Date : 2023-09-14

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 23I07-PTH03
Customer Identification : Petitgrain, - Paraguay - P60108R
Type : Essential Oil
Source : *Citrus aurantium subsp. amara*
Customer : Plant Therapy

Checked an 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

Méthode certifiée ISO 17025:2017 Certified method

Laboratoire PhytoChemia

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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
ISO
Results : See analysis summary (next page)
Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005
Date : 2023-09-12

Physicochemical data

Refractive index : 1.4597 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2023-09-08

Conclusion

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

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Analysis Summary - Consolidated Contents

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

Identification	%	Class
Ethanol	tr	Aliphatic alcohol
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
(3*Z*)-Hexenol	0.02	Aliphatic alcohol
Hexanol	0.02	Aliphatic alcohol
α-Thujene	0.01	Monoterpene
α-Pinene	0.08	Monoterpene
Camphene	0.01	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Sabinene	0.18	Monoterpene
β-Pinene	0.70	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
Myrcene	1.64	Monoterpene
α-Phellandrene	0.04	Monoterpene
cis-Dehydroxylinalool oxide	0.02	Monoterpenic ether
Δ3-Carene	0.53	Monoterpene
(3*Z*)-Hexenyl acetate	0.01	Aliphatic ester
α-Terpinene	0.03	Monoterpene
meta-Cymene	tr	Monoterpene
para-Cymene	0.03	Monoterpene
Limonene	0.98	Monoterpene
β-Phellandrene	0.05	Monoterpene
1,8-Cineole	0.07	Monoterpenic ether
(*Z*)-β-Ocimene	0.66	Monoterpene
(*E*)-β-Ocimene	1.94	Monoterpene
Unknown	0.01	Monoterpene
γ-Terpinene	0.04	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.06	Monoterpenic alcohol
Isoterpinolene	0.02	Monoterpene
para-Cymenene	tr	Monoterpene
Terpinolene	0.43	Monoterpene
trans-Linalool oxide (fur.)	0.05	Monoterpenic alcohol
Rosefuran	tr	Monoterpenic ether
Linalool	29.04	Monoterpenic alcohol
Hotrienol	0.04	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
allo-Ocimene	0.02	Monoterpene
trans-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
Linalyl methyl ether?	0.01	Monoterpenic ether
Benzeneacetonitrile	0.02	Simple phenolic

(*E*)-Myroxide	0.01	Monoterpenic ether
Isopulegol	tr	Monoterpenic alcohol
Citronellal	0.02	Monoterpenic aldehyde
Nerol oxide	0.03	Aliphatic ether
Terpinen-4-ol	0.12	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α-Terpineol	5.56	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.01	Monoterpenic alcohol
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.02	Monoterpenic alcohol
Nerol	1.06	Monoterpenic alcohol
6,7-Dihydro-7-hydroxylinalool	0.01	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
Neral	0.08	Monoterpenic aldehyde
Geraniol	3.11	Monoterpenic alcohol
Linalyl acetate	45.10	Monoterpenic ester
Geranial	0.13	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Geranyl formate	0.02	Monoterpenic ester
Methyl anthranilate	0.02	Phenolic ester
Linalyl propionate	0.05	Monoterpenic ester
Hodiendiol derivative	0.03	Oxygenated monoterpene
α-Terpinyl acetate	0.12	Monoterpenic ester
Unknown	0.05	Sesquiterpene
Neryl acetate	2.28	Monoterpenic ester
Geranyl acetate	3.52	Monoterpenic ester
β-Elemene	0.03	Sesquiterpene
Dimethyl anthranilate	0.01	Phenolic ester
β-Caryophyllene	0.79	Sesquiterpene
Aromadendrene	0.02	Sesquiterpene
α-Humulene	0.08	Sesquiterpene
allo-Aromadendrene	tr	Sesquiterpene
Geranylacetone	tr	Monoterpenic ketone
(*E*)-β-Farnesene	0.01	Sesquiterpene
Bicyclogermacrene	0.17	Sesquiterpene
α-Muurolene	0.02	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	tr	Sesquiterpene
γ-Cadinene	0.03	Sesquiterpene
trans-Calamenene	0.01	Sesquiterpene
δ-Cadinene	0.02	Sesquiterpene
(*E*)-Nerolidol	0.04	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Isospathulenol	0.01	Sesquiterpenic alcohol
τ-Cadinol	0.01	Sesquiterpenic alcohol

(2*E*,6*E*)-Farnesol	0.01	Sesquiterpenic alcohol
Mint sulfide?	tr	Sesquiterpenic sulfide
Phytol	0.02	Diterpenic alcohol
Consolidated total	**99.57**	

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.

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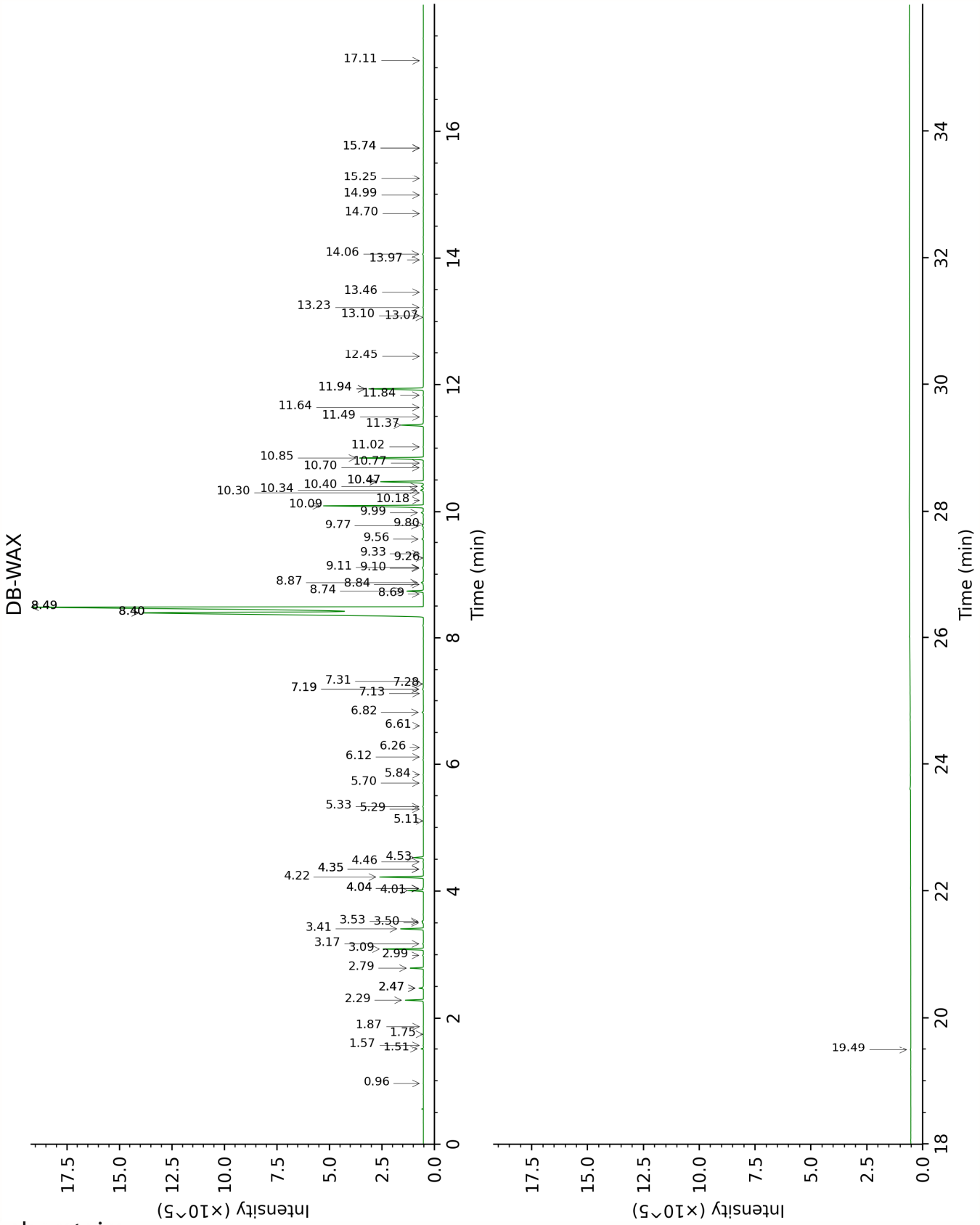
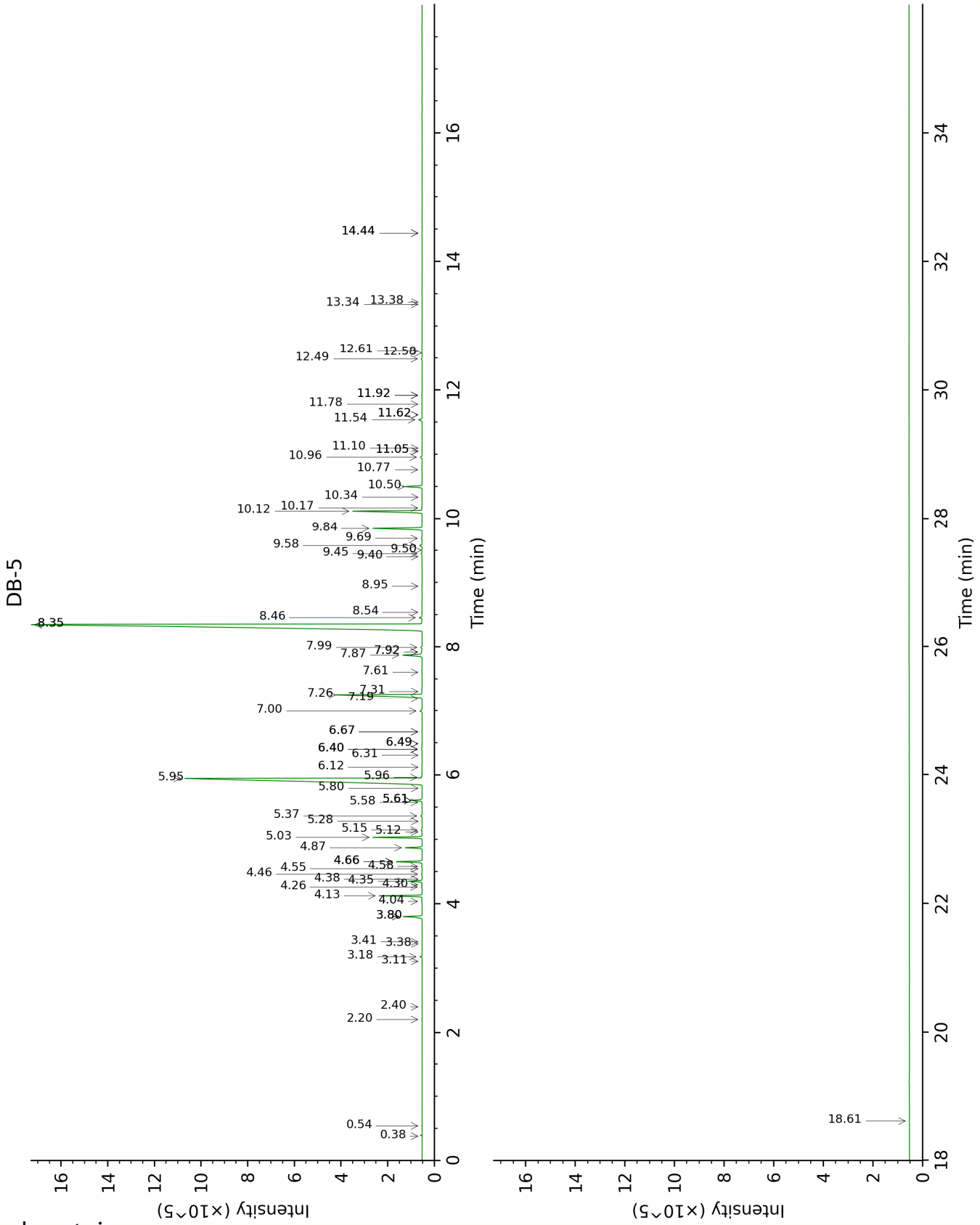

DB-WAX
Time (min)
Intensity (×10^5)
17.11
15.74
15.25
14.99
14.70
14.06
13.97
13.46
13.23
13.10
13.07
12.45
11.94
11.84
11.64
11.49
11.37
11.02
10.85
10.77
10.70
10.47
10.40
10.34
10.30
10.18
10.09
9.99
9.80
9.77
9.56
9.33
9.26
9.11
9.10
8.87
8.84
8.74
8.69
8.49
8.40
7.31
7.28
7.19
7.13
6.82
6.61
6.26
6.12
5.84
5.70
5.33
5.29
5.11
4.53
4.46
4.35
4.22
4.04
4.01
3.53
3.50
3.41
3.17
3.09
2.99
2.79
2.47
2.29
1.87
1.75
1.57
1.51
0.96
19.49


DB-5
Time (min)
Intensity (×10^5)
14.44
13.34
13.38
12.49
12.61
12.59
11.92
11.78
11.54
11.62
11.10
10.96
11.05
10.77
10.50
10.34
10.12
10.17
9.84
9.69
9.58
9.45
9.40
9.50
8.95
8.46
8.54
8.35
7.99
7.87
7.92
7.61
7.26
7.31
7.19
7.00
6.67
6.40
6.49
6.31
6.12
5.95
5.96
5.80
5.58
5.61
5.37
5.28
5.15
5.12
5.03
4.87
4.66
4.46
4.55
4.58
4.38
4.35
4.26
4.30
4.13
4.04
3.80
3.41
3.38
3.18
3.11
2.40
2.20
0.54
0.38
18.61

FULL ANALYSIS DATA

Ethanol	Column DB-WAX			Column DB-5		
	0.96	909.2	tr	0.38	501.8	tr
2-Methyl-3-buten-2-ol	1.75	1014.5	tr	0.54	607.7	0.01
(3*Z*)-Hexenol	6.12	1352.3	0.01	2.20	858.1	0.02
Hexanol	5.70	1322.9	0.02	2.40	874.3	0.02
α-Thujene	1.57	998.1	0.01	3.11	926.7	0.01
α-Pinene	1.51	990.4	0.07	3.18	931.4	0.08
Camphene	1.87	1025.8	0.01	3.38	944.5	0.01
Thuja-2,4(10)-diene	2.47*	1083.1	[0.20]	3.41	946.7	0.01
Sabinene	2.47*	1083.1	[0.20]	3.80*	972.3	[0.88]
β-Pinene	2.28	1065.2	0.70	3.80*	972.3	[0.88]
6-Methyl-5-hepten-2-one	5.33	1296.5	0.04	4.04	987.8	0.03
Myrcene	3.09	1132.4	1.63	4.13	993.5	1.64
α-Phellandrene	2.99	1124.7	0.04	4.26*†	1002.5	[0.04]
cis-Dehydroxylinalool oxide	4.04*	1205.2	[0.05]	4.30*†	1004.7	[0.02]
Δ3-Carene	2.79	1109.4	0.53	4.35	1008.2	0.53
(3*Z*)-Hexenyl acetate	5.11	1283.0	0.01	4.38	1010.1	0.01
α-Terpinene	3.17	1138.7	0.03	4.46	1015.0	0.03
meta-Cymene	4.35*	1227.4	[0.04]	4.55	1020.3	tr
para-Cymene	4.35*	1227.4	[0.04]	4.58	1022.5	0.03
Limonene	3.41	1156.9	0.98	4.66*	1027.1	[1.08]
β-Phellandrene	3.50	1164.1	0.05	4.66*	1027.1	[1.08]
1,8-Cineole	3.53	1166.0	0.07	4.66*	1027.1	[1.08]
(*Z*)-β-Ocimene	4.01	1203.0	0.67	4.87	1040.6	0.66
(*E*)-β-Ocimene	4.22	1218.4	1.94	5.03	1050.6	1.94
Unknown CUSE I [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	4.04*	1205.2	[0.05]	5.12	1055.8	0.01
γ-Terpinene	4.04*	1205.2	[0.05]	5.15	1057.7	0.04
cis-Sabinene hydrate	7.19*	1430.4	[0.06]	5.28	1066.2	0.01
cis-Linalool oxide (fur.)	6.82	1402.8	0.07	5.37	1071.3	0.06
Isoterpinolene	4.46	1235.9	0.02	5.58	1084.5	0.02
para-Cymenene	6.61	1387.3	tr	5.61*	1086.3	[0.46]
Terpinolene	4.53	1240.7	0.43	5.61*	1086.3	[0.46]
trans-Linalool oxide	7.19*	1430.4	[0.06]	5.61*	1086.3	[0.46]

(fur.)						
Rosefuran	6.26	1362.9	0.01	5.80	1098.1	tr
Linalool	8.40*†	1520.3	[33.53]	5.95	1107.8	29.04
Hotrienol	9.11	1575.2	0.05	5.96	1108.8	0.04
cis-para-Menth-2-en-1-ol	8.40*†	1520.3	[33.53]	6.12	1118.8	0.01
allo-Ocimene	5.84	1332.5	0.01	6.31	1130.6	0.02
trans-para-Menth-2-en-1-ol	9.26	1586.7	0.01	6.40*	1136.5	[0.06]
Linalyl methyl ether?	5.29	1296.6	0.01	6.40*	1136.5	[0.06]
Benzeneacetonitrile	12.45	1851.9	0.02	6.40*	1136.5	[0.06]
(*E*)-Myroxide	7.31	1439.4	0.01	6.49*	1142.0	[0.01]
Isopulegol	8.49*†	1527.2	[40.62]	6.49*	1142.0	[0.01]
Citronellal	7.28	1436.6	0.02	6.67*	1153.8	[0.03]
Nerol oxide	7.13	1425.5	0.03	6.67*	1153.8	[0.03]
Terpinen-4-ol	8.87	1556.9	0.10	7.00	1174.3	0.12
para-Cymen-8-ol	11.84	1798.3	0.02	7.19	1186.9	0.02
α-Terpineol	10.09	1653.4	5.54	7.26	1190.9	5.56
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	13.10	1909.5	0.02	7.31	1194.2	0.01
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	11.64	1781.7	0.03	7.61	1213.7	0.02
Nerol	11.36	1758.4	1.15	7.87	1231.5	1.06
6,7-Dihydro-7-hydroxylinalool	13.46	1943.2	0.01	7.92*	1234.6	[0.05]
Citronellol	11.02	1729.6	0.02	7.92*	1234.6	[0.05]
Neral	9.77	1627.3	0.08	7.99	1239.5	0.08
Geraniol	11.94*	1807.0	[2.81]	8.35*	1263.0	[48.22]
Linalyl acetate	8.49*†	1527.2	[40.62]	8.35*	1263.0	[48.22]
Geranial	10.40	1678.0	0.11	8.46	1270.3	0.13
2,6-Dimethyl-1,7-octadiene-3,6-diol	14.99	2086.0	0.01	8.54	1275.8	0.02
Geranyl formate	10.18	1660.2	0.01	8.94	1302.9	0.02
Methyl anthranilate	15.74*	2160.1	[0.01]	9.40	1335.1	0.02
Linalyl propionate	9.10	1574.3	0.02	9.45	1338.4	0.05
Hodiendiol derivative	13.23	1921.3	0.03	9.50	1342.2	0.03
α-Terpinyl acetate	9.99	1644.7	0.12	9.58	1347.3	0.12
Unknown PIMA XXVI [m/z 43, 81 (96), 95 (85), 67 (74), 69 (68), 41 (66)...204				9.69	1355.1	0.05

(1)]						
Neryl acetate	10.47*	1684.0	[2.28]	9.84	1366.0	2.28
Geranyl acetate	10.85	1714.9	3.51	10.12	1385.5	3.52
β-Elemene	8.69	1543.1	0.02	10.17	1389.1	0.03
Dimethyl anthranilate	13.97	1989.5	0.01	10.34	1400.8	0.01
β-Caryophyllene	8.74	1546.6	0.80	10.50	1412.9	0.79
Aromadendrene	8.84	1554.7	0.02	10.76	1432.4	0.02
α-Humulene	9.56	1610.4	0.08	10.96	1446.8	0.08
allo-Aromadendrene	9.33	1591.8	tr	11.05*	1453.7	[0.01]
Geranylacetone	11.94*	1807.0	[2.81]	11.05*	1453.7	[0.01]
(*E*)-β-Farnesene	9.80	1629.7	0.01	11.10	1457.3	0.01
Bicyclogermacrene	10.34	1673.1	0.16	11.54	1490.0	0.17
α-Muurolene	10.30	1669.9	0.02	11.62*	1495.7	[0.02]
(3*Z*,6*E*)-α-Farnesene	10.47*	1684.0	[2.28]	11.62*	1495.7	[0.02]
γ-Cadinene	10.70	1702.2	0.03	11.78	1508.1	0.03
trans-Calamenene	11.49	1769.1	0.01	11.92*	1518.9	[0.03]
δ-Cadinene	10.77	1708.2	0.02	11.92*	1518.9	[0.03]
(*E*)-Nerolidol	14.06	1998.1	0.04	12.49	1563.4	0.04
Spathulenol	14.70	2058.4	0.01	12.58	1570.6	0.01
Caryophyllene oxide	13.07	1907.2	0.02	12.61	1573.2	0.02
Isospathulenol	15.74*	2160.1	[0.01]	13.34	1631.5	0.01
τ-Cadinol	15.25	2111.9	0.01	13.38	1634.5	0.01
(2*E*,6*E*)-Farnesol	17.11	2300.8	0.01	14.44*	1723.4	[0.01]
Mint sulfide?				14.44*	1723.4	[0.01]
Phytol	19.49	2562.1	0.03	18.61	2112.1	0.02
Total reported		99.19%			99.56%	

*: 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

†: 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