

Date : September 20, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22114-PTH01


Customer identification : Patchouli - Indonesia - P20111R

Type : Essential oil

Source : *Pogostemon cablin*

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Amélie Simard, Analyste

Analysis date : September 19, 2022

Checked and approved by :

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Orange yellow liquid

Refractive index: 1.5091 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
5-Methyl-2-hexanone	0.01	Aliphatic ketone
α -Pinene	0.10	Monoterpene
Camphene	0.01	Monoterpene
Sabinene	tr	Monoterpene
β -Pinene	0.23	Monoterpene
Octen-3-ol	0.01	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
Myrcene	0.01	Monoterpene
Octan-3-ol	0.01	Aliphatic alcohol
Limonene	0.03	Monoterpene
Terpinolene	0.01	Monoterpene
Linalool	0.01	Monoterpenic alcohol
α -Terpineol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
δ -Elemene	0.14	Sesquiterpene
α -Copaene	0.01	Sesquiterpene
β -Patchoulene	2.57	Sesquiterpene
β -Bourbonene	0.01	Sesquiterpene
<i>cis</i> - β -Elemene	0.06	Sesquiterpene
β -Elemene	0.97	Sesquiterpene
Isocaryophyllene	0.03	Sesquiterpene
Cycloseychellene	0.40	Sesquiterpene
β -Caryophyllene	3.16	Sesquiterpene
Seychellene	6.20	Sesquiterpene
α -Guaiene	13.42	Sesquiterpene
Unknown	0.08	Sesquiterpene
Selina-5,11-diene	0.06	Sesquiterpene
α -Humulene	0.58	Sesquiterpene
α -Patchoulene	4.70	Sesquiterpene
Patchoulene analog I	1.77	Sesquiterpene
γ -Patchoulene	1.00	Sesquiterpene
9-epi- β -Caryophyllene	0.02	Sesquiterpene
Unknown	0.40	Sesquiterpene
Selina-4,11-diene	0.02	Sesquiterpene
Unknown	0.55	Sesquiterpene
β -Selinene	0.12	Sesquiterpene
Patchoulene analog II	0.01	Sesquiterpene
Unknown	0.39	Sesquiterpene
δ -Selinene	0.01	Sesquiterpene
Unknown	0.25	Sesquiterpene
α -Selinene	0.12	Sesquiterpene
Eudesma-2,4(15),11-triene	0.12	Sesquiterpene
Aciphyllene	2.87	Sesquiterpene
Pentadecane	0.30	Alkane
δ -Guaiene	16.70	Sesquiterpene

γ-Cadinene	0.46	Sesquiterpene
Nootkatene	0.02	Sesquiterpene
7-epi-α-Selinene	0.14	Sesquiterpene
Unknown	0.08	Sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.01	Sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Norpatchoulénol	0.64	Norsesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.32	Oxygenated sesquiterpene
Caryophyllene oxide isomer	0.07	Sesquiterpenic ether
Unknown	0.05	Oxygenated sesquiterpene
Caryophyllene oxide	0.36	Sesquiterpenic ether
Unknown	0.42	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Humulene epoxide II	0.05	Sesquiterpenic ether
Hexadecane	0.06	Alkane
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.23	Oxygenated sesquiterpene
Unknown	0.25	Oxygenated sesquiterpene
Unknown	0.63	Oxygenated sesquiterpene
Caryophylladiénol II	0.20	Sesquiterpenic alcohol
Hinesol	0.29	Sesquiterpenic alcohol
Pogostol	2.04	Sesquiterpenic alcohol
Patchoulol	28.62	Sesquiterpenic alcohol
Unknown	0.40	Oxygenated sesquiterpene
Unknown	0.14	Oxygenated sesquiterpene
Unknown	0.24	Oxygenated sesquiterpene
Unknown	0.07	Unknown
Unknown	0.04	Oxygenated sesquiterpene
Rotundone	0.20	Sesquiterpenic ketone
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
Pogostone	0.79	Terpenic lactone
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.15	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.15	Oxygenated sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Corymbolone analog	0.02	Sesquiterpenic alcohol

Corymbolone	0.05	Sesquiterpenic alcohol
Phytol	0.04	Diterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Consolidated total	96.33%	

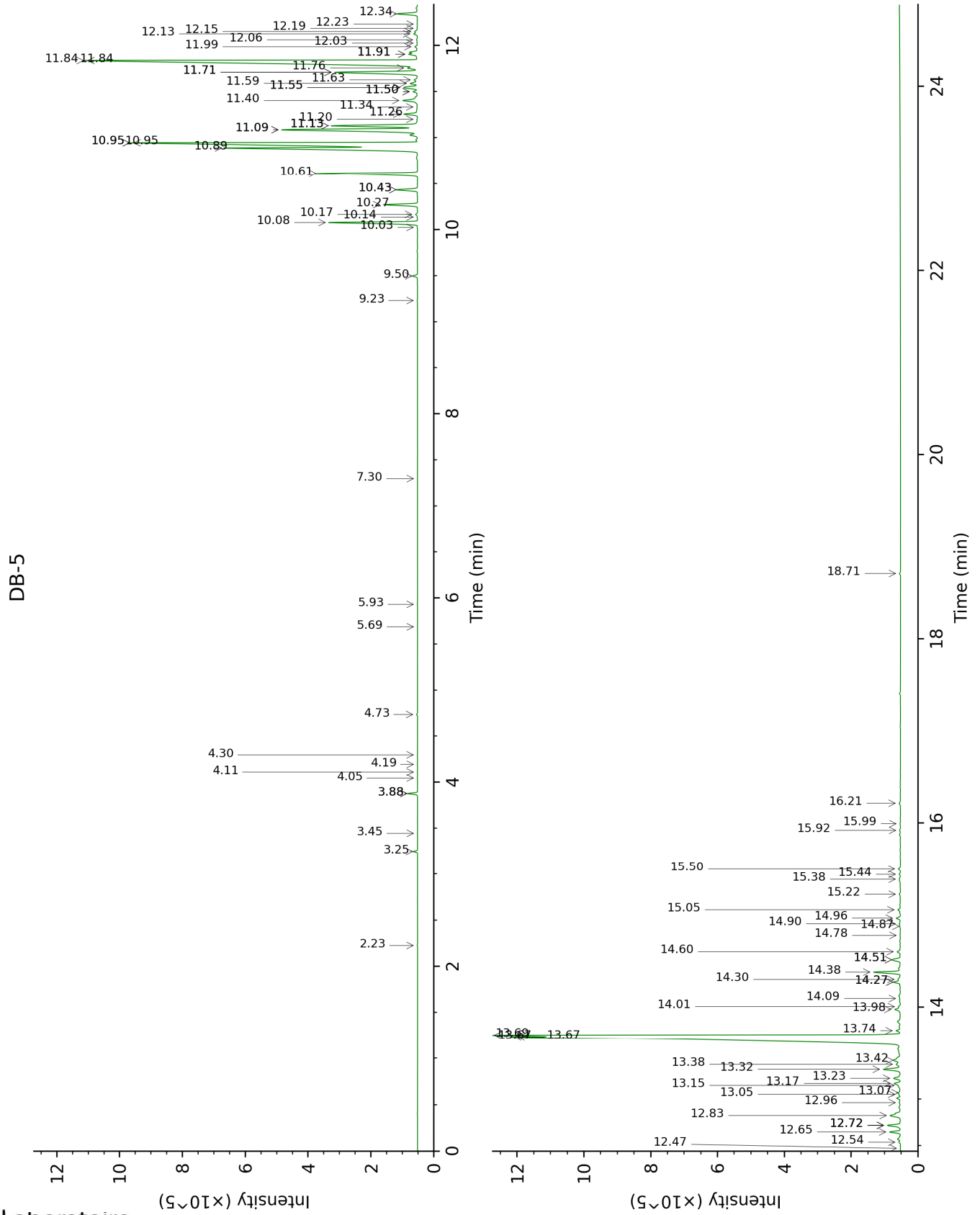
tr: The compound has been detected below 0.005% of total signal.

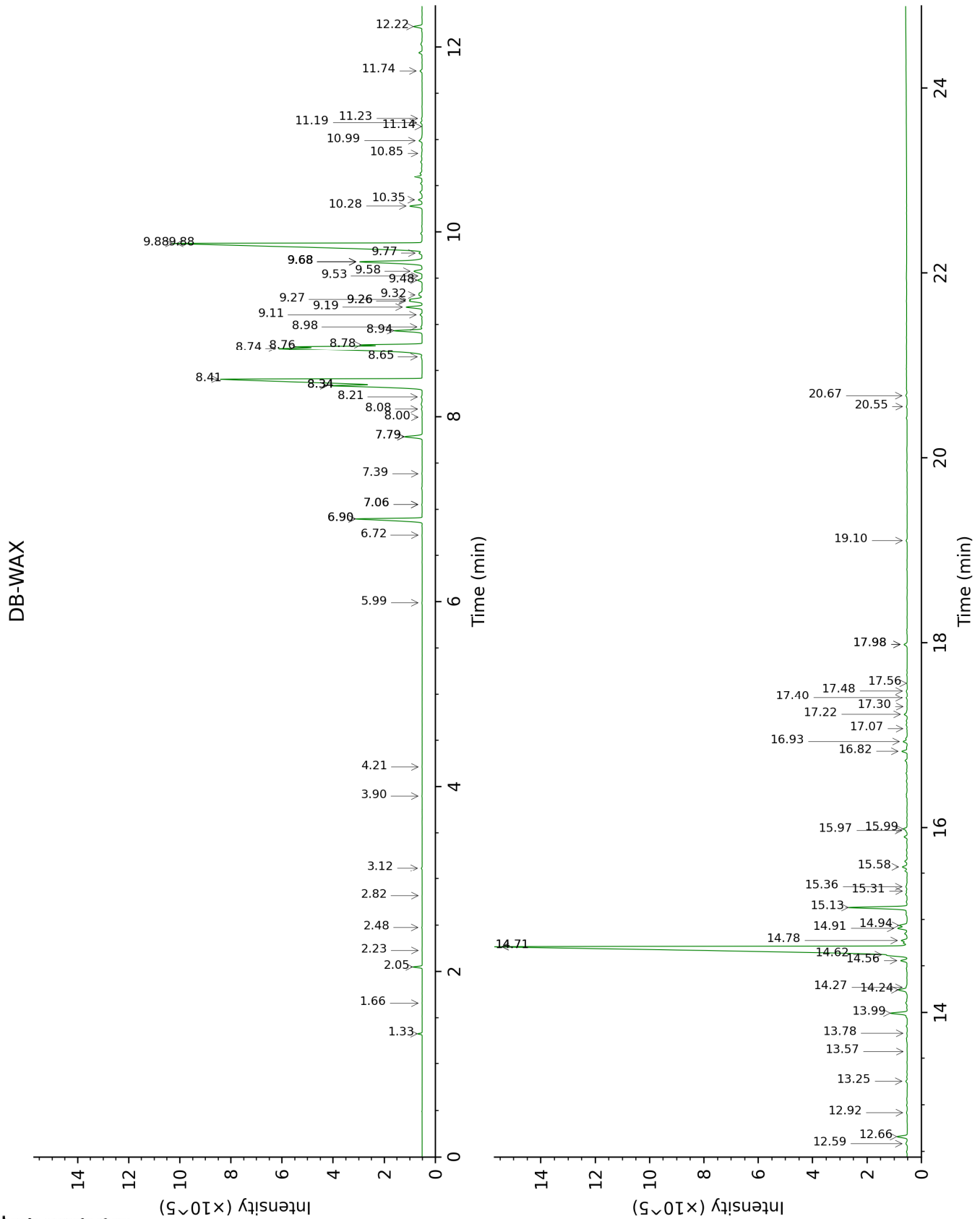
Note: no correction factor was applied

About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

Unknowns: Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
5-Methyl-2-hexanone	2.23	854	0.01	2.48	1106	0.01
α-Pinene	3.25	931	0.10	1.33	993	0.10
Camphene	3.45	944	0.01	1.66	1027	tr
Sabinene	3.88*	972	0.24	2.23	1084	tr
β-Pinene	3.88*	972	[0.24]	2.05	1066	0.23
Octen-3-ol	4.05	983	0.01	6.72	1422	0.01
Octan-3-one	4.11	987	0.01	3.90	1216	0.01
Myrcene	4.19	993	0.01	2.82	1133	tr
Octan-3-ol	4.30	1000	0.01	5.99	1368	0.01
Limonene	4.73	1027	0.03	3.12	1157	0.03
Terpinolene	5.69	1087	0.01	4.21	1239	0.01
Linalool	5.93	1102	0.01	8.00	1518	0.01
α-Terpineol	7.30	1189	0.01	9.68*	1651	2.92
Unknown [m/z 159, 117 (68), 132 (55), 200 (35)]	9.23	1316	0.01	7.06*	1447	0.02
δ-Elemene	9.50	1335	0.14	6.90*	1435	2.73
α-Copaene	10.02	1372	0.01	7.06*	1447	[0.02]
β-Patchoulene	10.08	1376	2.57	6.90*	1435	[2.73]
β-Bourbonene	10.14	1380	0.01	7.39	1471	0.01
cis-β-Elemene	10.17	1382	0.06	8.22	1535	0.04
β-Elemene	10.27	1390	0.97	8.34*†	1544	17.55
Isocaryophyllene	10.43*	1401	0.63	8.08	1524	0.03
Cycloseychellene	10.43*	1401	[0.63]	7.79*	1501	0.70
β-Caryophyllene	10.61	1414	3.16	8.34*†	1544	[17.55]
Seychellene	10.89†	1435	19.75	8.74†	1576	13.12
α-Guaiene	10.95*†	1439	[19.75]	8.41†	1550	[17.55]
Unknown [m/z 91, 93 (98), 79 (82), 81 (82), 105 (71), 107 (70)... 204 (38)]	10.95*†	1439	[19.75]	9.11	1604	0.08
Selina-5,11-diene	10.95*†	1439	[19.75]	8.65	1568	0.06
α-Humulene	11.09*	1450	5.28	9.19	1611	0.58
α-Patchoulene	11.09*	1450	[5.28]	8.76†	1577	[13.12]
Patchoulene analog I	11.13*	1453	2.77	8.78†	1579	[13.12]
γ-Patchoulene	11.13*	1453	[2.77]	8.94	1591	1.00
9-epi-β-Caryophyllene	11.20	1458	0.02	9.27†	1618	[1.06]
Unknown [m/z 159, 91 (88), 93 (72), 79 (69), 105 (68), 41 (66), 81 (54), 202? (50)...]	11.26	1462	0.40	9.26*†	1617	1.06
Selina-4,11-diene	11.34	1468	0.02	9.32†	1622	[1.06]

Unknown [m/z 147, 93 (87), 107 (77), 105 (77), 91 (73), 79 (63)... 204 (21)]	11.40	1474	0.55	9.26*†	1617	[1.06]
β-Selinene	11.50*	1481	0.13	9.77	1658	0.12
Patchoulene analog II	11.50*	1481	[0.13]	9.68*	1651	[2.92]
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.55*	1484	0.54	9.58	1643	0.39
δ-Selinene	11.55*	1484	[0.54]	9.53	1638	0.01
Unknown [m/z 161, 189 (96), 91 (74), 204 (73), 105 (69), 41 (52)]	11.59	1487	0.25	9.68*	1651	[2.92]
α-Selinene	11.63	1490	0.12	9.88*	1667	17.61
Eudesma-2,4(15),11-triene	11.71*	1496	2.99	10.99	1760	0.12
Aciphyllene	11.71*	1496	[2.99]	9.68*	1651	[2.92]
Pentadecane	11.76	1500	0.30	7.79*	1501	[0.70]
δ-Guaiene	11.84*	1506	17.16	9.88*	1667	[17.61]
γ-Cadinene	11.84*	1506	[17.16]	10.28	1700	0.46
Nootkatene	11.91*	1511	0.29	10.85	1749	0.02
7-epi-α-Selinene	11.91*	1511	[0.29]	10.35	1706	0.14
Unknown [m/z 159, 91 (81), 117 (68), 131 (51), 105 (46)... 202 (37)]	11.99	1518	0.08	9.48	1635	0.18
Unknown [m/z 41, 67 (95), 93 (92), 107 (91), 55 (77), 81 (77), 79 (73)... 205 (17)...]	12.03	1521	0.02	11.23	1781	0.03
Unknown [m/z 161, 119 (92), 91 (69), 105 (52), 145 (49)... 218 (6)]	12.06	1523	0.04	11.19	1777	0.06
Unknown [m/z 91, 105 (98), 108 (83), 93 (82), 133 (79), 77 (64), 79 (57), 41 (56), 145 (55)... 218? (5)]	12.13	1528	0.12			
Unknown [m/z 91, 105 (78), 93 (77), 107 (71), 79 (64), 41 (63), 77 (63), 145 (60)... 218 (17)]	12.15	1530	0.09			

Unknown [m/z 133, 105 (70), 146 (69), 145 (61), 91 (55), 131 (45), 187 (42), 159 (39), 119 (33), 202 (30)...]	12.19	1533	0.01	11.14	1773	0.01
Unknown [m/z 145, 131 (91), 91 (86), 105 (68), 146 (66), 43 (54)... 220? (5)]	12.23	1537	0.02			
Norpatchoulénol	12.34	1545	0.64	13.99	2031	0.61
Unknown [m/z 191, 159 (66), 133 (53), 91 (45), 41 (42), 177 (35), 105 (33), 220 (32)]	12.47	1556	0.02	13.57	1991	0.01
Unknown [m/z 41, 67 (90), 55 (87), 79 (85), 107 (84), 81 (84), 93 (84), 121 (77), 91 (74)... 220 (7)]	12.54	1561	0.06			
Unknown [m/z 43, 107 (94), 81 (71), 41 (63), 67 (58), 111 (58), 93 (55), 83 (54)... 205 (8), 220 (1)]	12.65	1569	0.32	12.22	1868	0.30
Caryophyllène oxide isomer	12.72*	1575	0.45	12.59	1902	0.07
Unknown isomer	12.72*	1575	[0.45]	14.27	2058	0.05
Caryophyllène oxide	12.72*	1575	[0.45]	12.66	1909	0.36
Unknown [m/z 43, 79 (44), 81 (41), 93 (40), 91 (40)... 220 (5)]	12.83	1583	0.42	14.24	2055	0.40
Unknown [m/z 43, 105 (77), 91 (71), 93 (68), 41 (62), 107 (6)... 205 (41), 220 (7)]	12.96	1594	0.07	14.56	2085	0.23
Humulène époxyde II	13.05†	1601	0.14	13.25	1962	0.05
Hexadécane	13.07†	1602	[0.14]	8.98	1594	0.06
Unknown [m/z 43, 161 (73), 91 (53), 95 (52), 79 (46), 119 (45)... 205 (29), 220? (1)]	13.15	1609	0.10	14.62	2091	0.60

Unknown [m/z 41, 91 (92), 55 (81), 93 (81), 79 (74), 43 (71), 95 (68), 123 (65)... 220 (17)]	13.17	1611	0.23	14.78	2106	0.21
Unknown [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	13.23	1615	0.25			
Unknown [m/z 41, 55 (92), 95 (80), 81 (76), 109 (76), 67 (66), 125 (65)... 220 (12)]	13.32	1623	0.63	14.71*†	2100	29.25
Caryophylladienol II	13.38	1628	0.20	15.99	2228	0.15
Hinesol	13.42	1631	0.29	14.91†	2119	0.69
Pogostol	13.67*†	1652	31.29	15.13	2142	2.04
Patchoulol	13.67*†	1652	[31.29]	14.71*†	2100	[29.25]
Unknown [m/z 175, 218 (59), 133 (49), 91 (43), 41 (38), 147 (36)]	13.69†	1654	[31.29]	14.94†	2122	[0.69]
Unknown [m/z 43, 41 (87), 91 (64), 55 (63), 81 (58), 95 (54), 107 (52)... 222 (12)]	13.74	1658	0.14			
Unknown [m/z 91, 41 (100), 107 (98), 108 (95), 95 (87), 93 (87), 105 (85), 79 (77), 119 (72)... 220? (15)]	13.98	1677	0.24	15.97	2226	0.04
Unknown [m/z 111, 250 (38), 126 (27), 139 (26), 43 (16), 41 (15), 166 (15)]	14.00	1679	0.07	11.74	1826	0.08
Unknown [m/z 43, 41 (95), 97 (89), 109 (71), 55 (71), 107 (70), 95 (69), 110 (65)... 222 (5)]	14.09	1687	0.04	15.31	2159	0.04
Rotundone	14.27*	1701	0.23	15.58	2186	0.20
Unknown [m/z 105, 107 (98), 91 (95), 166 (80), 248	14.27*	1701	[0.23]	12.92	1932	0.04

(80), 93 (76)... 233 (66)]						
Unknown [m/z 43, 41 (82), 137 (78), 109 (76), 95 (75), 91 (72), 55 (67)... 220? (14)]	14.30	1704	0.12			
Pogostone	14.38	1711	0.79			
Unknown [m/z 107, 93 (87), 41 (83), 81 (82), 67 (80), 55 (76)... 204 (53), 207 (34), 222 (9)]	14.51*	1722	0.36	16.82	2315	0.19
Unknown [m/z 83, 43 (85), 55 (39), 41 (29), 121 (27), 120 (25)... 218 (3)]	14.51*	1722	[0.36]	16.93	2326	0.15
Unknown [m/z 133, 148 (68), 147 (59), 91 (56), 79 (45), 105 (44)... 218 (8)]	14.60	1730	0.12	17.07	2342	0.02
Unknown [m/z 43, 83 (93), 55 (42), 41 (37), 121 (34), 111 (28)... 222? (1)]	14.78	1745	0.04	17.40	2377	0.04
Unknown [m/z 134, 107 (96), 91 (84), 93 (78), 79 (77), 41 (74), 43 (66), 77 (65)...]	14.87	1753	0.04	17.30	2367	0.01
Unknown [m/z 43, 191 (68), 41 (62), 91 (51), 95 (49), 110 (44)... 234 (22)]	14.90	1756	0.05			
Unknown [m/z 91, 105 (88), 95 (79), 93 (78), 81 (72), 79 (66)... 205 (33), 220 (7)...]	14.96	1761	0.15	17.56	2395	0.01
Unknown [m/z 149, 131 (54), 105 (48), 91 (46), 41 (30), 93 (27)... 218 (23)]	15.05	1769	0.10	17.22	2358	0.15
Unknown [m/z 43, 95 (58), 67 (50), 41 (47), 55	15.22	1783	0.06	17.98*	2442	0.13

(38), 109 (37)...						
221 (9)... 236? (3)]						
Unknown [m/z 219, 43 (67), 91 (46), 79 (42), 41 (41), 55 (36)... 234 (6)]	15.38	1797	0.09	17.98*	2442	[0.13]
Unknown [m/z 43, 91 (77), 79 (74), 109 (73), 110 (71)... 218 (52), 234? (1)]	15.44	1802	0.05	17.48	2386	0.04
Unknown [m/z 43, 91 (43), 41 (37), 79 (32), 219 (31)... 234 (14)]	15.50	1807	0.08	20.55	2747	0.03
Unknown [m/z 41, 110 (77), 55 (75), 69 (74), 43 (74), 95 (71), 97 (71), 123 (71), 67 (63), 136 (56)... 236? (7)]	15.92	1846	0.03	20.67	2762	0.05
Corymbolone analog	15.99	1852	0.02			
Corymbolone	16.21	1872	0.05			
Phytol	18.71	2111	0.04	19.10	2570	0.04
Unknown [m/z 41, 79 (97), 43 (97), 69 (72), 93 (70), 91 (62), 95 (58)... 220 (2)]				13.78	2011	0.02
Unknown [m/z 163, 119 (50), 91 (48), 95 (47), 41 (44), 105 (41)... 220 (18)]				15.36	2164	0.07
Total identified		91.85%			92.37%	
Total reported		96.96%			95.89%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied
R.T.: Retention time (minutes)
R.I.: Retention index