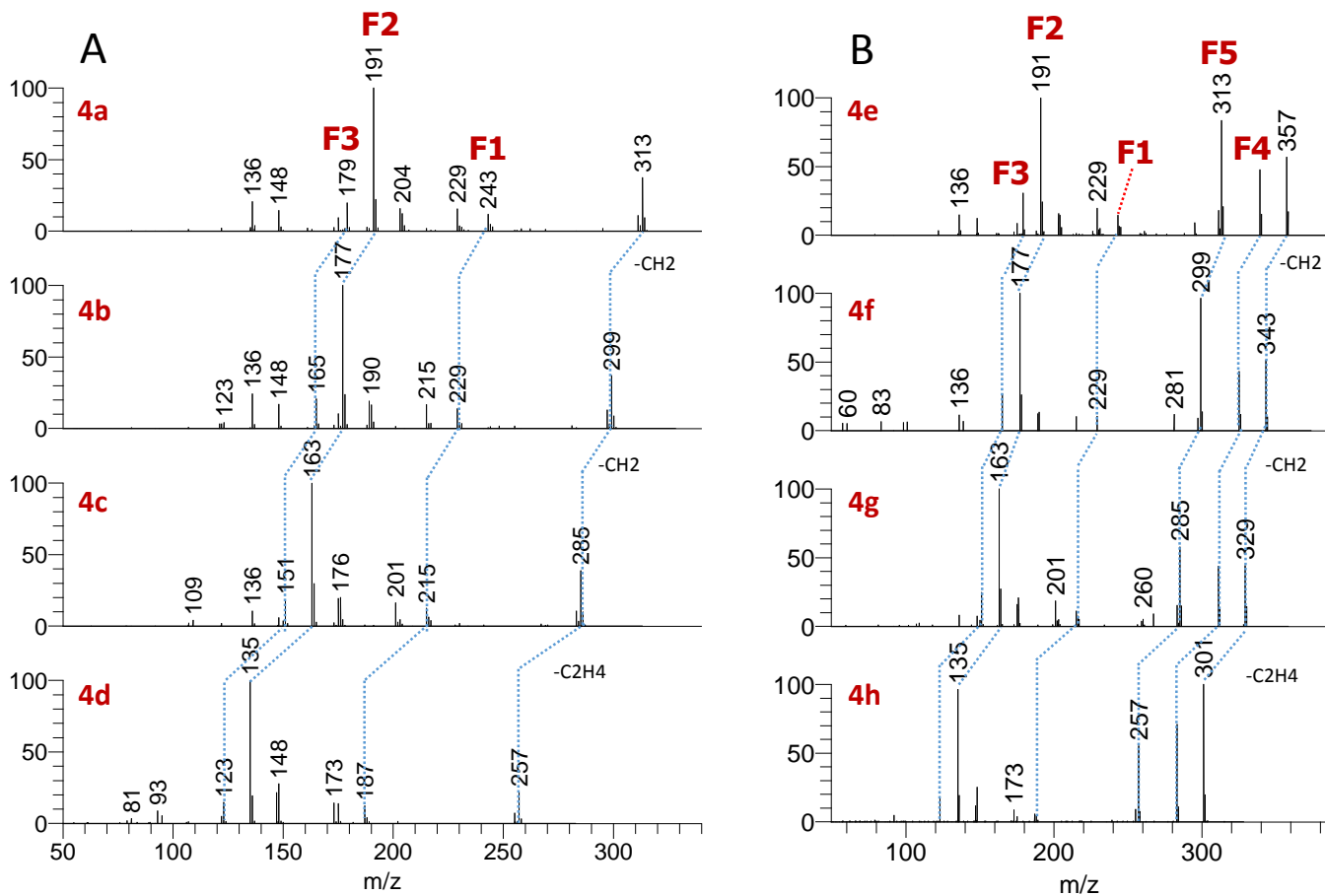


Figure S5. MS/MS spectral library of CBD-type phytocannabinoids. MS/MS spectra of the identified CBD type (**A**) neutral and (**B**) acid phytocannabinoids, (**C**) names, retention times and accurate masses, and (**D**) their fragmentation structures. Values of m/z in (**A**) and (**B**) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (**C**).



C

	Name	R1	R2	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-	[MF4-H]-	[MF5-H]-
4a	CBC ^a	C5H11	H	12.08	313.2173	243.1391	191.1078	179.1067	-	-
					C21H29O2	C16H19O2	C12H15O2	C11H15O2		
4b	CBC-C4 ^b	C4H9	H	11.05	299.2017	229.1234	177.0921	165.0921	-	-
					C20H27O2	C15H17O2	C11H13O2	C10H13O2		
4c	CBCV	C3H7	H	9.64	285.1860	215.1078	163.0765	151.0765	-	-
					C19H25O2	C14H15O2	C10H11O2	C9H11O2		
4d	CBCO	CH3	H	6.82	257.1547	187.0765	135.0452	123.0452	-	-
4e	CBCA	C5H11	COOH	13.23	357.2071	243.1391	191.1078	179.1067	339.1966	313.2173
					C22H29O4	C16H19O4	C12H15O4	C11H15O4	C22H27O3	C21H29O2
4f	CBCA-C4 ^b	C4H9	COOH	12.43	343.1915	229.1234	177.0921	165.0921	325.1809	299.2017
					C21H27O4	C15H17O4	C11H13O4	C10H13O4	C21H25O3	C20H27O2
4g	CBCVA	C3H7	COOH	11.48	329.1758	215.1078	163.0765	151.0765	311.1653	285.1860
					C20H25O4	C14H15O4	C10H11O4	C9H11O4	C20H23O3	C19H25O2
4h	CBCOA	CH3	COOH	9.36	301.1445	187.0765	135.0452	123.0452	283.1340	257.1547
					C18H21O4	C12H11O4	C8H7O4	C7H7O4	C18H19O3	C17H21O2

^aAnalytical standard

^bNon-isolated and identified phytocannabinoid in the literature

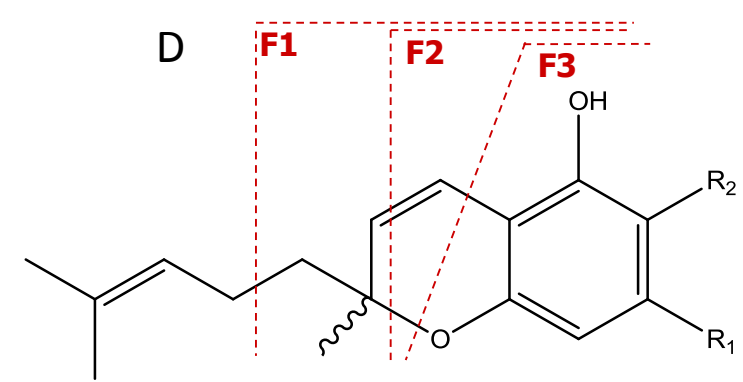
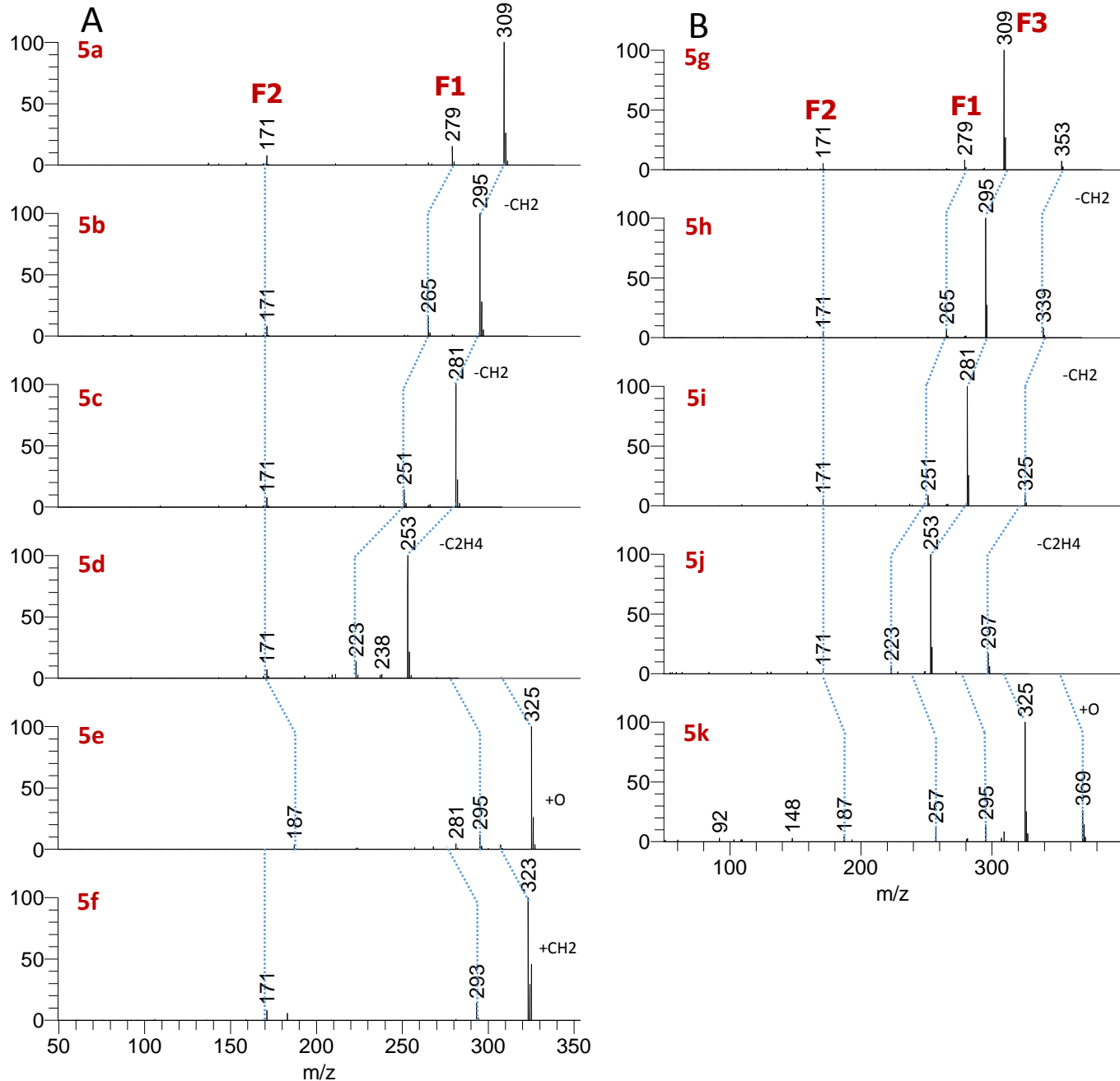


Figure S6. MS/MS spectral library of CBC-type phytocannabinoids. MS/MS spectra of the identified CBC type (A) neutral and (B) acid phytocannabinoids, (C) names, retention times and accurate masses, and (D) their fragmentation structures. Values of m/z in (A) and (B) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (C).



C

	Name	R1	R2	R3	R4	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-
5a	CBN ^a	C5H11	H	H	H	10.3	309.1860	279.1391	171.0815	-
							C21H25O2	C19H19O2	C12H11O	
5b	CBN-C4	C4H9	H	H	H	8.57	295.1703	265.1234	171.0815	-
							C20H23O2	C18H17O2	C12H11O	
5c	CBNV	C3H7	H	H	H	7.08	281.1547	251.1078	171.0815	-
							C19H21O2	C17H15O2	C12H11O	
5d	CBNO	CH3	H	H	H	5.20	253.1234	223.0765	171.0815	-
							C17H17O2	C15H11O2	C12H11O	
5e	8-OH-CBN	C5H11	H	H	OH	9.34	325.1809	295.1340	187.0765	-
							C21H25O3	C19H19O3	C12H11O2	
5f	CBNM	C5H11	H	CH3	H	11.55	323.2016	293.1547	171.0815	-
							C21H27O2	C20H21O2	C12H11O	
5g	CBNA	C5H11	COOH	H	H	12.11	353.1758	279.1391	171.0815	309.1860
							C22H25O4	C19H19O2	C12H11O	C21H25O2
5h	CBNA-C4 ^b	C4H9	COOH	H	H	11.03	339.1602	265.1234	171.0815	295.1703
							C21H23O4	C18H17O2	C12H11O	C20H23O2
5i	CBNVA ^b	C3H7	COOH	H	H	9.62	325.1445	251.1078	171.0815	281.1547
							C20H21O4	C17H15O2	C12H11O	C19H21O2
5j	CBNOA ^b	CH3	COOH	H	H	7.14	297.1132	223.0765	171.0815	253.1234
							C18H17O4	C15H11O2	C12H11O	C17H17O2
5k	8-OH-CBNA	C5H11	COOH	H	OH	12.06	369.1707	295.1340	187.0765	325.1809
							C22H25O5	C19H19O3	C12H11O2	C21H25O3

^aAnalytical standard

^bNon-isolated and identified phytocannabinoid in the literature

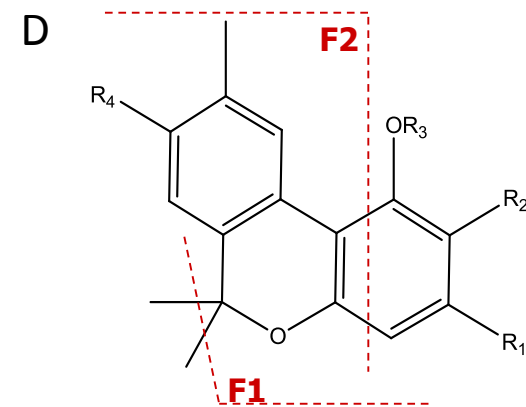
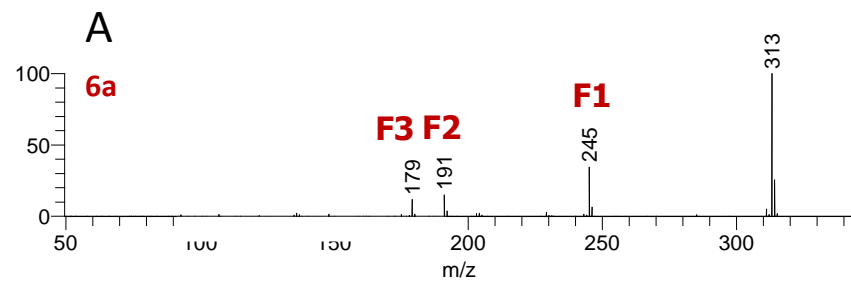


Figure S7. MS/MS spectral library of CBN-type phytocannabinoids. MS/MS spectra of the identified CBN type (**A**) neutral and (**B**) acid phytocannabinoids, (**C**) names, retention times and accurate masses, and (**D**) their fragmentation structures. Values of m/z in (**A**) and (**B**) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (**C**).



B

	Name	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-
6a	d8-THC ^a	11.41	313.2173 C ₂₁ H ₂₉ O ₂	245.1547 C ₁₆ H ₂₁ O ₂	191.1078 C ₁₂ H ₁₅ O ₂	179.1067 C ₁₁ H ₁₅ O ₂

^aAnalytical standard

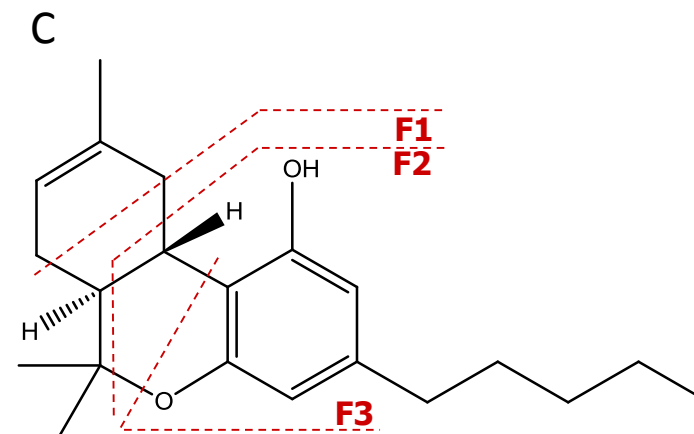
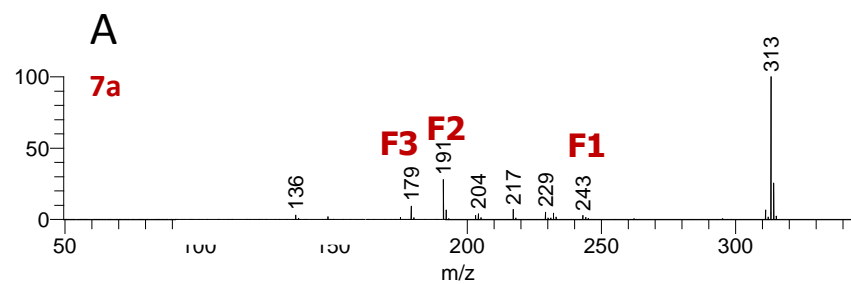


Figure S8. MS/MS spectral library of Δ^8 -THC. (A) MS/MS spectrum of Δ^8 -THC, (B) name, retention time and accurate mass, and (C) its fragmentation structure. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).



B

	Name	RT [min]	[M-H] ⁻	[MF1-H] ⁻	[MF2-H] ⁻	[MF3-H] ⁻
7a	CBL ^a	11.83	313.2173 C ₂₁ H ₂₉ O ₂	243.1391 C ₁₆ H ₁₉ O ₂	191.1078 C ₁₂ H ₁₅ O ₂	179.1067 C ₁₁ H ₁₅ O ₂

^aAnalytical standard

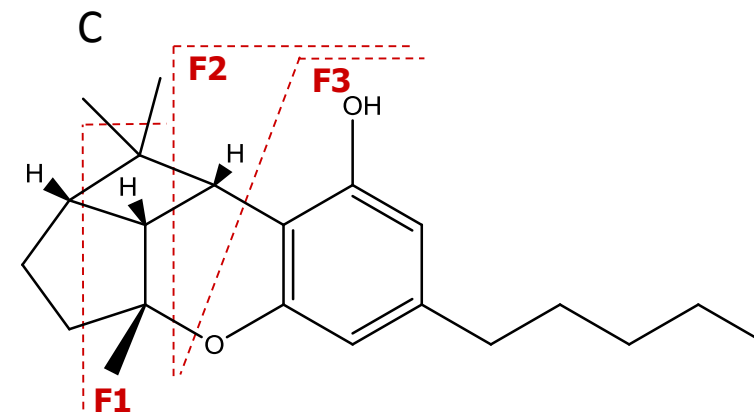


Figure S9. MS/MS spectral library of CBL. (A) MS/MS spectrum of CBL, (B) name, retention time and accurate mass, and (C) its fragmentation structure. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).

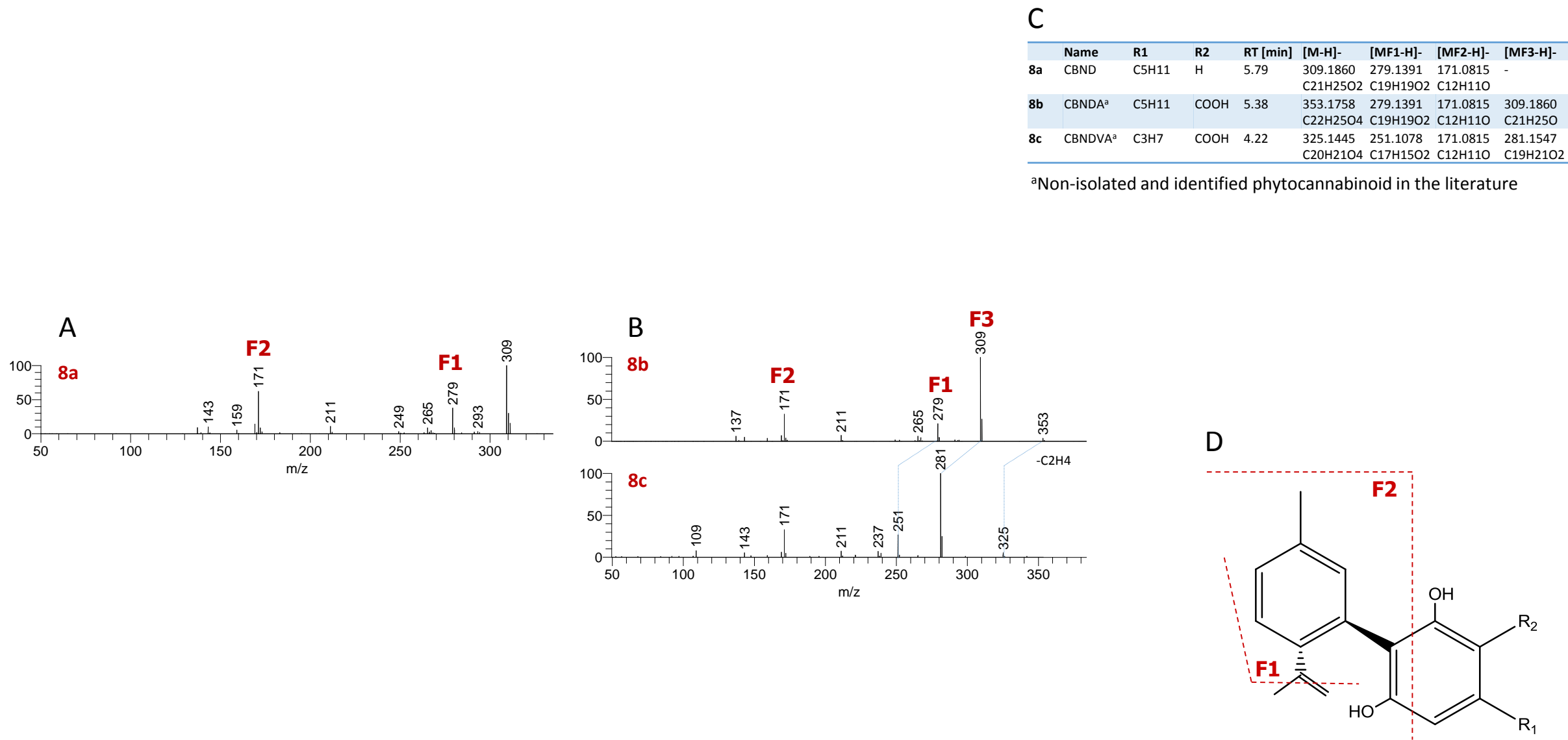
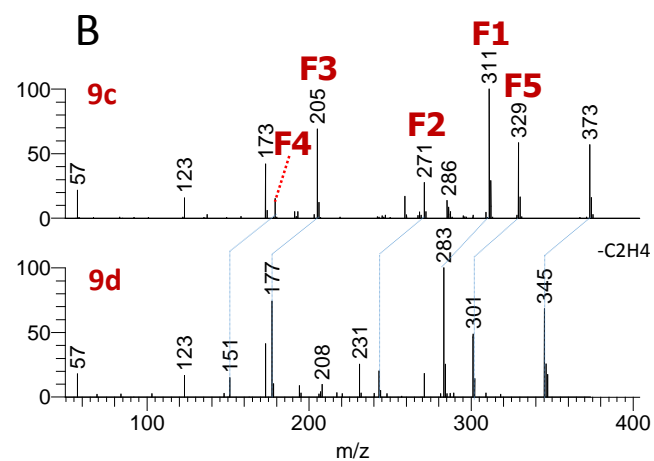
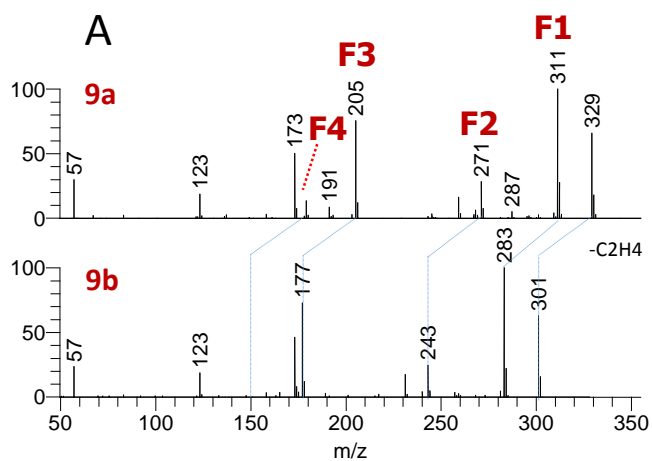


Figure S10. MS/MS spectral library of CBND-type phytocannabinoids. MS/MS spectra of the identified CBND type (**A**) neutral and (**B**) acid phytocannabinoids, (**C**) names, retention times and accurate masses, and (**D**) their fragmentation structures. Values of m/z in (**A**) and (**B**) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (**C**).



C

Name	R1	R2	RT [min]	[M-H] ⁻	[MF1-H] ⁻	[MF2-H] ⁻	[MF3-H] ⁻	[MF4-H] ⁻	[MF5-H] ⁻
9a	C5H11	H	6.64	329.2122	311.2017	271.1704	205.1234	179.1067	-
				C21H29O3	C21H27O2	C18H23O2	C13H17O2	C11H15O2	
9b	C3H7	H	4.80	301.1809	283.1704	243.1391	177.0921	151.0765	-
				C19H25O3	C19H23O2	C16H19O2	C11H13O2	C9H11O2	
9c	C5H11	COOH	6.74	373.2021	311.2017	271.1704	205.1234	179.1067	329.2122
				C21H29O5	C21H27O2	C18H23O2	C13H17O2	C11H15O2	C21H29O3
9d	C3H7	COOH	4.79	345.1707	283.1704	243.1391	177.0921	151.0765	301.1809
				C19H29O5	C19H23O2	C16H19O2	C11H13O2	C9H11O2	C19H25O3

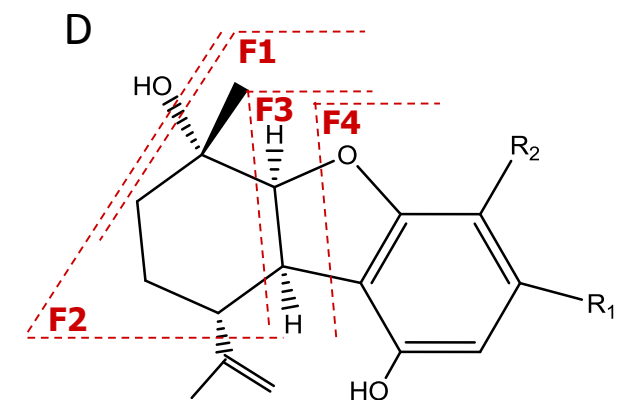


Figure S11. MS/MS spectral library of CBE-type phytocannabinoids. MS/MS spectra of the identified CBE type (**A**) neutral and (**B**) acid phytocannabinoids, (**C**) names, retention times and accurate masses, and (**D**) their fragmentation structures. Values of m/z in (**A**) and (**B**) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (**C**).

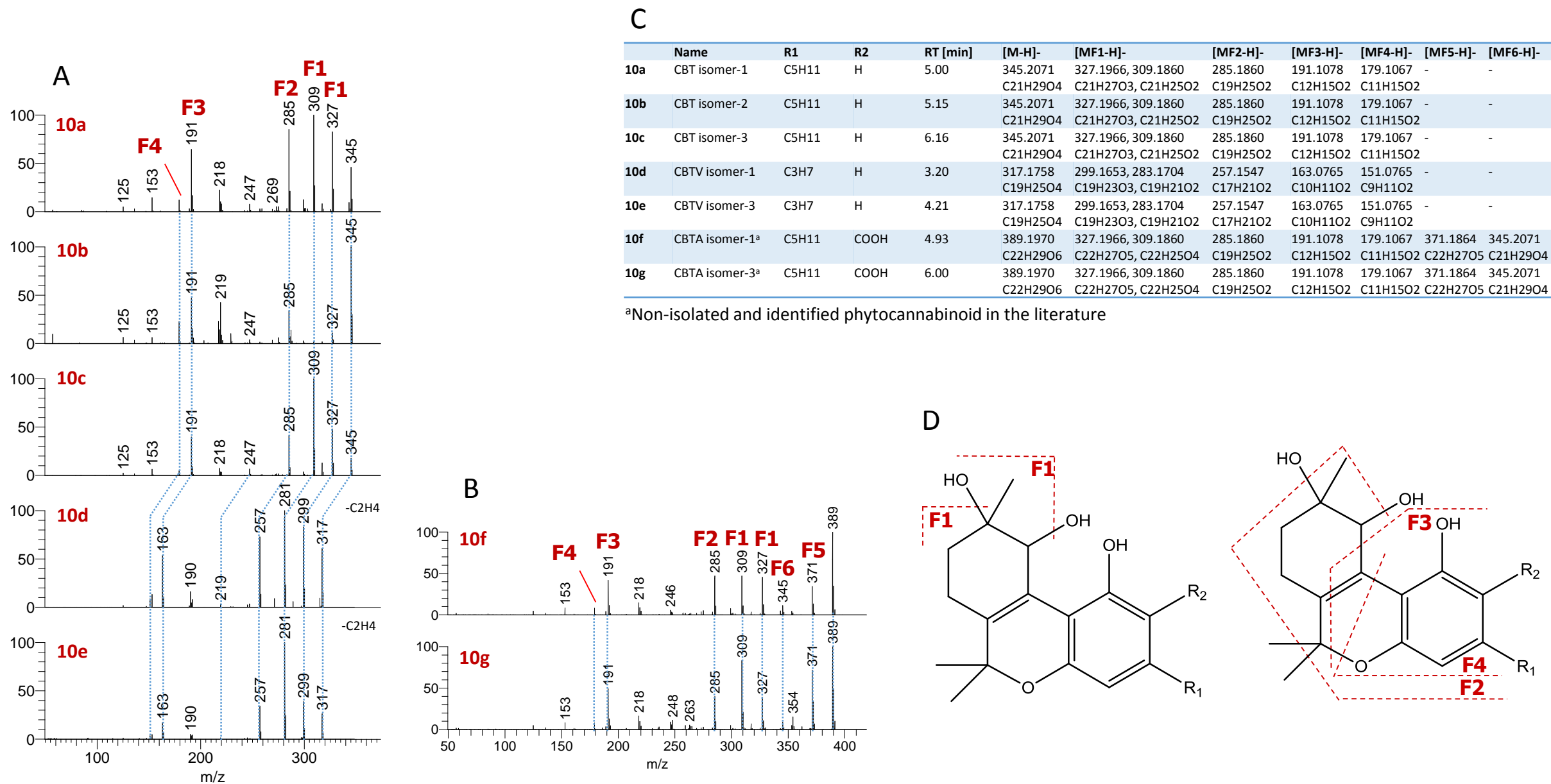
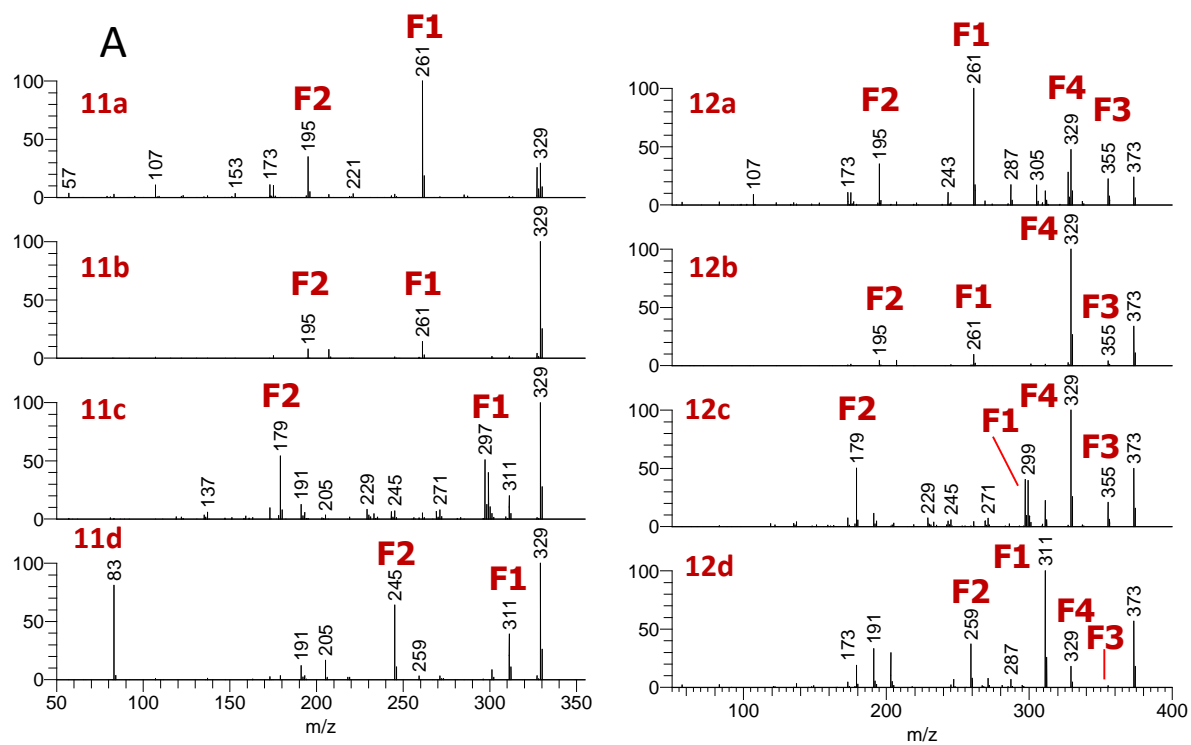
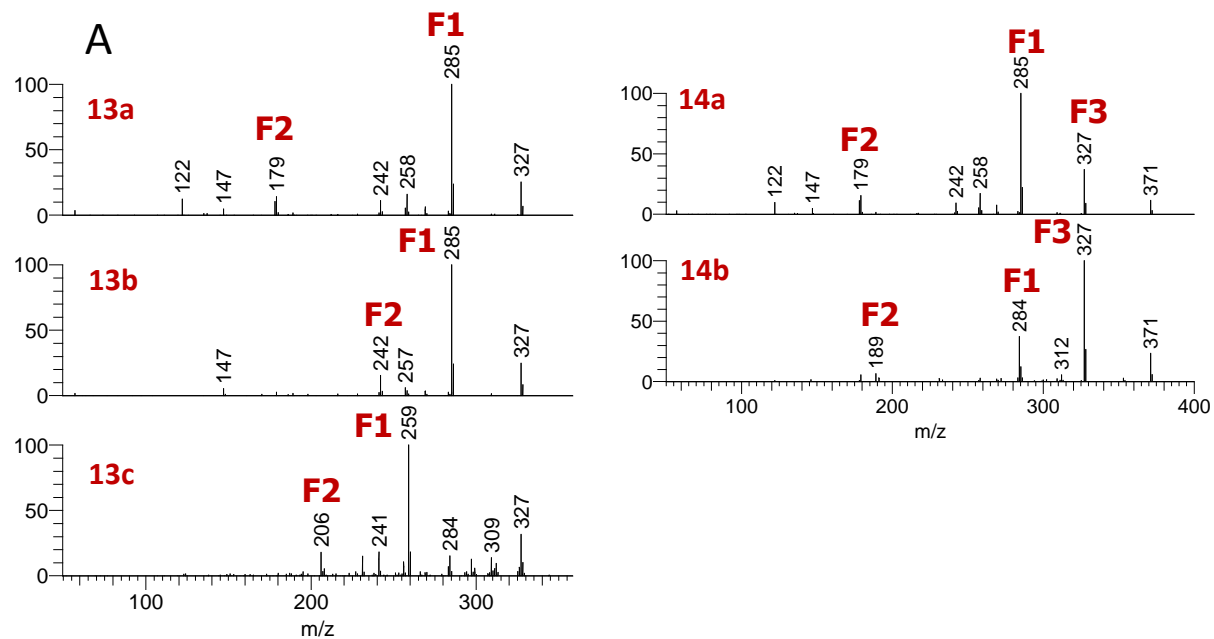


Figure S12. MS/MS spectral library of CBT-type phytocannabinoids. MS/MS spectra of the identified CBT type (A) neutral and (B) acid phytocannabinoids, (C) names, retention times and accurate masses, and (D) their fragmentation structures. Values of m/z in (A) and (B) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (C).



	Chemical formula	Acid-neutral pairing	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-	[MF4-H]-
11a	C21H30O3	A	4.04	329.2122	261.1496	195.1027	-	-
				C21H29O3	C16H21O3	C11H15O3		
11b	C21H30O3	B	5.06	329.2122	261.1496	195.1027	-	-
				C21H29O3	C16H21O3	C11H15O3		
11c	C21H30O3	C	5.15	329.2122	297.1860	179.1078	-	-
				C21H29O3	C20H25O2	C11H15O2		
11d	C21H30O3	-	9.26	329.2122	311.2017	245.1547	-	-
				C21H29O3	C21H27O2	C16H21O2		
12a	C22H30O5	A	4.41	373.2021	261.1496	195.1027	355.1915	329.2122
				C22H29O5	C16H21O3	C11H15O3	C22H27O4	C21H29O3
12b	C22H30O5	B	6.33	373.2021	261.1496	195.1027	355.1915	329.2122
				C22H29O5	C16H21O3	C11H15O3	C22H27O4	C21H29O3
12c	C22H30O5	C	5.64	373.2021	297.1860	179.1078	355.1915	329.2122
				C22H29O5	C20H25O2	C11H15O2	C22H27O4	C21H29O3
12d	C22H30O5	-	9.83	373.2021	311.2017	259.1704	355.1915	329.2122
				C22H29O5	C21H27O2	C16H21O2	C22H27O4	C21H29O3

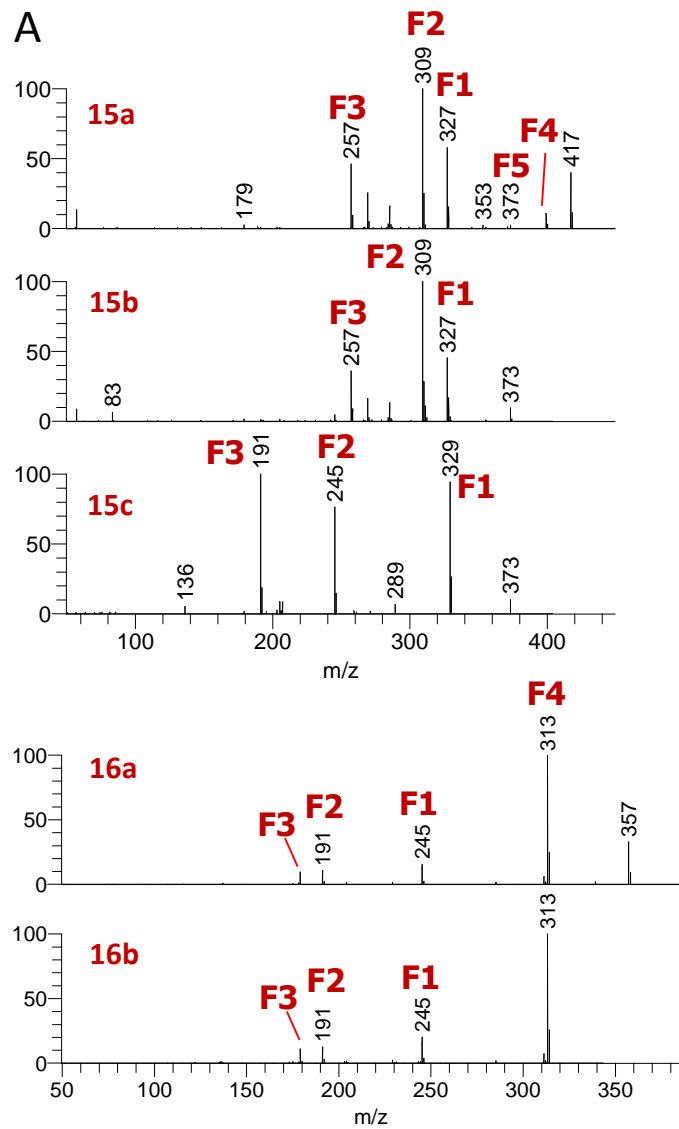
Figure S13. MS/MS spectral library of additional phytocannabinoids (Part I). (A) MS/MS spectra, and (B) names, retention times and accurate masses. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).



B

	Chemical formula	Acid-neutral pairing	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-
13a	C ₂₁ H ₂₈ O ₃	A	6.49	327.1966	285.1860	179.1078	-
				C ₂₁ H ₂₇ O ₃	C ₁₉ H ₂₅ O ₂	C ₁₁ H ₁₅ O ₂	
13b	C ₂₁ H ₂₈ O ₃	-	5.97	327.1966	285.1860	242.1312	-
				C ₂₁ H ₂₇ O ₃	C ₁₉ H ₂₅ O ₂	C ₁₆ H ₁₈ O ₂	
13c	C ₂₁ H ₂₈ O ₃	-	11.06	327.1966	259.1340	206.0948	-
				C ₂₁ H ₂₇ O ₃	C ₁₆ H ₁₉ O ₃	C ₁₂ H ₁₄ O ₃	
14a	C ₂₂ H ₂₈ O ₅	A	6.75	371.1864	285.1860	179.1078	327.1966
				C ₂₂ H ₂₇ O ₅	C ₁₉ H ₂₅ O ₂	C ₁₁ H ₁₅ O ₂	C ₂₁ H ₂₇ O ₃
14b	C ₂₂ H ₂₈ O ₅	-	8.04	371.1864	284.1418	189.0921	327.1966
				C ₂₂ H ₂₇ O ₅	C ₁₈ H ₂₀ O ₃	C ₁₂ H ₁₃ O ₂	C ₂₁ H ₂₇ O ₃

Figure S13. MS/MS spectral library of additional phytocannabinoids (Part II). (A) MS/MS spectra, and (B) names, retention times and accurate masses. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).



B

	Chemical formula	Acid-neutral pairing	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-	[MF4-H]-	[MF5-H]-
15a	C24H34O6	A	6.2	417.2283	327.1966	309.1860	257.1547	399.2177	373.2384
				C24H33O6	C21H27O3	C21H25O2	C17H21O2	C24H31O5	C23H33O4
15b	C23H34O4	A	7.48	373.2384	327.1966	309.1860	257.1547	-	-
				C23H33O4	C21H27O3	C21H25O2	C17H21O2	-	-
15c	C23H34O4	-	13.15	373.2384	329.2486	245.1547	191.1078	-	-
				C23H33O4	C22H33O2	C16H21O2	C12H15O2	-	-
16a	C22H30O4	B	12.31	357.2071	245.1547	191.1078	179.1067	-	313.2173
				C22H29O4	C16H21O2	C12H15O2	C11H15O2	-	C21H29O2
16b	C21H30O2	B	10.83	313.2173	245.1547	191.1078	179.1067	-	-
				C21H29O2	C16H21O2	C12H15O2	C11H15O2	-	-
17a	C21H30O5	-	6.43	361.2021	343.1915	325.1809	207.1027	179.1067	-
17b	C21H30O5	-	3.64	361.2021	333.2071	191.1078	179.1067	-	-
				C21H29O5	C20H29O4	C12H15O2	C11H15O2	-	-

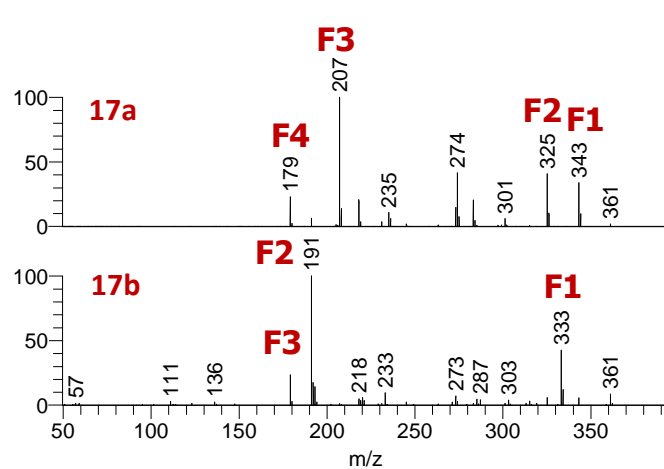
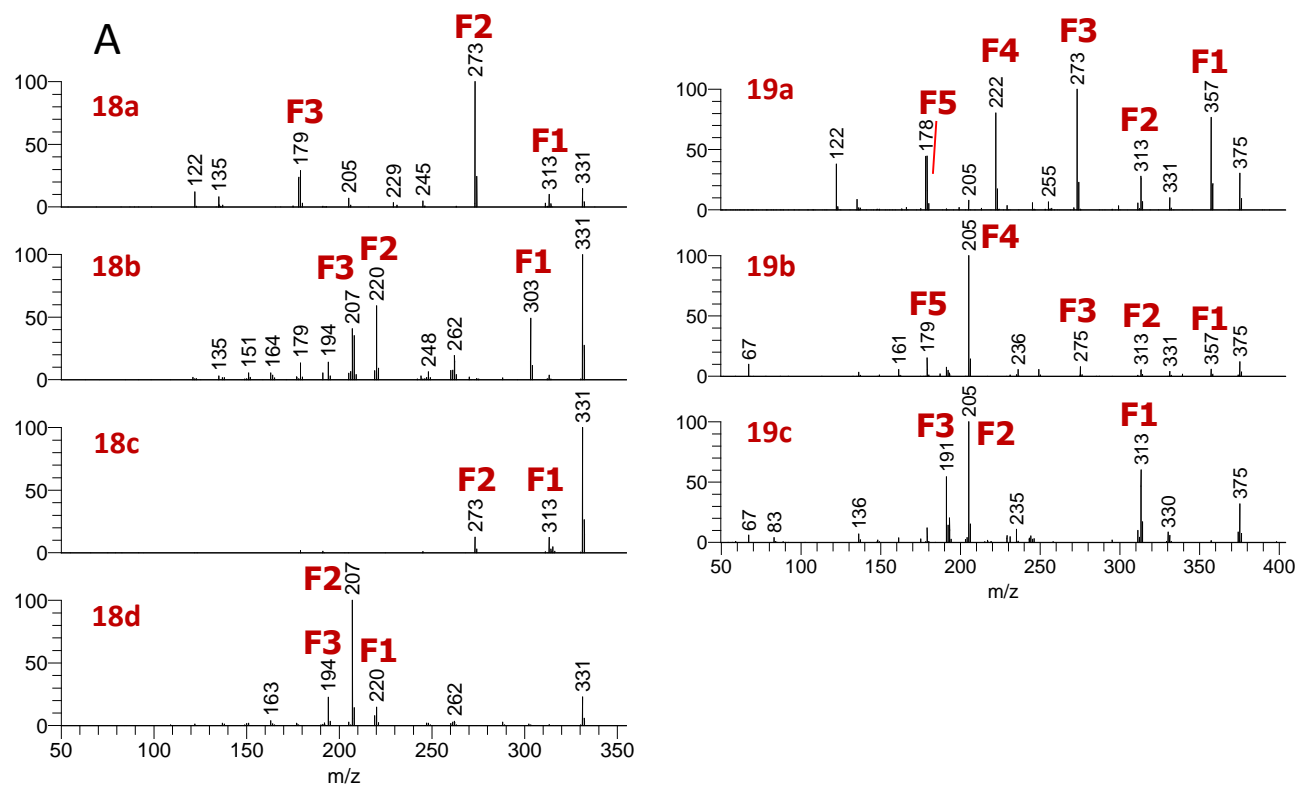


Figure S13. MS/MS spectral library of additional phytocannabinoids (Part III). (A) MS/MS spectra, and (B) names, retention times and accurate masses. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).



B

	Chemical formula	RT [min]	[M-H]-	[MF1-H]-	[MF2-H]-	[MF3-H]-	[MF4-H]-	[MF5-H]-
18a	C ₂₁ H ₃₂ O ₃	5.60	331.2279	313.2173	273.1860	179.1067	-	-
			C ₂₁ H ₃₁ O ₃	C ₂₁ H ₂₉ O ₂	C ₁₈ H ₂₅ O ₂	C ₁₁ H ₁₅ O ₂		
18b	C ₂₁ H ₃₂ O ₃	7.58	331.2279	303.2330	220.1105	207.1027	-	-
			C ₂₁ H ₃₁ O ₃	C ₂₀ H ₃₁ O ₂	C ₁₃ H ₁₆ O ₃	C ₁₂ H ₁₅ O ₃		
18c	C ₂₁ H ₃₂ O ₃	8.74	331.2279	313.2173	273.1860	-	-	
			C ₂₁ H ₃₁ O ₃	C ₂₁ H ₂₉ O ₂	C ₁₈ H ₂₅ O ₂			
18d	C ₂₁ H ₃₂ O ₃	10.12	331.2279	220.1105	207.1027	194.0948	-	-
			C ₂₁ H ₃₁ O ₃	C ₁₃ H ₁₆ O ₃	C ₁₂ H ₁₅ O ₃	C ₁₁ H ₁₄ O ₃		
19a	C ₂₂ H ₃₂ O ₅	4.80	375.2177	357.2071	313.2173	273.1860	222.0898	179.1067
			C ₂₂ H ₃₁ O ₅	C ₂₂ H ₂₉ O ₄	C ₂₁ H ₂₉ O ₂	C ₁₈ H ₂₅ O ₂	C ₁₂ H ₁₄ O ₄	C ₁₁ H ₁₅ O ₂
19b	C ₂₂ H ₃₂ O ₅	3.95	375.2177	357.2071	313.2173	275.2017	205.1234	179.1067
			C ₂₂ H ₃₁ O ₅	C ₂₂ H ₂₉ O ₄	C ₂₁ H ₂₉ O ₂	C ₁₃ H ₁₇ O ₂	C ₁₃ H ₁₇ O ₂	C ₁₁ H ₁₅ O ₂
19c	C ₂₂ H ₃₂ O ₅	9.06	375.2177	313.2173	205.1234	191.1078	-	-
			C ₂₂ H ₃₁ O ₅	C ₂₁ H ₂₉ O ₂	C ₁₃ H ₁₇ O ₂	C ₁₂ H ₁₅ O ₂		

Figure S13. MS/MS spectral library of additional phytocannabinoids (Part IV). (A) MS/MS spectra, and (B) names, retention times and accurate masses. Values of m/z in (A) are presented as nominal masses to improve interpretation of spectra. Accurate masses for the main fragments appear in (B).

Table S1. List of neutral and acid potential masses of phytocannabinoids used in data dependent MS/MS mode

Phytocannabinoid subclass	Neutral-type phytocannabinoids			Acid-type phytocannabinoids		
	Name	Chemical Formula	[M-H] ⁻	Name	Chemical Formula	[M-H] ⁻
CBN	Cannabiorcol-C1 (CBNO)	C17H18O2	253.12340	Cannabiorcolic acid-c1 (CBNOA)*	C18H18O4	297.11323
CBND	CBND-C1 (CBNDO)*	C17H18O2	253.12340	CBNDA-C1 (CBNDOA)*	C18H18O4	297.11323
Δ^9 -THC	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabiorcol-C1 (Δ^9 -THCO)	C17H22O2	257.15470	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabiorcolic acid-C1 (Δ^9 -THCOA)	C18H22O4	301.14453
CBD	Cannabidiol-C1 (CBDO)	C17H22O2	257.15470	Cannabidiolcolic acid-C1 (CBDOA)*	C18H22O4	301.14453
CBC	Cannabiorchromene-C1 (CBCO)	C17H22O2	257.15470	Cannabiorchromenic acid-C1 (CBCOA)	C18H22O4	301.14453
Δ^8 -THC	(-)- Δ^8 - <i>trans</i> -(6aR,10aR)-Tetrahydrocannabiorcol-C1 (Δ^8 -THCO)*	C17H22O2	257.15470	(-)- Δ^8 - <i>trans</i> -(6aR,10aR)-Tetrahydrocannabiorcolic acid-C1 (Δ^8 -THCOA)*	C18H22O4	301.14453
CBL	Cannabiorcyclo C1 (CBLO)	C17H22O2	257.15470	Cannabiorcycloic acid C1 (CBLOA)	C18H22O4	301.14453
CBG	CBG-C1 (CBGO)*	C17H24O2	259.17035	CBGA-C1 (CBGOA)*	C18H24O4	303.16018
CBN	Cannabinol-C2 (CBN-C2)	C18H20O2	267.13905	CBNA-C2*	C19H20O4	311.12888
CBND	CBND-C2*	C18H20O2	267.13905	CBNDA-C2*	C19H20O4	311.12888
Δ^9 -THC	Δ^9 -THC-C2*	C18H24O2	271.17035	Δ^9 -THCA-C2*	C19H24O4	315.16018
CBD	CBD-C2*	C18H24O2	271.17035	CBDA-C2*	C19H24O4	315.16018
CBC	CBC-C2*	C18H24O2	271.17035	CBCA-C2*	C19H24O4	315.16018
Δ^8 -THC	Δ^8 -THC-C2*	C18H24O2	271.17035	Δ^8 -THCA-C2*	C19H24O4	315.16018
CBL	CBL-C2*	C18H24O2	271.17035	CBLA-C2*	C19H24O4	315.16018
CBE	Bisnor-cannabielsoin-C1 (CBEO)	C17H22O3	273.14962	Bisnor-cannabielsoinic acid-C1 (CBEOA)	C18H22O5	317.13945
CBG	CBG-C2*	C18H26O2	273.18600	CBGA-C2*	C19H26O4	317.17583
CBN	Cannabivarin-C3 (CBNV)	C19H22O2	281.15470	CBNA-C3 (CBNVA)*	C20H22O4	325.14453
CBND	Cannabinodivarin-C3 (CBNDV)	C19H22O2	281.15470	CBNDA-C3 (CBNDVA)*	C20H22O4	325.14453
Δ^9 -THC	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabivarin-C3 (Δ^9 -THCV)	C19H26O2	285.18600	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabivarinic acid-C3 (Δ^9 -THCVA)	C20H26O4	329.17583

CBD	(-)-Cannabidivarin-C3 (CBDV)	C19H26O2	285.18600	Cannabidivarinic acid-C3 (CBDVA)	C20H26O4	329.17583
CBC	(±)-Cannabichromevarin-C3 (CBCV)	C19H26O2	285.18600	(±)-Cannabichromevarinic acid-C3 (CBCVA)	C20H26O4	329.17583
Δ^8 -THC	(-)- Δ^8 - <i>trans</i> -THC-C3 (Δ^8 -THCV)*	C19H26O2	285.18600	(-)- Δ^8 - <i>trans</i> -THCA-C3 (Δ^8 -THCVA)*	C20H26O4	329.17583
CBL	(±)-(1aS,3aR,8bR,8cR)-Cannabicyclovarin-C3 (CBLV)	C19H26O2	285.18600	Cannabicyclic acid-C3 (CBLVA)	C20H26O4	329.17583
CBC	2-Methyl-2-(4-methyl-2-pentenyl)-7-propyl-2H-1-benzopyran-5-ol	C19H26O2	285.18600	2-Methyl-2-(4-methyl-2-pentenyl)-7-propyl-2H-1-benzopyran-5-ol acid*	C20H26O4	329.17583
Miscellaneous	Δ^7 -tetrahydrocannabivarin-C3 (Δ^7 -THCV)	C19H26O2	285.18600	Δ^7 -tetrahydrocannabivarinic acid-C3 (Δ^7 -THCVA)*	C20H26O4	329.17583
CBE	CBE-C2*	C18H24O3	287.16527	CBEA-C2*	C19H24O5	331.15510
CBG	Cannabigerovarin-C3 (CBGV)	C19H28O2	287.20165	Cannabigerovarinic acid-C3 (CBGVA)	C20H28O4	331.19148
CBT	Cannabitol-C1 (CBTO)	C17H22O4	289.14453	Cannabitolic acid-C1 (CBTOA)*	C18H22O6	333.13436
CBN	Cannabinol-C4 (CBN-C4)	C20H24O2	295.17035	Cannabinolic acid-C4 (CBNA-C4)*	C21H24O4	339.16018
CBND	CBND-C4*	C20H24O4	295.17035	CBNDA-C4*	C21H24O4	339.16018
Δ^9 -THC	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinol-C4 (Δ^9 -THC-C4)	C20H28O2	299.20165	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinolic acid-C4 (Δ^9 -THCA-C4)	C21H28O4	343.19148
CBD	Cannabidiol-C4 (CBD-C4)	C20H28O2	299.20165	CBDA-C4*	C21H28O4	343.19148
CBC	CBC-C4*	C20H28O2	299.20165	CBCA-C4*	C21H28O4	343.19148
Δ^8 -THC	(-)- <i>trans</i> - Δ^8 -THC-C4*	C20H28O2	299.20165	(-)- <i>trans</i> - Δ^8 -THCA-C4*	C21H28O4	343.19148
CBL	CBL-C4*	C20H28O2	299.20165	CBLA-C4*	C21H28O4	343.19148
CBE	Cannabielsoin-C3 (CBEV)	C19H26O3	301.18092	Cannabielsoic acid-C3 (CBEVA)	C20H26O5	345.17075
CBG	CBG-C4*	C20H30O2	301.21730	CBGA-C4*	C21H30O4	345.20713
CBT	CBT-C2*	C18H24O4	303.16018	CBTA-C2*	C19H24O6	347.15001
Miscellaneous	Cannabichromanone-C3	C18H24O4	303.16018	Cannabichromanonic acid-C3*	C19H24O6	347.15001
Miscellaneous	Cannabiglendol-C3 (OH-iso-HHCV-C3)	C19H28O3	303.19657	Cannabiglendolic acid-C3 (OH-iso-HHCVA-C3)*	C20H28O5	347.18640
Miscellaneous	Cannabioxepane-C5 (CBX)	C21H22O2	305.15470	Cannabioxepanic acid-C5 (CBXA)*	C22H22O4	349.14453
Miscellaneous	Dehydrocannabifuran-C5 (DCBF)	C21H24O2	307.17035	Dehydrocannabifuranic acid-C5 (DCBFA)*	C22H24O4	351.16018
CBN	Cannabinol-C5 (CBN)	C21H26O2	309.18600	Cannabinolic acid-C5 (CBNA)	C22H26O4	353.17583
CBND	Cannabinodiol-C5 (CBND)	C21H26O2	309.18600	Cannabinodiolic acid-C5 (CBNDA)*	C22H26O4	353.17583

Miscellaneous	Cannabifuran-C5 (CBF)	C21H26O2	309.18600	Cannabifuranic acid-C5 (CBFA)*	C22H26O4	353.17583
Δ^9 -THC	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinol-C5 (Δ^9 -THC)	C21H30O2	313.21730	(-)- Δ^9 - <i>trans</i> -Tetrahydrocannabinolic acid-C5 (Δ^9 -THCA)	C22H30O4	357.20713
Δ^8 -THC	(-)- Δ^8 - <i>trans</i> -(6aR,10aR)-Tetrahydrocannabinol-C5 (Δ^8 -THC)	C21H30O2	313.21730	(-)- Δ^8 - <i>trans</i> -(6aR,10aR)-Tetrahydrocannabinolic acid-C5 (Δ^8 -THCA)	C22H30O4	357.20713
CBC	(\pm)-Cannabichromene-C5 (CBC)	C21H30O2	313.21730	(\pm)-Cannabichromenic acid-C5 (CBCA)	C22H30O4	357.20713
CBD	(-)-Cannabidiol-C5 (CBD)	C21H30O2	313.21730	Cannabidiolic acid-C5 (CBDA)	C22H30O4	357.20713
CBL	(\pm)-(1aS,3aR,8bR,8cR)-Cannabicyclol-C5 (CBL)	C21H30O2	313.21730	(\pm)-(1aS,3aR,8bR,8cR)-Cannabicyclolic acid-C5 (CBLA)	C22H30O4	357.20713
Miscellaneous	Cannabicitran-C5 (CBR)	C21H30O2	313.21730	Cannabicitranic acid-C5 (CBRA)*	C22H30O4	357.20713
Miscellaneous	(-)- Δ^9 -(6aS,10aR- <i>cis</i>)-Tetrahydrocannabinol-C5 ((-)- <i>cis</i> - Δ^9 -THC)	C21H30O2	313.21730	(-)- Δ^9 -(6aS,10aR- <i>cis</i>)-Tetrahydrocannabinolic acid-C5 ((-)- <i>cis</i> - Δ^9 -THCA)*	C22H30O5	357.20713
Miscellaneous	(-)- Δ^7 - <i>trans</i> -(1R,3R,6R)-Isotetrahydrocannabinol-C5 (<i>trans</i> -iso- Δ^7 -THC)	C21H30O2	313.21730	(-)- Δ^7 - <i>trans</i> -(1R,3R,6R)-Isotetrahydrocannabinolic acid-C5 (<i>trans</i> -iso- Δ^7 -THCA)*	C22H30O4	357.20713
CBE	CBE-C4*	C20H28O3	315.19657	CBEA-C4*	C21H28O5	359.18640
CBG	Cannabigerol-C5 (CBG)	C21H32O2	315.23295	Cannabigerolic acid-C5 (CBGA)	C22H32O4	359.22278
CBT	Cannabitrinol-C3 (CBTV)	C19H26O4	317.17583	CBTA-C3 (CBTVA)*	C20H26O6	361.16566
CBN	Cannabinol methyl ether-C5 (CBNM)	C22H28O2	323.20165	CBNMA-C5 (CBNMA)*	C23H28O4	367.19148
CBND	CBNDM-C5*	C22H28O2	323.20165	CBNDMA-C5 (CBNDMA)*	C23H28O4	367.19148
CBN	8-OH-CBN-C5 (OH-CBN)	C21H26O3	325.18092	8-OH-CBNA-C5 (OH-CBNA)	C22H26O5	369.17075
CBND	OH-CBND-C5 (OH-CBND)*	C21H26O3	325.18092	OH-CBNDA-C5 (OH-CBNDA)*	C22H26O5	369.17075
Miscellaneous	10-Oxo- $\Delta^{6a(10a)}$ -Tetrahydrocannabinol-C5 (OTHC)	C21H28O3	327.19657	10-Oxo- $\Delta^{6a(10a)}$ -Tetrahydrocannabinolic acid-C5 (OTHCA)*	C22H28O5	371.18640
Miscellaneous	Cannabichromanone D-C5	C21H28O3	327.19657	Cannabichromanonic acid D-C5*	C22H28O5	371.18640
Miscellaneous	Cannabicumaronone-C5 (CBCON-C5)	C21H28O3	327.19657	Cannabicumaronic acid-C5 (CBCONA)	C22H28O5	371.18640
CBD	Cannabidiol monomethyl ether-C5 (CBDM)	C22H32O2	327.23295	CBDMA-C5 (CBDMA)*	C23H32O4	371.22278
Δ^9 -THC	Δ^9 -THCM-C5*	C22H32O2	327.23295	Δ^9 -THCMA-C5 (Δ^9 -THCMA)*	C23H32O4	371.22278
CBC	(\pm)-3"-hydroxy- $\Delta^{4''}$ -cannabichromene-C5	C21H30O3	329.21222	(\pm)-3"-hydroxy- $\Delta^{4''}$ -cannabichromenic acid-C5*	C22H30O5	373.20205

CBE	(5aS,6S,9R,9aR)-Cannabielsoin-C5 (CBE)	C21H30O3	329.21222	(5aS,6S,9R,9aR)-Cannabielsoic acid-C5 (CBEA)	C22H30O5	373.20205
Miscellaneous	2-geranyl-5-hydroxy-3-n-pentyl-1,4-benzoquinone-C5	C21H30O3	329.21222	2-geranyl-5-hydroxy-3-n-pentyl-1,4-benzoquinonic acid-C5*	C22H30O5	373.20205
Δ^9 -THC	8 α -Hydroxy- Δ^9 -Tetrahydrocannabinol-C5 (8 α -OH- Δ^9 -THC)	C21H30O3	329.21222	8 α -Hydroxy- Δ^9 -Tetrahydrocannabinolic acid-C5 (8 α -OH- Δ^9 -THCA)*	C22H30O5	373.20205
Δ^9 -THC	8 β -Hydroxy- Δ^9 -Tetrahydrocannabinol-C5 (8 β -OH- Δ^9 -THC)	C21H30O3	329.21222	8 β -Hydroxy- Δ^9 -Tetrahydrocannabinolic acid-C5 (8 β -OH- Δ^9 -THCA)*	C22H30O5	373.20205
Δ^8 -THC	10 α -Hydroxy- Δ^8 -Tetrahydrocannabinol-C5 (10 α -OH- Δ^8 -THC)	C21H30O3	329.21222	10 α -Hydroxy- Δ^8 -Tetrahydrocannabinolic acid-C5 (10 α -OH- Δ^8 -THCA)*	C22H30O5	373.20205
Δ^8 -THC	10 β -Hydroxy- Δ^8 -Tetrahydrocannabinol-C5 (10 β -OH- Δ^8 -THC)	C21H30O3	329.21222	10 β -Hydroxy- Δ^8 -Tetrahydrocannabinolic acid-C5 (10 β -OH- Δ^8 -THCA)*	C22H30O5	373.20205
Δ^9 -THC	10 α -hydroxy- $\Delta^{9,11}$ -hexahydrocannabinol-C5	C21H30O3	329.21222	10 α -hydroxy- $\Delta^{9,11}$ -hexahydrocannabinolic acid-C5*	C22H30O5	373.20205
Δ^9 -THC	9 β ,10 β -Epoxyhexahydrocannabinol-C5	C21H30O3	329.21222	9 β ,10 β -Epoxyhexahydrocannabinolic acid-C5*	C22H30O5	373.20205
CBD	OH-CBD-C5 (OH-CBD)*	C21H30O3	329.21222	OH-CBDA-C5 (OH-CBDA)*	C22H30O5	373.20205
CBG	Cannabigerol monomethyl ether-C5 (CBGM)	C22H34O2	329.24860	Cannabigerolic acid monomethyl ether-C5 (CBGMA)	C23H34O4	373.23843
Miscellaneous	Cannabichromanone-C5	C20H28O4	331.19148	Cannabichromanonic acid-C5*	C21H28O6	375.18131
CBT	CBT-C4*	C20H28O4	331.19148	CBTA-C4*	C21H28O6	375.18131
CBG	(\pm)-6,7- <i>cis</i> -epoxycannabigerol-C5	C21H32O3	331.22787	(\pm)-6,7- <i>trans</i> -epoxycannabigerolic acid-C5	C22H32O5	375.21770
CBG	(\pm)-6,7- <i>trans</i> -epoxycannabigerol-C5	C21H32O3	331.22787	(\pm)-6,7- <i>cis</i> -epoxycannabigerolic acid-C5	C22H32O5	375.21770
CBC	(-)-7-hydroxycannabichromane-C5	C21H32O3	331.22787	(-)-7-hydroxycannabichromanonic acid-C5*	C22H32O5	375.21770
CBD	Cannabimovone-C5	C21H30O4	345.20713	Cannabimovonic acid-C5*	C22H30O6	389.19696
CBT	(-)- <i>trans</i> -Cannabitriol-C5 ((-)- <i>trans</i> -CBT)	C21H30O4	345.20713	(-)- <i>trans</i> -Cannabitriolic acid-C5 ((-)- <i>trans</i> -CBTA)*	C22H30O6	389.19696
CBT	(+)- <i>trans</i> -Cannabitriol-C5 ((+)- <i>trans</i> -CBT)	C21H30O4	345.20713	(+)- <i>trans</i> -Cannabitriolic acid-C5 ((+)- <i>trans</i> -CBTA)*	C22H30O6	389.19696
CBT	(\pm)- <i>cis</i> -Cannabitriol-C5 ((\pm)- <i>cis</i> -CBT)	C21H30O4	345.20713	(\pm)- <i>cis</i> -Cannabitriolic acid-C5 ((\pm)- <i>cis</i> -CBTA)*	C22H30O6	389.19696
CBT	(-)- <i>trans</i> -10-Ethoxy-9-hydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabivarin-C3 [(-)- <i>trans</i> -CBT-OEt]	C21H30O4	345.20713	(-)- <i>trans</i> -10-Ethoxy-9-hydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabivarinic acid-C3 ((-)- <i>trans</i> -CBT-OEt)*	C22H30O6	389.19696

Miscellaneous	(-)-(6aR,9S,10S,10aR)-9,10-Dihydroxyhexahydrocannabinol-C5 [(-)-Cannabiripsol] (CBR)	C21H32O4	347.22278	(-)-(6aR,9S,10S,10aR)-9,10-Dihydroxyhexahydrocannabinolic acid-C5 [(-)-Cannabiripsolic acid] (CBRA)*	C22H32O6	391.21261
Miscellaneous	Cannabichromanone C-C5	C21H28O5	359.18640	Cannabichromanonic acid C-C5*	C22H28O7	403.17623
Miscellaneous	(-)-6a,7,10a-Trihydroxy- Δ^9 -tetrahydrocannabinol-C5 [(-)-Cannabitetrol] (CBTT)	C21H30O5	361.20205	(-)-6a,7,10a-Trihydroxy- Δ^9 -tetrahydrocannabinolic acid-C5 ((-)-Cannabitetrol) (CBTTA)*	C22H30O7	405.19188
Miscellaneous	Cannabichromanone B-C5	C21H30O5	361.20205	Cannabichromanonic acid B-C5*	C22H30O7	405.19188
CBT	8,9-Dihydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabinol-C5 (8,9-Di-OH-CBT)	C21H30O5	361.20205	8,9-Dihydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabinolic acid-C5 (8,9-Di-OH-CBT)*	C22H30O7	405.19188
CBC	(\pm)-4-acetoxycannabichromene-C5	C23H32O4	371.22278	(\pm)-4-acetoxycannabichromenic acid-C5*	C24H32O6	415.21261
Miscellaneous	2-acetoxy-6-geranyl-3-n-pentyl-1,4-benzoquinone-C5	C23H32O4	371.22278	2-acetoxy-6-geranyl-3-n-pentyl-1,4-benzoquinonic acid-C5*	C24H32O6	415.21261
Miscellaneous	11-Acetoxy- Δ^9 -Tetrahydrocannabinol-C5 (11-OAc- Δ^9 -THC)*	C23H32O5	371.22278	11-Acetoxy- Δ^9 -Tetrahydrocannabinolic acid-C5 (11-OAc- Δ^9 -THCA)	C24H32O6	415.21261
CBG	5-acetyl-4-hydroxycannabigerol-C5	C23H34O4	373.23843	5-acetyl-4-hydroxycannabigerolic acid-C5*	C24H34O6	417.22826
CBG	4-acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenol-C5	C23H34O4	373.23843	4-acetoxy-2-geranyl-5-hydroxy-3-n-pentylphenolic acid-C5*	C24H34O6	417.22826
CBT	(-)- <i>trans</i> -10-Ethoxy-9-hydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabinol-C5 ((-)- <i>trans</i> -CBT-Oet)	C23H34O4	373.23843	(-)- <i>trans</i> -10-Ethoxy-9-hydroxy- $\Delta^{6a(10a)}$ -tetrahydrocannabinolic acid-C5 ((-)- <i>trans</i> -CBTA-Oet)*	C24H34O6	417.22826
	4-acetoxy-2-geranyl-5-hydroxy-3-n-propylphenol-C5	C23H34O4	373.23843	4-acetoxy-2-geranyl-5-hydroxy-3-n-propylphenolic acid-C5*	C24H34O6	417.22826
CBG	sesquicannabigerol-C5 (SesquiCBG)	C26H40O2	383.29555	Sesquicannabigerolic acid-C5 (SesquiCBGA)*	C27H40O4	427.28538
CBD	carmagerol-C5	C23H36O6	407.24391	Carmagerolic acid-C5*	C24H36O8	451.23374
CBN	4-terpenyl cannabinolate-C5	C32H42O4	489.30103			
Δ^9 -THC	β -fenchyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233			
Δ^9 -THC	α -fenchyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233			
Δ^9 -THC	epi-bornyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233			

Δ^9 -THC	bornyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233
Δ^9 -THC	α -terpenyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233
Δ^9 -THC	4-terpenyl- Δ^9 -tetrahydrocannabinolate-C5	C32H46O4	493.33233

*Additional potential phytocannabinoids that were added to the list according to their biosynthesis and decomposition pathways described in the literature.

Table S2. Correlation coefficients (R^2), limit of quantification (LOQ) and precision for the type I phytocannabinoids expressed as relative standard deviation (RSD)

Analyte	R^2	LOQ [ng/ml]	Concentration ^a [%]	Precision	
				Repeatability	Reproducibility
Δ^9 -THCA	0.9976	5	18.81 ^b	13.08 ^b	10.12 ^b
CBDA	0.9996	1	12.01	6.15	6.91
Δ^9 -THC	0.9979	2	0.98 ^b	8.17 ^b	11.04 ^b
CBDVA	0.9997	0.25	0.48	6.89	7.90
CBD	0.9995	1	0.41	4.62	8.66
CBGA	0.9933	2.5	0.19	5.96	6.74
CBG	0.9997	2	0.04	4.84	5.57
CBDV	0.9996	1.25	0.03	4.54	6.41
CBC	0.9991	0.25	0.03	4.09	8.82
Δ^9 -THCV	0.9999	0.25	0.02 ^b	9.16 ^b	9.81 ^b
CBN	0.9997	1.25	0.01 ^b	8.05 ^b	12.25 ^b
Δ^8 -THC	0.9977	1.25	<LOQ	-	-
CBL	0.9997	1.25	<LOQ	-	-

^a Average concentrations from ethanolic extractions of the same sample (n=5).

^b Precision values quantified according to a second sample.

Table S3. Ranges of absolute phytocannabinoid contents for the 36 *Cannabis* samples

Phyto. Abbreviation	Phyto. type	Calibration curve used	Minimum and maximum concentrations and deviations of the 36 <i>Cannabis</i> samples (Fig. 4)					
			Min conc. [% w/w]	Min deviation of Min conc. [% w/w]	Max deviation of Min conc. [% w/w]	Max conc. [% w/w]	Min deviation of Max conc. [% w/w]	Max deviation of Max conc. [% w/w]
Δ^9 -THCA*	I	-	0.2988	-	-	19.9701	-	-
Δ^9 -THC*	I	-	0.0152	-	-	4.2287	-	-
Δ^9 -THCA-C4	II	Δ^9 -THCA	0.0009	0.0004	0.0094	0.1185	0.0515	1.2492
Δ^9 -THC-C4	II	avg(Δ^9 -THC, Δ^9 -THCV)	0.0000	0.0000	0.0000	0.0107	0.0005	0.0121
Δ^9 -THCVA	II	Δ^9 -THCA	0.0021	0.0009	0.0217	0.4357	0.1892	4.5926
Δ^9 -THCV*	I	-	0.0000	-	-	0.0220	-	-
Δ^9 -THCOA	II	Δ^9 -THCA	0.0000	0.0000	0.0000	0.0632	0.0274	0.6662
Δ^9 -THCO	II	avg(Δ^9 -THC, Δ^9 -THCV)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Δ^9 -THCMA	II	Δ^9 -THCA	0.0000	0.0000	0.0000	0.0037	0.0016	0.0393
Δ^9 -THCM	II	avg(Δ^9 -THC, Δ^9 -THCV)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBDA*	I	-	0.0308	-	-	13.4860	-	-
CBD*	I	-	0.0000	-	-	2.0748	-	-
CBDA-C4	II	avg(CBDA,CBDVA)	0.0001	0.0001	0.0021	0.0779	0.0707	1.7171
CBD-C4	II	avg(CBD,CBDV)	0.0000	0.0000	0.0000	0.0055	0.0010	0.0247
CBDVA*	I	-	0.0001	0.0001	0.0032	1.0959	1.0959	26.6070
CBDV*	I	-	0.0000	-	-	0.0742	-	-
CBDOA	II	avg(CBDA,CBDVA)	0.0000	0.0000	0.0000	0.0166	0.0151	0.3655
CBDO	II	avg(CBD,CBDV)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBDMA	II	avg(CBDA,CBDVA)	0.0000	0.0000	0.0000	0.0091	0.0083	0.2015
CBDM	II	avg(CBD,CBDV)	0.0000	0.0000	0.0000	0.0013	0.0003	0.0061
CBGA*	I	-	0.0510	-	-	1.9291	-	-

CBG*	I	-	0.0213	-	-	0.1730	-	-
CBGA-C4	II	CBGA	0.0000	0.0000	0.0000	0.0031	0.0025	0.0613
CBG-C4	II	CBG	0.0000	0.0000	0.0000	0.0002	0.0001	0.0013
CBGVA	II	CBGA	0.0000	0.0000	0.0000	0.0239	0.0198	0.4809
CBGV	II	CBG	0.0000	0.0000	0.0000	0.0030	0.0007	0.0176
CBGOA	II	CBGA	0.0000	0.0000	0.0000	0.0036	0.0030	0.0721
CBGO	II	CBG	0.0000	0.0000	0.0000	0.0001	0.0000	0.0008
CBGMA	II	CBGA	0.0000	0.0000	0.0000	0.0002	0.0002	0.0044
CBGM	II	CBG	0.0000	0.0000	0.0000	0.0002	0.0001	0.0013
SesquiCBGA	II	CBGA	0.0001	0.0001	0.0026	0.0026	0.0022	0.0526
SesquiCBG	II	CBG	0.0022	0.0005	0.0129	0.0273	0.0067	0.1622
CBCA	II	CBDA	0.0328	0.0268	0.6501	0.3132	0.2553	6.1988
CBC*	I	-	0.0050	-	-	0.1096	-	-
CBCA-C4	II	CBDA	0.0000	0.0000	0.0000	0.0033	0.0027	0.0648
CBC-C4	II	CBC	0.0000	0.0000	0.0000	0.0007	0.0001	0.0035
CBCVA	II	CBDA	0.0004	0.0003	0.0077	0.0651	0.0531	1.2889
CBCV	II	CBC	0.0000	0.0000	0.0000	0.0136	0.0027	0.0647
CBCOA	II	CBDA	0.0000	0.0000	0.0000	0.0047	0.0038	0.0929
CBCO	II	CBC	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBNA	II	avg(Δ^9 -THCA,CBDA,CBGA) /avg(Δ^9 -THC,CBD,CBG)*CBN	0.0002	0.0002	0.0164	0.0809	0.0809	5.6388
CBN*	II	-	0.0000	-	-	0.1502	-	-
CBNA-C4	II	avg(Δ^9 -THCA,CBDA,CBGA) /avg(Δ^9 -THC,CBD,CBG)*CBN	0.0000	0.0000	0.0000	0.0004	0.0004	0.0281
CBN-C4	II	CBN	0.0000	0.0000	0.0000	0.0006	0.0004	0.0099
CBNVA	II	avg(Δ^9 -THCA,CBDA,CBGA) /avg(Δ^9 -THC,CBD,CBG)*CBN	0.0000	0.0000	0.0000	0.0011	0.0011	0.0736
CBNV	II	CBN	0.0000	0.0000	0.0000	0.0011	0.0008	0.0194
CBNOA	II	avg(Δ^9 -THCA,CBDA,CBGA) /avg(Δ^9 -THC,CBD,CBG)*CBN	0.0000	0.0000	0.0000	0.0001	0.0001	0.0101

CBNO	II	CBN	0.0000	0.0000	0.0000	0.0001	0.0000	0.0011
OH-CBNA	II	avg(Δ^9 -THCA,CBDA,CBGA) /avg(Δ^9 -THC,CBD,CBG)*CBN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
OH-CBN	II	CBN	0.0000	0.0000	0.0000	0.0009	0.0006	0.0150
CBNM	II	CBN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBEA	III	avg(acids)	0.0000	0.0000	0.0000	0.0275	0.0212	0.5141
CBE	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0037	0.0009	0.0211
CBEVA	III	avg(acids)	0.0000	0.0000	0.0000	0.0009	0.0007	0.0167
CBEV	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBNDA	III	avg(acids)	0.0000	0.0000	0.0000	0.0054	0.0042	0.1016
CBND	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBNDVA	III	avg(acids)	0.0000	0.0000	0.0000	0.0002	0.0002	0.0038
$\Delta 8$ -THC*	I	$\Delta 8$ -THC	0.0000	-	-	0.0004	-	-
CBL*	I	CBL	0.0000	-	-	0.0007	-	-
CBTA-1	III	avg(acids)	0.0000	0.0000	0.0000	0.0140	0.0107	0.2605
CBT-1	III	avg(neutrals)	0.0001	0.0000	0.0008	0.0711	0.0165	0.4002
CBTV-1	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0005	0.0001	0.0028
CBTA-3	III	avg(acids)	0.0002	0.0002	0.0043	0.0686	0.0528	1.2814
CBT-3	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0522	0.0121	0.2938
CBTV-3	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CBT-2	III	avg(neutrals)	0.0000	0.0000	0.0000	0.0104	0.0024	0.0586
329-11a	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0182	0.0042	0.1027
329-11b	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0089	0.0021	0.0499
329-11c	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0151	0.0035	0.0849
329-11d	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0026	0.0006	0.0144
373-12a	IV	avg(acids)	0.0000	0.0000	0.0000	0.0355	0.0273	0.6633
373-12b	IV	avg(acids)	0.0007	0.0005	0.0129	0.0047	0.0036	0.0879
373-12c	IV	avg(acids)	0.0000	0.0000	0.0000	0.0022	0.0017	0.0415

373-12d	IV	avg(acids)	0.0000	0.0000	0.0000	0.0064	0.0049	0.1192
327-13a	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0006	0.0001	0.0036
327-13b	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0004	0.0001	0.0022
327-13c	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0522	0.0121	0.2936
371-14a	IV	avg(acids)	0.0000	0.0000	0.0000	0.0011	0.0009	0.0208
371-14b	IV	avg(acids)	0.0000	0.0000	0.0000	0.0086	0.0066	0.1606
417-15a	IV	avg(acids)	0.0000	0.0000	0.0000	0.0073	0.0056	0.1371
373-15b	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0045	0.0010	0.0251
373-15c	IV	avg(acids)	0.0000	0.0000	0.0000	0.1718	0.1321	3.2081
357-16a	IV	avg(acids)	0.0023	0.0018	0.0438	0.0228	0.0175	0.4252
313-16b	IV	avg(neutrals)	0.0004	0.0001	0.0022	0.0630	0.0146	0.3546
361-17a	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0205	0.0047	0.1152
361-17b	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0006	0.0001	0.0035
331-18a	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.1020	0.0237	0.5745
331-18b	IV	avg(neutrals)	0.0275	0.0064	0.1549	0.2615	0.0606	1.4722
331-18c	IV	avg(neutrals)	0.0000	0.0000	0.0000	0.0023	0.0005	0.0129
331-18d	IV	avg(neutrals)	0.0220	0.0051	0.1239	0.1067	0.0248	0.6009
375-19a	IV	avg(acids)	0.0015	0.0012	0.0285	0.1482	0.1140	2.7677
375-19b	IV	avg(acids)	0.0000	0.0000	0.0000	0.0018	0.0014	0.0331
375-19c	IV	avg(acids)	0.0000	0.0000	0.0000	0.0030	0.0023	0.0559

*Analytical standard