Appendix to ML844/18

Metabolomic profiling of phytocannabinoids

Target screening of 243 phytocannabinoids saved in UCT database was performed using UHPL-HRMS method. In the ESI+ ionization mode, 120 compounds (unique combination of exact mass and respective retention time RT) were detected; in the ESI- ionization mode, 118 compounds (unique combination of exact mass and respective retention time RT) were detected. Considering the possible existence of isomeric forms, one detected substance may have several identities. All detected (tentative identification) phytocannabinoids are summarized in table I. Extracted ion chromatograms (XIC) illustrating the tested CBD oel (internal code ML844/18) are documented in figure 1 (ESI+) and figure 2 (ESI-). XICs with highlighted main phytocannabinoids (analytical standard available) are documented in figure 3 (ESI+) and figure 4 (ESI-). The results of target analysis of main phytocannabinoids are documented in certificate ML844/18.

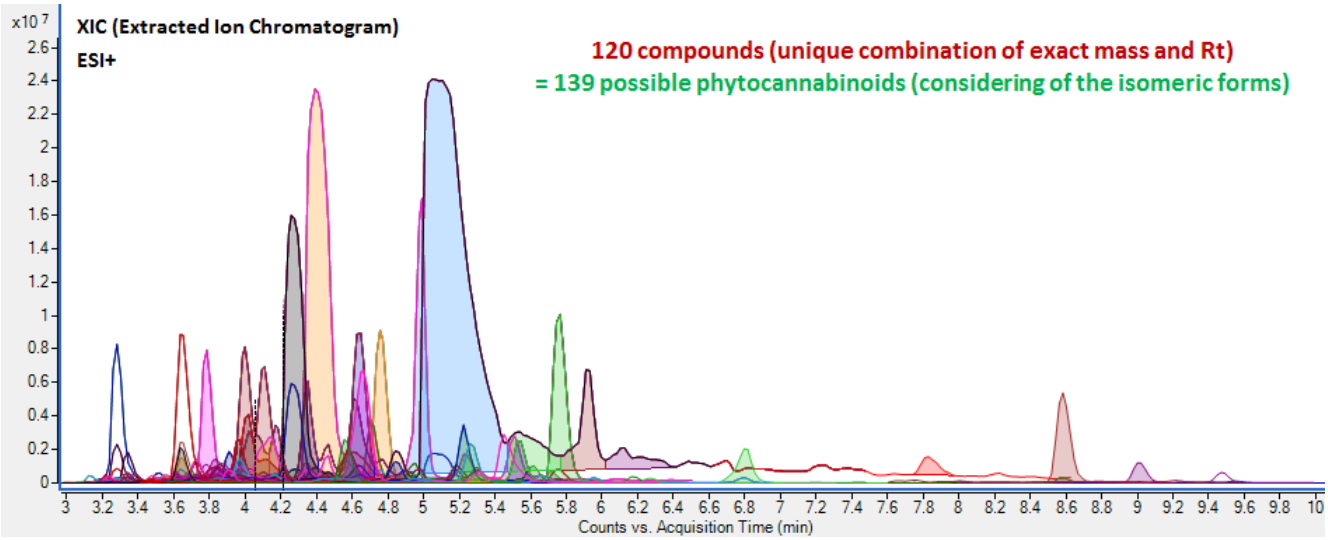

Figure 1: UHPLC-HRMS (ESI+) extracted ion chromatogram of 120 detected compounds with unique combination of exact mass and RT (ML844/18)

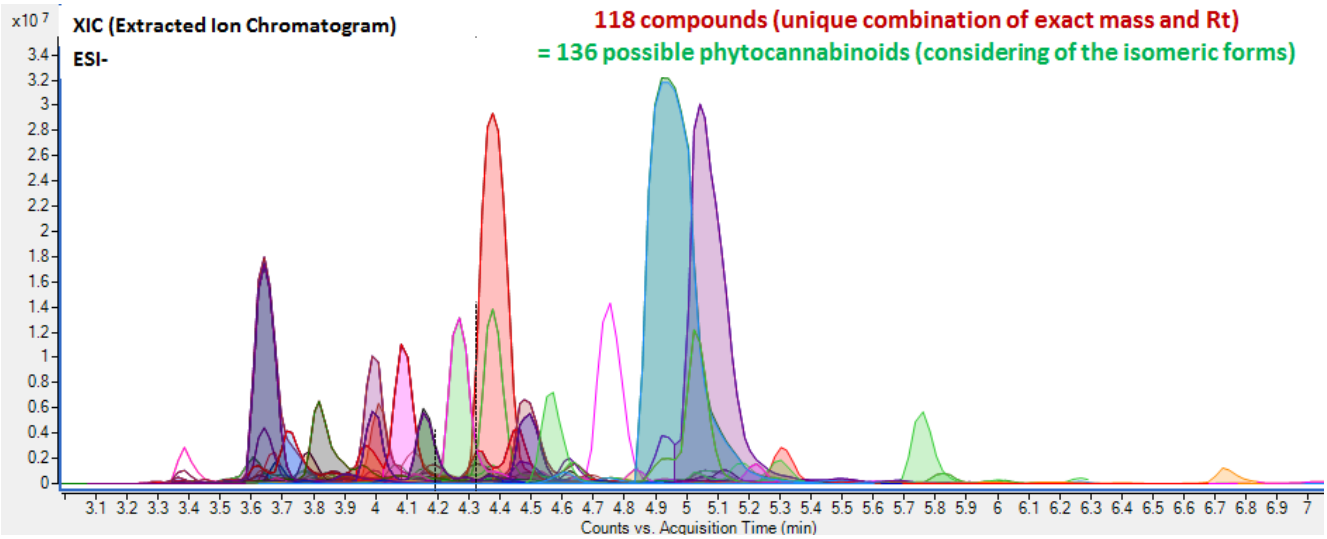

Figure 2: UHPLC-HRMS (ESI-) extracted ion chromatogram of 118 detected compounds with unique combination of exact mass and RT (ML844/18)

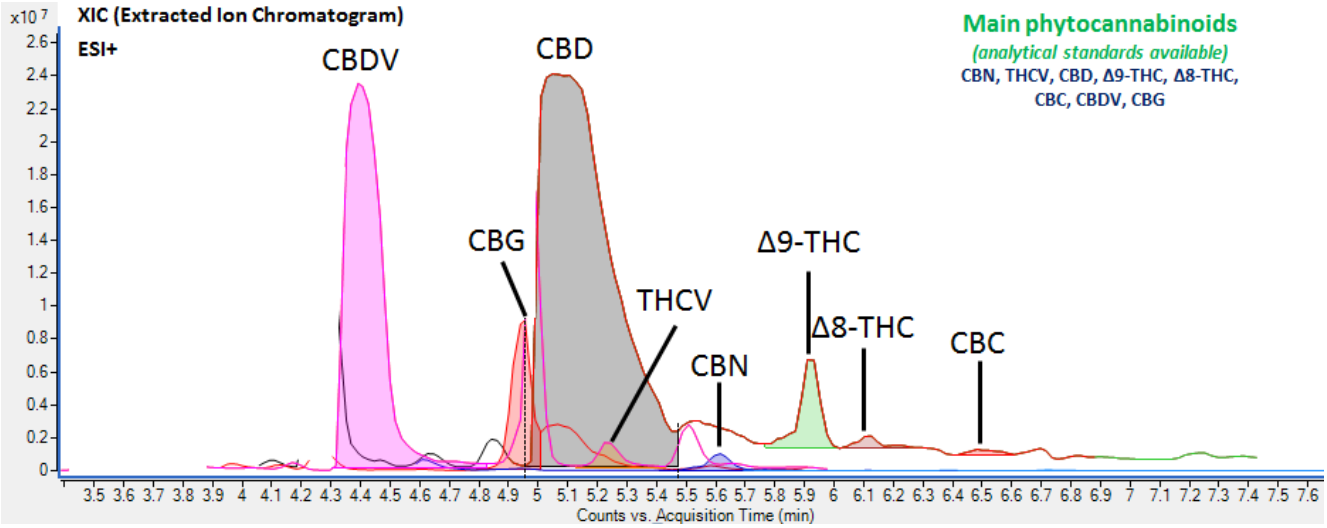

Figure 3: UHPLC-HRMS (ESI+) extracted ion chromatogram of detected main cannabinoids for which the analytical standards are available (ML844/18)

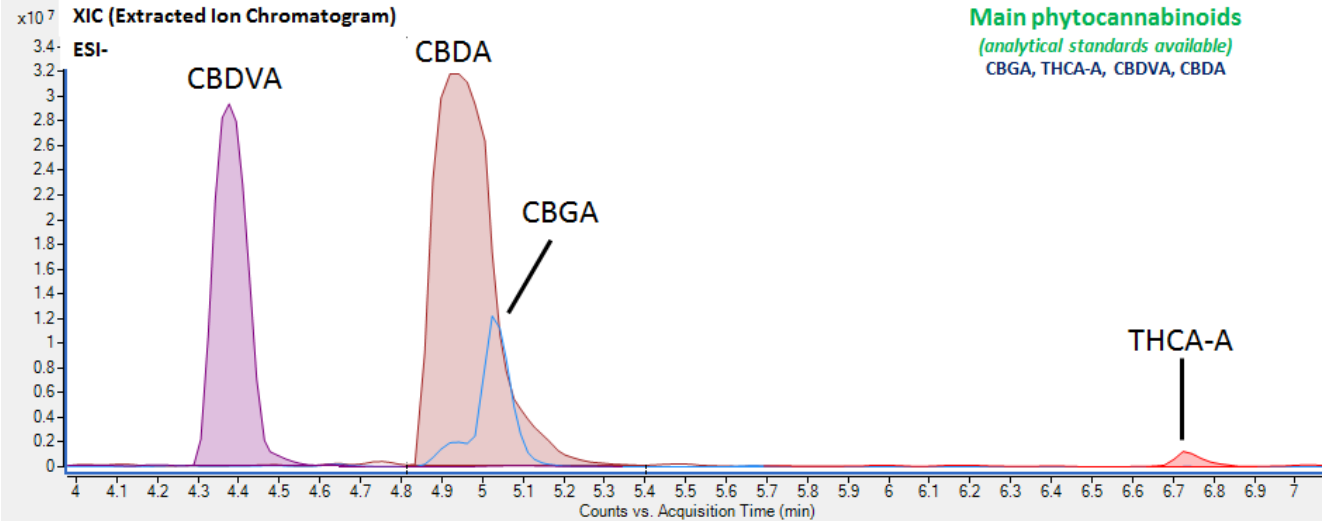

Figure 4: UHPLC-HRMS (ESI-) extracted ion chromatogram of detected main cannabinoids for which the analytical standards are available (ML844/18)

Table I: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
1	C17H18O2	254.1308	4.13	Cannabiorcol	1	Positive	93162
2	C17H22O2	258.1621	3.91	Cannabidiorcol/ Δ -9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	5	Positive	3130367
3	C17H22O2	258.1628	4.28			Positive	2023668
4	C17H22O2	258.1622	4.65			Positive	394151
5	C17H22O2	258.1628	9.02			Positive	137978
6	C17H22O2	258.1615	4.39			Negative	87700
7	C18H20O2	268.1463	3.73	Cannabinol-C2/56a/63a	3	Positive	64196
8	C18H20O2	268.1467	3.97			Positive	192256
9	C18H20O2	268.1465	5.69			Negative	29984
10	C18H20O3	284.1412	3.97	63h	1	Positive	259979
11	C18H20O3	284.1413	4.63	63h		Positive	124924
12	C18H22O4	302.1513	3.84	Δ -9-Tetrahydrocannabiorcolic acid A/ Δ -9-tetrahydrocannabiorcolic acid B/cannabiorcichromenic acid/anthopogochromenic acid/cannabiorcicyclolic acid/anthopogocyclolic acid	6	Positive	99404
13	C18H22O4	302.1521	4.43			Positive	94512
14	C18H22O4	302.1516	3.70			Negative	316740
15	C18H22O4	302.1516	4.23			Negative	58323
16	C18H22O4	302.1522	4.38			Negative	86912
17	C18H22O4	302.1514	5.24			Negative	106098
18	C18H24O4	304.1677	4.17	Cannabichromanone-C3	1	Positive	290968
19	C18H24O4	304.1674	3.77			Negative	207637
20	C18H24O4	304.1671	4.27			Negative	97795
21	C18H24O4	304.1672	4.64			Negative	59470
22	C18H26O4	306.1827	3.34	Amorfrutin 2	1	Negative	276054
23	C19H18O4	310.1207	3.38	69b	1	Negative	23761
24	C19H20O2	280.1471	3.60	Chiricanin A/araphyn-1/63k/68	4	Positive	314039
25	C19H20O2	280.1472	4.13			Positive	177126

*mass error < 5 ppm

**retention time

*** tentative identification of compounds was done based on available scientific article (Hanuš et al. 2016, Mechoulam 2002)

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
26	C19H20O3	296.1414	3.80	Trans-arachidin-2/arachidin-3/radulanin A/chiricanine B	4	Positive	29259
27	C19H20O3	296.1411	4.10			Negative	107133
28	C19H20O3	296.1412	4.38			Negative	110792
29	C19H22O2	282.1622	3.64	Cannabinodivarin/cannabivarin/demethyldecarboxyamorfrutin A/63b/63c	5	Positive	736814
30	C19H22O2	282.1620	3.85			Positive	640734
31	C19H22O2	282.1626	4.76			Positive	18155420
32	C19H22O2	282.1623	3.99			Positive	452698
33	C19H22O2	282.1626	6.38			Positive	355666
34	C19H22O2	282.1635	8.30			Positive	53692
35	C19H22O3	298.1565	3.60	Glepidotin C/64/66	3	Positive	946585
36	C19H22O3	298.1571	4.94			Positive	5646
37	C19H22O3	298.1583	4.04			Negative	301231
38	C19H22O3	298.1572	4.53			Negative	1328845
39	C19H22O4	314.1511	3.54	Araphyn-4/83	2	Positive	340667
40	C19H22O4	314.1528	3.80			Positive	221229
41	C19H22O4	314.1519	4.01			Negative	82219
42	C19H26O2	286.1941	4.39	CBDV	1	Positive	73242673
43	C19H26O2	286.1942	4.99	THCV	1	Positive	25085688
44	C19H26O2	286.1939	3.79	Δ 7-Trans-Isotetrahydrocannabivarin-C3/(1aS.3aR.8bR.8cR)-cannabicyclovarin/cannabivarichromene/2-methyl-2-(4-methyl-2-pentenyl)-7-propyl-2H-1-benzopyran-5-ol/delta7-1.2-cis-(1R.3R.6S)-isotetrahydrocannabivarin-C3/delta7-1.2-cis-(1S.3S.6R)-Isotetrahydrocannabivarin-C3.	6	Positive	13256741
45	C19H26O2	286.1938	5.22			Positive	4603465
46	C19H26O2	286.1937	5.51			Positive	6589975
47	C19H26O2	286.1933	6.72			Negative	2011279
48	C19H26O3	302.1887	3.65	C3-Cannabielsoin	1	Positive	1868804
49	C19H26O3	302.1883	3.89			Positive	780723
50	C19H26O3	302.1887	5.71			Positive	1452139
51	C19H26O3	302.1882	4.48			Negative	1641589
52	C19H26O3	302.1879	5.15			Negative	706950
53	C19H26O3	302.1878	5.28			Negative	313488

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
54	C19H26O4	318.1848	3.91	(9S.10S)-trans-Cannabitriol-C3/(9R.10R)-trans-cannabitriol-C3.	2	Positive	2117781
55	C19H26O4	318.1828	3.38			Negative	659631
56	C19H26O4	318.1833	3.61			Negative	3898492
57	C19H26O4	318.1832	3.77			Negative	1557334
58	C19H26O4	318.1834	3.84			Negative	1702280
59	C19H26O4	318.1830	5.13			Negative	158033
60	C19H28O3	304.2032	3.41	Cannabiglendol C3	1	Positive	785970
61	C19H28O3	304.2036	3.79			Negative	4187206
62	C19H28O3	304.2037	4.17			Negative	1258237
63	C19H28O3	304.2034	4.41			Negative	610181
64	C20H18O4	322.1204	4.12	Radulanin K	1	Negative	65854
65	C20H20O4	324.1354	3.50	59	1	Positive	112058
66	C20H20O4	324.1362	4.15			Negative	45127
67	C20H20O4	324.1360	4.25			Negative	30048
68	C20H20O5	340.1311	3.41	57a/Radulanin H	2	Negative	44869
69	C20H20O5	340.1307	3.71			Negative	94189
70	C20H22O4	326.1520	3.54	Demethylamorfrutin A/63d/65b/65c	4	Positive	1163646
71	C20H22O4	326.1516	3.89			Positive	215079
72	C20H22O4	326.1516	3.75			Negative	223265
73	C20H22O4	326.1520	4.44			Negative	12912
74	C20H24O5	344.1617	3.50	51	1	Positive	838952
75	C20H24O5	344.1622	3.86			Negative	503478
76	C20H24O5	344.1624	4.39			Negative	318226
77	C20H26O4	330.1831	3.67	Cannabichromevarinic acid/ Δ -9-tetrahydrocannabivarinic acid	2	Positive	802555
78	C20H26O4	330.1823	4.06			Positive	452389
79	C20H26O4	330.1820	3.86			Negative	460133
80	C20H26O4	330.1830	6.03			Negative	1200054
81	C20H26O4	330.1830	4.38	CBDVA	1	Negative	1.02E+08

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
82	C20H26O5	346.1781	3.36	(5aS.6S.9R.9aR)-C3-Cannabielsoic_acid_B/bis-nor-cannabielsoic acid B	2	Negative	564923
83	C20H26O5	346.1785	3.62			Negative	959703
84	C20H26O5	346.1778	3.92			Negative	926692
85	C20H28O2	300.2096	4.70	Δ -9-Tetrahydrocannabinol-C4/norCannabidiol	2	Positive	7467493
86	C20H28O2	300.2089	5.45			Positive	248160
87	C20H28O2	300.2082	5.15			Negative	329141
88	C20H28O4	332.2005	4.98	Cannabichromanone/cannabigerovarinic acid	2	Positive	612726
89	C20H28O4	332.1980	4.12			Negative	1411952
90	C20H28O4	332.1991	4.86			Negative	203211
91	C21H24O2	308.1781	5.11	Dehydrocannabifuran	1	Positive	484400
92	C21H24O2	308.1780	5.52			Positive	160783
93	C21H24O2	308.1781	7.18			Negative	16748
94	C21H24O4	340.1668	3.28	Amorfrutin A/65d	2	Positive	578366
95	C21H24O4	340.1677	3.91			Positive	1504557
96	C21H24O4	340.1682	4.01			Negative	85202
97	C21H24O5	356.1615	3.60	Amorfrutin 3	1	Positive	344334
98	C21H24O5	356.1629	3.38			Negative	202177
99	C21H26O2	310.1938	3.73	Cannabinodiol/cannabifuran	2	Positive	937219
100	C21H26O2	310.1941	4.39			Positive	2385191
101	C21H26O2	310.1937	4.61			Positive	1287718
102	C21H26O2	310.1938	5.62	CBN	1	Positive	2081908
103	C21H26O2	310.1929	5.60	Cannabinodiol/cannabifuran	2	Negative	375835
104	C21H26O3	326.1884	4.04	8-Hydroxycannabinol/7-hydroxycannabinol	2	Positive	953527
105	C21H26O3	326.1883	4.35			Positive	436688
106	C21H26O3	326.1885	4.84			Positive	967668
107	C21H26O3	326.1886	5.30			Positive	1120629
108	C21H26O3	326.1879	4.15			Negative	614627
109	C21H26O3	326.1883	5.30			Negative	5569614

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
110	C21H28O2	312.2090	3.84	7.8-Dihydrocannabinol	1	Positive	2298573
111	C21H28O2	312.2095	4.02			Positive	5277804
112	C21H28O2	312.2078	4.35			Positive	745273
113	C21H28O2	312.2093	4.61			Positive	5489026
114	C21H28O2	312.2093	4.99			Positive	1067798
115	C21H28O2	312.2087	4.92			Negative	469151
116	C21H28O3	328.2041	3.85	Cannabichromanone-D/cannabicoumaronone/10-oxo- Δ -6a(10a)-tetrahydrocannabinol/8-Oxo- Δ 9-trans-tetrahydrocannabinol/9.10-Anhydrocannabitriol/anhydrocannabimovone	6	Positive	1790986
117	C21H28O3	328.2040	4.17			Positive	4708012
118	C21H28O3	328.2047	4.35			Positive	8288911
119	C21H28O3	328.2040	4.96			Positive	1379763
120	C21H28O3	328.2046	5.77			Positive	17951929
121	C21H28O3	328.2036	3.73			Negative	4010150
122	C21H28O3	328.2040	3.99			Negative	7008806
123	C21H28O3	328.2037	4.46			Negative	2247342
124	C21H28O3	328.2040	5.76			Negative	9316028
125	C21H28O4	344.1986	3.97	10-Hydroxy-9-oxo- Δ -8-tetrahydrocannabinol/ Δ -9-tetrahydrocannabinolic acid-C4 A/ Δ -9-tetrahydrocannabinolic acid-C4 B	3	Positive	4620025
126	C21H28O4	344.1987	4.21			Positive	985498
127	C21H28O4	344.1984	4.41			Positive	835547
128	C21H28O4	344.1994	4.57			Positive	3890188
129	C21H28O4	344.2000	4.84			Positive	681613
130	C21H28O4	344.1978	3.71			Negative	719512
131	C21H28O4	344.1988	4.38			Negative	1793493
132	C21H28O4	344.1990	4.62			Negative	1593117
133	C21H28O4	344.1986	5.11			Negative	1950267
134	C21H28O5	360.1941	4.22	Cannabichromanone-C	1	Positive	520733
135	C21H28O5	360.1948	4.43			Positive	374977
136	C21H28O5	360.1934	3.66			Negative	1176113
137	C21H28O5	360.1939	4.38			Negative	817757

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
138	C21H30O2	314.2252	5.91	9-THC	1	Positive	15998152
139	C21H30O2	314.2253	6.13	8-THC	1	Positive	7453112
140	C21H30O2	314.2249	4.26	(1aS.3aR. 3R.8bR.8cR)-Cannabicyclol/cannabicitran/(-)- Δ 9-cis-(6aS.10aR)- Δ 9-tetrahydrocannabinol/(-) Δ 7 -trans-(1R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	4	Positive	44009335
141	C21H30O2	314.2251	4.84			Positive	4508911
142	C21H30O2	314.2252	5.13			Positive	3843428
143	C21H30O2	314.2251	5.55			Positive	18432863
144	C21H30O2	314.2250	7.63			Positive	1705718
145	C21H30O2	314.2256	5.13	CBD	1	Positive	1.45E+08
146	C21H30O2	314.2252	6.48	CBC	1	Positive	940965
147	C21H30O2	314.2244	4.46	(1aS.3aR.8bR.8cR)-Cannabicyclol/cannabicitran/(-)- Δ 9-cis-(6aS.10aR)- Δ 9-tetrahydrocannabinol/(-)- Δ 7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	5	Negative	1772027
148	C21H30O2	314.2245	4.92			Negative	2765288
149	C21H30O3	330.2200	4.11	8'-Hydroxyisocannabichromene/cannabielsoin/abnormal cannabigeroquinol/10α-hydroxy trans Δ-8-tetrahydrocannabinol/10β-hydroxy trans Δ-8-tetrahydrocannabinol/8α-hydroxy- Δ 9-trans-tetrahydrocannabinol/8β-hydroxy- Δ 9-trans-tetrahydrocannabinol/tetrahydrocannabinol epoxide/hydroxy Δ 9.11-hexahydrocannabinol	9	Positive	21070496
150	C21H30O3	330.2199	4.33			Positive	3105139
151	C21H30O3	330.2196	4.65			Positive	20108536
152	C21H30O3	330.2199	4.90			Positive	1499413
153	C21H30O3	330.2202	6.80			Positive	5367121
154	C21H30O3	330.2196	4.01			Negative	8698878
155	C21H30O3	330.2194	5.30			Negative	3406077
156	C21H30O4	346.2148	3.60	Trans-10-ethoxy-9-hydroxy-Δ6a(10a)-tetrahydrocannabivarin-C3/cannabimovone/(+)-(9S.10S)-trans-cannabitriol/(-)-(9R.10R)-trans-cannabitriol/(9S.10R)-cis-cannabitriol/(9R.10S)-cis-cannabitriol/ethoxy-cannabitriolvarin/isocannabitriol (8.9-dihydroxy-Δ-6a(10a)-tetrahydrocannabinol)	8	Positive	1433967
157	C21H30O4	346.2149	4.15			Positive	7777597
158	C21H30O4	346.2142	4.63			Positive	411015
159	C21H30O4	346.2144	3.71			Negative	7769253
160	C21H30O4	346.2143	3.97			Negative	6737645
161	C21H30O4	346.2146	4.08			Negative	17282687
162	C21H30O4	346.2146	4.33			Negative	3805253
163	C21H30O4	346.2145	4.46			Negative	7862193

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
164	C21H30O5	362.2083	3.91	Cannabichromanone-B/(-)-cannabitetrol/	2	Positive	922950
165	C21H30O5	362.2094	4.13			Positive	432146
166	C21H30O5	362.209	3.52			Negative	1142191
167	C21H30O5	362.2087	3.82			Negative	587437
168	C21H30O5	362.2089	3.89			Negative	726343
169	C21H30O5	362.2090	4.55			Negative	483018
170	C21H32O3	332.2348	3.80	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	3	Positive	2086630
171	C21H32O3	332.2354	4.84			Positive	2569042
172	C21H32O3	332.2354	5.09			Positive	367573
173	C21H32O3	332.2343	3.79			Negative	1269527
174	C21H32O3	332.2350	4.27			Negative	24835740
175	C21H32O3	332.2344	4.66			Negative	1205774
176	C21H32O3	332.2349	5.22			Negative	2993040
177	C21H32O4	348.2310	3.73	Cannabiripsol	1	Positive	1453713
178	C21H32O4	348.2297	3.82			Negative	10969949
179	C21H32O4	348.2298	3.96			Negative	3018422
180	C21H32O4	348.2291	4.19			Negative	1268793
181	C21H34O4	350.2457	3.82	Carmagerol		Positive	1108646
182	C21H30O2	316.2374	4.96	CBG	1	Positive	43371
183	C22H26O4	354.1834	3.97	Cannabinolic acid A	1	Positive	4605122
184	C22H26O4	354.1831	4.17			Positive	1416290
185	C22H26O4	354.1824	3.86			Negative	475910
186	C22H26O4	354.1830	4.14			Negative	1090909
187	C22H26O4	354.1831	4.50			Negative	291572
188	C22H26O4	354.1825	5.09			Negative	372755
189	C22H26O4	354.1824	6.27			Negative	277013

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
190	C22H26O5	370.1776	3.24	8-Hydroxycannabinolic acid A	1	Positive	690296
191	C22H26O5	370.1787	3.48			Positive	1777052
192	C22H26O5	370.1787	3.89			Negative	420898
193	C22H26O5	370.1783	4.12			Negative	1100022
194	C22H28O5	372.1940	3.97	Cannabicoumarononic acid	1	Positive	1018961
195	C22H28O5	372.1943	4.52			Positive	179169
196	C22H28O5	372.1941	3.77			Negative	371094
197	C22H28O5	372.1940	3.89			Negative	1672864
198	C22H28O5	372.1939	4.15			Negative	8158223
199	C22H28O5	372.1946	4.43			Negative	494563
200	C22H28O5	372.1935	5.06			Negative	1001592
201	C22H30O2	326.2251	8.58	Confluentin	1	Positive	709768
202	C22H30O3	342.2194	5.02	Ferruginene C/2-formyl-Δ9-trans-tetrahydrocannabinol	2	Negative	736123
203	C22H30O3	342.2197	5.82			Negative	1684866
204	C22H30O4	358.2149	4.94	CBDA	1	Negative	94483501
205	C22H30O4	358.2147	6.72	THCA	1	Negative	1746235
206	C22H30O4	358.2142	7.82	Ferruginene A/ferruginene B/Δ-9-tetrahydrocannabinolic acid B/cannabichromenic acid/cannabicyclolic acid/Δ-8-tetrahydrocannabinolic acid	6	Negative	411559
207	C22H30O5	374.2099	3.64	Cannabielsoic acid A/cannabielsoic acid B	2	Negative	24921910
208	C22H30O5	374.2096	3.99			Negative	7694483
209	C22H30O5	374.2095	4.38			Negative	922797
210	C22H30O5	374.2098	4.50			Negative	9078646
211	C22H30O5	374.2096	5.01			Negative	353197
212	C22H32O4	360.2294	4.48	Cannabinerolic acid	1	Negative	164644
213	C22H32O4	360.2295	5.67	CBGA	1	Negative	298903

Table I - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 1-4)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Ionization (mode polarity)	Peak area
214	C23H30O4	370.2145	3.84	Rhododaurichromanic acid A/daurichromenic acid	2	Positive	1900889
215	C23H30O4	370.2133	4.04			Positive	673347
216	C23H30O4	370.2148	4.50			Negative	393222
217	C23H30O4	370.2138	4.64			Negative	650399
218	C23H32O4	372.2308	5.26	(+/-)-4-Acetoxycannabichromene/acetyl cannabigeroquinol/7.8-dehydro-10-O-ethylcannabitriol	4	Positive	4975304
219	C23H32O4	372.2306	5.67			Positive	1183893
220	C23H32O4	372.2303	5.95			Positive	592742
221	C23H32O4	372.2293	5.78			Negative	70588
222	C23H32O4	372.2296	8.41			Negative	336131
223	C23H34O4	374.2464	4.66	(-)-(9R.10R)-trans-10-O-Ethylcannabitriol/5-acetyl-4-hydroxycannabigerol/acetyl abnormal cannabigeroquinol/cannabigerolic acid monomethylether	4	Positive	16071093
224	C23H34O4	374.2453	5.32			Positive	1626607
225	C23H34O4	374.2446	5.69			Negative	143855
226	C24H28O5	396.1918	3.64	54a (iBu)	1	Positive	2484654
227	C24H30O3	366.2191	4.41	Hydroxy helicannabigenol/55	2	Positive	38878
228	C24H30O3	366.2205	3.79			Negative	320149
229	C24H30O3	366.2192	4.71			Negative	293614
230	C24H32O6	416.2189	4.06	11-Acetoxy-Δ-8-tetrahydrocannabinoic acid	1	Negative	318680
231	C25H26O5	406.1777	4.64	72b/72c	2	Negative	198220
232	C26H28O6	436.1894	4.56	Desmodianone A/desmodianone D/desmodianone E	3	Positive	7665511
233	C26H28O6	436.1886	4.57			Negative	12181495
234	C26H30O6	438.2024	4.61	Desmodianone C	1	Negative	1444480
235	C26H32O4	408.2298	5.17	Amorfrutin B	1	Positive	4736
236	C26H40O2	384.3009	9.54	Sesquicannabigerol/O-propylcannabidiol/O-pentyl-Δ9-trans-tetrahydrocannabinol	3	Positive	169037
237	C37 H56O4	564.4162	9.00	γ-Eudesmyl cannabigerolate/ γ -cadinyl cannabigerolate	2	Positive	1705130
238	C43 H60O4	640.4503	8.58	Cannabisol	1	Positive	17144147

*mass error < 5 ppm

**retention time

*** tentative identification of compounds was done based on available scientific article (Hanuš et al. 2016, Mechoulam 2002)

Metabolomic profiling of non-cannabinoid biologically active compounds

Target screening of 151 non-cannabinoid biologically active compounds (terpenoids, phenols, bibenzyl stilbenes, fatty acids, amids, flavones, lignans, flavonoid glykosides, lingamide derivatives and quaternary ammonium cations) saved in UCT database was performed using UHPLC-HRMS method. In the ESI+ ionization mode, 47 compounds (unique combination of exact mass and respective retention time RT) were detected; in the ESI- ionization mode, 25 compounds (unique combination of exact mass and respective retention time RT) were detected. Considering the possible existence of isomeric forms, one detected substance may have several identities. All detected (tentative identification) non-cannabinoid biologically active compounds are summarized in table II. Extracted ion chromatograms (XIC) illustrating tested CBD oel (internal code ML844/18) are documented in figure 5 (ESI+) and figure 6 (ESI-).

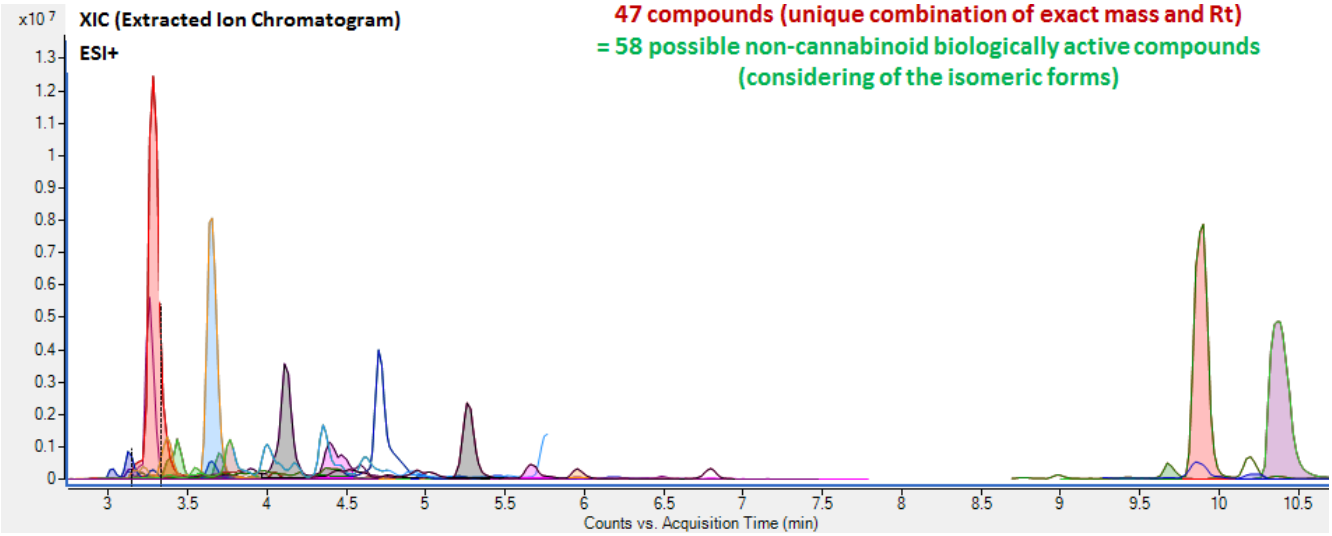

Figure 5: UHPLC-HRMS (ESI+) extracted ion chromatogram of 47 detected compounds with unique combination of exact mass and RT (ML844/18)

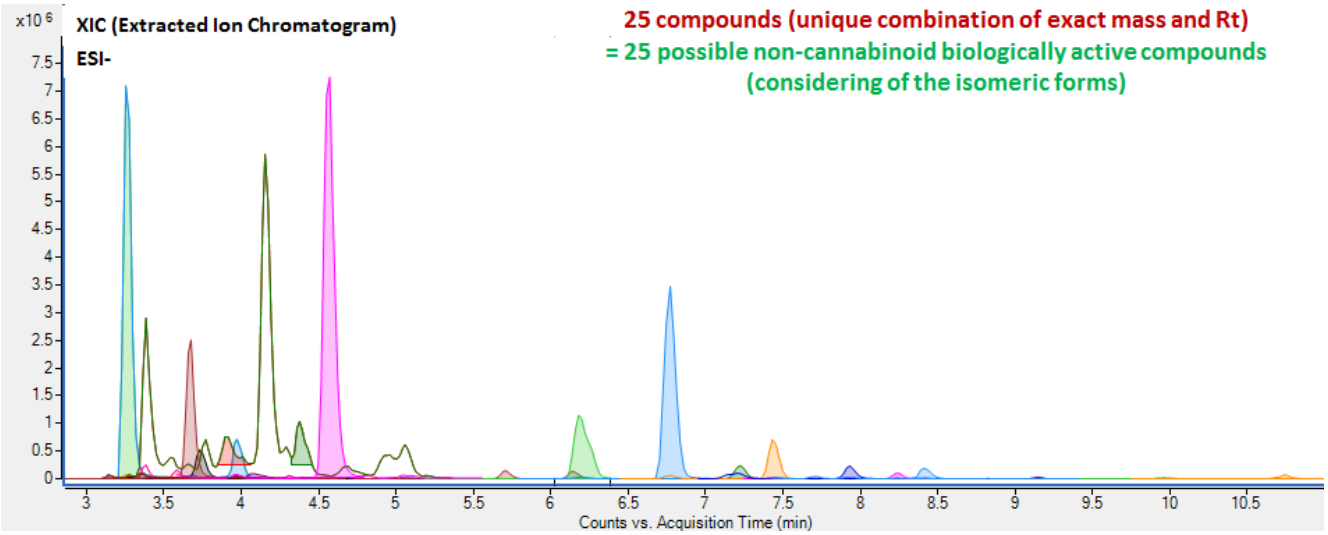

Figure 6: UHPLC-HRMS (ESI-) extracted ion chromatogram of 25 detected compounds with unique combination of exact mass and RT (ML844/18)

Table II: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 5-6)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Type of compounds	Ionization (mode polarity)	Peak area
1	C10H14	134.1099	3.22	p-cymene	1	terpenoid	Positive	87802
2	C10H14	134.1097	4.37				Positive	106263
3	C10H14	134.1097	5.03				Positive	162355
4	C10H16	136.1258	5.32	d-limonene / delta-3-carene / beta-myrcene / alpha-pinene / beta-pinene / trans-ocimene / cis-ocimene / beta-phellandrene / camphene / sabinene / alpha-thujene / terpinolene / gamma-terpinene	13	terpenoid	Positive	65877
5	C14H28O2	228.2088	6.14	myristic acid	1	fatty acid	Negative	237516
6	C15H14O3	242.0948	3.03	isocannabispiradienone / cannithrene-1	2	phenol	Positive	465700
7	C15H14O3	242.0944	3.30				Positive	148553
8	C15H18O3	246.1258	3.41	cannabispiran / isocannabispiran	2	phenol	Positive	280922
9	C15H18O3	246.1260	4.65				Positive	207792
10	C15H18O3	246.1260	5.73				Positive	101724
11	C15H18O3	246.1259	3.25				Negative	11422552
12	C15H18O3	246.1260	3.97				Negative	1286463
13	C15H20O3	248.1415	3.39	alpha-cannabispiranol	1	phenol	Positive	1201535
14	C15H20O3	248.1408	4.00				Positive	136399
15	C15H20O3	248.1409	6.80				Positive	92648
16	C15H20O3	248.1413	3.58				Negative	256662
17	C15H20O3	248.1412	4.31				Negative	85262
18	C15H24	204.1880	6.13	beta-caryophyllene / trans-gamma-bisabolene / cis-gamma-bisabolene / cis-beta-farnesene / allo-aromadendrene / viridiflorene / trans-alpha-farnesene / alpha-humulene (alpha-caryophyllene) / alpha-guaiene / beta-selinine / alpha-selinene / gamma-muurolene / gamma-curcumene / alpha-ylangene / beta-elemene / alpha-cis-bergamotene / alpha-trans-bergamotene / alpha-cadinene / alpha-longipinene / alpha-copaene	20	terpenoid	Positive	59406
19	C15H24 O	220.1824	3.58	caryophyllene oxide	1	terpenoid	Positive	675281
20	C15H24 O	220.1825	3.67				Positive	495697
21	C15H24 O	220.1818	3.97				Positive	530399

*mass error < 5 ppm

**retention time

*** tentative identification of compounds was done based on available scientific article (Hanuš and col. 2016, Mechoulam 2002)

Table II - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 5-6)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Type of compounds	Ionization (mode polarity)	Peak area
19	C15H24 O	220.1824	3.58	caryophyllene oxide	1	terpenoid	Positive	675281
20	C15H24 O	220.1825	3.67				Positive	495697
21	C15H24 O	220.1818	3.97				Positive	530399
22	C16H16O4	272.1054	3.43	cannithrene-2	1	phenol	Positive	2259372
23	C16H16O4	272.1057	3.70				Positive	1229956
24	C16H16O4	272.1053	3.91				Positive	195533
25	C16H18O3	258.1251	3.48	3-O-methylbatatasin III	1	bibenzyl stilbene	Positive	384630
26	C16H18O3	258.1259	3.82				Positive	139771
27	C16H18O3	258.1257	3.34				Negative	93723
28	C16H18O3	258.1255	3.96				Negative	91797
29	C16H32O2	256.2410	6.40	palmitic acid	1	fatty acid	Positive	56302
30	C16H32O2	256.2401	7.23				Negative	465176
31	C17H18O5	302.1161	3.28	4.5-dihydroxy-2.5-dihydroxy-2.3.6-trimethoxy-9.10- dihydrophenanthrene	1	new identified compounds	Positive	24704971
32	C17H18O5	302.1161	3.65				Positive	175087
33	C17H18O5	302.1156	5.04				Negative	15866
34	C17H20O5	304.1314	3.12	cannabistilbene-Iia / cannabistilbene-Iib	2	phenol	Positive	1366396
35	C17H20O5	304.1317	3.65				Positive	1078851
36	C17H20O5	304.1312	9.99				Positive	185956
37	C17H20O5	304.1317	10.37				Positive	17877395
38	C17H20O5	304.1317	10.89				Positive	85751
39	C18H20O5	316.1318	3.37	4-hydroxy-2.3.6.7-tetramethoxy-9	1	new identified compounds	Positive	2714935
40	C18H20O5	316.1318	3.65				Positive	15067190
41	C18H28O2	276.2095	4.11	stearidonic acid	1	fatty acid	Positive	8824190
42	C18H28O2	276.2098	4.39				Positive	4051419
43	C18H28O2	276.2086	4.08				Negative	801084
44	C18H28O2	276.2087	5.71				Negative	264891

Table II - continuation: Overview of compounds detected in the sample ML844/18 (corresponding with the figure 5-6)

Compound number	Formula	Exact mass* (neutral, monoisotopical)	RT** (min)	Possible identity (compound name)***	Number of possible compounds	Type of compounds	Ionization (mode polarity)	Peak area
45	C18H30O2	278.2228	3.65	alpha-linolenic acid / gamma-linolenic acid / isolinolenic acid	3	fatty acid	Positive	1875356
46	C18H30O2	278.2243	4.37				Positive	1569449
47	C18H30O2	278.2256	5.45				Positive	542341
48	C18H30O2	278.2247	6.18				Negative	3351029
49	C18H32O2	280.2405	6.77	linoleic acid	1	fatty acid	Negative	5561744
50	C18H34O2	282.2561	6.48	cis-vaccenic acid / oleic acid	2	fatty acid	Positive	201768
51	C18H34O2	282.2559	7.43				Negative	1012287
52	C18H36O2	284.2712	8.23	stearic acid	1	fatty acid	Negative	172491
53	C20H18O5	338.1156	3.70	6-prenylapigenin	1	flavone	Negative	92924
54	C20H24O3	312.1731	3.54	cannabistilbene-I	1	phenol	Positive	374591
55	C20H24O3	312.1733	3.77				Positive	1566779
56	C20H24O3	312.1733	4.77				Positive	417635
57	C20H24O3	312.1727	4.06				Negative	196543
58	C20H24O3	312.1732	4.38				Negative	1199977
59	C20H24O3	312.1723	7.93				Negative	353652
60	C20H40O2	312.3020	9.16	arachidic acid / isoarachidic acid	2	fatty acid	Negative	51621
61	C21H20O6	368.1260	3.68	cannflavin B	1	flavonoid	Negative	2982899
62	C22H44O2	340.3337	9.96	behenic acid	1	fatty acid	Negative	47441
63	C23H32O4	372.2308	5.26	5-acetoxy-6-geranyl-3-n-pentyl-1.4-benzoquinone	1	new identified compounds	Positive	4975304
64	C23H32O4	372.2306	5.67				Positive	1183893
65	C23H32O4	372.2303	5.95				Positive	592742
66	C23H32O4	372.2296	8.41				Negative	336131
67	C24H48O2	368.3645	10.74	lignoceric acid	1	fatty acid	Negative	120628
68	C26H28O6	436.1886	4.57	cannflavin A / cannflavin C	2	flavonoid	Negative	12181495
69	C29H48 O	412.3702	9.67	stigmasterol	1	phytosterol	Positive	774150
70	C29H48 O	412.3709	9.90				Positive	19119634
71	C29H50 O	414.3873	10.26	beta-sitosterol	1	phytosterol	Positive	129368
72	C31H64	436.4996	3.71	hentriacontane	1	hydrocarbon	Positive	114883

*mass error < 5 ppm

** retention time

*** tentative identification of compounds was done based on available scientific article (Hanuš and col. 2016, Mechoulam 2002)