

Date : April 18, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23D12-PTH02


Customer identification : Patchouli ORGANIC - India - PI0104R

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 : April 18, 2023

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

PHYSICOCHEMICAL DATA

Physical aspect: Bright orange liquid

Refractive index: 1.5087 ± 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	tr	Aliphatic ketone
α -Pinene	0.09	Monoterpene
Camphene	0.01	Monoterpene
β -Pinene	0.21	Monoterpene
Sabinene	0.01	Monoterpene
Octen-3-ol	0.01	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
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	0.15	Sesquiterpene
Eugenol	0.02	Phenylpropanoid
α -Copaene	0.02	Sesquiterpene
β -Patchoulene	2.55	Sesquiterpene
β -Bourbonene	0.02	Sesquiterpene
<i>cis</i> - β -Elemene	0.06	Sesquiterpene
β -Elemene	1.06	Sesquiterpene
Isocaryophyllene	0.03	Sesquiterpene
Cycloseychellene	0.38	Sesquiterpene
α -Gurjunene	0.11	Sesquiterpene
β -Caryophyllene	3.30	Sesquiterpene
Seychellene	8.68	Sesquiterpene
α -Guaiene	14.34	Sesquiterpene
Selina-5,11-diene	0.01	Sesquiterpene
Unknown	0.05	Sesquiterpene
α -Humulene	0.60	Sesquiterpene
α -Patchoulene	2.86	Sesquiterpene
Patchoulene analog I	1.60	Sesquiterpene
γ -Patchoulene	1.01	Sesquiterpene
9- <i>epi</i> - β -Caryophyllene	0.02	Sesquiterpene
Unknown	0.41	Sesquiterpene
Unknown	0.43	Sesquiterpene
Selina-4,11-diene	0.21	Sesquiterpene
β -Selinene	0.11	Sesquiterpene
Patchoulene analog II	0.13	Sesquiterpene
Unknown	0.14	Sesquiterpene
δ -Selinene	0.26	Sesquiterpene
α -Selinene	0.11	Sesquiterpene
Eudesma-2,4(15),11-triene	0.15	Sesquiterpene
Aciphyllene	2.93	Sesquiterpene
Pentadecane	0.23	Alkane
Nootkatene	0.02	Sesquiterpene

δ-Guaiene	17.56	Sesquiterpene
γ-Cadinene	0.27	Sesquiterpene
7-epi-α-Selinene	0.23	Sesquiterpene
Unknown	0.08	Sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.01	Sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Norpatchoulol	0.62	Norsesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.22	Oxygenated sesquiterpene
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Caryophyllene oxide	0.30	Sesquiterpenic ether
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.49	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Humulene epoxide II	0.05	Sesquiterpenic ether
Hexadecane	0.04	Alkane
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.23	Oxygenated sesquiterpene
Unknown	0.22	Oxygenated sesquiterpene
Unknown	0.56	Oxygenated sesquiterpene
Caryophylladienol I	0.04	Sesquiterpenic alcohol
Caryophylladienol II	0.20	Sesquiterpenic alcohol
Hinesol	0.29	Sesquiterpenic alcohol
Patchoulol	29.17	Sesquiterpenic alcohol
Pogostol	2.01	Sesquiterpenic alcohol
Unknown	0.11	Oxygenated sesquiterpene
Unknown	0.06	Unknown
Unknown	0.13	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Rotundone	0.14	Sesquiterpenic ketone
Unknown	0.10	Oxygenated sesquiterpene
Pogostone	1.12	Terpenic lactone
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.14	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.11	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene

Unknown	0.02	Oxygenated sesquiterpene
Corymbolone analog	0.01	Sesquiterpenic alcohol
Corymbolone	0.03	Sesquiterpenic alcohol
Phytol	0.03	Diterpenic alcohol
Consolidated total	98.32%	

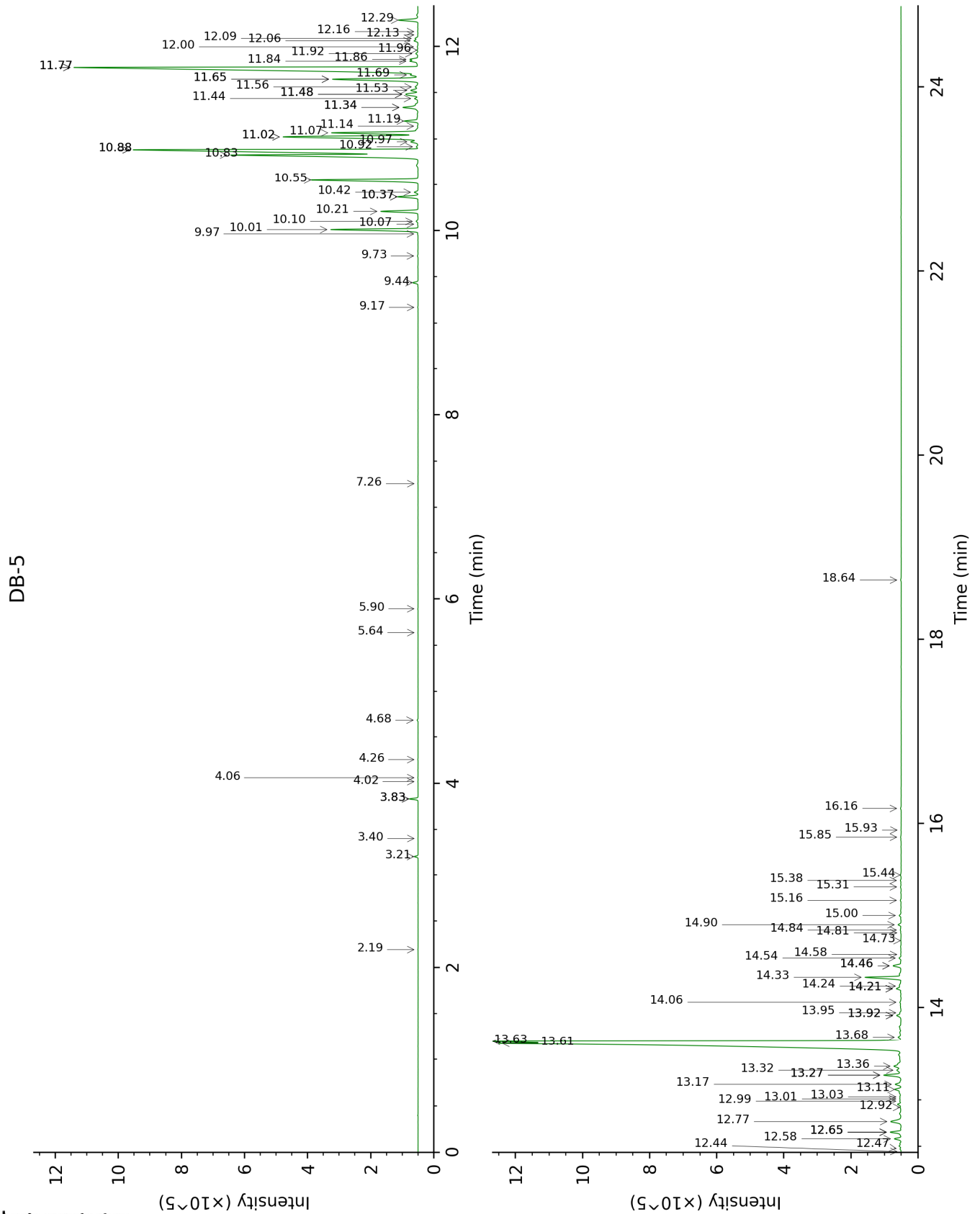
tr: The compound has been detected below 0.005% of total signal.

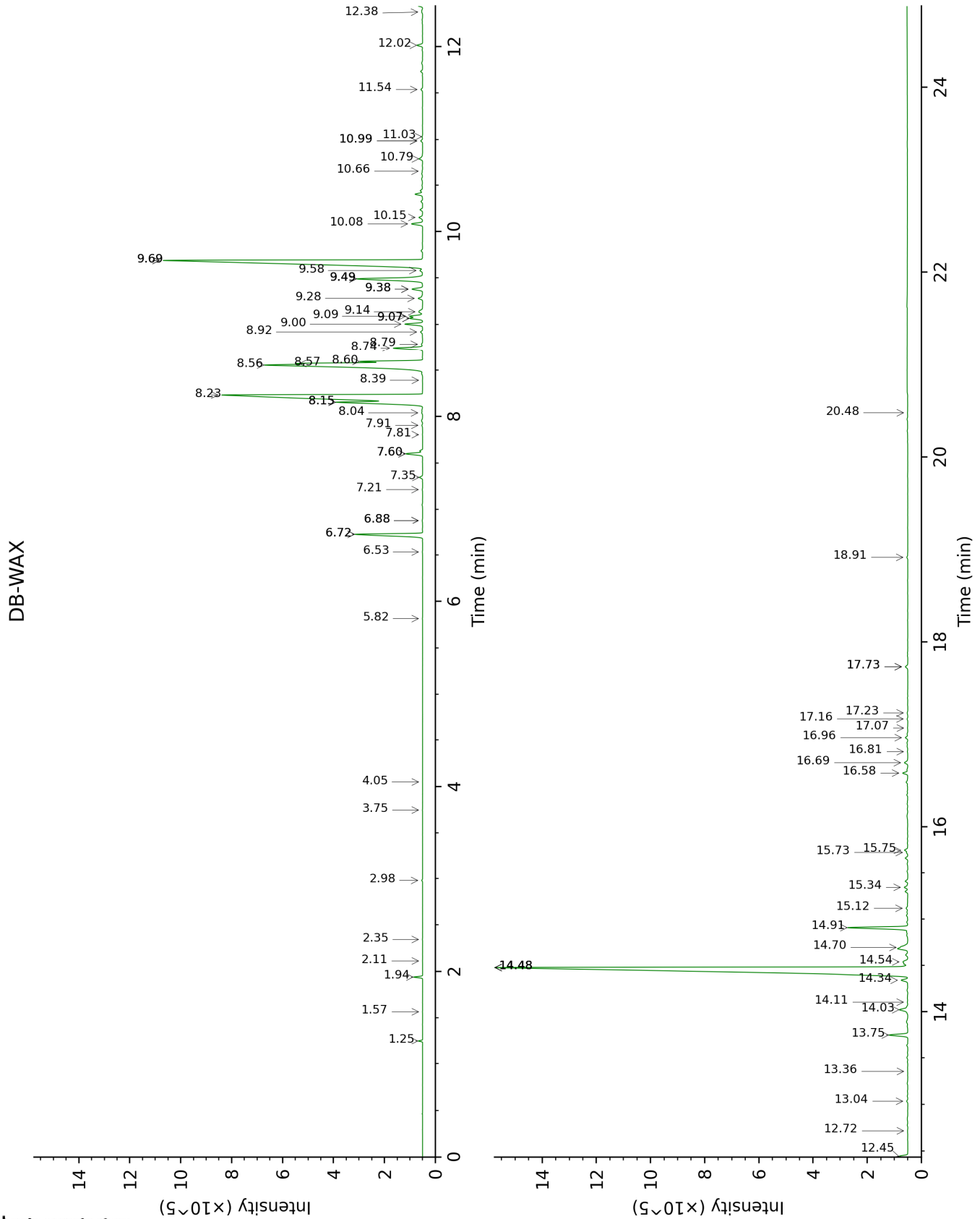
Note: no correction factor was applied

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.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
5-Methyl-2-hexanone	2.19	855	tr	2.34	1105	0.01
α-Pinene	3.21	931	0.09	1.25	990	0.08
Camphene	3.40	944	0.01	1.57	1026	tr
β-Pinene	3.83*	972	0.21	1.94	1064	0.21
Sabinene	3.83*	972	[0.21]	2.11	1083	0.01
Octen-3-ol	4.02	984	0.01	6.53	1420	0.01
Octan-3-one	4.06	987	0.01	3.75	1219	0.01
Octan-3-ol	4.26	1000	0.01	5.82	1367	0.01
Limonene	4.68	1027	0.03	2.98	1157	0.03
Terpinolene	5.64	1086	0.01	4.05	1242	0.01
Linalool	5.90	1102	0.01	7.81	1516	0.01
α-Terpineol	7.26	1189	0.01	9.49*	1650	3.06
Unknown [m/z 159, 117 (68), 132 (55), 200 (35)]	9.17	1317	0.01	6.88*	1446	0.02
δ-Elemene	9.44	1336	0.15	6.72*	1434	2.72
Eugenol	9.73	1356	0.02	14.48*	2097	29.76
α-Copaene	9.97	1373	0.02	6.88*	1446	[0.02]
β-Patchoulene	10.01	1376	2.55	6.72*	1434	[2.72]
β-Bourbonene	10.07	1380	0.02	7.21	1471	0.02
cis-β-Elemene	10.10	1382	0.06	8.04	1534	0.04
β-Elemene	10.21	1390	1.06	8.16*	1543	3.84
Isocaryophyllene	10.37*	1401	0.62	7.91	1524	0.03
Cycloseychellene	10.37*	1401	[0.62]	7.60*	1500	0.60
α-Gurjunene	10.42	1404	0.11	7.35	1481	0.11
β-Caryophyllene	10.55	1414	3.30	8.16*	1543	[3.84]
Seychellene	10.83†	1435	19.95	8.56	1575	8.68
α-Guaiene	10.88*†	1439	[19.95]	8.23	1549	14.34
Selina-5,11-diene	10.88*†	1439	[19.95]	8.39	1562	0.01
Unknown [m/z 91, 93 (98), 79 (82), 81 (82), 105 (71), 107 (70)... 204 (38)]	10.92	1442	0.05	8.92	1603	0.09
α-Humulene	10.97†	1446	8.36	9.00	1610	0.60
α-Patchoulene	11.02*†	1449	[8.36]	8.57	1576	2.86
Patchoulene analog I	11.02*†	1449	[8.36]	8.60	1578	1.60
γ-Patchoulene	11.07†	1453	[8.36]	8.74	1589	1.01
9-epi-β-Caryophyllene	11.14	1458	0.02	9.07*	1615	0.42
Unknown [m/z 159, 91 (88), 93 (72), 79 (69), 105 (68), 41 (66), 81 (54), 202? (50)...]	11.19	1462	0.41	9.07*	1615	[0.42]

Unknown [m/z 147, 93 (87), 107 (77), 105 (77), 91 (73), 79 (63)... 204 (21)]	11.34*	1473	0.56	9.09	1617	0.43
Selina-4,11-diene	11.34*	1473	[0.56]	9.14	1621	0.21
β-Selinene	11.44	1480	0.11	9.58	1657	0.10
Patchoulene analog II	11.48*	1484	0.54	9.49*	1650	[3.06]
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.48*	1484	[0.54]	9.38*	1641	0.40
δ-Selinene	11.53	1487	0.26	9.38*	1641	[0.40]
α-Selinene	11.56	1490	0.11	9.69*	1666	18.11
Eudesma-2,4(15),11-triene	11.65*	1496	3.08	10.79	1759	0.15
Aciphyllene	11.65*	1496	[3.08]	9.49*	1650	[3.06]
Pentadecane	11.69	1499	0.23	7.60*	1500	[0.60]
Nootkatene	11.77*	1505	17.58	10.66	1747	0.02
δ-Guaiene	11.77*	1505	[17.58]	9.69*	1666	[18.11]
γ-Cadinene	11.84	1511	0.27	10.08	1698	0.40
7-epi-α-Selinene	11.86	1512	0.23	10.15	1704	0.15
Unknown [m/z 159, 91 (81), 117 (68), 131 (51), 105 (46)... 202 (37)]	11.92	1517	0.08	9.28	1633	0.18
Unknown [m/z 41, 67 (95), 93 (92), 107 (91), 55 (77), 81 (77), 79 (73)... 205 (17)...]	11.96	1520	0.03	11.03	1779	0.02
Unknown [m/z 161, 119 (92), 91 (69), 105 (52), 145 (49)... 218 (6)]	12.00	1523	0.03	10.99*	1775	0.06
Unknown [m/z 91, 105 (98), 108 (83), 93 (82), 133 (79), 77 (64), 79 (57), 41 (56), 145 (55)... 218? (5)]	12.06	1528	0.12			
Unknown [m/z 91, 105 (78), 93 (77), 107 (71), 79 (64), 41 (63), 77 (63), 145 (60)... 218 (17)]	12.09	1530	0.10			
Unknown [m/z 133, 105 (70), 146 (69), 145 (61), 91	12.13	1533	0.01	10.99*	1775	[0.06]

(55), 131 (45), 187 (42), 159 (39), 119 (33), 202 (30)...						
Unknown [m/z 145, 131 (91), 91 (86), 105 (68), 146 (66), 43 (54)...	12.16	1536	0.02			
220? (5)] Norpatchoulenol	12.29	1546	0.62	13.75	2027	0.64
Unknown [m/z 191, 159 (66), 133 (53), 91 (45), 41 (42), 177 (35), 105 (33), 220 (32)]	12.44	1558	0.01	13.36	1989	0.01
Unknown [m/z 41, 67 (90), 55 (87), 79 (85), 107 (84), 81 (84), 93 (84), 121 (77), 91 (74)...	12.47	1560	0.04			
220 (7)] Unknown [m/z 43, 107 (94), 81 (71), 41 (63), 67 (58), 111 (58), 93 (55), 83 (54)...	12.58	1569	0.22	12.02	1866	0.19
205 (8), 220 (1)] Caryophyllene oxide isomer	12.66*	1574	0.37	12.38	1898	0.06
Caryophyllene oxide	12.66*	1574	[0.37]	12.45	1905	0.30
Unknown isomer	12.66*	1574	[0.37]	14.11	2061	0.02
Unknown [m/z 43, 79 (44), 81 (41), 93 (40), 91 (40)...	12.77	1583	0.49	14.02	2053	0.42
220 (5)] Unknown [m/z 43, 105 (77), 91 (71), 93 (68), 41 (62), 107 (6)...	12.92	1595	0.05	14.34	2084	0.25
205 (41), 220 (7)] Humulene epoxide II	12.99	1601	0.05	13.04	1959	0.04
Hexadecane	13.01	1602	0.04	8.79	1593	0.05
Unknown [m/z 43, 161 (73), 91 (53), 95 (52), 79 (46), 119 (45)...	13.03	1604	0.05	14.48*	2097	[29.76]
205 (29), 220? (1)] Unknown [m/z 41, 91 (92), 55 (81), 93 (81), 79 (74), 43 (71), 95	13.11	1611	0.23	14.54	2103	0.22

(68), 123 (65)... 220 (17)]						
Unknown [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	13.17	1615	0.22			
Unknown [m/z 41, 55 (92), 95 (80), 81 (76), 109 (76), 67 (66), 125 (65)... 220 (12)]	13.27*	1623	0.60	14.48*	2097	[29.76]
Caryophylladienol I	13.27*	1623	[0.60]	15.73	2224	0.04
Caryophylladienol II	13.32	1628	0.20	15.75	2226	0.13
Hinesol	13.36	1631	0.29	14.70	2119	0.26
Patchoulol	13.61†	1652	31.18	14.48*	2097	[29.76]
Pogostol	13.63†	1654	[31.18]	14.91	2140	2.01
Unknown [m/z 175, 218 (59), 133 (49), 91 (43), 41 (38), 147 (36)]	13.68	1658	0.11			
Unknown [m/z 111, 250 (38), 126 (27), 139 (26), 43 (16), 41 (15), 166 (15)]	13.92*	1677	0.19	11.54	1824	0.06
Unknown [m/z 95, 107 (99), 41 (85), 93 (82), 91 (82), 109 (71), 105 (71), 105 (71), 108 (66)... 220 (29)]	13.92*	1677	[0.19]			
Unknown [m/z 91, 41 (100), 107 (98), 108 (95), 95 (87), 93 (87), 105 (85), 79 (77), 119 (72)... 220? (15)]	13.95	1680	0.05			
Unknown [m/z 43, 41 (95), 97 (89), 109 (71), 55 (71), 107 (70), 95 (69), 110 (65)... 222 (5)]	14.06	1689	0.07	15.12	2162	0.07
Unknown [m/z 105, 107 (98), 91 (95), 166 (80), 248 (80), 93 (76)... 233 (66)]	14.21*	1701	0.16	12.72	1930	0.02
Rotundone	14.21*	1701	[0.16]	15.34	2184	0.14

Unknown [m/z 43, 41 (82), 137 (78), 109 (76), 95 (75), 91 (72), 55 (67)... 220? (14)]	14.24	1703	0.10			
Pogostone	14.33	1712	1.12			
Unknown [m/z 107, 93 (87), 41 (83), 81 (82), 67 (80), 55 (76)... 204 (53), 207 (34), 222 (9)]	14.46*	1722	0.31	16.58	2314	0.18
Unknown [m/z 83, 43 (85), 55 (39), 41 (29), 121 (27), 120 (25)... 218 (3)]	14.46*	1722	[0.31]	16.69	2326	0.14
Unknown [m/z 133, 148 (68), 147 (59), 91 (56), 79 (45), 105 (44)... 218 (8)]	14.54	1729	0.08	16.81	2339	0.02
Unknown [m/z 91, 108 (86), 107 (85), 93 (80), 120 (75), 105 (71), 95 (72)... 218 (37)]	14.58	1733	0.03			
Unknown [m/z 43, 83 (93), 55 (42), 41 (37), 121 (34), 111 (28)... 222? (1)]	14.73	1746	0.03	17.16	2377	0.02
Unknown [m/z 134, 107 (96), 91 (84), 93 (78), 79 (77), 41 (74), 43 (66), 77 (65)...]	14.81	1753	0.02	17.07	2366	0.02
Unknown [m/z 43, 191 (68), 41 (62), 91 (51), 95 (49), 110 (44)... 234 (22)]	14.84	1756	0.05			
Unknown [m/z 91, 105 (88), 95 (79), 93 (78), 81 (72), 79 (66)... 205 (33), 220 (7)...]	14.90	1761	0.11			
Unknown [m/z 149, 131 (54), 105 (48), 91 (46), 41 (30), 93 (27)... 218 (23)]	15.00	1769	0.08	16.96	2355	0.09

Unknown [m/z 43, 95 (58), 67 (50), 41 (47), 55 (38), 109 (37)... 221 (9)... 236? (3)]	15.16	1784	0.04	17.74*	2440	0.10
Unknown [m/z 219, 43 (67), 91 (46), 79 (42), 41 (41), 55 (36)... 234 (6)]	15.31	1796	0.03	17.74*	2440	[0.10]
Unknown [m/z 43, 91 (77), 79 (74), 109 (73), 110 (71)... 218 (52), 234? (1)]	15.38	1802	0.03	17.23	2384	0.03
Unknown [m/z 43, 91 (43), 41 (37), 79 (32), 219 (31)... 234 (14)]	15.44	1807	0.05			
Unknown [m/z 41, 110 (77), 55 (75), 69 (74), 43 (74), 95 (71), 97 (71), 123 (71), 67 (63), 136 (56)... 236? (7)]	15.85	1845	0.02			
Corymbolone analog	15.93	1852	0.01			
Corymbolone	16.16	1874	0.03	20.48	2764	0.01
Phytol	18.64	2112	0.03	18.91	2575	0.03
Total identified		94.82%			93.56%	
Total reported		97.91%			96.04%	

*: 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