

Date : October 11, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22J04-PTH03


Customer identification : Petitgrain - Paraguay - P60107R

Type : Essential oil

Source : *Citrus x aurantium*

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 : Amélie Simard, Analyste

Analysis date : October 07, 2022

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4599 ± 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
2-Methyl-3-buten-2-ol	0.02	Aliphatic alcohol
(3Z)-Hexenol	0.03	Aliphatic alcohol
(2E)-Hexenol	tr	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	0.15	Monoterpene
β -Pinene	0.76	Monoterpene
6-Methyl-5-hepten-2-one	0.04	Aliphatic ketone
Myrcene	2.53	Monoterpene
6-Methyl-5-hepten-2-ol	0.02	Aliphatic alcohol
Pseudolimonene	0.11	Monoterpene
α -Phellandrene	0.04	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
Δ^3 -Carene	0.45	Monoterpene
α -Terpinene	0.04	Monoterpene
para-Cymene	0.02	Monoterpene
1,8-Cineole	0.10*	Monoterpenic ether
β -Phellandrene	0.10*	Monoterpene
Limonene	2.21	Monoterpene
(Z)- β -Ocimene	0.59	Monoterpene
(E)- β -Ocimene	1.79	Monoterpene
Unknown	0.01	Monoterpene
γ -Terpinene	0.04	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.06	Monoterpenic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.38	Monoterpene
para-Cymenene	0.01	Monoterpene
Rosefuran	0.01	Monoterpenic ether
Linalool	26.97	Monoterpenic alcohol
Hotrienol	0.02	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
<i>cis</i> -para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
allo-Ocimene	0.01	Monoterpene
<i>trans</i> -para-Menth-2-en-1-ol	0.02	Monoterpenic alcohol
neo-allo-Ocimene	0.02	Monoterpene
Isopulegol	0.02	Monoterpenic alcohol
Citronellal	0.03	Monoterpenic aldehyde
Terpinen-4-ol	0.10	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
α -Terpineol	3.50	Monoterpenic alcohol
Hodiendiol	0.02	Monoterpenic alcohol

(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.01	Monoterpenic alcohol
Linalyl formate	0.01	Monoterpenic ester
Nerol	1.35	Monoterpenic alcohol
Citronellol	0.04	Monoterpenic alcohol
Neral	0.10	Monoterpenic aldehyde
Linalyl acetate	44.59	Monoterpenic ester
Geraniol	3.63	Monoterpenic alcohol
Geranial	0.16	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Isobornyl acetate	0.01	Monoterpenic ester
Bornyl acetate	0.01	Monoterpenic ester
4-Vinylguaiaacol	0.01	Simple phenolic
Methyl anthranilate	0.01	Phenolic ester
Linalyl propionate	0.06	Monoterpenic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
α -Terpinyl acetate	0.15	Monoterpenic ester
Eugenol	0.01	Phenylpropanoid
Unknown	0.05	Sesquiterpene
Neryl acetate	2.88	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
Geranyl acetate	3.89	Monoterpenic ester
β -Elemene	0.04	Sesquiterpene
Dimethyl anthranilate	0.02	Phenolic ester
β -Caryophyllene	1.12	Sesquiterpene
Aromadendrene	0.06	Sesquiterpene
α -Humulene	0.10	Sesquiterpene
Geranylacetone	0.01	Monoterpenic ketone
(E)- β -Farnesene	0.02	Sesquiterpene
γ -Muurolene	0.01	Sesquiterpene
Germacrene D	0.02	Sesquiterpene
Bicyclogermacrene	0.22	Sesquiterpene
α -Muurolene	0.02	Sesquiterpene
(3Z,6E)- α -Farnesene	0.02	Sesquiterpene
(3E,6E)- α -Farnesene	0.01	Sesquiterpene
γ -Cadinene	0.01	Sesquiterpene
δ -Cadinene	0.04	Sesquiterpene
(E)-Nerolidol	0.05	Sesquiterpenic alcohol
Spathulenol	tr	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
τ -Cadinol	0.01	Sesquiterpenic alcohol
Mint sulfide?	0.02	Sesquiterpenic sulfide
meta-Camphorene	0.16	Diterpene
Phytol	0.02	Diterpenic alcohol
Consolidated total	99.36%	

*: 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.

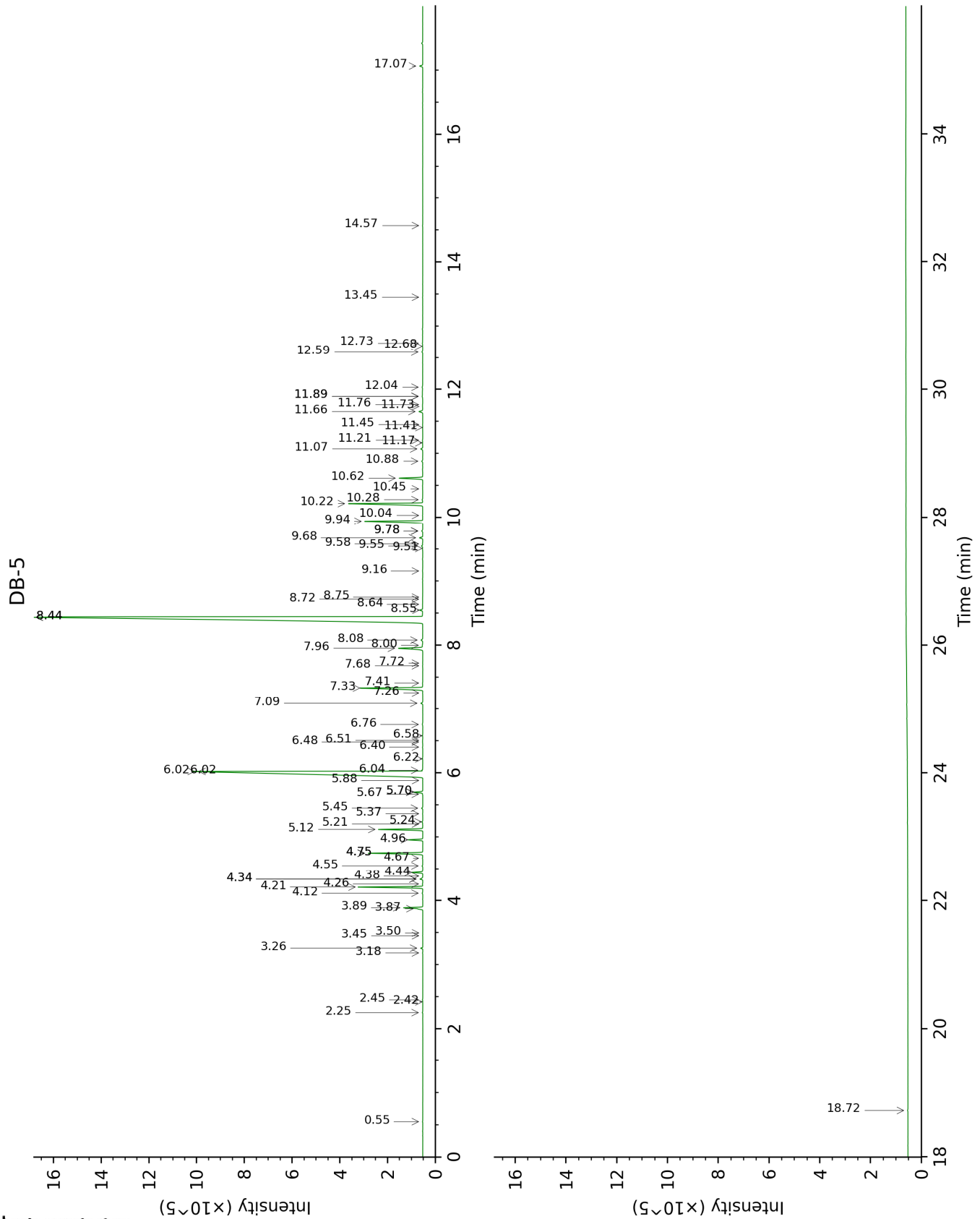
Note: no correction factor was applied

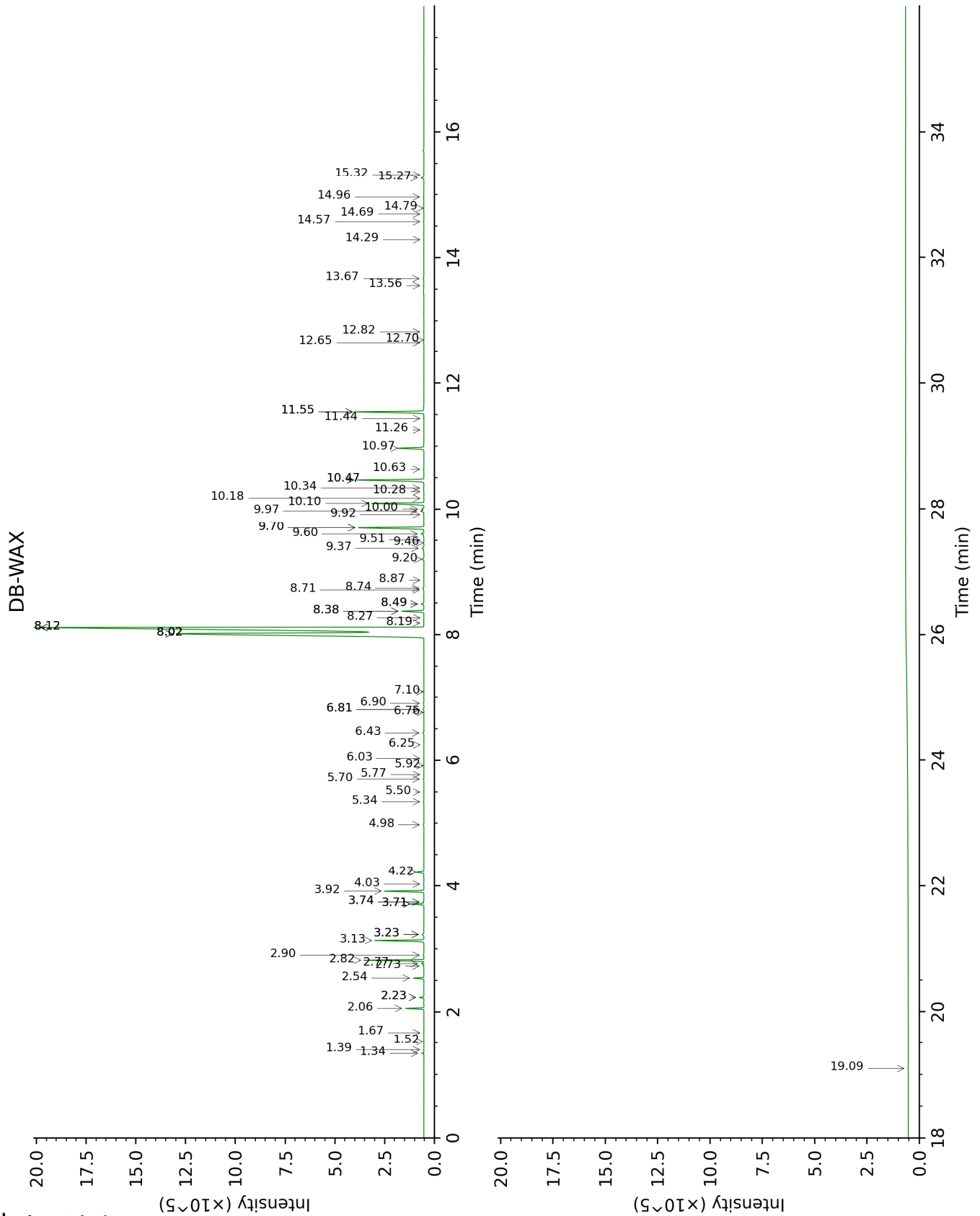
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2-Methyl-3-buten-2-ol	0.55	609	0.02	1.52	1013	tr
(3Z)-Hexenol	2.25	856	0.03	5.70	1347	0.03
(2E)-Hexenol	2.42	870	tr	6.03	1371	0.01
Hexanol	2.45	873	0.02	5.34	1321	0.02
α -Thujene	3.18	927	0.01	1.39	1000	0.01
α -Pinene	3.26	932	0.08	1.34	994	0.07
Camphene	3.45	944	0.01	1.67	1028	0.01
Thuja-2,4(10)-diene	3.50	947	0.01	2.23*	1085	0.17
Sabinene	3.87	972	0.15	2.23*	1085	[0.17]
β -Pinene	3.89	973	0.76	2.06	1067	0.73
6-Methyl-5-hepten-2-one	4.12	988	0.04	4.98	1295	0.04
Myrcene	4.21	994	2.53	2.82	1134	2.54
6-Methyl-5-hepten-2-ol	4.26	997	0.02	6.81*	1428	0.04
Pseudolimonene	4.34*	1002	0.14	2.77	1129	0.11
α -Phellandrene	4.34*	1002	[0.14]	2.73	1126	0.04
<i>cis</i> -Dehydroxylinalool oxide	4.38	1005	0.01	3.74*	1205	0.04
Δ 3-Carene	4.44	1009	0.45	2.54	1111	0.43
α -Terpinene	4.55	1016	0.04	2.90	1140	0.04
para-Cymene	4.67	1023	0.02	4.03	1226	0.02
1,8-Cineole	4.75*	1028	2.31	3.23*	1166	0.12
β -Phellandrene	4.75*	1028	[2.31]	3.23*	1166	[0.12]
Limonene	4.75*	1028	[2.31]	3.13	1158	2.21
(Z)- β -Ocimene	4.96	1041	0.59	3.71*	1203	0.60
(E)- β -Ocimene	5.12	1051	1.79	3.92	1218	1.80
Unknown [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	5.20	1057	0.01	3.71*	1203	[0.60]
γ -Terpinene	5.24	1059	0.04	3.74*	1205	[0.04]
<i>cis</i> -Sabinene hydrate	5.36	1067	0.01	6.76	1425	0.01
<i>cis</i> -Linalool oxide (fur.)	5.45	1072	0.06	6.43	1400	0.06
<i>trans</i> -Linalool oxide (fur.)	5.67	1086	0.02	6.81*	1428	[0.04]
Terpinolene	5.70*	1088	0.40	4.22	1240	0.38
para-Cymenene	5.70*	1088	[0.40]	6.25	1386	0.01
Rosefuran	5.88	1099	0.01	5.92	1363	tr
Linalool	6.02*	1108	27.00	8.02*†	1519	71.68
Hotrienol	6.02*	1108	[27.00]	8.71	1573	0.02

(Z)-6-Methyl-3,5-heptadien-2-one	6.04	1109	0.03	8.12*†	1527	[71.68]
cis-para-Menth-2-en-1-ol	6.22	1121	0.01	8.02*†	1519	[71.68]
allo-Ocimene	6.40	1132	0.01	5.50	1332	0.02
trans-para-Menth-2-en-1-ol	6.48	1137	0.02	8.87	1585	0.01
neo-allo-Ocimene	6.51	1139	0.02	5.77	1352	0.01
Isopulegol	6.58	1144	0.02	8.02*†	1519	[71.68]
Citronellal	6.76	1155	0.03	6.90	1435	0.04
Terpinen-4-ol	7.09	1176	0.10	8.49*	1556	0.14
para-Cymen-8-ol	7.26	1187	0.01	11.44	1799	0.01
α-Terpineol	7.34	1192	3.50	9.70*	1653	3.53
Hodiendiol	7.41	1197	0.02	12.70	1912	0.01
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.68	1214	0.01	11.26	1783	tr
Linalyl formate	7.72	1217	0.01	8.27	1539	0.01
Nerol	7.96	1232	1.35	10.97	1758	1.39
Citronellol	8.00	1236	0.04	10.64	1730	0.02
Neral	8.08	1241	0.10	9.37	1626	0.10
Linalyl acetate	8.44*	1265	48.21	8.12*†	1527	[71.68]
Geraniol	8.44*	1265	[48.21]	11.55*	1808	3.64
Geranial	8.55	1272	0.16	10.00	1677	0.13
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.64	1278	0.02	14.57	2086	0.02
Isobornyl acetate	8.72	1284	0.01	8.19	1533	0.02
Bornyl acetate	8.75	1286	0.01	8.12*†	1527	[71.68]
4-Vinylguaiaacol	9.16	1311	0.01	14.96	2125	0.03
Methyl anthranilate	9.51	1336	0.01	15.32	2160	0.01
Linalyl propionate	9.55	1339	0.06	8.74	1575	0.06
Hodiendiol derivative	9.58	1341	0.02	12.82	1924	0.02
α-Terpinyl acetate	9.68	1348	0.15	9.60	1644	0.15
Eugenol	9.78*	1355	0.06	14.69	2098	0.01
Unknown [m/z 43, 81 (96), 95 (85), 67 (74), 69 (68), 41 (66)...204 (1)]	9.78*	1355	[0.06]			
Neryl acetate	9.94	1367	2.88	10.10	1685	2.89
α-Copaene	10.04	1373	0.01	7.10	1450	0.01
Geranyl acetate	10.22	1386	3.89	10.47*	1716	3.90
β-Elemene	10.28	1390	0.04	8.38*	1547	1.14
Dimethyl anthranilate	10.45	1402	0.02	13.56	1990	0.01
β-Caryophyllene	10.62	1415	1.12	8.38*	1547	[1.14]
Aromadendrene	10.88	1434	0.06	8.49*	1556	[0.14]
α-Humulene	11.07	1449	0.10	9.20	1612	0.10
Geranylacetone	11.17	1456	0.01	11.55*	1808	[3.64]
(E)-β-Farnesene	11.21	1459	0.02	9.46	1633	0.02
γ-Murolene	11.41	1474	0.01	9.51	1637	0.01

Germacrene D	11.45	1477	0.02	9.70*	1653	[3.53]
Bicyclogermacrene	11.66	1492	0.22	9.97	1675	0.19
α-Muurolene	11.73	1498	0.02	9.92	1670	0.02
(3Z,6E)-α-Farnesene	11.76	1500	0.02	10.18	1691	0.01
(3E,6E)-α-Farnesene	11.89*	1510	0.04	10.47*	1716	[3.90]
γ-Cadinene	11.89*	1510	[0.04]	10.28	1700	0.01
δ-Cadinene	12.04	1522	0.04	10.34	1705	0.03
(E)-Nerolidol	12.59	1564	0.05	13.67	2001	0.05
Spathulenol	12.68	1572	tr	14.29	2059	0.01
Caryophyllene oxide	12.73	1576	0.01	12.65	1908	0.02
τ-Cadinol	13.45	1634	0.01	14.79	2107	0.02
Mint sulfide?	14.57	1727	0.02			
meta-Camphorene	17.06	1951	0.16	15.27	2155	0.15
Phytol	18.72	2113	0.02	19.09	2570	0.03
Total identified		99.38%			99.24%	
Total reported		99.39%			99.24%	

*: 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