

Date : June 09, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23E26-NPA06


Customer identification : Patchouli - Indonesia - NPS00056 - Lot # NP0140

Type : Essential oil

Source : *Pogostemon cablin*

Customer : Nature Packaged

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 : Sylvain Mercier, M. Sc., Chimiste 2014-005

Analysis date : June 06, 2023

Checked and approved by :



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

Notes: 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.

This report is an update from the first version issued on June 9, 2023, to format it for online publication.

PHYSICOCHEMICAL DATA

Physical aspect: Orange brownish 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	0.11	Monoterpene
β -Pinene	0.25	Monoterpene
Sabinene	tr	Monoterpene
Octen-3-ol	tr	Aliphatic alcohol
Octan-3-one	tr	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	0.14	Sesquiterpene
Eugenol	0.02	Phenylpropanoid
α -Copaene	0.01	Sesquiterpene
β -Patchoulene	2.52	Sesquiterpene
<i>cis</i> - β -Elemene	0.02	Sesquiterpene
β -Elemene	0.89	Sesquiterpene
Isocaryophyllene	0.02	Sesquiterpene
Cycloseychellene	0.61	Sesquiterpene
α -Gurjunene	0.01	Sesquiterpene
β -Caryophyllene	3.15	Sesquiterpene
Seychellene	6.04	Sesquiterpene
α -Guaiene	13.85	Sesquiterpene
Unknown	0.25	Sesquiterpene
α -Patchoulene	4.79	Sesquiterpene
α -Humulene	0.57	Sesquiterpene
Patchoulene analog I	1.58	Sesquiterpene
γ -Patchoulene	1.02	Sesquiterpene
9-epi- β -Caryophyllene	0.02	Sesquiterpene
Unknown	0.38	Sesquiterpene
Selina-4,11-diene	0.24	Sesquiterpene
Unknown	0.31	Sesquiterpene
β -Selinene	0.13	Sesquiterpene
Patchoulene analog II	0.10	Sesquiterpene
Unknown	0.14	Sesquiterpene
δ -Selinene	0.24	Sesquiterpene
α -Selinene	0.12	Sesquiterpene
Aciphyllene	2.81	Sesquiterpene
Eudesma-2,4(15),11-triene	0.15	Sesquiterpene
δ -Guaiene	16.43	Sesquiterpene
γ -Cadinene	0.51	Sesquiterpene
Pentadecane	0.01	Alkane
Nootkatene	0.32	Sesquiterpene
7-epi- α -Selinene	0.21	Sesquiterpene

Unknown	0.09	Sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.11	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Norpatchoulénol	0.63	Norsesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.35	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Caryophyllène oxide	0.42	Sesquiterpenic ether
Caryophyllène oxide isomer	0.08	Sesquiterpenic ether
Unknown	0.52	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Hexadécane	0.12	Alkane
Humulène époxyde II	0.07	Sesquiterpenic ether
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.24	Oxygenated sesquiterpene
Unknown	0.28	Oxygenated sesquiterpene
Unknown	0.13	Oxygenated sesquiterpene
Caryophylladiénol I	0.06	Sesquiterpenic alcohol
Caryophylladiénol II	0.20	Sesquiterpenic alcohol
Hinesol	0.30	Sesquiterpenic alcohol
Patchoulol	29.86	Sesquiterpenic alcohol
Pogostol	1.99	Sesquiterpenic alcohol
Unknown	0.16	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.08	Unknown
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Rotundone	0.27	Sesquiterpenic ketone
Unknown	0.09	Oxygenated sesquiterpene
Pogostone	0.59	Terpenic lactone
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.21	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.14	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Corymbolone analog	0.02	Sesquiterpenic alcohol
Corymbolone	0.07	Sesquiterpenic alcohol

Consolidated total	96.45%	
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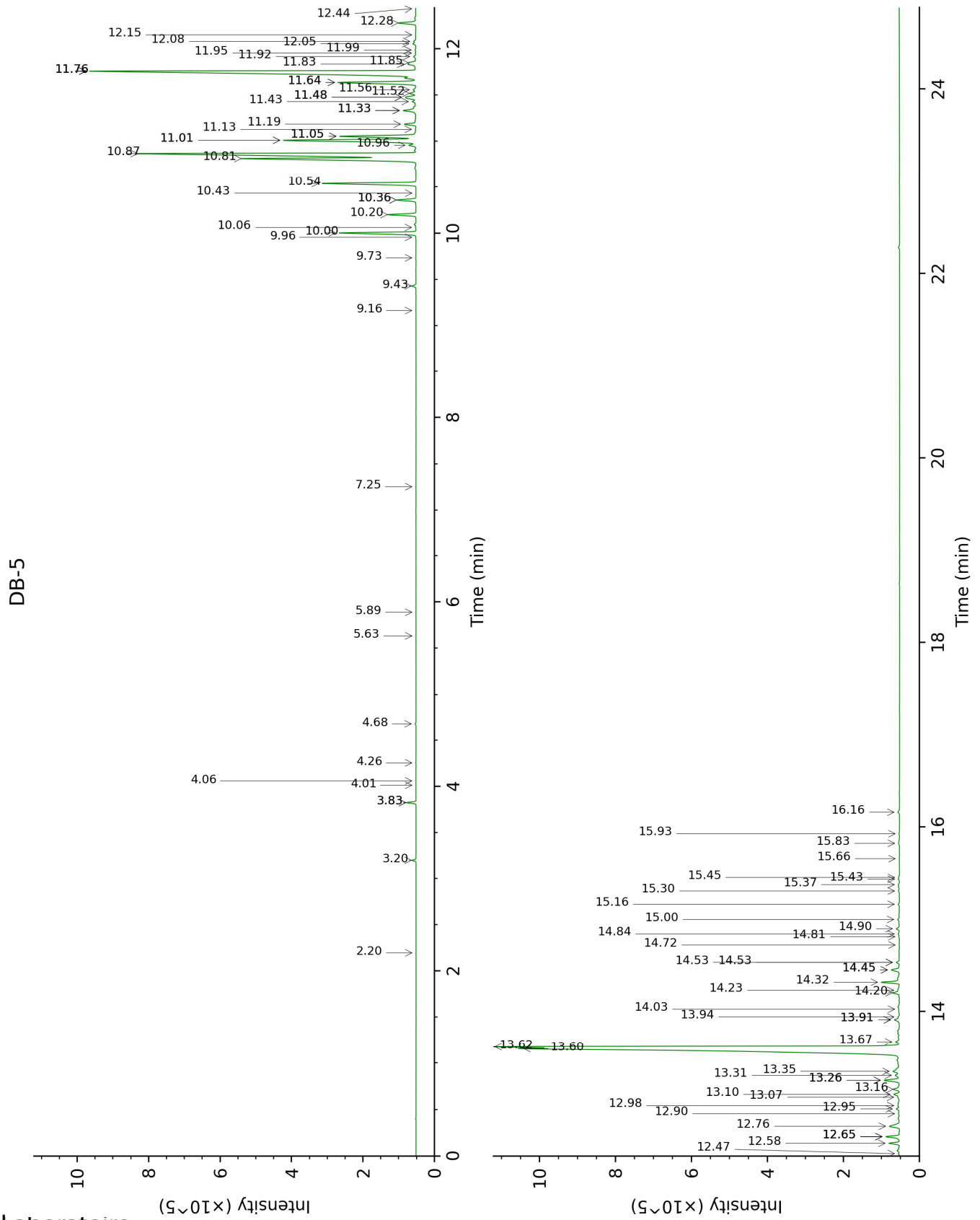
tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

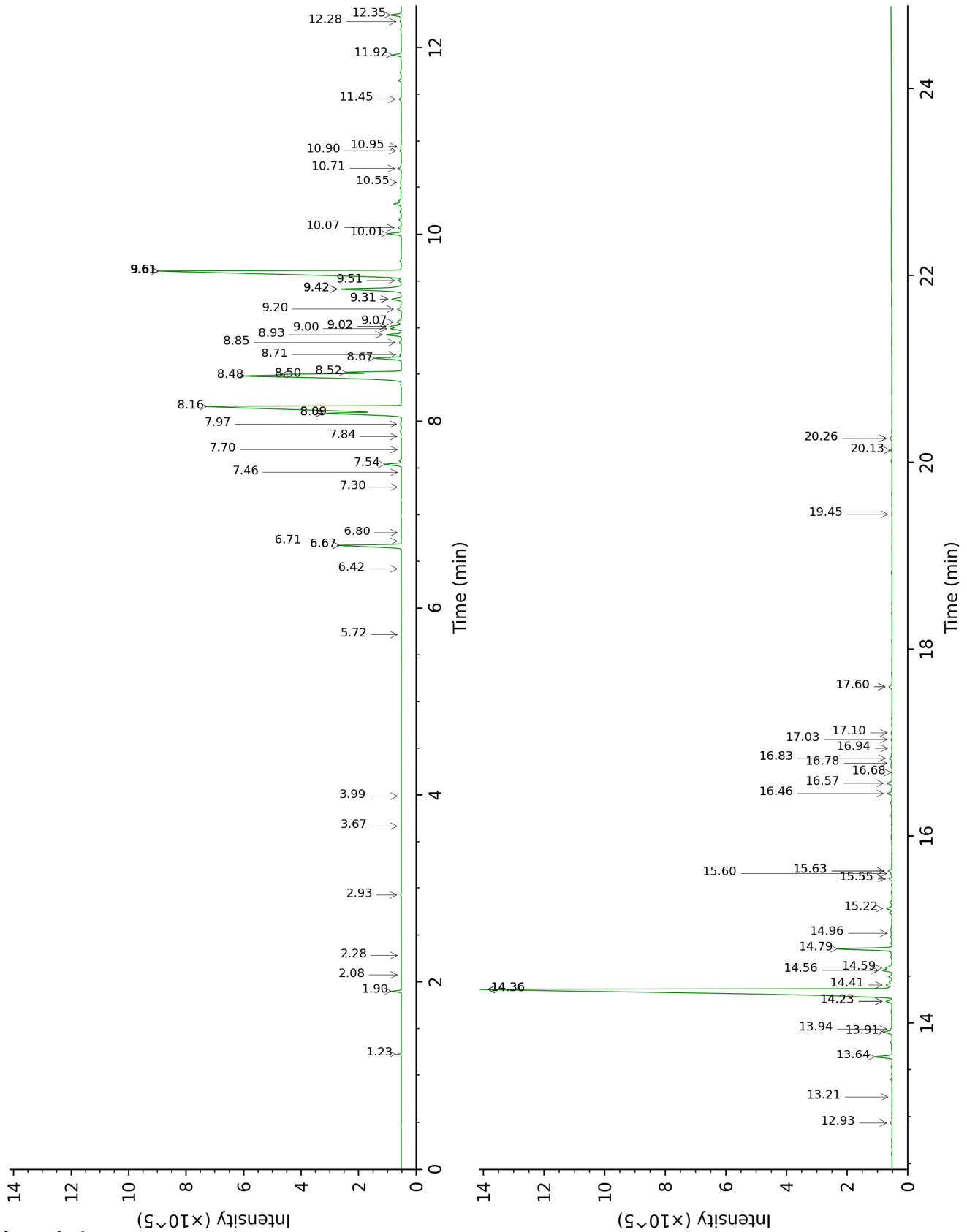
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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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DB-WAX



FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
5-Methyl-2-hexanone	2.20	855	0.01	2.28	1106	0.01
α-Pinene	3.20	931	0.11	1.23	993	0.10
β-Pinene	3.83*	972	0.26	1.90	1067	0.25
Sabinene	3.83*	972	[0.26]	2.08	1085	tr
Octen-3-ol	4.01	984	tr	6.42	1419	tr
Octan-3-one	4.06	987	tr	3.67	1220	0.01
Octan-3-ol	4.26	1000	0.01	5.72	1367	0.01
Limonene	4.68	1026	0.03	2.93	1159	0.03
Terpinolene	5.64	1086	0.01	3.99	1244	0.01
Linalool	5.89	1102	0.01	7.70	1516	tr
α-Terpineol	7.25	1189	0.01	9.42*	1654	2.92
Unknown [m/z 159, 117 (68), 132 (55), 200 (35)]	9.16	1316	0.01	6.71	1442	0.01
δ-Elemene	9.43	1335	0.14	6.67*	1438	2.66
Eugenol	9.73	1356	0.02	14.36*	2101	30.01
α-Copaene	9.96	1372	0.01	6.80	1448	0.01
β-Patchoulene	10.00	1375	2.52	6.67*	1438	[2.66]
cis-β-Elemene	10.06	1380	0.02	7.97	1538	0.04
β-Elemene	10.20	1389	0.89	8.09*	1547	3.46
Isocaryophyllene	10.36*	1400	0.64	7.84	1527	0.02
Cycloseychellene	10.36*	1400	[0.64]	7.54	1504	0.61
α-Gurjunene	10.43	1406	0.01	7.30	1486	0.01
β-Caryophyllene	10.54	1414	3.15	8.09*	1547	[3.46]
Seychellene	10.81†	1434	19.89	8.48†	1578	11.72
α-Guaiene	10.87†	1438	[19.89]	8.16	1553	13.85
Unknown [m/z 91, 93 (98), 79 (82), 81 (82), 105 (71), 107 (70)... 204 (38)]	10.96	1445	0.25	8.85	1607	0.09
α-Patchoulene	11.01*	1449	5.36	8.50†	1579	[11.72]
α-Humulene	11.01*	1449	[5.36]	8.93	1614	0.57
Patchoulene analog I	11.06*	1452	2.75	8.52	1581	1.58
γ-Patchoulene	11.06*	1452	[2.75]	8.67	1593	1.02
9-epi-β-Caryophyllene	11.13	1458	0.02	9.02*†	1621	[0.82]
Unknown [m/z 159, 91 (88), 93 (72), 79 (69), 105 (68), 41 (66), 81 (54), 202? (50)...]	11.19	1462	0.38	9.00†	1619	0.82
Selina-4,11-diene	11.33*	1473	0.54	9.07	1625	0.24
Unknown [m/z 147, 93 (87), 107 (77), 105 (77), 91	11.33*	1473	[0.54]	9.02*†	1621	[0.82]

(73), 79 (63)... 204 (21)]						
β-Selinene	11.43	1480	0.13	9.51	1661	0.12
Patchoulene analog II	11.48*	1483	0.55	9.42*	1654	[2.92]
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.48*	1483	[0.55]	9.31*	1645	0.38
δ-Selinene	11.52	1486	0.24	9.31*	1645	[0.38]
α-Selinene	11.56	1489	0.12	9.61*	1670	17.31
Aciphyllene	11.64*	1495	2.96	9.42*	1654	[2.92]
Eudesma-2,4(15),11-triene	11.64*	1495	[2.96]	10.71	1763	0.15
δ-Guaiene	11.76*	1504	16.95	9.61*	1670	[17.31]
γ-Cadinene	11.76*	1504	[16.95]	10.01	1703	0.51
Pentadecane	11.76*	1504	[16.95]	7.46	1498	0.01
Nootkatene	11.83	1510	0.32	10.55	1750	0.06
7-epi-α-Selinene	11.85	1511	0.21	10.07	1708	0.14
Unknown [m/z 159, 91 (81), 117 (68), 131 (51), 105 (46)... 202 (37)]	11.92	1517	0.09	9.20	1636	0.16
Unknown [m/z 41, 67 (95), 93 (92), 107 (91), 55 (77), 81 (77), 79 (73)... 205 (17)...]	11.95	1520	0.02	10.94	1783	0.03
Unknown [m/z 161, 119 (92), 91 (69), 105 (52), 145 (49)... 218 (6)]	11.99	1522	0.03	10.90	1779	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	0.11			
Unknown [m/z 91, 105 (78), 93 (77), 107 (71), 79 (64), 41 (63), 77 (63), 145 (60)... 218 (17)]	12.08	1529	0.08			
Unknown [m/z 145, 131 (91), 91 (86), 105 (68), 146 (66), 43 (54)... 220? (5)]	12.15	1535	0.02			
Norpatchoulenol	12.28	1545	0.63	13.64	2030	0.65

Unknown [m/z 191, 159 (66), 133 (53), 91 (45), 41 (42), 177 (35), 105 (33), 220 (32)]	12.44	1557	0.01	13.21	1989	0.01
Unknown [m/z 41, 67 (90), 55 (87), 79 (85), 107 (84), 81 (84), 93 (84), 121 (77), 91 (74)... 220 (7)]	12.47	1560	0.05			
Unknown [m/z 43, 107 (94), 81 (71), 41 (63), 67 (58), 111 (58), 93 (55), 83 (54)... 205 (8), 220 (1)]	12.58	1569	0.35	11.92	1870	0.33
Unknown isomer	12.65*	1574	0.50	13.94	2060	0.05
Caryophyllene oxide	12.65*	1574	[0.50]	12.35	1908	0.42
Caryophyllene oxide isomer	12.65*	1574	[0.50]	12.28	1902	0.08
Unknown [m/z 43, 79 (44), 81 (41), 93 (40), 91 (40)... 220 (5)]	12.76	1583	0.52	13.91	2056	0.38
Unknown [m/z 43, 105 (77), 91 (71), 93 (68), 41 (62), 107 (6)... 205 (41), 220 (7)]	12.90	1594	0.05	14.23*	2088	0.25
Hexadecane	12.95	1598	0.12	8.71	1596	0.06
Humulene epoxide II	12.98	1600	0.07	12.93	1963	0.06
Unknown [m/z 43, 161 (73), 91 (53), 95 (52), 79 (46), 119 (45)... 205 (29), 220? (1)]	13.07	1608	0.08	14.23*	2088	[0.25]
Unknown [m/z 41, 91 (92), 55 (81), 93 (81), 79 (74), 43 (71), 95 (68), 123 (65)... 220 (17)]	13.10	1610	0.24	14.41	2106	0.25
Unknown [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	13.16	1614	0.28			
Unknown [m/z 41, 55 (92), 95	13.26*	1622	0.62	14.36*	2101	[30.01]

(80), 81 (76), 109 (76), 67 (66), 125 (65)... 220 (12)]						
Caryophylladienol I	13.26*	1622	[0.62]	15.55*	2222	0.12
Caryophylladienol II	13.31	1627	0.20	15.60	2228	0.05
Hinesol	13.35	1630	0.30	14.56	2121	0.41
Patchoulol	13.60†	1651	31.85	14.36*	2101	[30.01]
Pogostol	13.62†	1652	[31.85]	14.79	2145	1.99
Unknown [m/z 175, 218 (59), 133 (49), 91 (43), 41 (38), 147 (36)]	13.67	1657	0.16	14.59	2124	0.29
Unknown [m/z 95, 107 (99), 41 (85), 93 (82), 91 (82), 109 (71), 105 (71), 105 (71), 108 (66)... 220 (29)]	13.91*	1677	0.24	15.63*	2231	0.16
Unknown [m/z 111, 250 (38), 126 (27), 139 (26), 43 (16), 41 (15), 166 (15)]	13.91*	1677	[0.24]	11.45	1827	0.08
Unknown [m/z 91, 41 (100), 107 (98), 108 (95), 95 (87), 93 (87), 105 (85), 79 (77), 119 (72)... 220? (15)]	13.94	1679	0.05	15.55*	2222	[0.12]
Unknown [m/z 43, 41 (95), 97 (89), 109 (71), 55 (71), 107 (70), 95 (69), 110 (65)... 222 (5)]	14.03	1686	0.03	14.96	2162	0.04
Rotundone	14.20	1701	0.27	15.22	2188	0.23
Unknown [m/z 43, 41 (82), 137 (78), 109 (76), 95 (75), 91 (72), 55 (67)... 220? (14)]	14.23	1703	0.09			
Pogostone	14.32	1710	0.59			
Unknown [m/z 107, 93 (87), 41 (83), 81 (82), 67 (80), 55 (76)... 204 (53), 207 (34), 222 (9)]	14.45*	1722	0.36	16.46	2318	0.18
Unknown [m/z 83, 43 (85), 55	14.45*	1722	[0.36]	16.57	2330	0.21

(39), 41 (29), 121 (27), 120 (25)... 218 (3)] Unknown [m/z 91, 108 (86), 107 (85), 93 (80), 120 (75), 105 (71), 95 (72)... 218 (37)]	14.53*	1729	0.12	15.63*	2231	[0.16]
Unknown [m/z 133, 148 (68), 147 (59), 91 (56), 79 (45), 105 (44)... 218 (8)]	14.53*	1729	[0.12]	16.68	2343	0.02
Unknown [m/z 43, 83 (93), 55 (42), 41 (37), 121 (34), 111 (28)... 222? (1)]	14.72	1745	0.02	17.03	2382	0.04
Unknown [m/z 134, 107 (96), 91 (84), 93 (78), 79 (77), 41 (74), 43 (66), 77 (65)...]	14.81	1753	0.03	16.94	2371	0.02
Unknown [m/z 43, 191 (68), 41 (62), 91 (51), 95 (49), 110 (44)... 234 (22)]	14.84	1756	0.06			
Unknown [m/z 91, 105 (88), 95 (79), 93 (78), 81 (72), 79 (66)... 205 (33), 220 (7)...]	14.90	1760	0.14			
Unknown [m/z 149, 131 (54), 105 (48), 91 (46), 41 (30), 93 (27)... 218 (23)]	15.00	1769	0.08	16.83	2360	0.11
Unknown [m/z 43, 95 (58), 67 (50), 41 (47), 55 (38), 109 (37)... 221 (9)... 236? (3)]	15.16	1783	0.05	17.60*	2445	0.13
Unknown [m/z 219, 43 (67), 91 (46), 79 (42), 41 (41), 55 (36)... 234 (6)]	15.30	1796	0.05	17.60*	2445	[0.13]
Unknown [m/z 43, 91 (77), 79 (74), 109 (73), 110	15.37	1802	0.04	17.10	2390	0.04

(71)... 218 (52), 234? (1)] Unknown [m/z 43, 91 (43), 41 (37), 79 (32), 219 (31)... 234 (14)]	15.43	1807	0.04	20.13	2746	0.04
Unknown [m/z 91, 41 (79), 43 (74), 79 (72), 105 (65), 77 (64), 147 (64), 93 (61)... 218 (26), 234 (14)]	15.45	1809	0.03	16.78	2354	0.04
Unknown [m/z 43, 69 (60), 41 (55), 55 (40), 95 (33), 163 (27)... 234 (17)]	15.66	1828	0.01	19.45	2662	0.02
Unknown [m/z 41, 110 (77), 55 (75), 69 (74), 43 (74), 95 (71), 97 (71), 123 (71), 67 (63), 136 (56)... 236? (7)]	15.83	1843	0.07	20.26*	2763	0.08
Corymbolone analog	15.93	1852	0.02			
Corymbolone	16.16	1873	0.07	20.26*	2763	[0.08]
Total identified		93.83%			92.51%	
Total reported		97.35%			95.80%	

*: 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