

Date : 2023-09-28

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23I21-PTH03

Customer Identification : Douglas Fir - New Zealand - DC0105R

Type : Essential Oil

Source : *Pseudotsuga menziesii* var. *menziesii* ("Coastal")

Customer : Plant Therapy

Checked and approved by:

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

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID



Results : See analysis summary (next page)

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

Date : 2023-09-25

PHYSICOCHEMICAL DATA

Refractive index : 1.4742 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cindy Caron B. Sc.

Date : 2023-09-22

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
3-Methylcyclopentene	0.02	Alkene
3-Pentanone	tr	Aliphatic ketone
Toluene	0.02	Simple phenolic
Octane	0.02	Alkane
Unknown	tr	Alkene
Ethyl 2-methylbutyrate	0.05	Aliphatic ester
(2E)-Hexenal	0.06	Aliphatic aldehyde
(3Z)-Hexenol	0.06	Aliphatic alcohol
Hexanol	0.04	Aliphatic alcohol
Santene	0.01	Normonoterpene
Styrene	0.01	Simple phenolic
Bornylene	0.01	Monoterpene
Ethanol	tr	Aliphatic alcohol
Tricyclene	0.08	Monoterpene
α -Thujene	1.15	Monoterpene
α -Pinene	15.87	Monoterpene
Camphene	0.67	Monoterpene
α -Fenchene	0.02	Monoterpene
Thuja-2,4(10)-diene	0.03	Monoterpene
β -Pinene	21.26	Monoterpene
Sabinene	11.33	Monoterpene
3-Methyl-3-cyclohexenone	0.02	Aliphatic ketone
Dehydro-1,8-cineole	0.01	Monoterpenic ether
Myrcene	2.18	Monoterpene
α -Phellandrene	0.27	Monoterpene
Pseudolimonene	0.02	Monoterpene
Ethyl hexanoate	0.01	Aliphatic ester
Δ^3 -Carene	10.52	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
α -Terpinene	2.29	Monoterpene
Carvomenthene	0.03	Aliphatic alcohol
para-Cymene	0.85	Monoterpene
1,8-Cineole	[1.51]	Monoterpenic ether
Limonene	2.57	Monoterpene
β -Phellandrene	[1.51]	Monoterpene
(Z)- β -Ocimene	0.10	Monoterpene
(E)- β -Ocimene	0.37	Monoterpene
Unknown	0.04	Unknown
γ -Terpinene	3.81	Monoterpene
cis-Sabinene hydrate	0.07	Monoterpenic alcohol

Unknown	0.01	Unknown
Terpinolene isomer	0.01	Monoterpene
Terpinolene	11.19	Monoterpene
<i>para</i> -Cymenene	0.22	Monoterpene
α -Pinene oxide	0.01	Monoterpenic ether
<i>trans</i> -Sabinene hydrate	0.04	Monoterpenic alcohol
Linalool	0.21	Monoterpenic alcohol
Unknown	0.04	Oxygenated monoterpene
Unknown	0.01	Monoterpenic alcohol
<i>para</i> -Menta-1,3,8-triene	0.04	Monoterpene
<i>cis</i> -Rose oxide	0.02	Monoterpenic ether
endo-Fenchol	0.05	Monoterpenic alcohol
(E)-4,8-Dimethylnona-1,3,7-triene	0.01	Terpene derivative
<i>cis</i> - <i>para</i> -Menth-2-en-1-ol	0.13	Monoterpenic alcohol
Methyl octanoate	0.01	Aliphatic ester
Cosmene	0.01	Monoterpene
1-Terpineol	0.02	Monoterpenic alcohol
<i>trans</i> -Pinocarveol	0.09	Monoterpenic alcohol
<i>trans</i> - <i>para</i> -Menth-2-en-1-ol	0.10	Monoterpenic alcohol
Camphene hydrate	0.05	Monoterpenic alcohol
Epoxyterpinolene	0.03	Monoterpenic ether
Pinocamphone	0.02	Monoterpenic ketone
Citronellal	0.11	Monoterpenic aldehyde
Pinocarvone	0.03	Monoterpenic ketone
Borneol	0.06	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Terpinen-4-ol	4.33	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
<i>para</i> -Cymen-8-ol	0.13	Monoterpenic alcohol
α -Terpineol	0.57	Monoterpenic alcohol
Methyl salicylate	0.03	Phenolic ester
Myrtenol	0.05	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene
Ethyl octanoate	0.05	Aliphatic ester
Verbenone	0.03	Monoterpenic ketone
<i>trans</i> -Piperitol	0.06	Monoterpenic alcohol
Unknown	0.02	Oxygenated monoterpene
Citronellol	0.50	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Thymol methyl ether	0.11	Monoterpenic ether
Neral	0.02	Monoterpenic aldehyde
Piperitone	0.03	Monoterpenic ketone
Geraniol	0.04	Monoterpenic alcohol
<i>trans</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Unknown	0.03	Unknown

Unknown	0.02	Oxygenated monoterpene
Bornyl acetate	0.30	Monoterpenic ester
(E)-Anethole	0.03	Phenylpropanoid
<i>trans</i> -Pinocarvyl acetate	0.03	Monoterpenic ester
Unknown	0.01	Monoterpenic alcohol
Methyl geranate	0.02	Monoterpenic ester
Methyl decanoate	0.02	Aliphatic ester
Citronellic acid	0.01	Monoterpenic acid
δ-Elemene	0.05	Sesquiterpene
α-Longipinene	0.02	Sesquiterpene
Citronellyl acetate	1.65	Monoterpenic ester
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Ethyl (4E)-decenoate	0.02	Aliphatic ester
Geranyl acetate	0.81	Monoterpenic ester
β-Elemene	0.05	Sesquiterpene
allo-Isolongifolene	0.01	Sesquiterpene
Longifolene	0.10	Sesquiterpene
Ethyl decanoate	0.15	Aliphatic ester
β-Caryophyllene	0.08	Sesquiterpene
<i>trans</i> -α-Bergamotene	0.03	Sesquiterpene
6,9-Guaiadiene	0.04	Sesquiterpene
Unknown	0.02	Sesquiterpene
α-Humulene	0.09	Sesquiterpene
Selina-4(15),7-diene	0.08	Sesquiterpene
(E)-β-Farnesene	0.02	Sesquiterpene
γ-Muurolene	0.04	Sesquiterpene
Germacrene D	0.24	Sesquiterpene
δ-Selinene	0.03	Sesquiterpene
Unknown	0.05	Sesquiterpene
α-Muurolene	0.05	Sesquiterpene
Methyl (E)-isoeugenol	0.01	Phenylpropanoid
(Z)-α-Bisabolene	0.03	Sesquiterpene
γ-Cadinene	tr	Sesquiterpene
(3E,6E)-α-Farnesene	0.07	Sesquiterpene
δ-Cadinene	0.13	Sesquiterpene
Methyl laurate?	0.02	Aliphatic ester
(E)-α-Bisabolene	0.05	Sesquiterpene
(E)-Nerolidol	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
Ethyl dodecanoate	0.02	Aliphatic ester
Humulene epoxide II	0.01	Sesquiterpenic ether
Selin-6-en-4a-ol isomer	0.06	Sesquiterpenic alcohol
Alismol	0.01	Sesquiterpenic alcohol
γ-Eudesmol	0.02	Sesquiterpenic alcohol

τ-Cadinol	0.01	Sesquiterpenic alcohol
Cubenol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.03	Sesquiterpenic alcohol
(2E,6E)-Farnesyl acetate	0.01	Sesquiterpenic ester
Cembrene?	0.04	Diterpene
Thunbergol?	0.02	Diterpenic alcohol
(Z)-Abienol	0.10	Diterpenic alcohol
Consolidated total	98.82	

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

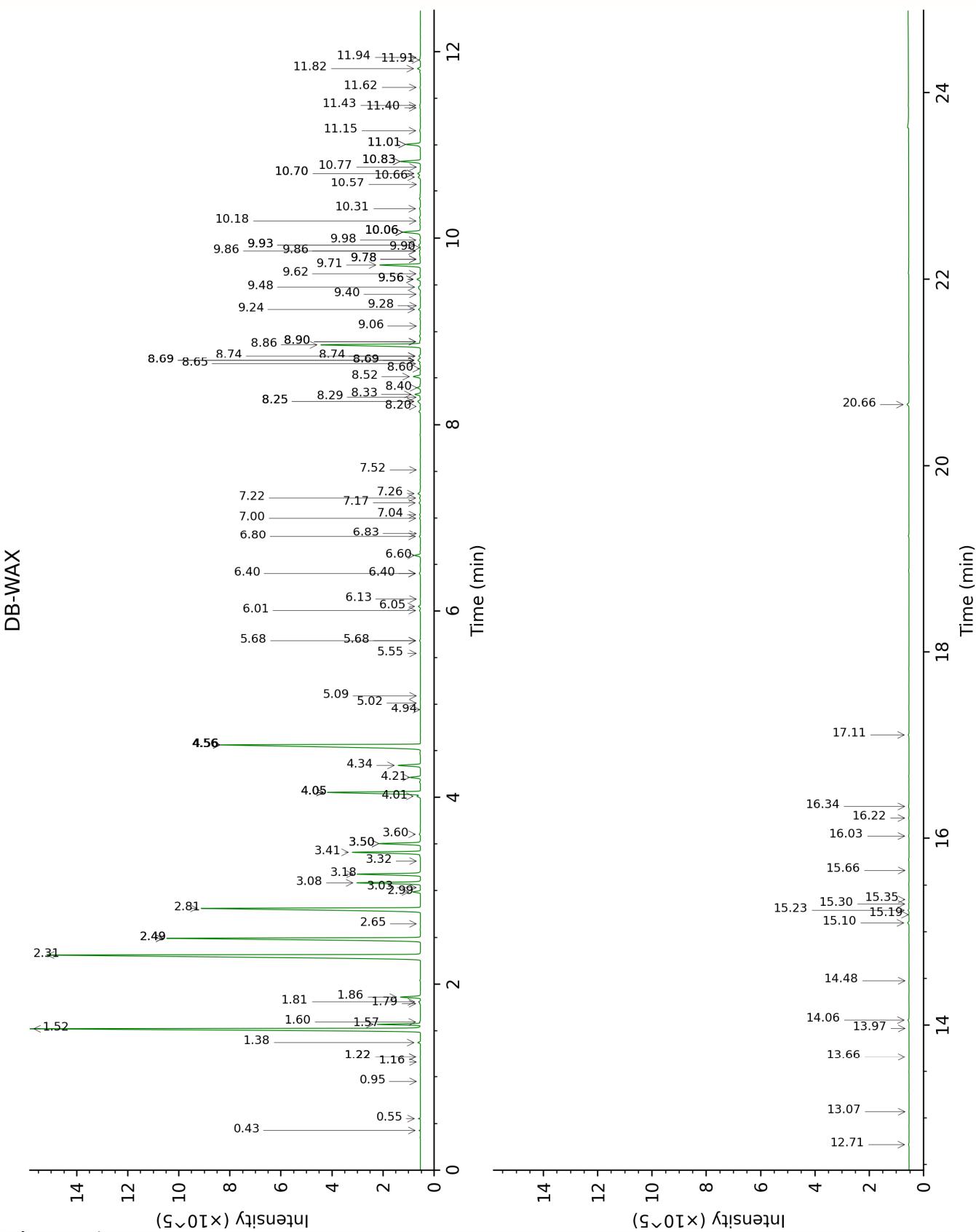
Note: no correction factor was applied

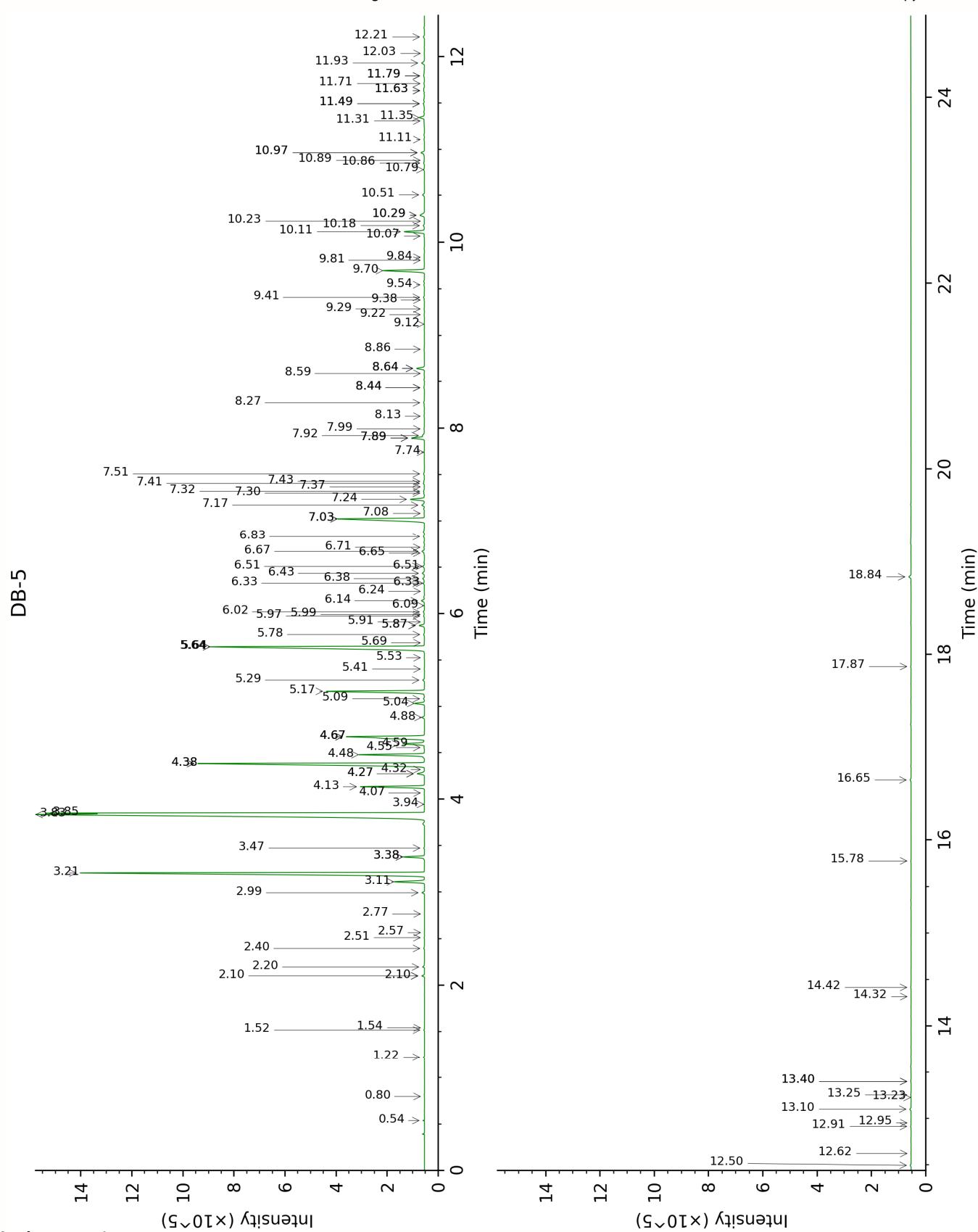
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

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





FULL ANALYSIS DATA

3- Methylcyclopentene	Column DB-WAX			Column DB-5		
	0.43	669.7	0.02	0.54	607.2	0.02
3-Pentanone	1.16	938.7	0.01	0.80	693.9	tr
Toluene	1.60	1000.3	0.02	1.22	759.5	0.02
Octane	0.55	781.0	0.03	1.52	799.8	0.02
Unknown BODA II [m/z 109, 67 (33), 41 (16), 81 (13)... 124 (8)]				1.54	803.2	tr
Ethyl 2-methylbutyrate	1.81	1020.5	0.05	2.10*	849.7	[0.08]
(2E)-Hexenal	3.60	1171.9	0.06	2.10*	849.7	[0.08]
(3Z)-Hexenol	6.05	1347.6	0.08	2.20	857.5	0.06
Hexanol	5.68*	1321.5	[0.04]	2.40	873.8	0.04
Santene	1.22*	947.3	[0.01]	2.51	883.3	0.01
Styrene	4.05*	1205.9	[3.81]	2.57	887.7	0.01
Bornylene	1.22*	947.3	[0.01]	2.77	904.1	0.01
Ethanol	0.95	907.8	tr			
Tricyclene	1.38	970.7	0.08	2.99	919.2	0.08
α-Thujene	1.57	997.9	1.14	3.11	926.9	1.15
α-Pinene	1.52	992.7	15.80	3.21	933.2	15.87
Camphene	1.86	1025.3	0.67	3.38*	944.5	[0.72]
α-Fenchene	1.79	1018.7	0.02	3.38*	944.5	[0.72]
Thuja-2,4(10)-diene	2.49*	1084.8	[11.26]	3.47	950.7	0.03
β-Pinene	2.31	1067.8	21.26	3.83*†	974.3	[24.21]
Sabinene	2.49*	1084.8	[11.26]	3.85*†	975.3	[8.38]
3-Methyl-3-cyclohexenone	6.40*	1372.8	[0.05]	3.94	981.5	0.02
Dehydro-1,8-cineole	3.32	1149.8	0.01	4.07	989.5	0.01
Myrcene	3.08	1132.0	2.26	4.13	994.0	2.18
α-Phellandrene	2.99	1124.5	0.27	4.27*	1003.1	[0.31]
Pseudolimonene	3.03	1128.1	0.02	4.27*	1003.1	[0.31]
Ethyl hexanoate	4.01	1202.9	0.14	4.32	1006.0	0.01
Δ3-Carene	2.81	1111.0	10.52	4.38*	1010.0	[10.56]
(3Z)-Hexenyl acetate	5.09	1281.9	0.01	4.38*	1010.0	[10.56]
α-Terpinene	3.18	1139.1	2.32	4.48	1015.9	2.29
Carvomenthene	2.65	1098.4	0.02	4.55	1020.7	0.03
para-Cymene	4.34	1226.9	0.84	4.59	1023.2	0.85
1,8-Cineole	3.50*	1164.3	[1.51]	4.67*	1027.9	[4.07]
Limonene	3.41	1157.1	2.57	4.67*	1027.9	[4.07]
β-Phellandrene	3.50*	1164.3	[1.51]	4.67*	1027.9	[4.07]
(Z)-β-Ocimene	4.05*	1205.9	[3.81]	4.88	1040.9	0.10
(E)-β-Ocimene	4.21	1217.6	0.38	5.04	1050.7	0.37
Unknown PSME I [m/z 115, 97 (84), 155]	4.56*	1242.9	[11.17]	5.09	1053.9	0.04

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Plus que des analyses... des conseils

(69), 55 (51), 69 (50), 43 (46)...						
γ-Terpinene	4.05*	1205.9	[3.81]	5.17	1058.9	3.81
cis-Sabinene hydrate	7.16	1428.4	0.06	5.29	1066.3	0.07
Unknown PSME III [m/z 101, 88 (98), 43 (54), 55 (44), 41 (40), 95 (40), 73 (36)...]	4.94	1270.5	0.01	5.40	1073.8	0.01
Terpinolene isomer	4.56*	1242.9	[11.17]	5.53	1081.3	0.01
Terpinolene	4.56*	1242.9	[11.17]	5.64*	1088.7	[11.41]
para-Cymenene	6.60	1386.6	0.22	5.64*	1088.7	[11.41]
α-Pinene oxide	5.68*	1321.5	[0.04]	5.69	1091.3	0.01
trans-Sabinene hydrate	8.25*	1509.1	[0.15]	5.78	1096.9	0.04
Linalool	8.33	1514.9	0.21	5.87*	1102.9	[0.21]
Unknown CEDE I [m/z 95, 150 (45), 110 (35), 107 (23), 109 (21)]	6.01	1344.5	0.04	5.87*	1102.9	[0.21]
Unknown ORMA I [m/z 119, 109 (94), 43 (61), 95 (56), 91 (48), 77 (32), 152 (32), 137 (31), 134 (24)]	8.74*	1546.9	[0.07]	5.91	1105.4	0.01
para-Mentha-1,3,8-triene	6.40*	1372.8	[0.05]	5.97	1109.3	0.04
cis-Rose oxide	5.55	1311.8	0.01	5.99	1110.5	0.02
endo-Fenchol	8.65	1540.1	0.04	6.02	1112.2	0.05
(E)-4,8-Dimethylnona-1,3,7-triene	5.02	1276.2	0.01	6.09	1116.5	0.01
cis-para-Menth-2-en-1-ol	8.40	1520.4	0.12	6.14	1119.8	0.13
Methyl octanoate	6.13	1353.2	0.01	6.24	1126.3	0.01
Cosmene	6.83	1403.7	0.01	6.33*	1131.8	[0.05]
1-Terpineol	8.60	1536.0	0.02	6.33*	1131.8	[0.05]
trans-Pinocarveol	9.48	1604.0	0.08	6.38	1134.9	0.09
trans-para-Menth-2-en-1-ol	9.28	1588.2	0.01	6.43	1138.6	0.10
Camphene hydrate	8.74*	1546.9	[0.07]	6.51*	1143.3	[0.08]
Epoxyterpinolene	7.00	1416.2	0.03	6.51*	1143.3	[0.08]
Pinocamphone	7.52	1454.4	0.01	6.65	1152.4	0.02
Citronellal	7.26	1435.7	0.11	6.67	1153.6	0.11
Pinocarvone	8.20	1505.0	0.02	6.71	1156.4	0.03
Borneol	10.06*	1651.0	[0.83]	6.83	1163.8	0.06
Unknown CASA XVIII	9.93*	1639.9	[0.08]	7.03*	1176.2	[4.36]

[m/z 69, 84 (62), 41 (30), 123 (26), 97 (24), 109 (23)…]						
Terpinen-4-ol	8.86	1556.2	4.33	7.03*	1176.2	[4.36]
Unknown PSME IV						
[m/z 96, 119 (99), 96 (86), 91 (81), 43 (65), 41 (49), 67 (45)…]				7.08	1180.0	0.03
para-Cymen-8-ol	11.82	1796.8	0.12	7.17	1185.6	0.13
α-Terpineol	10.06*	1651.0	[0.83]	7.24	1189.6	0.57
Methyl salicylate	10.77	1708.2	0.01	7.30	1193.8	0.03
Myrtenol	11.16	1740.8	0.05	7.32	1195.1	0.05
Unknown MISC XV						
[m/z 121, 43 (99), 91 (85), 77 (73), 93 (41), 136 (33)… 166 (3)]				7.37	1198.1	0.01
Ethyl octanoate	6.80	1401.4	0.04	7.41	1200.5	0.05
Verbenone	9.90	1637.7	0.01	7.43	1201.9	0.03
trans-Piperitol	10.66	1699.1	0.12	7.51	1207.2	0.06
Unknown MISC XVI						
[m/z 122, 91 (56), 79 (33), 95 (33), 107 (31), 43 (30), 77 (30), 135 (27)… 150 (9)]	9.62	1615.4	0.03	7.74	1222.6	0.02
Citronellol	11.01*	1728.5	[0.63]	7.89*	1232.8	[0.52]
Unknown CIAU II						
[m/z 137, 152 (28), 43 (25), 91 (24), 109 (23), 119 (19)]	11.62	1779.7	0.03	7.89*	1232.8	[0.52]
Thymol methyl ether	8.69*	1542.9	[0.14]	7.92	1234.6	0.11
Neral	9.78*	1627.8	[0.03]	7.99	1239.4	0.02
Piperitone	10.18	1660.6	0.03	8.13	1248.5	0.03
Geraniol	11.91	1804.9	0.05	8.27	1258.1	0.04
trans-Ascaridole glycol	14.48	2037.5	0.01	8.44*	1268.9	[0.04]
Unknown PSME V						
[m/z 88, 101 (61), 55 (39), 41 (34), 83 (30), 70 (24), 43 (24)…]				8.44*	1268.9	[0.04]
Unknown CIAU V						
[m/z 95, 67 (45), 41 (42), 110 (42), 43 (41), 59 (36)]	12.72	1875.2	0.02	8.59	1279.1	0.02
Bornyl acetate	8.52	1529.5	0.30	8.64*	1282.7	[0.32]
(E)-Anethole	11.43	1763.5	0.03	8.64*	1282.7	[0.32]

<i>trans</i> -Pinocarvyl acetate	9.40	1597.9	0.03	8.86	1296.9	0.03
Unknown MEAL I [m/z 97, 112 (92), 83 (62), 43 (44), 41 (25)... 170? (4)]	15.30	2116.6	0.01	9.12	1315.4	0.01
Methyl geranate	10.06*	1651.0	[0.83]	9.22	1322.5	0.02
Methyl decanoate	8.90*	1558.7	[0.05]	9.29	1326.9	0.02
Citronellic acid	16.34	2221.1	0.04	9.38	1333.6	0.01
δ -Elemene	7.22	1432.2	0.04	9.41	1335.6	0.05
α -Longipinene	7.04	1419.1	0.03	9.54	1345.0	0.02
Citronellyl acetate	9.71	1622.9	1.69	9.70	1355.7	1.65
Unknown PSME VIII [m/z 43, 95 (53), 121 (47), 107 (38), 93 (36), 41 (35), 67 (31)...]				9.81	1363.5	0.02
Unknown PSME IX [m/z 69, 43 (79), 93 (68), 41 (66), 111 (43), 55 (41), 68 (37)...]				9.84	1365.7	0.02
Ethyl (4E)-decenoate	9.78*	1627.8	[0.03]	10.07	1381.7	0.02
Geranyl acetate	10.83*	1713.3	[0.83]	10.11	1385.0	0.81
β -Elemene	8.69*	1542.9	[0.14]	10.18	1389.6	0.05
allo-Isolongifolene	8.30	1512.5	0.02	10.23	1392.9	0.01
Longifolene	8.25*	1509.1	[0.15]	10.29*	1397.3	[0.25]
Ethyl decanoate	9.56*	1610.7	[0.16]	10.29*	1397.3	[0.25]
β -Caryophyllene	8.69*	1542.9	[0.14]	10.51	1413.3	0.08
<i>trans</i> - α -Bergamotene	8.69*	1542.9	[0.14]	10.78	1433.9	0.03
6,9-Guaiadiene	8.90*	1558.7	[0.05]	10.86	1439.1	0.04
Unknown BOCA IV [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	9.06	1571.5	0.01	10.89	1441.3	0.02
α -Humulene	9.56*	1610.7	[0.16]	10.97*	1447.4	[0.18]
Selina-4(15),7-diene	9.24	1585.2	0.08	10.97*	1447.4	[0.18]
(E)- β -Farnesene	9.86*	1634.9	[0.05]	11.11	1457.9	0.02
γ -Muurolene	9.86*	1634.9	[0.05]	11.31	1472.7	0.04
Germacrene D	10.06*	1651.0	[0.83]	11.34	1475.4	0.24
δ -Selinene	9.98	1644.2	0.03	11.49*	1486.5	[0.08]
Unknown POCA VI [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	9.93*	1639.9	[0.08]	11.49*	1486.5	[0.08]
α -Muurolene	10.31	1671.1	0.05	11.63*	1496.9	[0.04]

Methyl (<i>E</i>)-isoeugenol	15.35	2121.4	0.01	11.63*	1496.9	[0.04]
(<i>Z</i>)- α -Bisabolene	10.57	1691.9	0.01	11.71	1502.5	0.03
γ -Cadinene	10.70*	1702.4	[0.14]	11.79*	1509.0	[0.07]
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	10.83*	1713.3	[0.83]	11.79*	1509.0	[0.07]
δ -Cadinene	10.70*	1702.4	[0.14]	11.93	1519.8	0.13
Methyl laurate?	11.40	1761.4	0.02	12.03	1527.9	0.02
(<i>E</i>)- α -Bisabolene	11.01*	1728.5	[0.63]	12.21	1541.7	0.05
(<i>E</i>)-Nerolidol	14.06	1997.6	0.05	12.50	1564.0	0.04
Caryophyllene oxide	13.07	1906.9	0.01	12.62	1574.1	0.01
Ethyl dodecanoate	11.94	1807.3	0.02	12.92	1596.9	0.02
Humulene epoxide II	13.66	1960.8	0.01	12.95	1599.9	0.01
Selin-6-en-4 α -ol isomer	15.10	2096.7	0.06	13.10	1611.8	0.06
Alismol	16.03	2188.7	0.02	13.23	1622.2	0.01
γ -Eudesmol	15.23	2110.0	0.04	13.25	1624.5	0.02
τ -Cadinol	15.18	2105.4	0.01	13.40*	1636.4	[0.02]
Cubenol	13.97	1989.1	0.01	13.40*	1636.4	[0.02]
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	15.66	2152.1	0.01	14.32	1712.6	0.01
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	17.11	2300.1	0.03	14.42	1721.2	0.03
(2 <i>E</i> ,6 <i>E</i>)-Farnesyl acetate	16.22	2208.4	0.02	15.78	1840.6	0.01
Cembrene?				16.65	1920.4	0.04
Thunbergol?				17.87	2038.5	0.02
(<i>Z</i>)-Abienol	20.66	2699.7	0.09	18.84	2135.4	0.10
Total reported		98.31%			98.82%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is taken into account in the consolidated total

t: 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