

Date : March 21, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21L21-PTH04

Customer identification : Orange 5 Fold - OR0100

Type : Essential oil

Source : *Citrus sinensis* ct. rectified

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 : Seydou Ka, Ph. D.

Analysis date : January 03, 2022

Checked and approved by :

Sylvain Mercier, M. Sc., Chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

This report is an update of the version first issued on January 12, 2022 to correct a mistake in the lot number.

PHYSICOCHEMICAL DATA

Physical aspect: Bright orange brownish liquid

Refractive index: 1.4765 ± 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
Heptanal	0.01	Aliphatic aldehyde
α -Pinene	0.06	Monoterpene
Sabinene	0.11	Monoterpene
β -Pinene	0.01	Monoterpene
Myrcene	0.83	Monoterpene
α -Phellandrene	0.02	Monoterpene
Octanal	0.17	Aliphatic aldehyde
Δ^3 -Carene	0.07	Monoterpene
Limonene	87.33	Monoterpene
β -Phellandrene	0.23	Monoterpene
(Z)- β -Ocimene	tr	Monoterpene
(E)- β -Ocimene	0.03	Monoterpene
γ -Terpinene	0.01	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Octanol	0.05	Aliphatic alcohol
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.04	Monoterpene
6,7-Epoxymyrcene	tr	Monoterpenic ether
<i>trans</i> -Sabinene hydrate	tr	Monoterpenic alcohol
Linalool	1.82	Monoterpenic alcohol
Hotrienol	0.01	Monoterpenic alcohol
Nonanal	0.10	Aliphatic aldehyde
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.10	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.09	Monoterpenic ether
<i>cis</i> -para-Mentha-2,8-dien-1-ol	0.16	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.01	Monoterpenic alcohol
Citronellal	0.22	Monoterpenic aldehyde
Nonanol	0.01	Aliphatic alcohol
Unknown	0.04	Oxygenated monoterpene
Cryptone	0.01	Normonoterpenic ketone
para-Cymen-8-ol	0.01	Monoterpenic alcohol
α -Terpineol	0.16	Monoterpenic alcohol
Unknown	0.05	Unknown
Unknown	0.06	Unknown
<i>trans</i> -Isopiperitenol	0.04	Monoterpenic alcohol
Decanal	1.49	Aliphatic aldehyde
Octyl acetate	0.04	Aliphatic ester
<i>trans</i> -Carveol	0.12	Monoterpenic alcohol
<i>cis</i> -Carveol	0.08	Monoterpenic alcohol
Citronellol	0.05	Monoterpenic alcohol
Neral	0.17	Monoterpenic aldehyde
Carvone	0.08	Monoterpenic ketone
Geraniol	0.02	Monoterpenic alcohol
(2E)-Decenal	0.02	Aliphatic aldehyde

Perillaldehyde	0.10	Monoterpenic aldehyde
Geranial	0.36	Monoterpenic aldehyde
Limonen-10-ol	0.08	Monoterpenic alcohol
Undecanal	0.06	Aliphatic aldehyde
<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide	tr	Monoterpenic peroxide
(2 <i>E</i> ,4 <i>E</i>)-Decadienal	0.02	Aliphatic aldehyde
para-Mentha-1,8-diene-4-hydroperoxide	0.04	Monoterpenic peroxide
Limonene <i>trans</i> -glycol	0.05	Monoterpenic alcohol
Neryl acetate	0.03	Monoterpenic ester
α -Copaene	0.11	Sesquiterpene
β -Cubebene	0.09	Sesquiterpene
Geranyl acetate	0.13	Monoterpenic ester
Capric acid	tr	Aliphatic acid
β -Elemene	0.08	Sesquiterpene
Dodecanal	0.27	Aliphatic aldehyde
β -Caryophyllene	0.09	Sesquiterpene
β -Copaene	0.17	Sesquiterpene
α -Humulene	0.04	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.05	Sesquiterpene
γ -Muurolene	0.02	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
Valencene	0.35	Sesquiterpene
α -Muurolene	0.05	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	0.05	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
γ -Cadinene	0.04	Sesquiterpene
δ -Cadinene	0.11	Sesquiterpene
α -Elemol	0.04	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.02	Sesquiterpenic ether
δ -Undecalactone	0.01	Aliphatic lactone
Tetradecanal	0.02	Aliphatic aldehyde
Unknown	0.01	Oxygenated sesquiterpene
β -Sinensal	0.16	Sesquiterpenic aldehyde
α -Sinensal	0.10	Sesquiterpenic aldehyde
Nootkatone	0.06	Sesquiterpenic ketone
Hexadecanal	0.04	Aliphatic aldehyde
meta-Camphorene	0.01	Diterpene
Palmitic acid	0.22	Aliphatic acid
Octadecanal	0.03	Aliphatic aldehyde
Methyl stearate	0.02	Aliphatic ester
Linoleic acid	0.16	Aliphatic acid
Oleic acid	0.15	Aliphatic acid
<i>cis</i> -Vaccenic acid	0.15	Aliphatic acid
Stearic acid	0.26	Aliphatic acid
Pentamethoxyflavone isomer	0.15	Flavonoid
Tetramethoxyflavone isomer	0.20	Flavonoid
3-Methoxynobiletin (3,5,6,7,8,3',4'-heptamethoxyflavone)	0.35	Flavonoid
Nobiletin	0.29	Flavonoid

Consolidated total	98.95%	
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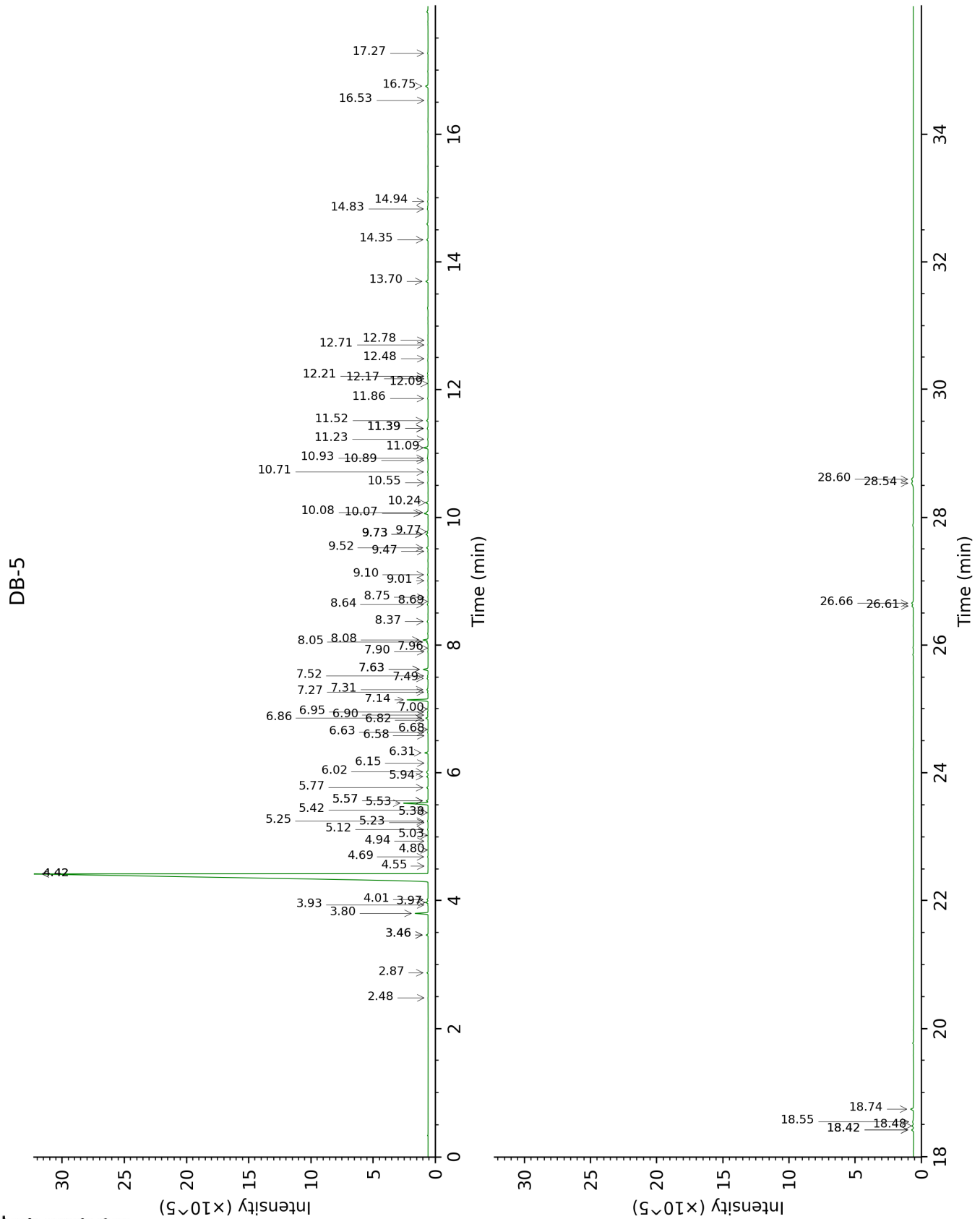
tr: The compound has been detected below 0.005% of total signal.

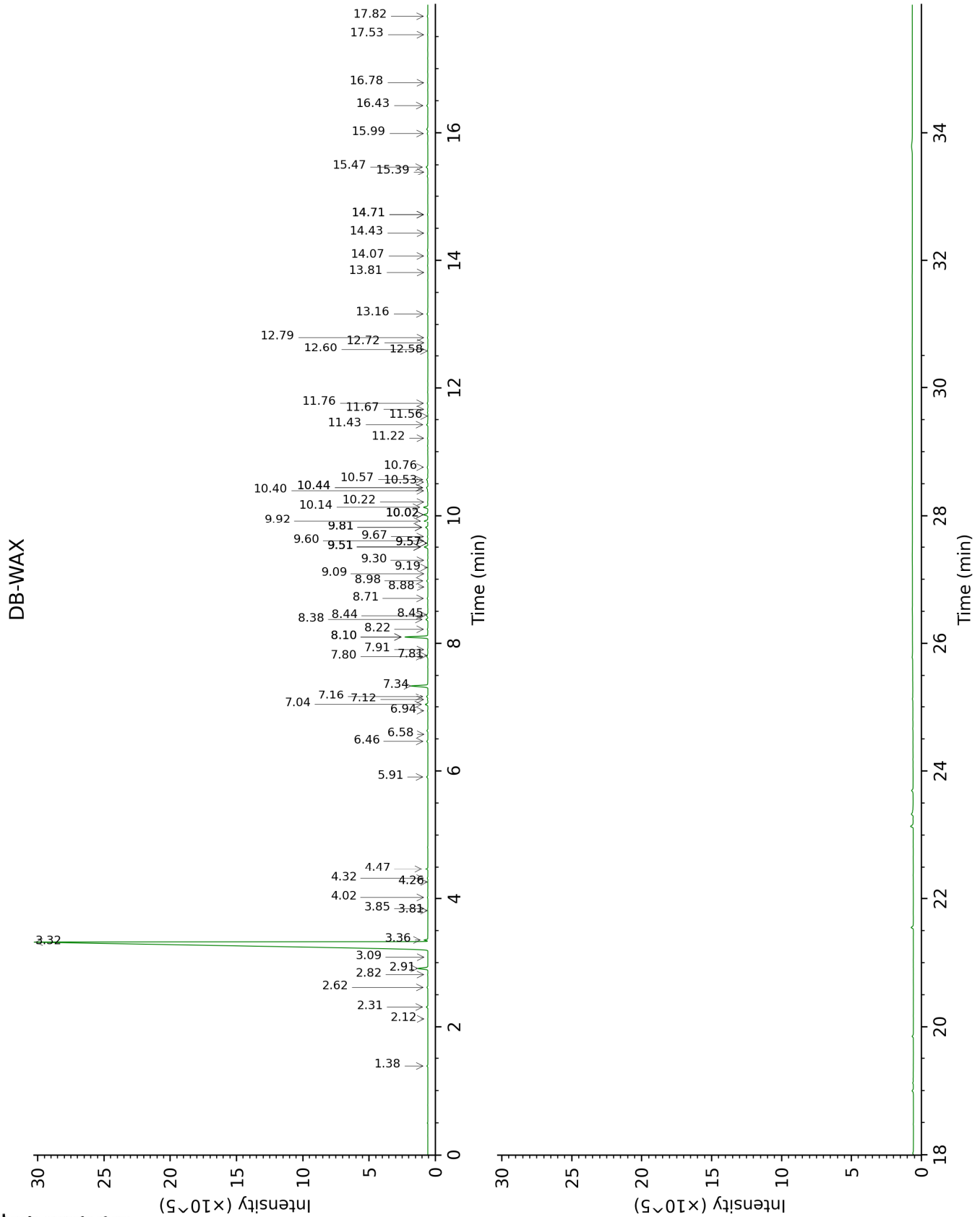
Note: no correction factor was applied

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	%
Heptanal	2.48	903	0.01	3.09	1149	0.01
α -Pinene	2.87	930	0.06	1.38	992	0.07
Sabinene	3.46*	970	0.12	2.31	1085	0.11
β -Pinene	3.46*	970	[0.12]	2.12	1067	0.01
Myrcene	3.80	993	0.83	2.91	1135	0.83
α -Phellandrene	3.93	1002	0.02	2.82	1127	0.02
Octanal	3.97	1004	0.17	4.47	1254	0.17
Δ^3 -Carene	4.02	1007	0.07	2.62	1112	0.07
Limonene	4.42*	1033	86.65	3.32	1167	87.33
β -Phellandrene	4.42*	1033	[86.65]	3.36	1170	0.23
(Z)- β -Ocimene	4.55	1041	tr	3.81	1206	0.01
(E)- β -Ocimene	4.69	1050	0.03	4.02	1221	0.03
γ -Terpinene	4.80	1057	0.01	3.85	1208	0.01
<i>cis</i> -Sabinene hydrate	4.94	1066	0.01	6.94	1430	0.03
<i>cis</i> -Linalool oxide (fur.)	5.03	1072	0.01	6.58	1403	0.01
Octanol	5.12	1077	0.05	8.22	1527	0.05
Isoterpinolene	5.23	1084	0.01	4.26	1239	0.01
Terpinolene	5.25	1086	0.04	4.32	1243	0.05
6,7-Epoxymyrcene	5.38	1094	tr			
<i>trans</i> -Sabinene hydrate	5.42	1096	tr	7.91	1502	0.03
Linalool	5.53	1103	1.82	8.10*	1518	1.85
Hotrienol	5.57*	1106	0.11	8.88	1578	0.01
Nonanal	5.57*	1106	[0.11]	5.91	1355	0.10
<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.77	1119	0.10	8.98	1586	0.10
<i>cis</i> -Limonene oxide	5.94	1130	0.09	6.46	1395	0.09
<i>cis</i> -para-Mentha-2,8-dien-1-ol	6.02	1135	0.16	9.51*	1628	0.33
<i>trans</i> -Verbenol	6.15	1143	0.01	9.60	1636	0.02
Citronellal	6.31	1154	0.22	7.04	1438	0.21
Nonanol	6.58	1171	0.01	9.51*	1628	[0.33]
Unknown [m/z 69, 84 (62), 41 (30), 123 (26), 97 (24), 109 (23)...]	6.63	1174	0.04	9.67	1641	0.05
Cryptone	6.68	1177	0.01	9.19	1602	0.01
para-Cymen-8-ol	6.82	1186	0.01	11.56	1799	0.01
α -Terpineol	6.86	1188	0.16	9.81*	1653	0.23
Unknown [m/z 121, 79 (98), 93 (87), 94 (73), 91 (63), 105 (45)...]	6.90	1192	0.05	7.81	1495	0.04
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	6.95	1195	0.06	8.10*	1518	[1.85]
<i>trans</i> -Isopiperitenol	7.00	1198	0.04	10.44*	1704	0.14
Decanal	7.14	1207	1.49	7.34	1460	1.42
Octyl acetate	7.27	1216	0.04	7.12	1443	0.04
<i>trans</i> -Carveol	7.31	1218	0.12	11.43	1788	0.11

<i>cis</i> -Carveol	7.48	1230	0.08	11.76	1817	0.06
Citronellol	7.52	1233	0.05	10.76	1731	0.07
Neral	7.63*	1240	0.39	9.51*	1628	[0.33]
Carvone	7.63*	1240	[0.39]	10.02*	1670	0.41
Geraniol	7.90	1258	0.02	11.67	1808	0.03
(2 <i>E</i>)-Decenal	7.96	1262	0.02	9.09	1594	0.02
Perillaldehyde	8.05	1268	0.10			
Geranial	8.08	1270	0.36	10.14	1679	0.37
Limonen-10-ol	8.37	1290	0.08	13.16	1943	0.07
Undecanal	8.64	1308	0.06	8.71	1564	0.06
<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide	8.68	1311	tr			
(2 <i>E</i> ,4 <i>E</i>)-Decadienal	8.75	1316	0.02	11.22	1770	0.04
para-Mentha-1,8-diene-4-hydroperoxide	9.01	1334	0.04			
Limonene <i>trans</i> -glycol	9.10	1340	0.05	15.99	2219	0.06
Neryl acetate	9.47	1366	0.03	10.22	1686	0.02
α -Copaene	9.52	1370	0.11	7.16	1447	0.12
β -Cubebene	9.73*	1385	0.20	7.80	1494	0.09
Geranyl acetate	9.73*	1385	[0.20]	10.57	1715	0.13
Capric acid	9.73*	1385	[0.20]			
β -Elemene	9.77	1388	0.08	8.45	1545	0.06
Dodecanal	10.07	1409	0.27	10.02*	1670	[0.41]
β -Caryophyllene	10.08	1410	0.09	8.44	1543	0.10
β -Copaene	10.24	1422	0.17	8.38	1539	0.17
α -Humulene	10.55	1445	0.04	9.30	1611	0.03
(<i>E</i>)- β -Farnesene	10.71	1457	0.05	9.57*	1633	0.06
γ -Muurolene	10.90	1471	0.02	9.57*	1633	[0.06]
Germacrene D	10.93	1473	0.08	9.81*	1653	[0.23]
Valencene	11.09	1486	0.35	9.92	1662	0.33
α -Muurolene	11.23	1496	0.05	10.02*	1670	[0.41]
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	11.39*	1508	0.09	10.53	1712	0.05
Cubebol	11.39*	1508	[0.09]	12.58	1889	0.01
γ -Cadinene	11.39*	1508	[0.09]	10.40	1700	0.04
δ -Cadinene	11.52	1518	0.11	10.44*	1704	[0.14]
α -Elemol	11.86	1545	0.04	14.07	2028	0.03
(<i>E</i>)-Nerolidol	12.09	1564	0.02	13.81	2003	0.02
Spathulenol	12.17	1569	0.03	14.42	2062	0.03
Caryophyllene oxide isomer	12.21*	1572	0.04	12.72	1902	0.01
Caryophyllene oxide	12.21*	1572	[0.04]	12.80	1909	0.02
δ -Undecalactone	12.48	1594	0.01			
Tetradecanal	12.71	1612	0.02	12.60	1891	0.02
Unknown [m/z 161, 43 (74), 105 (57), 121 (45), 81 (43)... 204 (31)...]	12.78	1618	0.01	14.71*	2090	0.04
β -Sinensal	13.70	1694	0.16	15.47	2165	0.17
α -Sinensal	14.35	1750	0.10	16.43	2264	0.09
Nootkatone	14.83	1792	0.06	17.82	2414	0.06
Hexadecanal	14.94	1802	0.04	14.71*	2090	[0.04]

meta-Camphorene	16.53	1948	0.01	15.39	2158	0.01
Palmitic acid	16.75	1970	0.22			
Octadecanal	17.27	2019	0.03	16.78	2301	0.03
Methyl stearate	18.42*	2135	0.18	17.53	2382	0.02
Linoleic acid	18.42*	2135	[0.18]			
Oleic acid	18.48	2142	0.15			
cis-Vaccenic acid	18.55	2148	0.15			
Stearic acid	18.74	2169	0.26			
Pentamethoxyflavone isomer	26.61	3136	0.15			
Tetramethoxyflavone isomer	26.66	3141	0.20			
3-Methoxynobiletin (3,5,6,7,8,3',4'-heptamethoxyflavone)	28.54	3326	0.35			
Nobiletin	28.60	3331	0.29			
Total identified		98.02%			96.67%	
Total reported		98.19%			96.76%	

*: Two or more compounds are coeluting on this column

[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

R.T.: Retention time (minutes)

R.I.: Retention index