Date : 2024-05-13

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 24D29-PTH03
Customer Identification : Petitgrain - Paraguay - P60109R
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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 : 2024-05-07

Physicochemical data

Refractive index : 1.4596 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2024-04-29

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	0.02	Aliphatic alcohol
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
(3*Z*)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
α-Thujene	0.01	Monoterpene
α-Pinene	0.09	Monoterpene
Camphene	tr	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
Sabinene	0.19	Monoterpene
β-Pinene	0.76	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
Myrcene	1.83	Monoterpene
α-Phellandrene	0.04	Monoterpene
Δ3-Carene	0.58	Monoterpene
(3*Z*)-Hexenyl acetate	0.01	Aliphatic ester
α-Terpinene	0.03	Monoterpene
para-Cymene	0.02	Monoterpene
Limonene	1.23	Monoterpene
β-Phellandrene	0.05	Monoterpene
(*Z*)-β-Ocimene	0.75	Monoterpene
(*E*)-β-Ocimene	2.20	Monoterpene
Unknown	0.01	Monoterpene
γ-Terpinene	0.05	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.07	Monoterpenic alcohol
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.50	Monoterpene
para-Cymenene	0.01	Monoterpene
Linalool	28.84	Monoterpenic alcohol
Hotrienol	0.06	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.01	Monoterpene
allo-Ocimene	0.02	Monoterpene
trans-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
neo-allo-Ocimene	0.02	Monoterpene
(*E*)-Myroxide	tr	Monoterpenic ether
Isopulegol	0.03	Monoterpenic alcohol
Citronellal	0.03	Monoterpenic aldehyde
Terpinen-4-ol	0.14	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol

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α-Terpineol	4.50	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.02	Monoterpenic alcohol
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.02	Monoterpenic alcohol
Octyl acetate	0.02	Aliphatic ester
Nerol	1.35	Monoterpenic alcohol
Neral	0.07	Monoterpenic aldehyde
Geraniol	3.60	Monoterpenic alcohol
Linalyl acetate	42.93	Monoterpenic ester
Geranial	0.17	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.03	Monoterpenic alcohol
Bornyl acetate	0.06	Monoterpenic ester
Geranyl formate	0.02	Monoterpenic ester
Methyl anthranilate	0.02	Phenolic ester
Linalyl propionate	0.06	Monoterpenic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
α-Terpinyl acetate	0.14	Monoterpenic ester
Neryl acetate	2.81	Monoterpenic ester
Geranyl acetate	4.04	Monoterpenic ester
β-Elemene	0.04	Sesquiterpene
Dimethyl anthranilate	0.02	Phenolic ester
β-Caryophyllene	0.97	Sesquiterpene
Aromadendrene	0.04	Sesquiterpene
α-Humulene	0.09	Sesquiterpene
Geranylacetone	0.01	Monoterpenic ketone
(*E*)-β-Farnesene	0.02	Sesquiterpene
Bicyclogermacrene	0.19	Sesquiterpene
α-Muurolene	0.01	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	tr	Sesquiterpene
γ-Cadinene	0.03	Sesquiterpene
δ-Cadinene	0.03	Sesquiterpene
(*E*)-Nerolidol	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
(2*E*,6*E*)-Farnesol	0.02	Sesquiterpenic alcohol
meta-Camphorene	0.01	Diterpene
Phytol	0.02	Diterpenic alcohol
Consolidated total	**99.19**	

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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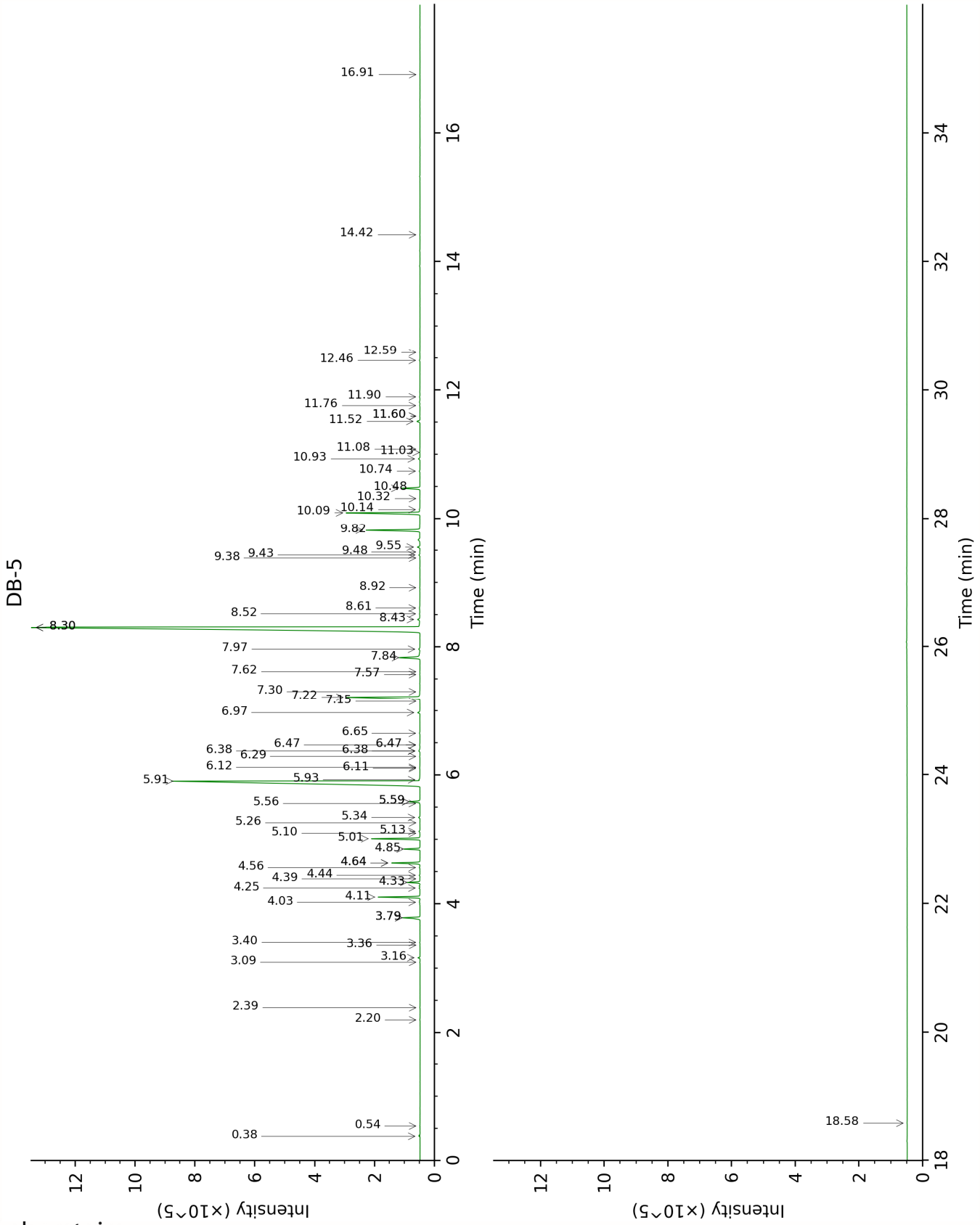
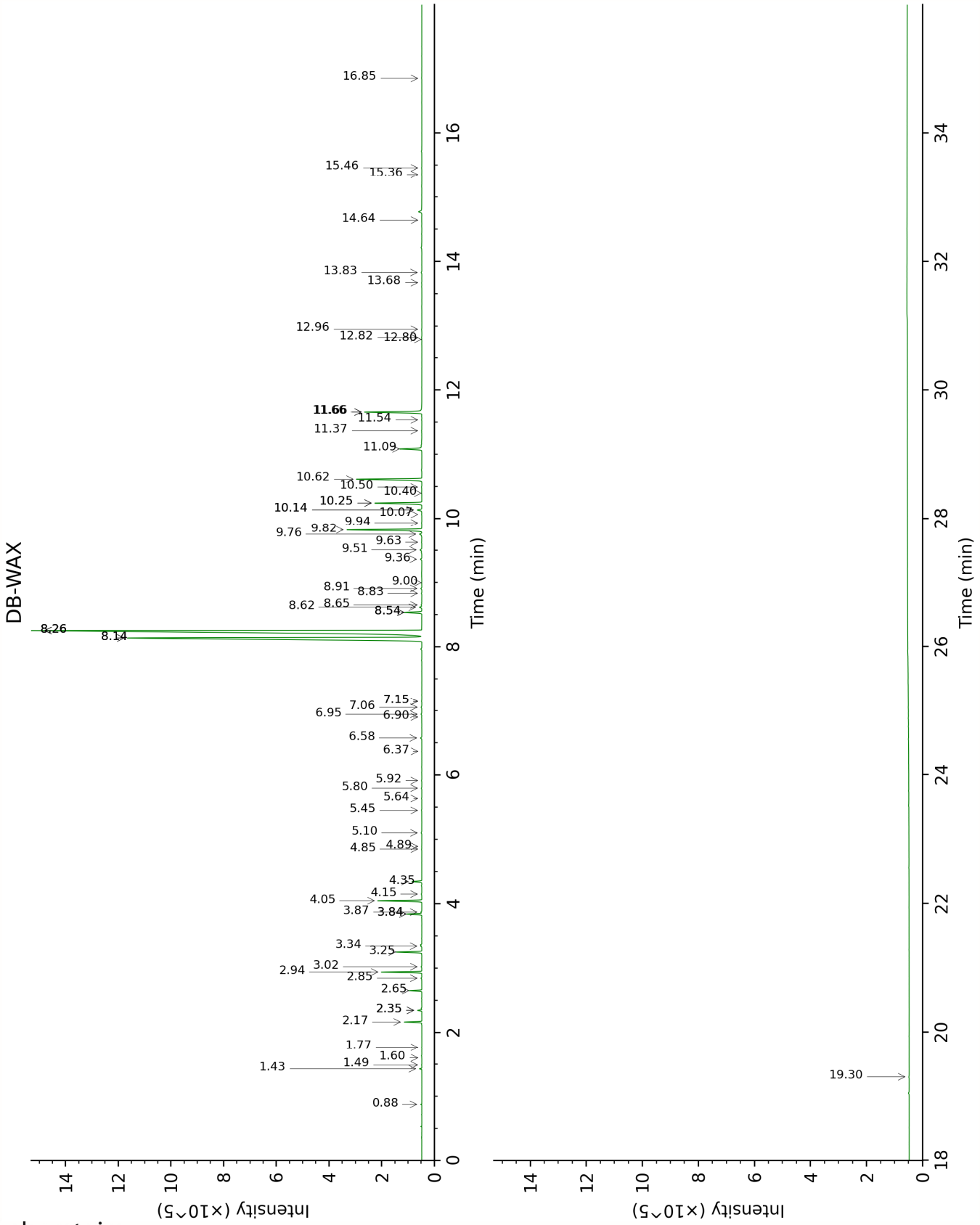

DB-5
16.91
14.42
12.59
12.46
11.90
11.76
11.60
11.52
11.08
11.03
10.93
10.74
10.48
10.32
10.14
10.09
9.82
9.55
9.48
9.43
9.38
8.92
8.61
8.52
8.43
8.30
7.97
7.84
7.62
7.57
7.30
7.22
7.15
6.97
6.65
6.47
6.47
6.38
6.38
6.29
6.12
6.11
5.93
5.91
5.59
5.56
5.34
5.26
5.13
5.10
5.01
4.85
4.64
4.56
4.44
4.39
4.33
4.25
4.11
4.03
3.79
3.40
3.36
3.16
3.09
2.39
2.20
0.54
0.38
Time (min)
Intensity (×10^5)
18.58
Time (min)
Intensity (×10^5)


DB-WAX
Intensity (×10^5)
Time (min)
16.85
15.46
15.36
14.64
13.83
13.68
12.96
12.82
12.80
11.66
11.54
11.37
11.09
10.62
10.50
10.40
10.25
10.14
10.07
9.94
9.82
9.76
9.63
9.51
9.36
9.00
8.91
8.83
8.65
8.62
8.54
8.26
8.14
7.15
7.06
6.95
6.90
6.58
6.37
5.92
5.80
5.64
5.45
5.10
4.89
4.85
4.35
4.15
4.05
3.87
3.84
3.34
3.25
3.02
2.94
2.85
2.65
2.35
2.17
1.77
1.60
1.49
1.43
0.88
19.30

FULL ANALYSIS DATA

	Column DB-5			Column DB-WAX		
Ethanol	0.38	500.9	0.02	0.88	911.3	0.03
2-Methyl-3-buten-2-ol	0.54	606.8	tr	1.60	1016.1	tr
(3*Z*)-Hexenol	2.20	858.5	0.01	5.80	1343.6	0.03
Hexanol	2.39	874.1	0.01	5.45	1318.4	0.02
α-Thujene	3.09	926.9	0.01	1.49	1003.1	0.01
α-Pinene	3.16	931.6	0.09	1.43	994.2	0.08
Camphene	3.36	944.4	tr	1.77	1031.7	0.01
Thuja-2,4(10)-diene	3.40	947.2	0.02	2.35*	1085.9	[0.18]
Sabinene	3.78*	972.5	[0.95]	2.35*	1085.9	[0.18]
β-Pinene	3.78*	972.5	[0.95]	2.17	1068.9	0.76
6-Methyl-5-hepten-2-one	4.02	988.3	0.03	5.10	1292.7	0.05
Myrcene	4.11	993.6	1.83	2.94	1135.1	1.83
α-Phellandrene	4.25	1002.9	0.04	2.85	1127.9	0.04
Δ3-Carene	4.33	1008.5	0.58	2.65	1113.4	0.56
(3*Z*)-Hexenyl acetate	4.39	1011.9	0.01	4.89	1277.8	0.01
α-Terpinene	4.44	1015.4	0.03	3.02	1141.2	0.04
para-Cymene	4.56	1022.9	0.02	4.15	1225.2	0.04
Limonene	4.64*	1027.4	[1.33]	3.25	1158.5	1.23
β-Phellandrene	4.64*	1027.4	[1.33]	3.34	1165.4	0.05
(*Z*)-β-Ocimene	4.85	1040.9	0.75	3.84*	1203.1	[0.76]
(*E*)-β-Ocimene	5.01	1051.0	2.20	4.05	1217.9	2.22
Unknown CUSE I [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	5.10	1056.2	0.01	3.84*	1203.1	[0.76]
γ-Terpinene	5.13	1058.1	0.05	3.87	1205.3	0.05
cis-Sabinene hydrate	5.26	1066.4	0.01	6.90	1424.6	0.02
cis-Linalool oxide (fur.)	5.34	1071.6	0.07	6.58	1400.4	0.08
trans-Linalool oxide (fur.)	5.56	1085.2	0.02	6.95	1427.9	0.05
Terpinolene	5.59*	1086.9	[0.54]	4.35	1239.0	0.50
para-Cymenene	5.59*	1086.9	[0.54]	6.37	1385.2	0.01
Linalool	5.91	1106.9	28.84	8.14*†	1518.1	[28.69]
Hotrienol	5.93	1108.3	0.06	8.83	1572.5	0.03
cis-para-Menth-2-en-1-ol	6.10	1119.6	0.01	8.14*†	1518.1	[28.69]

(*E*)-4,8-Dimethyl-1,3,7-nonatriene	6.12	1120.6	0.01	4.85	1274.8	0.01
allo-Ocimene	6.29	1131.5	0.02	5.64	1331.9	0.02
trans-para-Menth-2-en-1-ol	6.38*	1136.8	[0.10]	9.00	1585.4	0.01
neo-allo-Ocimene	6.38*	1136.8	[0.10]	5.92	1352.2	0.02
(*E*)-Myroxide	6.47*	1142.8	[0.03]	7.15*	1443.1	[0.02]
Isopulegol	6.47*	1142.8	[0.03]	8.26*†	1527.2	[42.79]
Citronellal	6.65	1154.4	0.03	7.06	1436.1	0.05
Terpinen-4-ol	6.97	1174.9	0.14	8.62	1555.5	0.13
para-Cymen-8-ol	7.15	1186.4	0.01	11.54	1796.2	0.01
α-Terpineol	7.22	1190.6	4.50	9.82	1651.9	4.48
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	7.30	1196.1	0.02	12.82	1910.4	0.02
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.57	1213.6	0.02	11.37	1781.8	0.01
Octyl acetate	7.62	1216.6	0.02	7.15*	1443.1	[0.02]
Nerol	7.84	1231.2	1.35	11.09	1757.6	1.38
Neral	7.97	1240.0	0.07	9.51	1626.1	0.12
Geraniol	8.30*	1262.5	[46.53]	11.66*	1806.6	[3.61]
Linalyl acetate	8.30*	1262.5	[46.53]	8.26*†	1527.2	[42.79]
Geranial	8.43	1270.9	0.17	10.14*	1677.8	[0.29]
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.52	1276.7	0.03	14.64	2082.7	0.01
Bornyl acetate	8.61	1282.8	0.06	8.26*†	1527.2	[42.79]
Geranyl formate	8.92	1303.9	0.02	9.94	1661.0	0.02
Methyl anthranilate	9.38	1336.3	0.02	15.36	2153.3	0.01
Linalyl propionate	9.43	1339.6	0.06	8.91	1578.4	0.06
Hodiendiol derivative	9.48	1342.9	0.02	12.96	1922.6	0.02
α-Terpinyl acetate	9.55	1348.3	0.14	9.76	1646.2	0.14
Neryl acetate	9.82	1367.0	2.81	10.25*	1686.6	[2.81]
Geranyl acetate	10.09	1386.5	4.04	10.62	1717.3	4.07
β-Elemene	10.14	1390.1	0.04	8.54*	1549.3	[0.98]
Dimethyl anthranilate	10.32	1402.2	0.02	13.68	1989.8	0.02
β-Caryophyllene	10.48	1413.9	0.97	8.54*	1549.3	[0.98]
Aromadendrene	10.74	1433.6	0.04	8.65	1558.3	0.04
α-Humulene	10.93	1447.9	0.09	9.36	1614.1	0.08
Geranylacetone	11.03	1455.3	0.01	11.66*	1806.6	[3.61]
(*E*)-β-Farnesene	11.08	1459.0	0.02	9.63	1635.9	0.01
Bicyclogermacrene	11.52	1491.2	0.19	10.14*	1677.8	[0.29]

α-Muurolene	11.60*	1497.2	[0.02]	10.07	1672.0	0.01
(3*Z*,6*E*)-α-Farnesene	11.60*	1497.2	[0.02]	10.25*	1686.6	[2.81]
γ-Cadinene	11.76	1509.6	0.03	10.40	1699.2	0.02
δ-Cadinene	11.90	1520.2	0.03	10.50	1707.0	0.02
(*E*)-Nerolidol	12.46	1564.8	0.04	13.83	2004.5	0.05
Caryophyllene oxide	12.59	1574.6	0.02	12.80	1908.2	0.01
(2*E*,6*E*)-Farnesol	14.42	1724.8	0.02	16.85	2308.0	0.02
meta-Camphorene	16.91	1949.7	0.01	15.46	2164.0	0.02
Phytol	18.58	2112.9	0.02	19.30	2581.7	0.03
Total reported		99.34%			98.77%	

*: 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

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