

Date : May 06, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22D27-PTH06

Customer identification : Patchouli (Aging) - P20104R

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 : Seydou Ka, Ph. D.

Analysis date : May 04, 2022

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow orange liquid

Refractive index: 1.5080 ± 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
β-Pinene	0.21	Monoterpene
Sabinene	tr	Monoterpene
Octen-3-ol	0.01	Aliphatic alcohol
Octan-3-one	tr	Aliphatic ketone
Limonene	0.02	Monoterpene
Linalool	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
δ-Elemene	0.16	Sesquiterpene
α-Copaene	0.41	Sesquiterpene
β-Patchoulene	2.70	Sesquiterpene
β-Bourbonene	0.01	Sesquiterpene
cis-β-Elemene	0.06	Sesquiterpene
β-Elemene	1.10	Sesquiterpene
Cycloseychellene	0.28	Sesquiterpene
Isocaryophyllene	0.03	Sesquiterpene
β-Caryophyllene	3.57	Sesquiterpene
Selina-5,11-diene	0.04	Sesquiterpene
Seychellene	6.13	Sesquiterpene
α-Guaiene	14.15	Sesquiterpene
Unknown	0.07	Sesquiterpene
α-Patchoulene	4.71	Sesquiterpene
α-Humulene	0.62	Sesquiterpene
Patchoulene analog I	1.89	Sesquiterpene
γ-Patchoulene	0.98	Sesquiterpene
9-epi-β-Caryophyllene	0.02	Sesquiterpene
Unknown	0.43	Sesquiterpene
Unknown	0.64*	Sesquiterpene
Selina-4,11-diene	0.64*	Sesquiterpene
β-Selinene	0.13	Sesquiterpene
Patchoulene analog II	0.10	Sesquiterpene
δ-Selinene	0.53*	Sesquiterpene
Unknown	0.53*	Sesquiterpene
α-Selinene	0.25	Sesquiterpene
Eudesma-2,4(15),11-triene	0.16	Sesquiterpene
Aciphyllene	3.02	Sesquiterpene
Pentadecane	0.30	Alkane
γ-Cadinene	0.11	Sesquiterpene
δ-Guaiene	18.41	Sesquiterpene
7-epi-α-Selinene	0.15	Sesquiterpene
Nootkatene	0.01	Sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.11	Oxygenated sesquiterpene

Unknown	0.09	Oxygenated sesquiterpene
Norpatchoulenol	0.57	Norsesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.16	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Caryophyllene oxide	0.23	Sesquiterpenic ether
Unknown	0.29	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Hexadecane	0.02	Alkane
Humulene epoxide II	0.03	Sesquiterpenic ether
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.17	Oxygenated sesquiterpene
Caryophylladienol I	0.54	Sesquiterpenic alcohol
Caryophylladienol II	0.13	Sesquiterpenic alcohol
Hinesol	0.38	Sesquiterpenic alcohol
Pogostol	2.01	Sesquiterpenic alcohol
Patchoulol	28.72	Sesquiterpenic alcohol
Unknown	0.19	Oxygenated sesquiterpene
Unknown	0.13	Unknown
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Rotundone	0.12	Sesquiterpenic ketone
Unknown	0.05	Oxygenated sesquiterpene
Pogostone	1.32	Terpenic lactone
Unknown	0.21	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Phytol	0.03	Diterpenic alcohol
Consolidated total	98.04%	

*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered

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

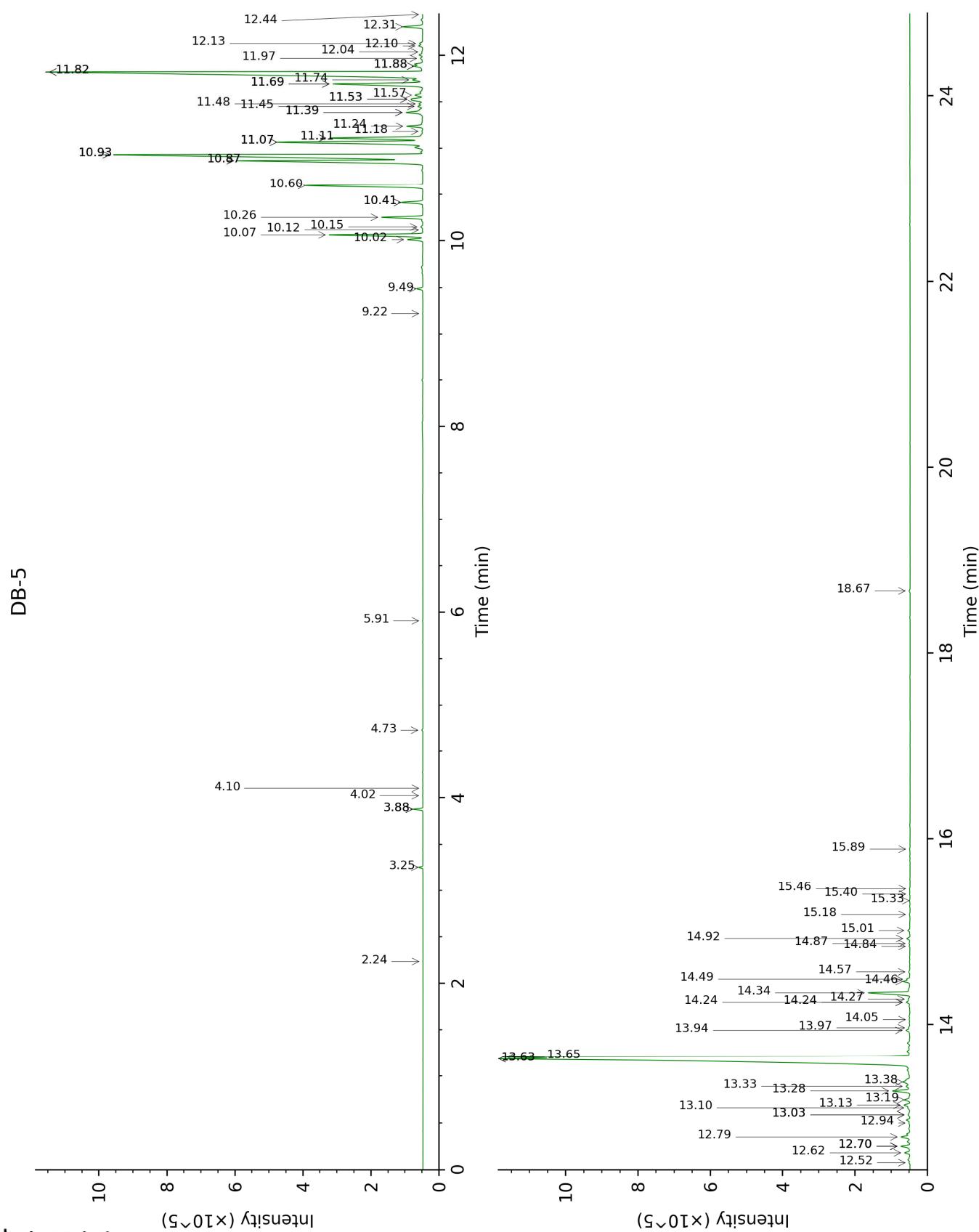
tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

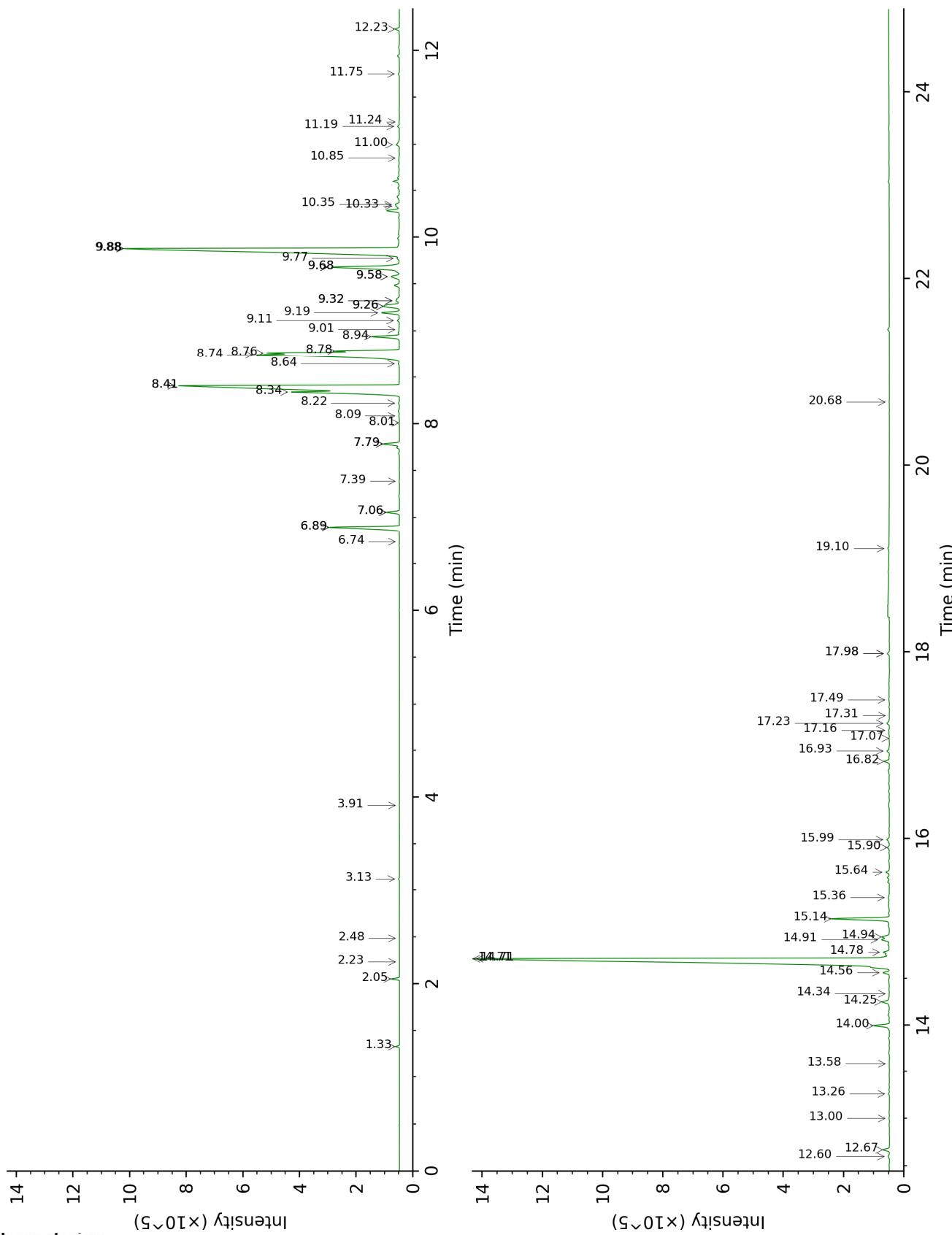
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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



DB-WAX



FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
5-Methyl-2-hexanone	2.24	854	tr	2.48	1106	tr
α-Pinene	3.26	930	0.09	1.33	990	0.09
β-Pinene	3.88*	971	0.21	2.05	1065	0.21
Sabinene	3.88*	971	[0.21]	2.23	1084	tr
Octen-3-ol	4.02	980	0.01	6.74	1422	0.01
Octan-3-one	4.10	986	tr	3.91	1218	0.01
Limonene	4.73	1026	0.02	3.13	1157	0.02
Linalool	5.91	1100	0.01	8.01	1518	0.01
Unknown [m/z 159, 117 (68), 132 (55), 200 (35)]	9.22	1317	0.01	7.06*	1446	0.43
δ-Elemene	9.49	1336	0.16	6.90*	1434	2.89
α-Copaene	10.02	1373	0.41	7.06*	1446	[0.43]
β-Patchoulene	10.07	1377	2.70	6.90*	1434	[2.89]
β-Bourbonene	10.12	1380	0.01	7.39	1471	0.01
cis-β-Elemene	10.15	1383	0.06	8.22	1534	0.03
β-Elemene	10.26	1390	1.10	8.34†	1543	18.83
Cycloseychellene	10.41*	1401	0.60	7.79*	1500	0.58
Isocaryophyllene	10.41*	1401	[0.60]	8.08	1523	0.03
β-Caryophyllene	10.60	1415	3.57	8.41*†	1548	[18.83]
Selina-5,11-diene	10.87*†	1435	20.40	8.64	1567	0.04
Seychellene	10.87*†	1435	[20.40]	8.74†	1574	12.95
α-Guaiene	10.93*†	1440	[20.40]	8.41*†	1548	[18.83]
Unknown [m/z 91, 93 (98), 79 (82), 81 (82), 105 (71), 107 (70)... 204 (38)]	10.93*†	1440	[20.40]	9.11	1603	0.07
α-Patchoulene	11.07*	1450	5.33	8.76†	1576	[12.95]
α-Humulene	11.07*	1450	[5.33]	9.19	1610	0.62
Patchoulene analog I	11.11*	1453	2.86	8.78†	1578	[12.95]
γ-Patchoulene	11.11*	1453	[2.86]	8.94	1590	0.98
9-epi-β-Caryophyllene	11.18	1459	0.02	9.32*†	1620	[1.09]
Unknown [m/z 159, 91 (88), 93 (72), 79 (69), 105 (68), 41 (66), 81 (54), 202? (50)...]	11.24	1463	0.43	9.26*†	1615	1.09
Unknown [m/z 147, 93 (87), 107 (77), 105 (77), 91 (73), 79 (63)... 204 (21)]	11.39*	1474	0.64	9.26*†	1615	[1.09]
Selina-4,11-diene	11.39*	1474	[0.64]	9.32*†	1620	[1.09]
β-Selinene	11.45	1479	0.13	9.77	1657	0.08

Patchoulene analog II	11.48	1481	0.10	9.68*	1649	3.26
δ-Selinene	11.53*	1484	0.53	9.58*	1641	0.40
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.53*	1484	[0.53]	9.58*	1641	[0.40]
α-Selinene	11.57	1488	0.25	9.88*	1665	19.08
Eudesma-2,4(15),11-triene	11.69*	1497	3.18	11.00	1758	0.16
Aciphylene	11.69*	1497	[3.18]	9.68*	1649	[3.26]
Pentadecane	11.74	1500	0.30	7.79*	1500	[0.58]
γ-Cadinene	11.82*	1506	18.52	10.33	1702	0.11
δ-Guaiene	11.82*	1506	[18.52]	9.88*	1665	[19.08]
7-epi-α-Selinene	11.88*	1511	0.26	10.35	1704	0.15
Nootkatene	11.88*	1511	[0.26]	10.85	1746	0.01
Unknown [m/z 41, 67 (95), 93 (92), 107 (91), 55 (77), 81 (77), 79 (73)... 205 (17)...]	11.97	1518	0.07	11.24	1779	0.01
Unknown [m/z 161, 119 (92), 91 (69), 105 (52), 145 (49)... 218 (6)]	12.04	1523	0.02	11.19	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)]	12.10	1528	0.11			
Unknown [m/z 91, 105 (78), 93 (77), 107 (71), 79 (64), 41 (63), 77 (63), 145 (60)... 218 (17)]	12.13	1530	0.09			
Norpatchoulenol	12.31	1544	0.57	14.00	2030	0.60
Unknown [m/z 191, 159 (66), 133 (53), 91 (45), 41 (42), 177 (35), 105 (33), 220 (32)]	12.44	1555	0.01	13.58	1990	0.01
Unknown [m/z 41, 67 (90), 55 (87), 79 (85), 107 (84), 81 (84), 93 (84), 121 (77), 91 (74)... 220 (7)]	12.52	1561	0.03			
Unknown [m/z 43, 107 (94), 81	12.62	1570	0.16	12.23	1866	0.14

(71), 41 (63), 67 (58), 111 (58), 93 (55), 83 (54)... 205 (8), 220 (1)]					
Unknown isomer	12.70*	1575	0.28	14.34	2062
Caryophyllene oxide isomer	12.70*	1575	[0.28]	12.60	1899
Caryophyllene oxide	12.70*	1575	[0.28]	12.67	1906
Unknown [m/z 43, 79 (44), 81 (41), 93 (40), 91 (40)... 220 (5)]	12.79	1583	0.29	14.25	2054
Unknown [m/z 43, 105 (77), 91 (71), 93 (68), 41 (62), 107 (6)... 205 (41), 220 (7)]	12.94	1594	0.04	14.56	2084
Hexadecane	13.03*	1601	0.08	9.01	1595
Humulene epoxide II	13.03*	1601	[0.08]	13.26	1960
Unknown [m/z 43, 161 (73), 91 (53), 95 (52), 79 (46), 119 (45)... 205 (29), 220? (1)]	13.10	1607	0.07	14.71*†	2098
Unknown [m/z 41, 91 (92), 55 (81), 93 (81), 79 (74), 43 (71), 95 (68), 123 (65)... 220 (17)]	13.13	1610	0.19	14.78	2105
Unknown [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	13.19	1614	0.17		
Caryophylladienol I	13.28	1622	0.54		
Caryophylladienol II	13.33	1626	0.13	15.99	2228
Hinesol	13.38	1630	0.38	14.91†	2119
Pogostol	13.63*†	1651	30.28	15.14	2141
Patchoulol	13.63*†	1651	[30.28]	14.71*†	2098
Unknown [m/z 175, 218 (59), 133 (49), 91 (43), 41 (38), 147 (36)]	13.65†	1653	[30.28]	14.94†	2122
Unknown [m/z 111, 250 (38), 126 (27), 139 (26), 43	13.94	1676	0.13	11.75	1824
					0.04

(16), 41 (15), 166 (15)]						
Unknown [m/z 91, 41 (100), 107 (98), 108 (95), 95 (87), 93 (87), 105 (85), 79 (77), 119 (72)... 220? (15)]	13.97	1678	0.05	15.90	2220	0.08
Unknown [m/z 43, 41 (95), 97 (89), 109 (71), 55 (71), 107 (70), 95 (69), 110 (65)... 222 (5)]	14.05	1686	0.02	15.36	2164	0.07
Unknown [m/z 105, 107 (98), 91 (95), 166 (80), 248 (80), 93 (76)... 233 (66)]	14.24*	1701	0.13	13.00	1936	0.02
Rotundone	14.24*	1701	[0.13]	15.64	2192	0.12
Unknown [m/z 43, 41 (82), 137 (78), 109 (76), 95 (75), 91 (72), 55 (67)... 220? (14)]	14.27	1704	0.05			
Pogostone	14.34	1710	1.32			
Unknown [m/z 107, 93 (87), 41 (83), 81 (82), 67 (80), 55 (76)... 204 (53), 207 (34), 222 (9)]	14.46	1720	0.21	16.82	2316	0.18
Unknown [m/z 83, 43 (85), 55 (39), 41 (29), 121 (27), 120 (25)... 218 (3)]	14.49	1722	0.08	16.94	2328	0.09
Unknown [m/z 133, 148 (68), 147 (59), 91 (56), 79 (45), 105 (44)... 218 (8)]	14.57	1729	0.04	17.07	2343	0.02
Unknown [m/z 134, 107 (96), 91 (84), 93 (78), 79 (77), 41 (74), 43 (66), 77 (65)...]	14.84	1753	0.02	17.31	2369	0.02
Unknown [m/z 43, 191 (68), 41 (62), 91 (51), 95 (49), 110 (44)... 234 (22)]	14.87	1756	0.03			

Unknown [m/z 91, 105 (88), 95 (79), 93 (78), 81 (72), 79 (66)... 205 (33), 220 (7)...]	14.92	1760	0.09			
Unknown [m/z 149, 131 (54), 105 (48), 91 (46), 41 (30), 93 (27)... 218 (23)]	15.01	1768	0.06	17.23	2360	0.11
Unknown [m/z 43, 95 (58), 67 (50), 41 (47), 55 (38), 109 (37)... 221 (9)... 236? (3)]	15.18	1783	0.02	17.98*	2444	0.08
Unknown [m/z 219, 43 (67), 91 (46), 79 (42), 41 (41), 55 (36)... 234 (6)]	15.33	1796	0.02	17.98*	2444	[0.08]
Unknown [m/z 43, 91 (77), 79 (74), 109 (73), 110 (71)... 218 (52), 234? (1)]	15.40	1802	0.01	17.49	2388	0.01
Unknown [m/z 91, 41 (79), 43 (74), 79 (72), 105 (65), 77 (64), 147 (64), 93 (61)... 218 (26), 234 (14)]	15.46	1807	0.02	17.16	2352	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)]	15.89	1846	0.01	20.68	2763	0.01
Phytol	18.67	2112	0.03	19.10	2572	0.04
Total identified		95.27%			94.76%	
Total reported		97.81%			96.45%	

*: 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