

Date : January 14, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20L21-PSC01

Customer identification : Petitgrain Orange - CISI-2020-01

Type : Essential oil

Source : *Citrus sinensis*

Customer : Pacha Soap Co.

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 : Sylvain Mercier, M. Sc., Chimiste

Analysis date : January 13, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4736 ± 0.0003 (20 °C; method PC-MAT-016)

Optical rotation: +67.5° (21 °C, methanol, $c = 1.1$)

CONCLUSION

Limonene content of this sample is too high for a genuine orange petitgrain oil. Literature reports that limonene in sweet orange petitgrain oil should account for less than 17% of total volatiles.¹

REFERENCE

(1) Dugo, G.; Cotroneo, A.; Bonaccorsi, I. Composition of Petitgrain Oils. In *Citrus oils: Composition, advanced analytical techniques, contaminants, and biological activity*; Dugo, G., Mondello, L., Eds.; CRC Press: Boca Raton, FL, 2011; pp 253–331.

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
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	0.01	Furan
(2E)-Hexenal	0.01	Aliphatic aldehyde
(3Z)-Hexenol	0.04	Aliphatic alcohol
(2E)-Hexenol	0.02	Aliphatic alcohol
Hexanol	0.14	Aliphatic alcohol
Tricyclene	0.01	Monoterpene
α -Thujene	0.35	Monoterpene
α -Pinene	1.32	Monoterpene
Camphene	0.03	Monoterpene
α -Fenchene	0.01	Monoterpene
Sabinene	12.97	Monoterpene
β -Pinene	1.03	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
Myrcene	3.19	Monoterpene
2-Carene	0.01	Monoterpene
α -Phellandrene	0.48	Monoterpene
Pseudolimonene	0.05	Monoterpene
Octanal	0.02	Aliphatic aldehyde
Δ^3 -Carene	5.62	Monoterpene
α -Terpinene	1.29	Monoterpene
ortho-Cymene	0.01	Monoterpene
para-Cymene	0.18	Monoterpene
Limonene	50.11	Monoterpene
β -Phellandrene	0.81	Monoterpene
1,8-Cineole	0.05	Monoterpenic ether
(Z)- β -Ocimene	0.20	Monoterpene
(E)- β -Ocimene	4.93	Monoterpene
Unknown	0.08	Monoterpene
γ -Terpinene	2.09	Monoterpene
cis-Sabinene hydrate	0.02	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Octanol	0.03	Aliphatic alcohol
α -Pinene oxide analog	0.01	Monoterpenic ether
Isoterpinolene	0.16	Monoterpene
Terpinolene	1.29	Monoterpene
trans-Linalool oxide (fur.)	tr	Monoterpenic alcohol
para-Cymenene	0.03	Monoterpene
trans-Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	2.18	Monoterpenic alcohol
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
cis-para-Mentha-2-en-1-ol	0.08	Monoterpenic alcohol
cis-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol

<i>trans</i> -Limonene oxide	0.02	Monoterpenic ether
<i>trans</i> -para-Menth-2-en-1-ol	0.03	Monoterpenic alcohol
Unknown	0.04	Oxygenated normonoterpene
Isopulegol	0.03	Monoterpenic alcohol
Citronellal	0.22	Monoterpenic aldehyde
Isoneral	0.01	Monoterpenic aldehyde
Terpinen-4-ol	3.21	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α -Terpineol	0.22	Monoterpenic alcohol
<i>cis</i> -Piperitol	0.04	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene
<i>trans</i> -Piperitol	0.02	Monoterpenic alcohol
Decanal	0.04	Aliphatic aldehyde
Nerol	0.18	Monoterpenic alcohol
Citronellol	0.48	Monoterpenic alcohol
Neral	0.08	Monoterpenic aldehyde
Geraniol	0.18	Monoterpenic alcohol
Geranial	0.11	Monoterpenic aldehyde
Thymol	0.01	Monoterpenic alcohol
Methyl geranate	0.03	Monoterpenic ester
Citronellyl acetate	0.19	Monoterpenic ester
Neryl acetate	0.11	Monoterpenic ester
α -Copaene	0.05	Sesquiterpene
<i>cis</i> - β -Elemene	0.06	Sesquiterpene
Geranyl acetate	0.06	Monoterpenic ester
β -Elemene	1.65	Sesquiterpene
β -Caryophyllene	0.74	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
α -Humulene	0.29	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.10	Sesquiterpene
γ -Murolene	0.06	Sesquiterpene
Germacrene D	0.03	Sesquiterpene
β -Selinene	0.11	Sesquiterpene
α -Selinene	0.16	Sesquiterpene
Germacrene A	0.56	Sesquiterpene
γ -Cadinene	0.04	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	0.09	Sesquiterpene
δ -Cadinene	0.06	Sesquiterpene
β -Sesquiphellandrene	0.02	Sesquiterpene
α -Elemol	0.02	Sesquiterpenic alcohol
<i>cis</i> -Sesquisabinene hydrate	0.01	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Unknown	0.05	Oxygenated sesquiterpene
β -Sinensal	0.16	Sesquiterpenic aldehyde
α -Sinensal	0.08	Sesquiterpenic aldehyde
Phytone	0.01	Terpenic ketone
Phytol	0.03	Diterpenic alcohol
Consolidated total	98.72%	

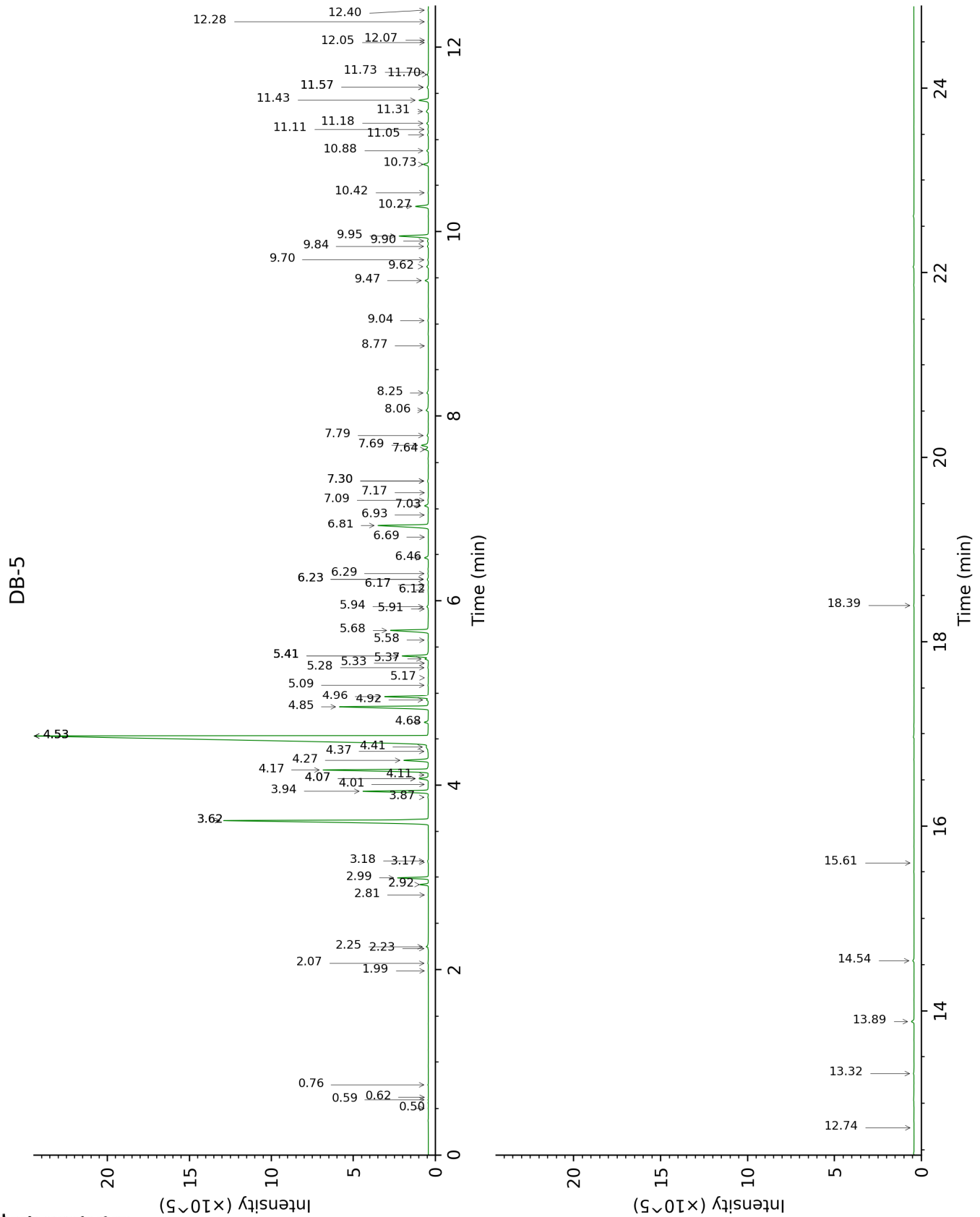
tr: The compound has been detected below 0.005% of total signal.

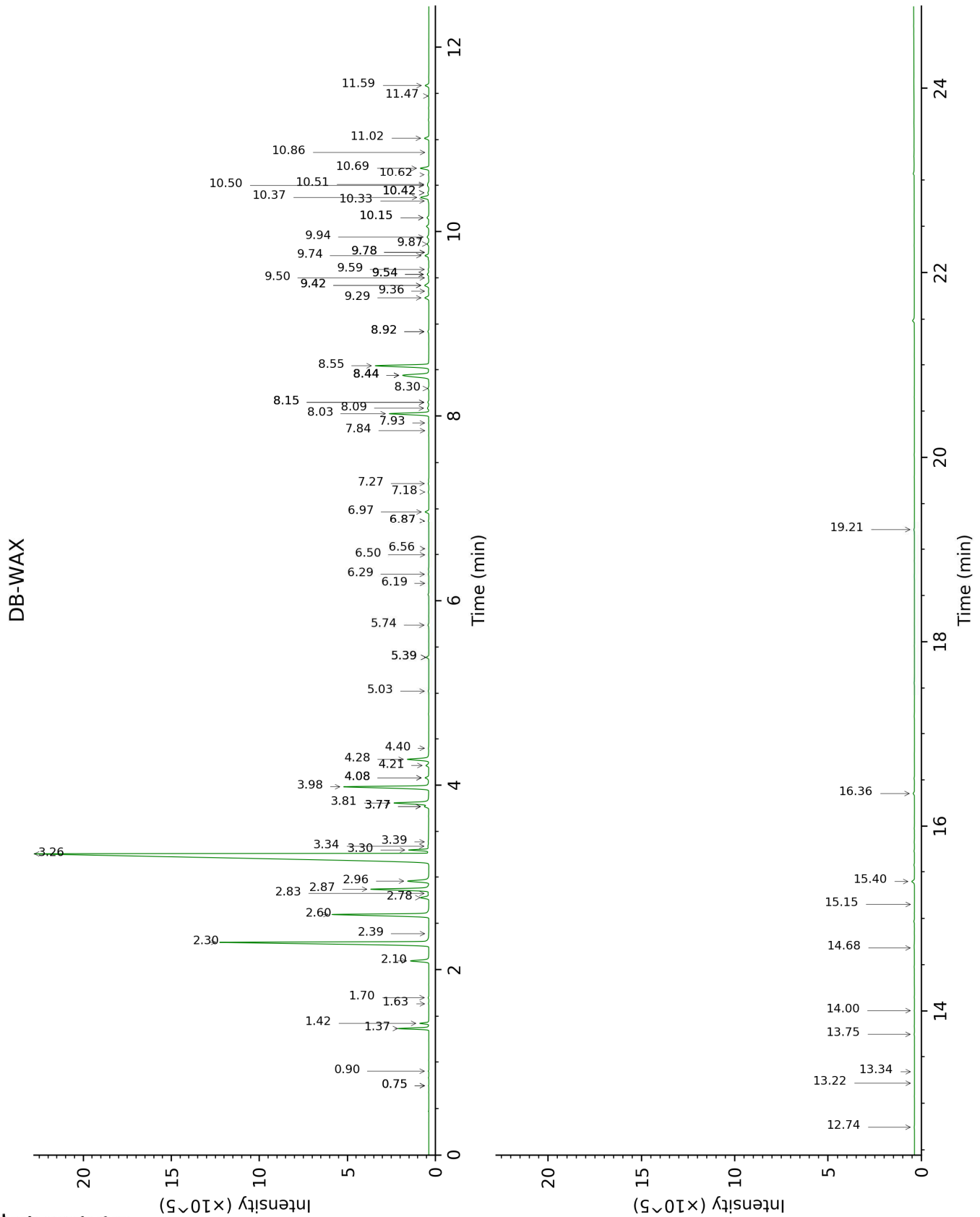
Note: no correction factor was applied

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	0.50	589	tr			
Isovaleral	0.60	639	0.01	0.75*	883	0.01
2-Methylbutyral	0.62	651	tr	0.75*	883	[0.01]
2-Ethylfuran	0.76	710	0.01	0.90	916	0.01
(2E)-Hexenal	1.99	855	0.01	3.39	1174	0.02
(3Z)-Hexenol	2.07	861	0.04	5.74	1344	0.06
(2E)-Hexenol	2.23	875	0.02	6.19	1377	0.02
Hexanol	2.25	876	0.14	5.39*	1320	0.14
Tricyclene	2.81	919	0.01			
α-Thujene	2.92	927	0.35	1.42	999	0.37
α-Pinene	2.99	931	1.32	1.37	992	1.29
Camphene	3.17†	943	0.05	1.70	1027	0.03
α-Fenchene	3.18†	944	[0.05]	1.63	1020	0.01
Sabinene	3.62*	973	14.06	2.30	1086	12.97
β-Pinene	3.62*	973	[14.06]	2.10	1066	1.03
6-Methyl-5-hepten-2-one	3.87	989	0.03	5.02	1297	0.03
Myrcene	3.94	994	3.19	2.87	1133	3.21
2-Carene	4.01	998	0.01	2.39	1096	0.01
α-Phellandrene	4.07*	1003	0.50	2.78	1126	0.48
Pseudolimonene	4.07*	1003	[0.50]	2.83	1130	0.05
Octanal	4.11	1005	0.02	4.40	1251	0.02
Δ3-Carene	4.17	1008	5.62	2.60	1112	5.57
α-Terpinene	4.27	1015	1.29	2.96	1140	1.32
ortho-Cymene	4.37	1021	0.01	4.08*	1227	0.23
para-Cymene	4.41	1024	0.18	4.08*	1227	[0.23]
Limonene	4.53*	1031	51.26	3.26	1164	50.11
β-Phellandrene	4.53*	1031	[51.26]	3.30	1168	0.81
1,8-Cineole	4.53*	1031	[51.26]	3.34	1171	0.05
(Z)-β-Ocimene	4.68	1041	0.20	3.77*†	1204	2.34
(E)-β-Ocimene	4.85	1051	4.93	3.98	1220	4.91
Unknown [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	4.92	1056	0.08	3.77*†	1204	[2.34]
γ-Terpinene	4.96	1058	2.09	3.81†	1207	[2.34]
cis-Sabinene hydrate	5.09	1066	0.02	6.87*	1427	0.03
cis-Linalool oxide (fur.)	5.17	1071	0.01	6.50	1399	0.02
Octanol	5.28	1078	0.03	8.15*	1523	0.06
α-Pinene oxide analog	5.33	1081	0.01	5.39*	1320	[0.14]
Isoterpinolene	5.37	1084	0.16	4.22	1237	0.16
Terpinolene	5.40*	1086	1.35	4.28	1242	1.29
trans-Linalool oxide (fur.)	5.40*	1086	[1.35]	6.87*	1427	[0.03]

para-Cymenene	5.40*	1086	[1.35]	6.29	1384	0.03
trans-Sabinene hydrate	5.58	1097	0.02	7.93	1506	0.02
Linalool	5.68	1104	2.18	8.03	1514	2.21
trans-para-Mentha-2,8-dien-1-ol	5.91	1118	0.01	8.92*	1583	0.06
cis-para-Menth-2-en-1-ol	5.94	1120	0.08	8.09	1518	0.11
cis-para-Mentha-2,8-dien-1-ol	6.12	1131	0.02	9.50	1629	0.03
trans-Limonene oxide	6.17	1135	0.02	6.56	1404	0.01
trans-para-Menth-2-en-1-ol	6.23*	1139	0.07	8.92*	1583	[0.06]
Unknown [m/z 41, 69 (87), 82 (66), 67 (55), 109 (46)... 142 (18)]	6.23*	1139	[0.07]	9.36	1618	0.04
Isopulegol	6.29	1143	0.03	8.15*	1523	[0.06]
Citronellal	6.46	1154	0.22	6.97	1434	0.21
Isoneral	6.69	1168	0.01	7.84	1500	0.01
Terpinen-4-ol	6.81	1176	3.21	8.55	1554	3.20
para-Cymen-8-ol	6.93	1184	0.02	11.47	1793	0.02
α-Terpineol	7.03	1191	0.22	9.74	1649	0.24
cis-Piperitol	7.09	1195	0.04	9.54*	1632	0.10
Unknown [m/z 109, 91 (100), 81 (88), 94 (75), 119 (74), 96 (73), 41 (63)... 150 (2)]	7.18	1200	0.01	10.86	1742	0.01
trans-Piperitol	7.30*	1208	0.06	10.42*	1704	0.08
Decanal	7.30*	1208	[0.06]	7.27	1457	0.04
Nerol	7.64	1231	0.18	11.02	1754	0.26
Citronellol	7.69	1234	0.48	10.69	1727	0.49
Neral	7.79	1242	0.08	9.42*	1623	0.33
Geraniol	8.06	1260	0.18	11.59	1803	0.22
Geranial	8.25	1273	0.11	10.15*	1682	0.13
Thymol	8.77	1304	0.01	15.15	2135	0.01
Methyl geranate	9.04	1323	0.03	9.78*	1652	0.04
Citronellyl acetate	9.47	1354	0.19	9.42*	1623	[0.33]
Neryl acetate	9.62	1365	0.11	10.15*	1682	[0.13]
α-Copaene	9.70	1370	0.05	7.18	1450	0.03
cis-β-Elemene	9.84	1381	0.06	8.30	1535	0.05
Geranyl acetate	9.90	1385	0.06	10.51	1712	0.06
β-Elemene	9.95	1389	1.65	8.44*	1546	2.26
β-Caryophyllene	10.27	1412	0.74	8.44*	1546	[2.26]
β-Copaene	10.42	1423	0.02	8.44*	1546	[2.26]
α-Humulene	10.74	1447	0.29	9.29	1612	0.27
(E)-β-Farnesene	10.88	1458	0.10	9.54*	1632	[0.10]
γ-Murolene	11.05	1471	0.06	9.59	1637	0.04
Germacrene D	11.11	1475	0.03	9.78*	1652	[0.04]
β-Selinene	11.18	1480	0.11	9.87	1659	0.11

α-Selinene	11.31	1490	0.16	9.94	1665	0.13
Germacrene A	11.43	1499	0.56	10.37	1700	0.56
γ-Cadinene	11.57*	1510	0.11	10.33	1696	0.04
(3E,6E)-α-Farnesene	11.57*	1510	[0.11]	10.50	1711	0.09
δ-Cadinene	11.70	1521	0.06	10.42*	1704	[0.08]
β-Sesquiphellandrene	11.73	1523	0.02	10.62	1721	0.03
α-Elemol	12.05	1548	0.02	14.00	2023	0.01
cis-Sesquisabinene hydrate	12.08	1550	0.01	13.22	1949	0.01
(E)-Nerolidol	12.28	1566	0.02	13.75	1999	0.02
Caryophyllene oxide	12.40	1576	0.02	12.74	1906	0.02
Humulene epoxide II	12.74	1602	0.01	13.34	1961	0.01
Unknown [m/z 43, 81 (79), 93 (77), 91 (70), 161 (68), 107 (67), 95 (65)...]	13.32	1650	0.05			
β-Sinensal	13.89	1697	0.16	15.40	2160	0.17
α-Sinensal	14.54	1754	0.08	16.36	2258	0.08
Phytone	15.61	1848	0.01	14.68	2088	0.01
Phytol	18.39	2112	0.03	19.21	2574	0.04
Total identified		98.92%			98.52%	
Total reported		99.06%			98.57%	

*: 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