Appendix No. 1 – ML 4910/21

Records documenting analysis of the sample using U-HPLC-HRMS/MS metabolomic profiling (targeted screening) method

Sample description

Lab code	Sample name (provided by the client)	Sample description
ML 4910/21	Olejek konopny 30% CBD Dekoktum	Hemp oil

Testing strategy

Metabolomic profiling (targeted screening) strategy was selected for the testing of the sample (laboratory code ML 4910/21). This type of analytical approach is based on UCT internal databases of compounds which may occur in *Cannabis sativa* L. and products thereof; the first UCT database (A) includes molecular spectral information for 246 minor phytocannabinoids, the second UCT database (B) includes molecular spectral information for 151 other (non-cannabinoid) biologically active compounds (e.g. terpenoids, phenols, bibenzyl stilbenes, fatty acids, amides, flavones, lignans, flavonoid glycosides, lignanamide derivatives). The analysis of the given sample was performed by ultra-high performance liquid chromatography coupled to high resolution tandem mass spectrometry (ISO 17025 accredited method KM 15, system E: U-HPLC-HRMS/MS (Q-TOF)). Detailed description of analytical procedures and conditions (SOP) are available at Laboratory.

Testing conditions

Sample preparation consisted of sample dissolution in ethanol and following dilution. Subsequently, a reversed-phase chromatographic column was used for the compound's separation; quadrupole/time of flight mass analyzer (Agilent 6560 Q-TOF) with electrospray ionization source was used for their detection. Each sample was injected into U-HPLC – HRMS/MS system in several dilutions to overcome matrix effects including column and/or detector saturation for particular compounds. The data were recorded and evaluated separately for both the positive and negative electrospray ionization mode (ESI+ and ESI-). For the data processing, Agilent MassHunter Profinder and Agilent MassHunter Qualitative Analysis softwares were used.

Test results and interpretation

The overall chemical compositions of the sample detectable under given method conditions are illustrated by total compound chromatograms (TCC) (**Figure 1 - 2**) recorded in ESI+ and ESI- ionization mode. The TCC shows all features (compounds) detected in the sample, non-filtered by the UCT databases.

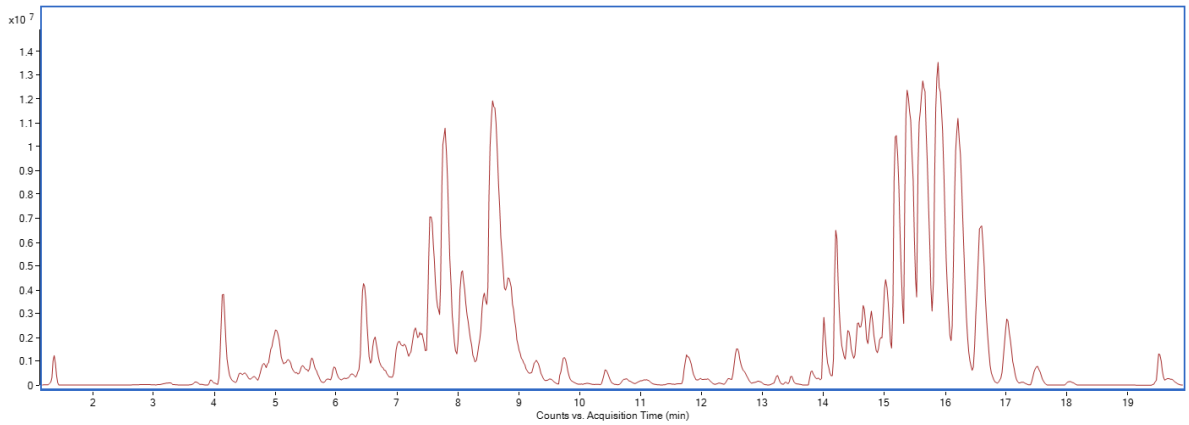

Figure 1: ML 4910/21 - UHPLC-HRMS/MS total compound chromatogram obtained for undiluted sample in ESI+

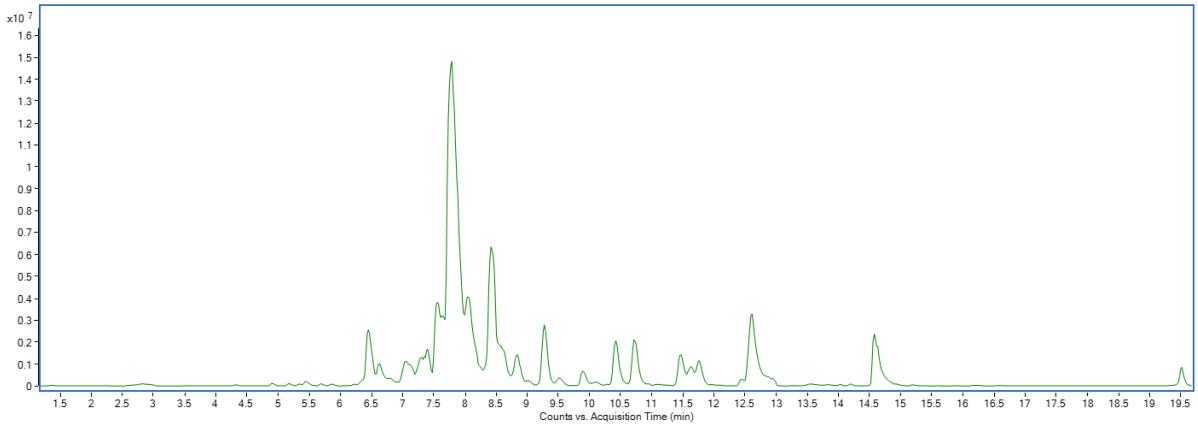

Figure 2: ML 4910/21 - UHPLC-HRMS/MS total compound chromatogram obtained for undiluted sample in ESI-

A) Targeted screening of phytocannabinoids

The following amounts of major phytocannabinoids (**Table I**) characterized by unique combination of exact mass and retention time RT, whose identities were confirmed by certified standards, were detected.

Table I: Number of major phytocannabinoids detected in the sample in ESI+ and ESI-

Sample name	Number of major phytocannabinoids detected in ESI+	Number of major phytocannabinoids detected in ESI-
ML 4910/21	5	8

Extracted ion chromatograms (XIC) of these compounds in both ionization modes (ESI+, ESI-) are documented on **Figures 3 – 4** and their overview is also summarized in **Table II**.

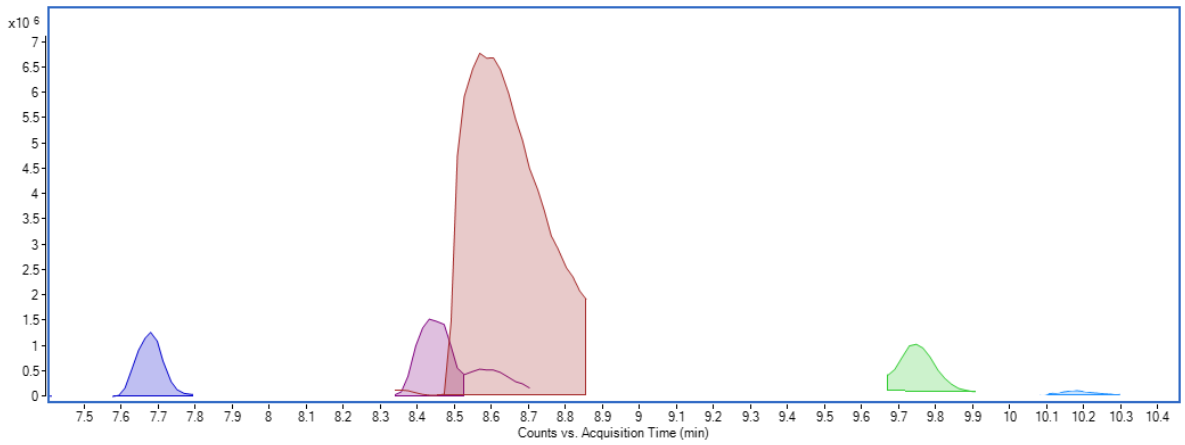

Figure 3: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of major phytocannabinoids detected in ESI+ (obtained for undiluted sample)

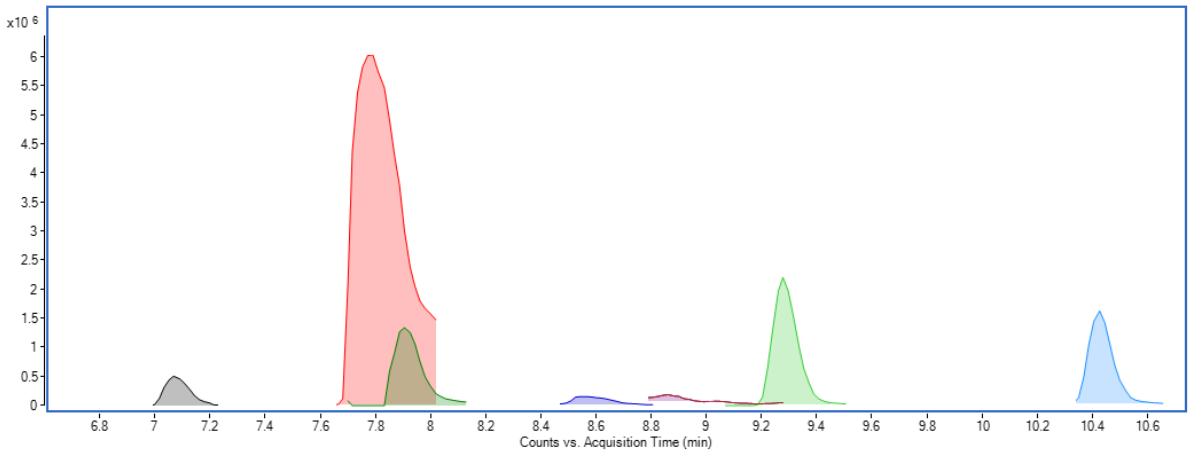

Figure 4: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of major phytocannabinoids detected in ESI- (obtained for undiluted sample)

Table II: Overview of major phytocannabinoids detected in ESI+ and ESI- (corresponding with the Figures 3 - 4)

Measured exact mass[a] (neutral, monoisotopical)	Elemental formula[b]	RT[c] (min)	Ionization mode	Identity (confirmed by certified standards)	Peak area[d]
330.1832	C20 H26 O4	7.08	ESI-	CBDVA	3.3E+06
286.1937	C19 H26 O2	7.67	ESI+	CBDV	1.1E+07
358.2143	C22 H30 O4	7.79	ESI-	CBDA	3.0E+08
360.2296	C22 H32 O4	7.91	ESI-	CBGA	8.1E+06
316.2398	C21 H32 O2	8.44	ESI+	CBG	2.0E+07
314.2252	C21 H30 O2	8.58	ESI+	CBD	1.3E+09
286.1930	C19 H26 O2	8.58	ESI-	THCV	3.8E+06
358.2143	C22 H30 O4	8.89	ESI-	Δ^9-THCA-A	1.0E+06
358.2141	C22 H30 O4	9.06	ESI-	CBLA	2.1E+05
310.1933	C21 H26 O2	9.28	ESI-	CBN	1.4E+07
314.2253	C21 H30 O2	9.74	ESI+	Δ^9-THC	6.7E+06
314.2251	C21 H30 O2	10.18	ESI+	CBL	4.6E+05
314.2248	C21 H30 O2	10.43	ESI-	CBC	9.6E+06

[a] *Mass error compared the theoretical exact mass < 5 ppm*
[b] *Match of isotopic pattern confirmed*
[c] *Retention time*
[d] *Peak area related to the undiluted sample prepared according to stated procedure*

The following amounts of minor phytocannabinoids (**Table III**) characterized by unique combination of exact mass *m/z* and retention time RT were detected.

Table III: Number of minor phytocannabinoids detected in the sample in ESI+ and ESI-

Sample name	Number of minor phytocannabinoids detected in ESI+	Number of minor phytocannabinoids detected in ESI-
ML 4910/21	16	48

Extracted ion chromatograms (XIC) of the detected compounds in both ionization modes (ESI+, ESI-) are documented on **Figures 5 - 6**. All detected phytocannabinoids (tentative identification) are also summarized in **Table IV** (ESI+) and **Table V** (ESI-). Considering the possible existence of isomeric forms, one detected compound may have several identities.

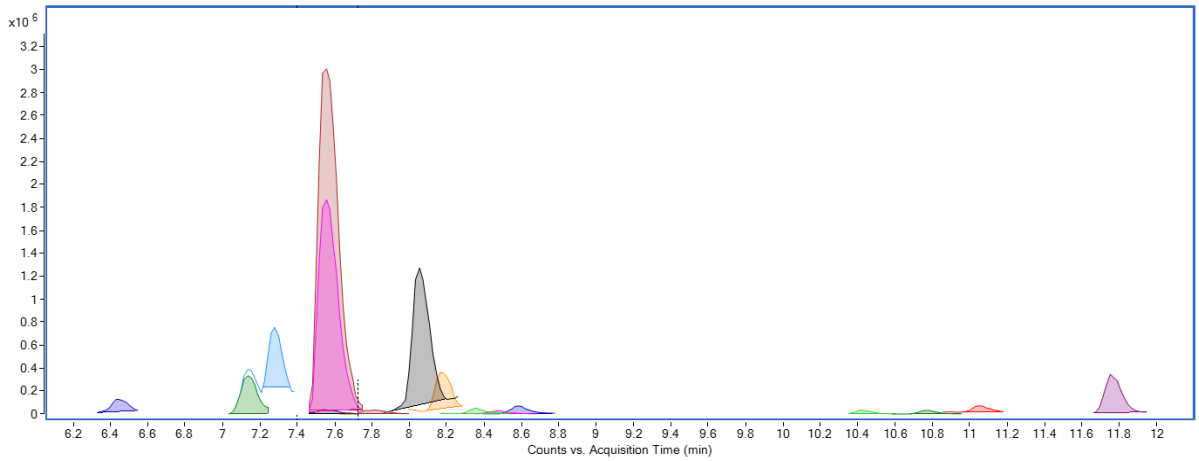

Figure 5: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of 16 compounds with unique combination of exact mass and RT detected in ESI+ (obtained for undiluted sample)

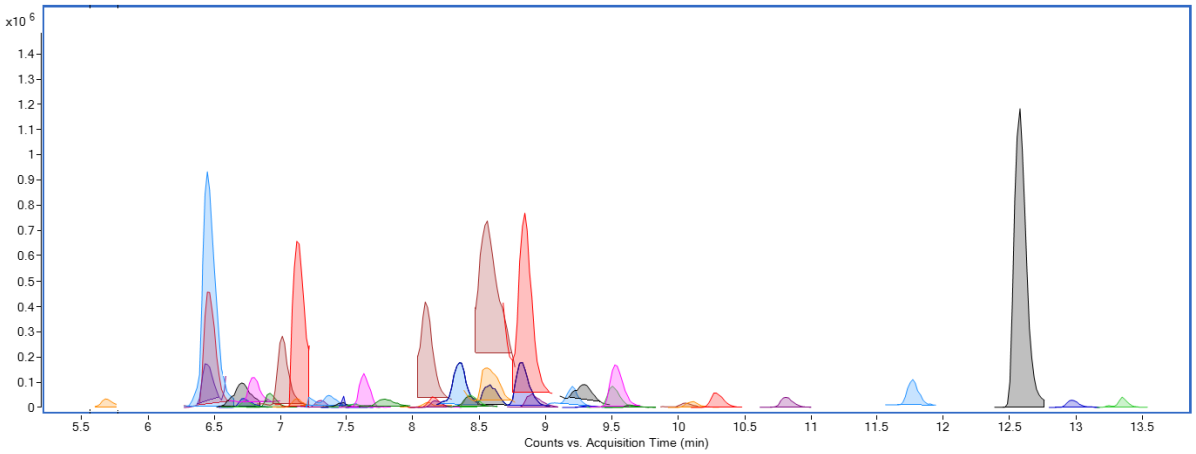

Figure 6: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of 48 compounds with unique combination of exact mass and RT detected in ESI- (obtained for undiluted sample)

Table IV: Overview of compounds detected in ESI+ (corresponding with the Figure 5)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Peak area[e]
1	346.2149	C21 H30 O4	6.43	Trans-10-ethoxy-9-hydroxy-delta6a(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-delta-6a(10a)-tetrahydrocannabinol)	8.7E+05
2	312.2091	C21 H28 O2	7.13	7.8-Dihydrocannabinol	2.1E+06
3	330.2200	C21 H30 O3	7.28	8'-Hydroxyisocannabichromene/ cannabielsoin/abnormal cannabigeroquinol/10alpha-hydroxy trans delta-8-tetrahydrocannabinol/10 beta-hydroxy trans delta-8-tetrahydrocannabinol/8 alpha-hydroxy-delta9-trans-tetrahydrocannabinol/8 beta-hydroxy-delta9-trans-tetrahydrocannabinol/tetrahydrocannabinol epoxide/hydroxy delta9.11-hexahydrocannabinol	3.0E+06
4	258.1622	C17 H22 O2	7.54	Cannabidiorcol/delta-9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	2.9E+05
5	314.2254	C21 H30 O2	7.55	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	3.6E+07
6	332.2357	C21 H32 O3	7.55	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	2.2E+07
7	436.1890	C26 H28 O6	7.81	Desmodianone A/desmodianone D/desmodianone E	3.3E+05
8	330.2203	C21 H30 O3	8.06	8'-Hydroxyisocannabichromene/ cannabielsoin/abnormal cannabigeroquinol/10alpha-hydroxy trans delta-8-tetrahydrocannabinol/10 beta-hydroxy trans delta-8-tetrahydrocannabinol/8 alpha-hydroxy-delta9-trans-tetrahydrocannabinol/8 beta-hydroxy-delta9-trans-tetrahydrocannabinol/tetrahydrocannabinol epoxide/hydroxy delta9.11-hexahydrocannabinol	8.7E+06
9	314.2247	C21 H30 O2	8.18	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	2.2E+06
10	346.2147	C21 H30 O4	8.36	Trans-10-ethoxy-9-hydroxy-delta6a(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-delta-6a(10a)-tetrahydrocannabinol)	2.6E+05

Table IV - continuation: Overview of compounds detected in ESI+ (corresponding with the Figure 5)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Peak area[e]
11	286.1935	C19 H26 O2	8.49	(delta)-?7 -trans-(1R. 3R. 6R)-isotetrahydrocannabivarin-C3 (?7-trans-Isotetrahydrocannabivarin)/(1aS.3aR.8bR.8cR)-Cannabicyclovarin/Cannabivarichromene ((RS)-Cannabichromevarin)/delta-9-trans-tetrahydrocannabivarin/2-Methyl-2-(4-methyl-2-pentenyl)-7-propyl-2H-1-benzopyran-5-ol/delta7-1.2-cis-(1R.3R.6S)-Isotetrahydrocannabivarin-C3 (?7-cis-Isotetrahydrocannabivarin)/delta7-1.2-cis-(1S.3S.6R)-Isotetrahydrocannabivarin-C3/delta 9-cis-Tetrahydrocannabidivarin	1.6E+05
12	258.1622	C17 H22 O2	8.59	Cannabidiorcol/delta-9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	5.0E+05
13	258.1622	C17 H22 O2	10.42	Cannabidiorcol/delta-9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	2.1E+05
14	330.2559	C22 H34 O2	10.77	O-Methylcannabigerol	2.1E+05
15	314.2252	C21 H30 O2	11.05	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	4.9E+05
16	314.2250	C21 H30 O2	11.75	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	2.1E+06

[a] *Mass error compared the theoretical exact mass < 5 ppm*

[b] *Match of isotopic pattern confirmed*

[c] *Retention time*

[d] *Tentative identification of compounds based on available scientific articles (Hanuš et al. 2016, Mechoulam 2002); possible identities are separated by the symbol "/"*

[e] *Peak area related to the undiluted sample prepared according to stated procedure*

Table V: Overview of compounds detected in ESI- (corresponding with the Figure 6)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Peak area[e]
1	330.1822	C20 H26 O4	5.69	Cannabichromevarinic acid/delta-9-tetrahydrocannabivarinic acid	1.7E+05
2	282.1617	C19 H22 O2	6.46	Cannabinodivarin/cannabivarin/demethyldecarboxyamorfrutin A/63b/63c	2.8E+06
3	328.2036	C21 H28 O3	6.46	Cannabichromanone-D/cannabicoumaronone/10-oxo-delta-6a(10a)-tetrahydrocannabinol/8-Oxo-delta9-trans-tetrahydrocannabinol/9.10-Anhydrocannabitriol/anhydrocannabimovone/Cannabidiol Hydroxyquinone	9.1E+05
4	374.2091	C22 H30 O5	6.47	Cannabielsoic acid A/cannabielsoic acid B	6.2E+06
5	332.2344	C21 H32 O3	6.71	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	9.2E+05
6	294.1616	C20 H22 O2	6.73	Radulanin J	2.5E+05
7	304.2032	C19 H28 O3	6.74	Cannabiglendol C3	1.4E+05
8	348.2293	C21 H32 O4	6.81	Cannabiripsol	5.8E+05
9	258.1619	C17 H22 O2	6.93	Cannabidiorcol/delta-9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	3.1E+05
10	374.2092	C22 H30 O5	7.02	Cannabielsoic acid A/cannabielsoic acid B	1.5E+06
11	358.2138	C22 H30 O4	7.14	Ferruginene A/ferruginene B/delta-9-tetrahydrocannabinolic acid B/delta-8-tetrahydrocannabinolic acid	2.0E+05
12	330.2188	C21 H30 O3	7.15	8'-Hydroxyisocannabichromene/ cannabielsoin/abnormal cannabigeroquinol/10alpha-hydroxy trans delta-8-tetrahydrocannabinol/10 beta-hydroxy trans delta-8-tetrahydrocannabinol/8 alpha-hydroxy-delta9-trans-tetrahydrocannabinol/8 beta-hydroxy-delta9-trans-tetrahydrocannabinol/tetrahydrocannabinol epoxide/hydroxy delta9.11-hexahydrocannabinol	3.9E+06
13	362.1891	C24 H26 O3	7.32	Machaeridiol C/machaeriol B	1.6E+05
14	348.2290	C21 H32 O4	7.38	Cannabiripsol	2.5E+05
15	318.1829	C19 H26 O4	7.49	(9S.10S)-trans-Cannabitriol-C3/(9R.10R)-trans-cannabitriol-C3	8.1E+04
16	332.1989	C20 H28 O4	7.50	Cannabichromanone/cannabigerovarinic acid	7.4E+04
17	350.2237	C24 H30 O2	7.56	Heli-cannabigerol/63f	5.9E+04
18	310.1929	C21 H26 O2	7.64	Cannabinodiol/cannabifuran	7.3E+05
19	314.2245	C21 H30 O2	7.79	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	8.6E+05
20	300.2083	C20 H28 O2	8.10	delta-9-Tetrahydrocannabinol-C4/norCannabidiol	2.3E+06

Table V - continuation: Overview of compounds detected in ESI- (corresponding with the Figure 6)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Peak area[e]
21	316.2394	C21 H32 O2	8.10	Cannabinerol/abnormal cannabigerol/hexahydrocannabinol	1.3E+05
22	282.1618	C19 H22 O2	8.15	Cannabinodivarin/cannabivarin/demethyldecarboxyamorfrutin A/63b/63c	2.3E+05
23	258.1617	C17 H22 O2	8.17	Cannabidiorcol/delta-9-trans-tetrahydrocannabiorcol/cannabiorcitran/cannabiorcicyclol/cannabiorcichromene	1.7E+05
24	332.2345	C21 H32 O3	8.37	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	1.1E+06
25	308.1774	C21 H24 O2	8.44	Dehydrocannabifuran	3.4E+05
26	348.2288	C21 H32 O4	8.44	Cannabiripsol	3.2E+05
27	288.2081	C19 H28 O2	8.45	Cannabigerovarin	2.6E+05
28	358.2145	C22 H30 O4	8.57	Ferruginene A/ferruginene B/delta-9-tetrahydrocannabinolic acid B/delta-8-tetrahydrocannabinolic acid	4.2E+06
29	346.2141	C21 H30 O4	8.58	Trans-10-ethoxy-9-hydroxy-delta6a(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-delta-6a(10a)-tetrahydrocannabinol)	3.7E+06
30	332.2346	C21 H32 O3	8.59	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	6.1E+05
31	332.2347	C21 H32 O3	8.84	rac-6'-Epoxycannabigerol (2'S*. 3'R*)/rac-6'-epoxycannabigerol (2'R*. 3'R*)/(-)-7-Hydroxycannabichromane	1.2E+06
32	316.2401	C21 H32 O2	8.85	Cannabinerol/abnormal cannabigerol/hexahydrocannabinol	4.5E+06
33	372.2297	C23 H32 O4	8.90	(+/-)-4-Acetoxycannabichromene/acetyl cannabigeroquinol/7.8-dehydro-10-O-ethylcannabitriol/	3.9E+05
34	286.1929	C19 H26 O2	9.20	(delta)-7 -trans-(1R. 3R. 6R)-isotetrahydrocannabivarin-C3 (?7-trans-Isotetrahydrocannabivarin)/(1aS.3aR.8bR.8cR)-Cannabicyclovarin/Cannabivarichromene ((RS)-Cannabichromevarin)/delta-9-trans-tetrahydrocannabivarin/2-Methyl-2-(4-methyl-2-pentenyl)-7-propyl-2H-1-benzopyran-5-ol/delta7-1.2-cis-(1R.3R.6S)-Isotetrahydrocannabivarin-C3 (?7-cis-Isotetrahydrocannabivarin)/delta7-1.2-cis-(1S.3S.6R)-Isotetrahydrocannabivarin-C3/delta 9-cis-Tetrahydrocannabidivarin	4.9E+05
35	316.2390	C21 H32 O2	9.30	Cannabinerol/abnormal cannabigerol/hexahydrocannabinol	8.2E+05
36	268.1467	C18 H20 O2	9.31	Cannabinol-C2/56a/63a	5.5E+04

Table V - continuation: Overview of compounds detected in ESI- (corresponding with the Figure 6)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Peak area[e]
37	314.2241	C21 H30 O2	9.43	Cannabicitran/(-)-delta9-cis-(6aS.10aR)-delta9-tetrahydrocannabinol/(â')-delta7 -trans-(1R. 3R. 6R)-isotetrahydrocannabinol-C5/cannabigeroquinone	9.7E+05
38	342.2190	C22 H30 O3	9.51	Ferruginene C/2-formyl-delta9-trans-tetrahydrocannabinol	5.5E+05
39	328.2037	C21 H28 O3	9.53	Cannabichromanone-D/ cannabicoumaronone/10-oxo-delta-6a(10a)-tetrahydrocannabinol/8-Oxo-delta9-trans-tetrahydrocannabinol/9.10-Anhydrocannabitriol/anhydrocannabimovone/Cannabidiol Hydroxyquinone	1.2E+06
40	342.2545	C23 H34 O2	9.64	(-)-trans-9-tetrahydrocannabiphorol/cannabidiphorol	6.3E+04
41	330.2192	C21 H30 O3	10.06	8'-Hydroxyisocannabichromene/ cannabielsoin/abnormal cannabigeroquinol/10alpha-hydroxy trans delta-8-tetrahydrocannabinol/10 beta-hydroxy trans delta-8-tetrahydrocannabinol/8 alpha-hydroxy-delta9-trans-tetrahydrocannabinol/8 beta-hydroxy-delta9-trans-tetrahydrocannabinol/tetrahydrocannabinol epoxide/hydroxy delta9.11-hexahydrocannabinol	1.0E+05
42	372.2295	C23 H32 O4	10.11	(+/-)-4-Acetoxycannabichromene/acetyl cannabigeroquinol/7.8-dehydro-10-O-ethylcannabitriol/	1.6E+05
43	384.3021	C26 H40 O2	10.29	Sesquicannabigerol/O-propylcannabidiol/O-pentyl-delta9-trans-tetrahydrocannabinol	4.0E+05
44	384.3019	C26 H40 O2	10.81	Sesquicannabigerol/O-propylcannabidiol/O-pentyl-delta9-trans-tetrahydrocannabinol	2.6E+05
45	358.2140	C22 H30 O4	11.75	Ferruginene A/ferruginene B/delta-9-tetrahydrocannabinolic acid B/delta-8-tetrahydrocannabinolic acid	5.8E+05
46	640.4486	C43 H60 O4	12.57	Cannabisol	7.5E+06
47	686.4178	C43 H58 O7	12.98	cannabidiolic acid tetrahydrocannabitriol ester	1.7E+05
48	494.3386	C32 H46 O4	13.35	beta-Fenchyl delta 9 -tetrahydrocannabinolate/epi-bornyl delta 9 -tetrahydrocannabinolate/alpha -terpenyl delta 9 -tetrahydrocannabinolate/4-terpenyl delta 9 -tetrahydrocannabinolate/bornyl delta 9 -tetrahydrocannabinolate/alpha -fenchyl delta 9 -tetrahydrocannabinolate	1.9E+05

[a] *Mass error compared the theoretical exact mass < 5 ppm*

[b] *Match of isotopic pattern confirmed*

[c] *Retention time*

[d] *Tentative identification of compounds based on available scientific articles (Hanuš et al. 2016, Mechoulam 2002); possible identities are separated by the symbol "/"*

[e] *Peak area related to the undiluted sample prepared according to stated procedure*

B) Targeted screening of other (non-cannabinoid) biologically active compounds

In the tested samples, the following amounts of other (non-cannabinoid) biologically active compounds (**Table VI**) characterized by unique combination of exact mass and retention time RT were detected.

Table VI: Number of other biologically active compounds detected in the sample in ESI+ and ESI-

Sample name	Number of other biologically active compounds detected in ESI+	Number of other biologically active compounds detected in ESI-
ML 4910/21	9	20

Extracted ion chromatograms (XIC) of the detected compounds in both ionization modes (ESI+, ESI-) are documented on **Figures 7 - 8**. All detected non-cannabinoid biologically active compounds (tentative identification) are also summarized in **Table VII** (ESI+) and **Table VIII** (ESI-). Considering the possible existence of isomeric forms, one detected compound may have several identities.

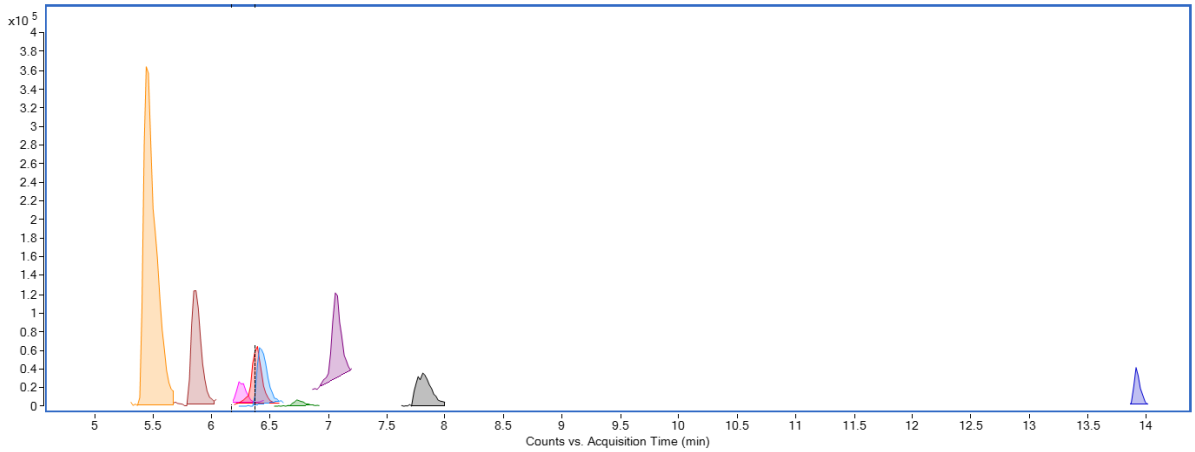

Figure 7: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of 9 compound with unique combination of exact mass and RT detected in ESI+ (obtained for undiluted sample)

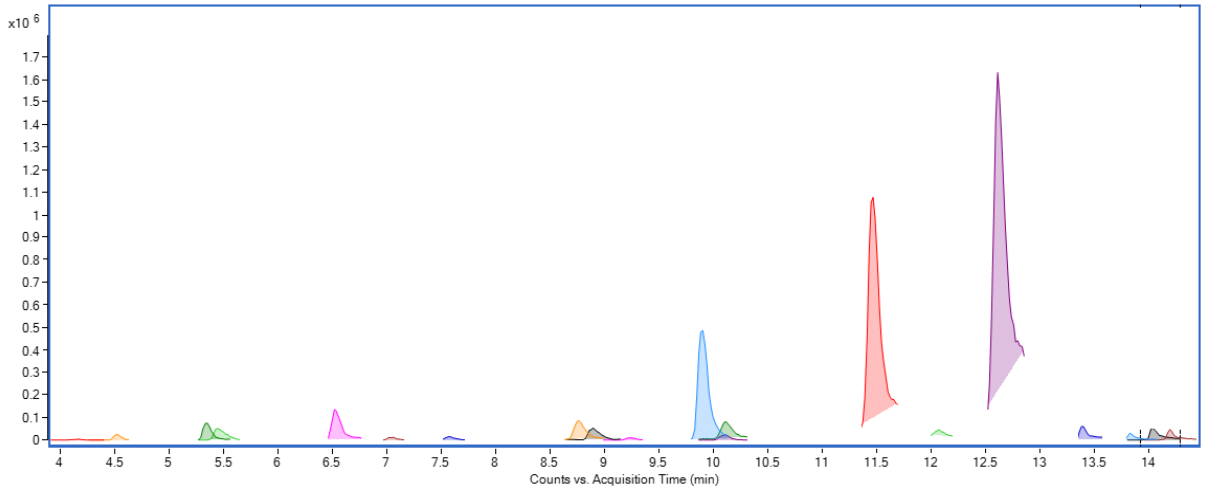

Figure 8: ML 4910/21 - UHPLC-HRMS/MS extracted ion chromatogram of 20 compounds with unique combination of exact mass and RT detected in ESI- (obtained for undiluted sample)

Table VII: Overview of compounds detected in ESI+ (corresponding with the Figure 7)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Compound group	Peak area[e]
1	302.1158	C17 H18 O5	5.49	4.5-dihydroxy-2.5-dihydroxy-2.3.6-trimethoxy-9.10-dihydrophenanthrene	new non-cannabinoid constituent[f]	2.6E+06
2	272.1054	C16 H16 O4	5.86	cannithrene-2	phenol	7.4E+05
3	220.1820	C15 H24 O	6.25	caryophyllene oxide	terpenoid	1.3E+05
4	316.1315	C18 H20 O5	6.39	4-hydroxy-2.3.6.7-tetramethoxy-9	new non-cannabinoid constituent[f]	3.6E+05
5	368.1266	C21 H20 O6	6.42	cannflavin / isocannflavin B	flavonoid	4.2E+05
6	222.1985	C15 H26 O	6.73	guajol / trans-nerolidol / gamma-eudesmol / beta-eudesmol / alpha-eudesmol / epi-alpha-bisabolol	terpenoid	5.0E+04
7	312.1740	C20 H24 O3	7.06	cannabistilbene-I	phenol	5.4E+05
8	436.1890	C26 H28 O6	7.81	cannflavin A / cannflavin C	flavonoid	3.3E+05
9	412.3701	C29 H48 O	13.91	stigmasterol	phytosterol	1.4E+05

[a] *Mass error compared the theoretical exact mass < 5 ppm*
[b] *Match of isotopic pattern confirmed*
[c] *Retention time*
[d] *Possible identities are separated by the symbol "/"*
[e] *Peak area related to the undiluted sample prepared according to stated procedure*
[f] *Mohamed M. Radwan et al. 2008*

Table VIII: Overview of compounds detected in ESI- (corresponding with the Figure 8)

Cmp. number	Measured exact mass[a] (neutral, monoisotopical)	Estimated elemental formula[b]	RT[c] (min)	Tentative identity (name of possible compounds)[d]	Compound group	Peak area[e]
1	188.1048	C9 H16 O4	4.15	azealic acid	fatty acid	1.5E+05
2	242.0941	C15 H14 O3	4.51	isocannabispiradienone / cannithrene-1	phenol	1.3E+05
3	246.1255	C15 H18 O3	5.33	cannabispiran / isocannabispiran	phenol	4.3E+05
4	242.0940	C15 H14 O3	5.48	isocannabispiradienone / cannithrene-1	phenol	4.0E+05
5	144.1151	C8 H16 O2	6.52	caprylic acid	fatty acid	4.2E+05
6	158.1307	C9 H18 O2	7.04	pelargonic acid	fatty acid	6.5E+05
7	172.1463	C10 H20 O2	7.58	capric acid	fatty acid	4.0E+05
8	200.1777	C12 H24 O2	8.76	lauric acid	fatty acid	8.9E+05
9	372.2296	C23 H32 O4	8.90	5-acetoxy-6-geranyl-3-n-pentyl-1.4-benzoquinone	new non-cannabinoid constituent[f]	3.9E+05
10	276.2084	C18 H28 O2	9.24	stearidonic acid	fatty acid	6.1E+04
11	278.2248	C18 H30 O2	9.90	alpha-linolenic acid / gamma-linolenic acid / isolinolenic acid	fatty acid	3.5E+06
12	372.2294	C23 H32 O4	10.10	5-acetoxy-6-geranyl-3-n-pentyl-1.4-benzoquinone	new non-cannabinoid constituent[f]	1.6E+05
13	228.2089	C14 H28 O2	10.11	myristic acid	fatty acid	8.9E+04
14	256.2405	C16 H32 O2	11.46	palmitic acid	fatty acid	6.8E+07
15	270.2557	C17 H34 O2	12.06	margaric acid	fatty acid	5.4E+04
16	284.2719	C18 H36 O2	12.61	stearic acid	fatty acid	1.0E+08
17	312.3024	C20 H40 O2	13.39	arachidic acid / isoarachidic acid	fatty acid	4.6E+04
18	340.3335	C22 H44 O2	13.83	behenic acid	fatty acid	2.0E+05
19	414.3849	C29 H50 O	14.04	beta-sitosterol	phytosterol	3.1E+04
20	368.3647	C24 H48 O2	14.20	lignoceric acid	fatty acid	9.4E+04

[a] *Mass error compared the theoretical exact mass < 5 ppm*
[b] *Match of isotopic pattern confirmed*
[c] *Retention time*
[d] *Possible identities are separated by the symbol "/"*
[e] *Peak area related to the undiluted sample prepared according to stated procedure*
[f] *Mohamed M. Radwan et al. 2008*

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End of the appendix

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