Date : September 23, 2020

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 20I14-PTH04
Customer identification : Petitgrain - P60106810R
Type : Essential oil
Source : *Citrus x aurantium*
Customer : Plant Therapy

Analysis

Method: PC-MAT-014 ISO - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.
Analyst : Fanny Charlier, B. Sc., chimiste à l'entraînement
Analysis date : September 17, 2020

Checked and approved by :

Alexis St-Gelais, M. Sc., chimiste 2013-174

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Méthode certifiée ISO 17025:2017 Certified method

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid
Refractive index: 1.4593 ± 0.0003 (20 °C; method PC-MAT-016)

ISO 8901:2004 - OIL OF BITTER ORANGE PETITGRAIN, CULTIVATED

Compound	Min. %	Max. %	Observed %	Complies?
Geranyl acetate	1.5	5.5	3.9	Yes
Geraniol	1	4	3	Yes
α-Terpineol	1	7	6	Yes
Linalyl acetate	40	72	47	Yes
Linalool	10	32	26	Yes
(E)-β-Ocimene	1	4	2	Yes
Limonene	1	6	1	Yes
Refractive index	1.4550	1.4720	1.4593	Yes

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
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isoamyl alcohol	tr	Aliphatic alcohol
Toluene	0.01	Simple phenolic
(3*Z*)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.02	Aliphatic alcohol
α-Thujene	0.03	Monoterpene
α-Pinene	0.11	Monoterpene
Camphene	0.01	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
β-Pinene	1.05	Monoterpene
Sabinene	0.15	Monoterpene
6-Methyl-5-hepten-2-one	0.05	Aliphatic ketone
Myrcene	1.82	Monoterpene
α-Phellandrene	0.04	Monoterpene
Octanal	0.03	Aliphatic aldehyde
Δ3-Carene	0.36	Monoterpene
α-Terpinene	0.04	Monoterpene
para-Cymene	0.03	Monoterpene
Limonene	0.83	Monoterpene
1,8-Cineole	0.05	Monoterpenic ether
β-Phellandrene	0.04	Monoterpene
(*Z*)-β-Ocimene	0.74	Monoterpene
(*E*)-β-Ocimene	2.17	Monoterpene
Unknown	0.01	Monoterpene
γ-Terpinene	0.06	Monoterpene
cis-Sabinene hydrate	0.02	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.05	Monoterpenic alcohol
Terpinolene	0.43	Monoterpene
trans-Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Linalool	25.53	Monoterpenic alcohol
Hotrienol	0.04	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
allo-Ocimene	0.02	Monoterpene
Camphor	0.01	Monoterpenic ketone
trans-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
neo-allo-Ocimene	0.01	Monoterpene
Benzeneacetonitrile	0.01	Simple phenolic
Isopulegol	0.02	Monoterpenic alcohol
Camphene hydrate	0.01	Monoterpenic alcohol
Citronellal	0.04	Monoterpenic aldehyde
Borneol	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.16	Monoterpenic alcohol
α-Terpineol	5.78	Monoterpenic alcohol
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.01	Monoterpenic alcohol
Linalyl formate	0.02	Monoterpenic ester

Nerol	1.21	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
Neral	0.09	Monoterpenic aldehyde
Linalyl acetate	46.52	Monoterpenic ester
Geraniol	3.04	Monoterpenic alcohol
Geranial	0.15	Monoterpenic aldehyde
Bornyl acetate	0.01	Monoterpenic ester
4-Vinylguaiacol	0.02	Simple phenolic
Methyl anthranilate	0.02	Phenolic ester
Linalyl propionate	0.04	Monoterpenic ester
Hodiendiol derivative	0.01	Oxygenated monoterpene
α-Terpinyl acetate	0.10	Monoterpenic ester
Unknown	0.03	Sesquiterpene
Neryl acetate	2.27	Monoterpenic ester
Geranyl acetate	3.91	Monoterpenic ester
β-Elemene	0.03	Sesquiterpene
Dimethyl anthranilate	0.01	Phenolic ester
β-Caryophyllene	0.71	Sesquiterpene
α-Humulene	0.08	Sesquiterpene
(*E*)-β-Farnesene	0.02	Sesquiterpene
γ-Muurolene	0.01	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Bicyclogermacrene	0.24	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	0.01	Sesquiterpene
α-Muurolene	0.01	Sesquiterpene
γ-Cadinene	0.04	Sesquiterpene
trans-Calamenene	0.01	Sesquiterpene
δ-Cadinene	0.01	Sesquiterpene
(*E*)-Nerolidol	0.06	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
τ-Cadinol	0.01	Sesquiterpenic alcohol
α-Cadinol	0.01	Sesquiterpenic alcohol
Mint sulfide?	0.03	Sesquiterpenic sulfide
meta-Camphorene	0.01	Diterpene
Phytol	0.03	Diterpenic alcohol
Consolidated total	**98.73%**	

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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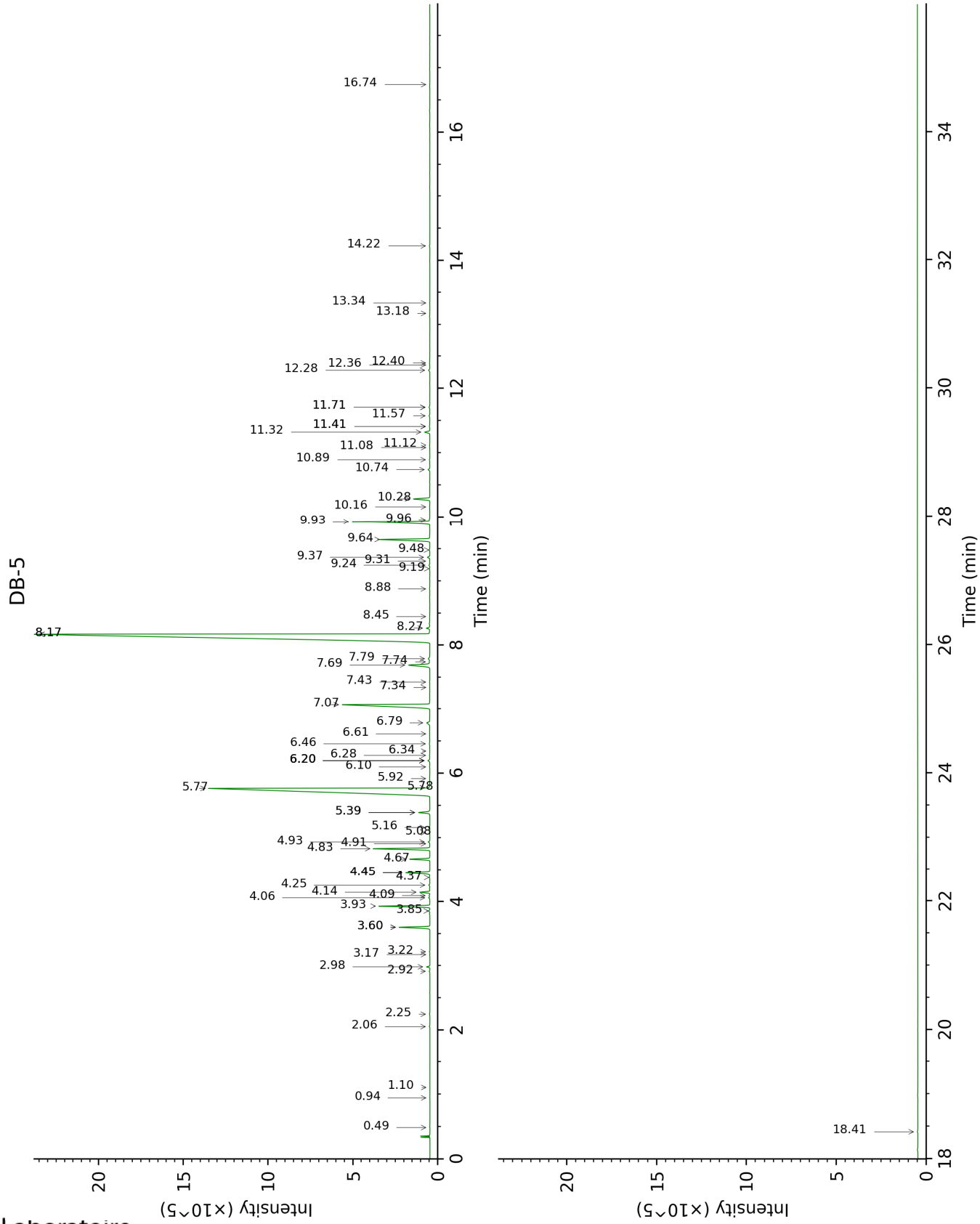
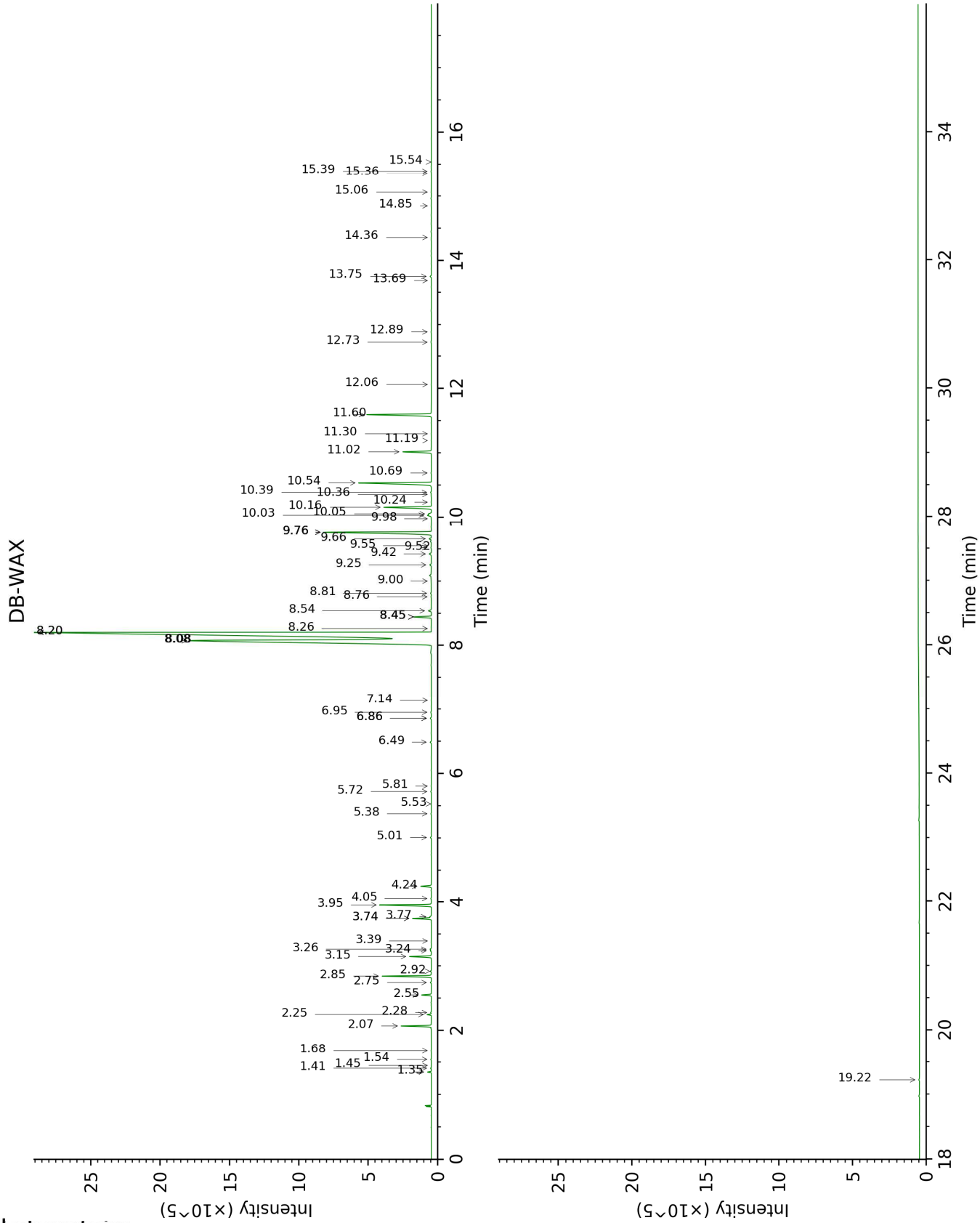

DB-5
16.74
14.22
13.34
13.18
12.28
12.36
12.40
11.71
11.57
11.32
11.41
11.08
11.12
10.89
10.74
10.28
10.16
9.93
9.96
9.64
9.37
9.48
9.24
9.31
9.19
8.88
8.45
8.27
8.17
7.69
7.79
7.74
7.43
7.34
7.07
6.79
6.61
6.46
6.34
6.28
6.20
6.10
5.92
5.78
5.77
5.39
5.16
5.08
4.93
4.83
4.91
4.67
4.45
4.37
4.25
4.14
4.09
4.06
3.93
3.85
3.60
3.17
3.22
2.98
2.92
2.25
2.06
1.10
0.94
0.49
18.41
Time (min)
Intensity (×10^5)


DB-WAX
Intensity (×10^5)
Time (min)
8.20
8.08
8.26
8.54
8.81
8.76
8.45
9.00
9.25
9.76
9.66
9.55
9.42
9.52
10.03
10.16
10.05
9.98
10.39
10.54
10.36
10.24
10.69
11.02
11.30
11.19
11.60
12.06
12.73
12.89
13.75
13.69
14.36
14.85
15.06
15.39
15.36
15.54
19.22
6.95
6.86
7.14
6.49
5.72
5.81
5.53
5.38
5.01
3.95
4.05
3.74
3.77
4.24
3.26
3.15
3.39
3.24
2.85
2.75
2.92
2.55
2.25
2.28
2.07
1.68
1.41
1.45
1.54
1.35

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2-Methyl-3-buten-2-ol	0.49	604	tr	1.54	1012	0.02
Isoamyl alcohol	0.94	734	tr	3.39	1175	tr
Toluene	1.10	757	0.01	1.45	1003	0.01
(3*Z*)-Hexenol	2.06	858	0.03	5.72	1342	0.03
Hexanol	2.25	874	0.02	5.38	1317	0.02
α-Thujene	2.92	925	0.03	1.41	999	0.02
α-Pinene	2.98	930	0.11	1.35	990	0.10
Camphene	3.17	942	0.01	1.68	1026	0.01
Thuja-2,4(10)-diene	3.22	945	0.02	2.28	1086	0.03
β-Pinene	3.60*	971	1.20	2.07	1065	1.05
Sabinene	3.60*	971	[1.20]	2.25	1082	0.15
6-Methyl-5-hepten-2-one	3.85	988	0.05	5.01	1293	0.04
Myrcene	3.93	992	1.82	2.85	1132	1.80
α-Phellandrene	4.06	1001	0.04	2.75	1124	0.04
Octanal	4.09	1003	0.03			
Δ3-Carene	4.14	1007	0.36	2.55	1109	0.35
α-Terpinene	4.25	1014	0.04	2.92	1138	0.04
para-Cymene	4.37	1021	0.03	4.05	1224	0.02
Limonene	4.45*	1026	0.93	3.15	1156	0.83
1,8-Cineole	4.45*	1026	[0.93]	3.26	1165	0.05
β-Phellandrene	4.45*	1026	[0.93]	3.24	1163	0.04
(*Z*)-β-Ocimene	4.67	1040	0.74	3.74*	1202	0.74
(*E*)-β-Ocimene	4.83	1050	2.17	3.95	1217	2.14
Unknown [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	4.91	1054	0.01	3.74*	1202	[0.74]
γ-Terpinene	4.94	1056	0.06	3.77	1204	0.06
cis-Sabinene hydrate	5.08	1065	0.02	6.86*	1426	0.05
cis-Linalool oxide (fur.)	5.16	1070	0.05	6.49	1398	0.06
Terpinolene	5.39*	1085	0.47	4.24	1238	0.43
trans-Linalool oxide (fur.)	5.39*	1085	[0.47]	6.86*	1426	[0.05]
Linalool	5.77	1108	25.53	8.08*†	1517	72.09
Hotrienol	5.78	1109	0.04	8.76	1570	0.02
cis-para-Menth-2-en-1-ol	5.92	1118	0.01	8.08*†	1517	[72.09]
allo-Ocimene	6.10	1130	0.02	5.53	1328	0.01
Camphor	6.20*	1136	0.09	7.14	1446	0.01
trans-para-Menth-2-en-1-ol	6.20*	1136	[0.09]	9.00	1589	0.01
neo-allo-Ocimene	6.20*	1136	[0.09]	5.81	1348	0.01
Benzeneacetonitrile	6.20*	1136	[0.09]	12.06	1846	0.01
Isopulegol	6.28	1141	0.02	8.20*†	1527	[72.09]

Camphene hydrate	6.34	1145	0.01	8.44*	1546	0.74
Citronellal	6.46	1152	0.04	6.95	1433	0.04
Borneol	6.61	1162	0.02	9.76*	1650	5.78
Terpinen-4-ol	6.78	1173	0.16	8.54	1553	0.14
α-Terpineol	7.07	1191	5.78	9.76*	1650	[5.78]
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.34	1209	0.01	11.30	1779	0.01
Linalyl formate	7.43	1215	0.02	8.44*	1546	[0.74]
Nerol	7.69	1232	1.21	11.02	1755	1.25
Citronellol	7.74	1236	0.02	10.69	1727	0.02
Neral	7.79	1239	0.09	9.42	1623	0.11
Linalyl acetate	8.17*	1264	49.63	8.20*†	1527	[72.09]
Geraniol	8.17*	1264	[49.63]	11.60	1805	3.04
Geranial	8.27	1271	0.15	10.06	1674	0.12
Bornyl acetate	8.45	1282	0.01	8.26	1532	0.01
4-Vinylguaiacol	8.88	1311	0.02	15.06	2126	0.01
Methyl anthranilate	9.19	1333	0.02	15.39	2159	0.02
Linalyl propionate	9.24	1337	0.04	8.81	1574	0.04
Hodiendiol derivative	9.31	1341	0.01	12.89	1920	0.02
α-Terpinyl acetate	9.37	1346	0.10	9.66	1642	0.10
Unknown [m/z 43, 81 (96), 95 (85), 67 (74), 69 (68), 41 (66)...204 (1)]	9.48	1354	0.03			
Neryl acetate	9.64	1365	2.27	10.16	1683	2.28
Geranyl acetate	9.93	1385	3.91	10.54	1714	3.97
β-Elemene	9.96	1387	0.03	8.44*	1546	[0.74]
Dimethyl anthranilate	10.16	1401	0.01	13.69	1993	0.01
β-Caryophyllene	10.28	1411	0.71	8.44*	1546	[0.74]
α-Humulene	10.74	1445	0.08	9.25	1609	0.07
(*E*)-β-Farnesene	10.89	1456	0.02	9.52	1631	0.02
γ-Muurolene	11.08	1470	0.01	9.55	1633	0.01
Germacrene D	11.12	1473	0.01	9.76*	1650	[5.78]
Bicyclogermacrene	11.32	1488	0.24	10.03	1673	0.21
(3*Z*,6*E*)-α-Farnesene	11.41*	1494	0.03	10.24	1689	0.01
α-Muurolene	11.41*	1494	[0.03]	9.98	1668	0.01
γ-Cadinene	11.58	1507	0.04	10.39	1702	0.04
trans-Calamenene	11.71*	1518	0.05	11.19	1770	0.01
δ-Cadinene	11.71*	1518	[0.05]	10.36	1699	0.01
(*E*)-Nerolidol	12.28	1563	0.06	13.75	2000	0.06
Spathulenol	12.36	1569	0.01	14.36	2058	0.01
Caryophyllene oxide	12.40	1572	0.02	12.73	1905	0.03
τ-Cadinol	13.18	1635	0.01	14.85	2105	0.01
α-Cadinol	13.34	1648	0.01	15.54	2174	0.01
Mint sulfide?	14.22	1722	0.03			
meta-Camphorene	16.74	1951	0.01	15.36	2156	0.01
Phytol	18.41	2116	0.03	19.22	2573	0.04
Total identified		**98.88%**			**98.56%**	

Total reported	**98.92%**	**98.56%**

*: 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

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