

Date : August 16, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22H09-PTH03


Customer identification : Neroli - Tunisia/Morocco - N10110R

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 : August 11, 2022

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.4693 ± 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
Ethyl acetate	tr	Aliphatic ester
Isoamyl alcohol	tr	Aliphatic alcohol
(3Z)-Hexenol	0.01	Aliphatic alcohol
(2E)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Tricyclene	0.01	Monoterpene
α -Thujene	0.02	Monoterpene
α -Pinene	1.27	Monoterpene
Camphene	0.04	Monoterpene
α -Fenchene	tr	Monoterpene
β -Pinene	8.41	Monoterpene
Sabinene	2.27	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.14	Monoterpene
α -Phellandrene	0.13	Monoterpene
Octanal	0.01	Aliphatic aldehyde
Δ^3 -Carene	0.02	Monoterpene
(3Z)-Hexenyl acetate	0.02	Aliphatic ester
α -Terpinene	0.03	Monoterpene
(2E)-Hexenyl acetate	0.01	Aliphatic ester
para-Cymene	0.04	Monoterpene
β -Phellandrene	0.06	Monoterpene
1,8-Cineole	0.12	Monoterpenic ether
Limonene	13.99	Monoterpene
(Z)- β -Ocimene	1.57	Monoterpene
(E)- β -Ocimene	4.19	Monoterpene
γ -Terpinene	0.06	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.16	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene isomer	0.01	Monoterpene
Terpinolene	0.33	Monoterpene
trans-Linalool oxide (fur.)	0.16	Monoterpenic alcohol
α -Pinene oxide	0.01	Monoterpenic ether
trans-Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	41.92	Monoterpenic alcohol
Phenylethyl alcohol	0.12	Simple phenolic
cis-para-Menth-2-en-1-ol	0.04	Monoterpenic alcohol
cis-Limonene oxide	0.01	Monoterpenic ether
allo-Ocimene	0.12	Monoterpene
Benzeneacetonitrile	0.06	Simple phenolic
(Z)-Myroxide	0.03	Monoterpenic ether
Camphor	0.09	Monoterpenic ketone
neo-allo-Ocimene	0.01	Monoterpene
(E)-Myroxide	0.05	Monoterpenic ether

Epoxyterpinolene	0.01	Monoterpenic ether
Citronellal	0.01	Monoterpenic aldehyde
Borneol	0.05	Monoterpenic alcohol
δ -Terpineol	0.03	Monoterpenic alcohol
Terpinen-4-ol	0.14	Monoterpenic alcohol
<i>trans</i> -Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
α -Terpineol	4.45	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Lilac alcohol A	0.01	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.02	Monoterpenic alcohol
Linalyl formate	0.02	Monoterpenic ester
Nerol	0.93	Monoterpenic alcohol
Citronellol	0.04	Monoterpenic alcohol
6,7-Dihydro-7-hydroxylinalool	0.01	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Phenylethyl acetate	0.10	Phenolic ester
Geraniol	2.02	Monoterpenic alcohol
Linalyl acetate	5.29	Monoterpenic ester
(<i>trans</i> ?) -Linalool oxide acetate (fur.)?	0.01	Monoterpenic ester
Geranial	0.06	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.03	Monoterpenic alcohol
Bornyl acetate	0.03	Monoterpenic ester
Indole	0.23	Indole
Methyl anthranilate	0.39	Phenolic ester
Linalyl propionate	0.01	Monoterpenic ester
Hodiendiol derivative	0.01	Oxygenated monoterpene
α -Terpinyl acetate	0.03	Monoterpenic ester
Eugenol	0.01	Phenylpropanoid
Neryl acetate	1.30	Monoterpenic ester
Geranyl acetate	2.60	Monoterpenic ester
β -Elemene	0.03	Sesquiterpene
(<i>Z</i>)-Jasmone	0.01	Jasmonate
Dimethyl anthranilate	0.03	Phenolic ester
β -Caryophyllene	0.59	Sesquiterpene
α -Humulene	0.05	Sesquiterpene
Geranylacetone	0.01	Monoterpenic ketone
(<i>E</i>)- β -Farnesene	0.04	Sesquiterpene
Germacrene D	0.03	Sesquiterpene
Bicyclogermacrene	0.07	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i>)- α -Farnesene	0.01	Sesquiterpene
γ -Cadinene	0.03	Sesquiterpene
δ -Cadinene	0.02	Sesquiterpene
(<i>Z</i>)-Nerolidol	0.01	Sesquiterpenic alcohol
α -Elemol	0.03	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	1.56	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.07	Sesquiterpenic ether
α -Cadinol	tr	Sesquiterpenic alcohol
α -Bisabolol	0.02	Sesquiterpenic alcohol
2,3-Dihydrofarnesol	0.01	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>Z</i>)-Farnesol	0.02	Sesquiterpenic alcohol

Heptadecane	0.02	Alkane
(2E,6E)-Farnesol	1.41	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Octadecane	0.03	Alkane
(2E,6E)-Farnesyl acetate	0.02	Sesquiterpenic ester
Unknown	0.07	Unknown
Unknown	0.05	Unknown
Eicosane	0.01	Alkane
Heneicosane	0.01	Alkane
Phytol	0.01	Diterpenic alcohol
Tricosane	0.02	Alkane
Pentacosane	0.01	Alkane
Heptacosane	0.01	Alkane
Squalene	0.01	Triterpene
Consolidated total	98.91%	

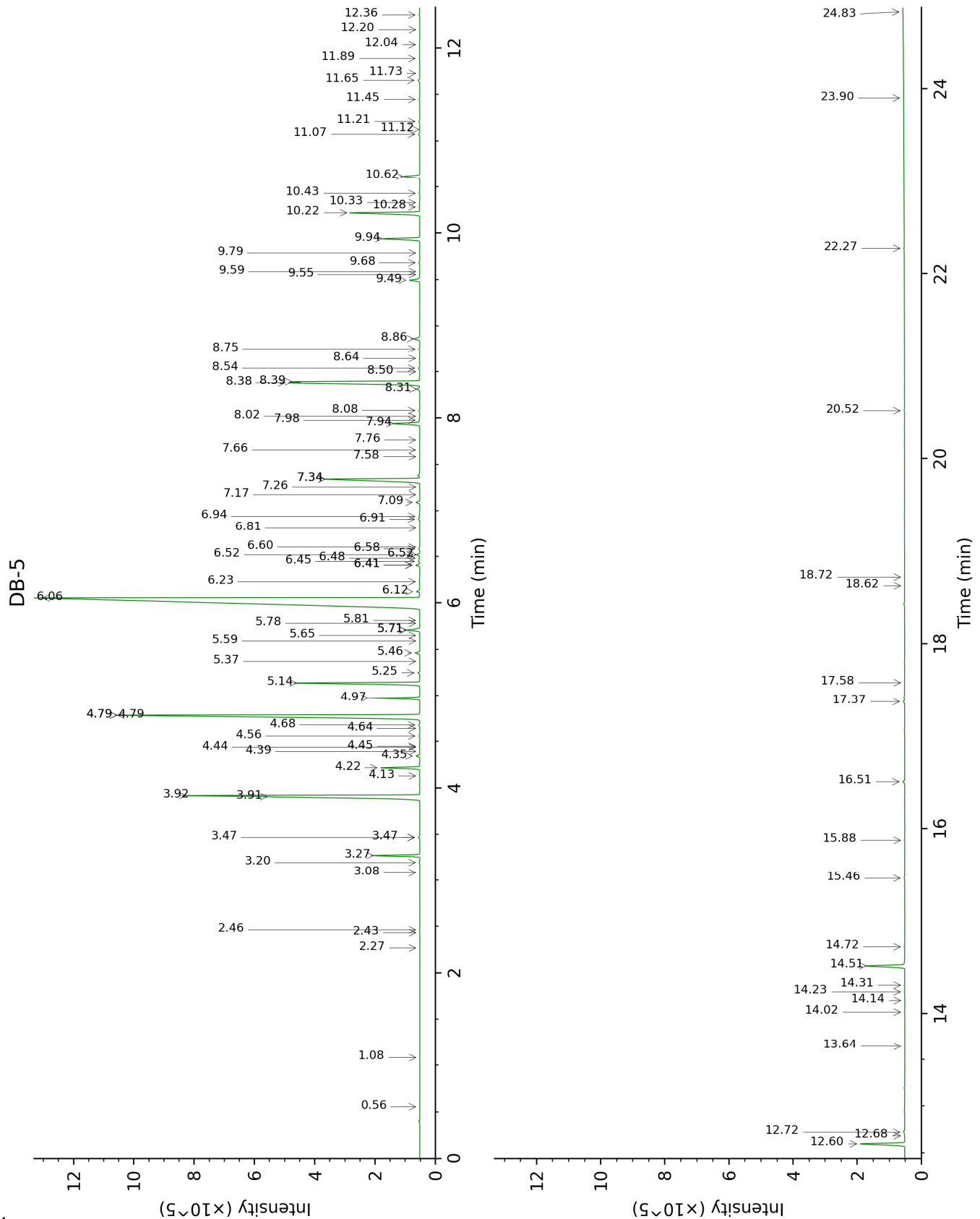
tr: The compound has been detected below 0.005% of total signal.

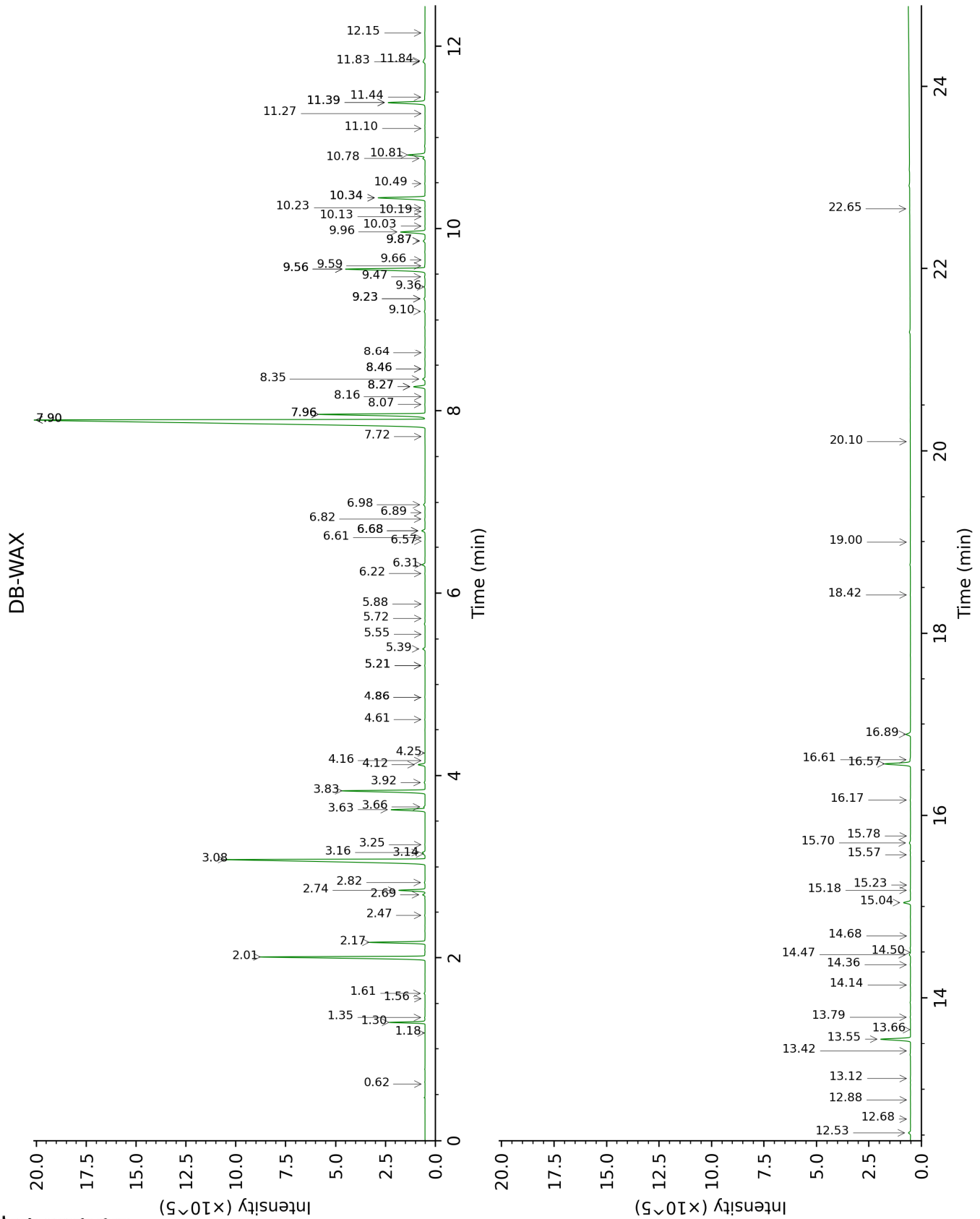
Note: no correction factor was applied

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	%
Ethyl acetate	0.56	607	tr	0.62	852	tr
Isoamyl alcohol	1.08	734	tr	3.25	1174	0.01
(3Z)-Hexenol	2.27	858	0.01	5.55	1342	0.01
(2E)-Hexenol	2.43	871	0.01	5.88	1366	0.01
Hexanol	2.46	873	0.01	5.21*	1317	0.02
Tricyclene	3.08	920	0.01	1.18	974	tr
α -Thujene	3.20	927	0.02	1.35	1002	0.02
α -Pinene	3.27	932	1.27	1.30	994	1.27
Camphene	3.47*	945	0.05	1.61	1030	0.04
α -Fenchene	3.47*	945	[0.05]	1.56	1024	tr
β -Pinene	3.91†	974	10.72	2.01	1069	8.41
Sabinene	3.92†	974	[10.72]	2.17	1085	2.27
6-Methyl-5-hepten-2-one	4.13	988	0.02	4.86*	1296	0.03
Myrcene	4.22	994	1.14	2.74	1134	1.13
α -Phellandrene	4.35	1002	0.13	2.69	1130	0.11
Octanal	4.39	1005	0.01	4.25	1250	0.01
Δ 3-Carene	4.44†	1008	0.03	2.47	1112	0.02
(3Z)-Hexenyl acetate	4.45†	1009	[0.03]	4.61	1278	0.02
α -Terpinene	4.56	1016	0.03	2.82	1141	0.03
(2E)-Hexenyl acetate	4.64	1021	0.01	4.86*	1296	[0.03]
para-Cymene	4.68	1023	0.04	3.92	1227	0.04
β -Phellandrene	4.78*	1030	14.19	3.14	1166	0.06
1,8-Cineole	4.78*	1030	[14.19]	3.16	1167	0.12
Limonene	4.78*	1030	[14.19]	3.08	1161	13.99
(Z)- β -Ocimene	4.97	1041	1.57	3.63	1204	1.57
(E)- β -Ocimene	5.14	1052	4.19	3.84	1220	4.21
γ -Terpinene	5.25	1058	0.06	3.66	1207	0.06
cis-Sabinene hydrate	5.37	1066	0.01	6.68*	1426	0.18
cis-Linalool oxide (fur.)	5.46	1072	0.16	6.31	1398	0.16
Octanol	5.59	1080	0.02	7.96*†	1523	[47.27]
Terpinolene isomer	5.65	1084	0.01	4.16	1244	0.01
Terpinolene	5.71*	1087	0.49	4.12	1241	0.33
trans-Linalool oxide (fur.)	5.71*	1087	[0.49]	6.68*	1426	[0.18]
α -Pinene oxide	5.78	1092	0.01	5.21*	1317	[0.02]
trans-Sabinene hydrate	5.81	1094	0.01	7.72	1504	0.01
Linalool	6.06	1109	41.92	7.90*†	1518	47.27
Phenylethyl alcohol	6.12	1113	0.12	11.83	1846	0.10
cis-para-Menth-2-en-1-ol	6.23	1120	0.04	7.90*†	1518	[47.27]
cis-Limonene oxide	6.41*	1131	0.13	6.22	1391	0.01
allo-Ocimene	6.41*	1131	[0.13]	5.39	1330	0.12

Benzeneacetonitrile	6.45	1134	0.06	11.84	1847	0.07
(Z)-Myroxide	6.48	1136	0.03	6.61	1420	0.01
Camphor	6.52*	1138	0.10	6.98	1448	0.09
neo-allo-Ocimene	6.52*	1138	[0.10]	5.72	1355	0.01
(E)-Myroxide	6.58	1143	0.05	6.89	1441	0.01
Epoxyterpinolene	6.60	1144	0.01	6.57	1417	0.01
Citronellal	6.81	1157	0.01	6.82	1436	0.02
Borneol	6.91	1163	0.05	9.56*	1651	4.50
δ-Terpineol	6.94	1165	0.03	9.23*	1624	0.07
Terpinen-4-ol	7.09	1175	0.14	8.35	1554	0.12
trans-Linalool oxide (pyr.)	7.18	1180	0.01	10.34*	1716	2.63
para-Cymen-8-ol	7.26	1185	0.01	11.26	1796	tr
α-Terpineol	7.34*	1191	4.45	9.56*	1651	[4.50]
Myrtenal	7.34*	1191	[4.45]	8.46*	1563	0.02
Lilac alcohol A	7.58	1206	0.01	9.66	1660	0.01
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.66	1211	0.02	11.10	1782	0.01
Linalyl formate	7.76	1218	0.02	8.16	1539	0.01
Nerol	7.94	1230	0.93	10.81	1757	0.95
Citronellol	7.98	1233	0.04	10.49	1729	0.02
6,7-Dihydro-7-hydroxylinalool	8.02	1235	0.01	12.88	1942	0.01
Neral	8.08	1240	0.04	9.23*	1624	[0.07]
Phenylethyl acetate	8.31	1255	0.10	10.78	1754	0.11
Geraniol	8.38†	1260	7.32	11.39*	1806	2.03
Linalyl acetate	8.39†	1260	[7.32]	7.96*†	1523	[47.27]
(trans?)-Linalool oxide acetate (fur.)?	8.50	1267	0.01	8.46*	1563	[0.02]
Geranial	8.54	1270	0.06	9.87*	1677	0.10
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.64	1277	0.03	14.36	2083	0.03
Bornyl acetate	8.75	1284	0.03	8.07	1532	0.02
Indole	8.86	1292	0.23	16.89	2344	0.26
Methyl anthranilate	9.49	1335	0.39	15.04	2151	0.39
Linalyl propionate	9.55	1340	0.01	8.64	1577	0.01
Hodiendiol derivative	9.59	1342	0.01	12.68	1923	0.01
α-Terpinyl acetate	9.68	1349	0.03	9.47	1644	0.03
Eugenol	9.79	1356	0.01	14.50	2096	0.01
Neryl acetate	9.94	1367	1.30	9.96	1685	1.29
Geranyl acetate	10.22	1386	2.60	10.34*	1716	[2.63]
β-Elemene	10.28	1391	0.03	8.27*	1547	0.60
(Z)-Jasmone	10.33	1394	0.01	12.15	1874	0.03
Dimethyl anthranilate	10.43	1401	0.03	13.42	1992	0.02
β-Caryophyllene	10.62	1415	0.59	8.27*	1547	[0.60]
α-Humulene	11.07	1449	0.05	9.10	1613	0.04
Geranylacetone	11.12	1453	0.01	11.39*	1806	[2.03]
(E)-β-Farnesene	11.21	1459	0.04	9.36	1635	0.04
Germacrene D	11.45	1477	0.03	9.59	1654	0.03

Bicyclogermacrene	11.65	1492	0.07	9.87*	1677	[0.10]
(3Z,6E)- α -Farnesene	11.73	1498	0.01	10.03	1690	0.01
γ -Cadinene	11.89	1510	0.03	10.19	1703	0.01
δ -Cadinene	12.04	1522	0.02	10.23	1706	0.01
(Z)-Nerolidol	12.20	1534	0.01	13.12	1964	0.02
α -Elemol	12.36	1547	0.03	13.79	2028	0.02
(E)-Nerolidol	12.60	1565	1.56	13.55	2005	1.56
Spathulenol	12.68	1572	0.02	14.14	2062	0.02
Caryophyllene oxide	12.72	1575	0.07	12.53	1909	0.11
α -Cadinol	13.64	1650	tr	15.24	2170	0.01
α -Bisabolol	14.02	1680	0.02	15.18	2165	0.02
2,3-Dihydrofarnesol	14.14	1691	0.01	15.78	2226	0.01
(2E,6Z)-Farnesol	14.23	1698	0.02	16.17	2268	0.02
Heptadecane	14.31	1704	0.02	10.13	1699	0.01
(2E,6E)-Farnesol	14.51	1722	1.41	16.57	2309	1.47
(2E,6E)-Farnesal	14.72	1740	0.02	15.57	2205	0.02
Octadecane	15.46	1804	0.03	11.44	1811	0.05
(2E,6E)-Farnesyl acetate	15.88	1842	0.02	15.70	2218	0.08
Unknown [m/z 93, 69 (93), 109 (84), 135 (82), 203 (74), 41 (49)...]	16.51	1899	0.07	14.47	2094	0.07
Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	17.37	1981	0.05			
Eicosane	17.58	2001	0.01	13.66	2014	0.02
Heneicosane	18.62	2104	0.01	14.68	2114	0.01
Phytol	18.72	2114	0.01	19.00	2581	0.01
Tricosane	20.52	2304	0.02	16.61	2314	0.03
Pentacosane	22.28	2505	0.01	18.42	2514	0.02
Heptacosane	23.90	2705	0.01	20.10	2714	0.01
Squalene	24.83	2826	0.01	22.65	3042	0.01
Total identified		98.84%			98.82%	
Total reported		98.96%			98.89%	

*: 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