

**Date :** June 09, 2023

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 23F02-PTH02

**Customer identification :** Neroli - Egypt - N10111R

**Type :** Essential oil

**Source :** *Citrus aurantium* subsp. *amara*

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

**Analysis date :** June 07, 2023

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4671 \pm 0.0003$  (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
Ethanol	0.02	Aliphatic alcohol
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanol	0.03	Aliphatic alcohol
$\alpha$ -Thujene	0.02	Monoterpene
$\alpha$ -Pinene	0.39	Monoterpene
Camphene	0.02	Monoterpene
$\alpha$ -Fenchene	tr	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.50	Monoterpene
$\beta$ -Pinene	5.31	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.91	Monoterpene
$\alpha$ -Phellandrene	0.01	Monoterpene
Pseudolimonene	0.01	Monoterpene
$\Delta^3$ -Carene	0.03	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
$\alpha$ -Terpinene	0.05	Monoterpene
meta-Cymene	0.02	Monoterpene
para-Cymene	0.05	Monoterpene
Limonene	8.86	Monoterpene
$\beta$ -Phellandrene	0.11	Monoterpene
(Z)- $\beta$ -Ocimene	0.78	Monoterpene
(E)- $\beta$ -Ocimene	4.69	Monoterpene
$\gamma$ -Terpinene	0.10	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.17	Monoterpenic alcohol
$\alpha$ -Pinene oxide analog	0.01	Monoterpenic ether
Terpinolene	0.37	Monoterpene
trans-Linalool oxide (fur.)	0.08	Monoterpenic alcohol
$\alpha$ -Pinene oxide	0.01	Monoterpenic ether
Rosefuran	0.01	Monoterpenic ether
Linalool	46.24	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.05	Aliphatic ketone
Phenylethyl alcohol	0.04	Simple phenolic
cis-para-Menth-2-en-1-ol	0.05	Monoterpenic alcohol
allo-Ocimene	0.02	Monoterpene
(Z)-Myroxide	0.01	Monoterpenic ether
Benzeneacetonitrile	0.14	Simple phenolic
neo-allo-Ocimene	0.02	Monoterpene
(E)-Myroxide	0.02	Monoterpenic ether
Lilac aldehyde A	0.02	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.23	Monoterpenic alcohol

para-Cymen-8-ol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	5.12	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.04	Monoterpenic alcohol
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.04	Monoterpenic alcohol
Nerol	1.13	Monoterpenic alcohol
Unknown	0.02	Oxygenated monoterpene
Citronellol	0.01	Monoterpenic alcohol
6,7-Dihydro-7-hydroxylinalool	0.01	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Phenylethyl acetate	0.08	Phenolic ester
Linalyl acetate	9.54	Monoterpenic ester
Geraniol	3.13	Monoterpenic alcohol
Geranial	0.06	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.01	Monoterpenic alcohol
Bornyl acetate	0.02	Monoterpenic ester
1-Nitro-2-phenylethane	0.01	Simple phenolic
Indole	0.08	Indole
Methyl anthranilate	0.12	Phenolic ester
Linalyl propionate	0.03	Monoterpenic ester
Hodiendiol derivative	0.01	Oxygenated monoterpene
$\alpha$ -Terpinyl acetate	0.08	Monoterpenic ester
Eugenol	0.02	Phenylpropanoid
Neryl acetate	1.60	Monoterpenic ester
Geranyl acetate	3.09	Monoterpenic ester
$\beta$ -Elemene	0.03	Sesquiterpene
(Z)-Jasmone	0.03	Jasmonate
Dimethyl anthranilate	0.01	Phenolic ester
$\beta$ -Caryophyllene	0.59	Sesquiterpene
Aromadendrene	0.01	Sesquiterpene
$\alpha$ -Humulene	0.07	Sesquiterpene
Geranylacetone	0.03	Monoterpenic ketone
allo-Aromadendrene	0.01	Sesquiterpene
(E)- $\beta$ -Farnesene	0.08	Sesquiterpene
Germacrene D	0.07	Sesquiterpene
Bicyclogermacrene	0.20	Sesquiterpene
(3Z,6E)- $\alpha$ -Farnesene	0.02	Sesquiterpene
$\gamma$ -Cadinene	0.01	Sesquiterpene
(3E,6E)- $\alpha$ -Farnesene	0.01	Sesquiterpene
$\delta$ -Cadinene	0.01	Sesquiterpene
<i>trans</i> -Calamenene	0.01	Sesquiterpene
(E)-Nerolidol	1.47	Sesquiterpenic alcohol
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.03	Sesquiterpenic ether
Viridiflorol	0.02	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.02	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.02	Sesquiterpenic alcohol
(8Z)-Heptadecene	0.03	Alkene
2,3-Dihydrofarnesol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.03	Sesquiterpenic alcohol
Heptadecane	0.01	Alkane

(2E,6Z)-Farnesal	0.02	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.95	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
(2E,6E)-Farnesyl acetate	0.03	Sesquiterpenic ester
Unknown	0.07	Unknown
Tricosane	0.05	Alkane
Pentacosane	0.03	Alkane
Heptacosane	0.02	Alkane
Squalene	0.01	Triterpene
<b>Consolidated total</b>	<b>98.87%</b>	

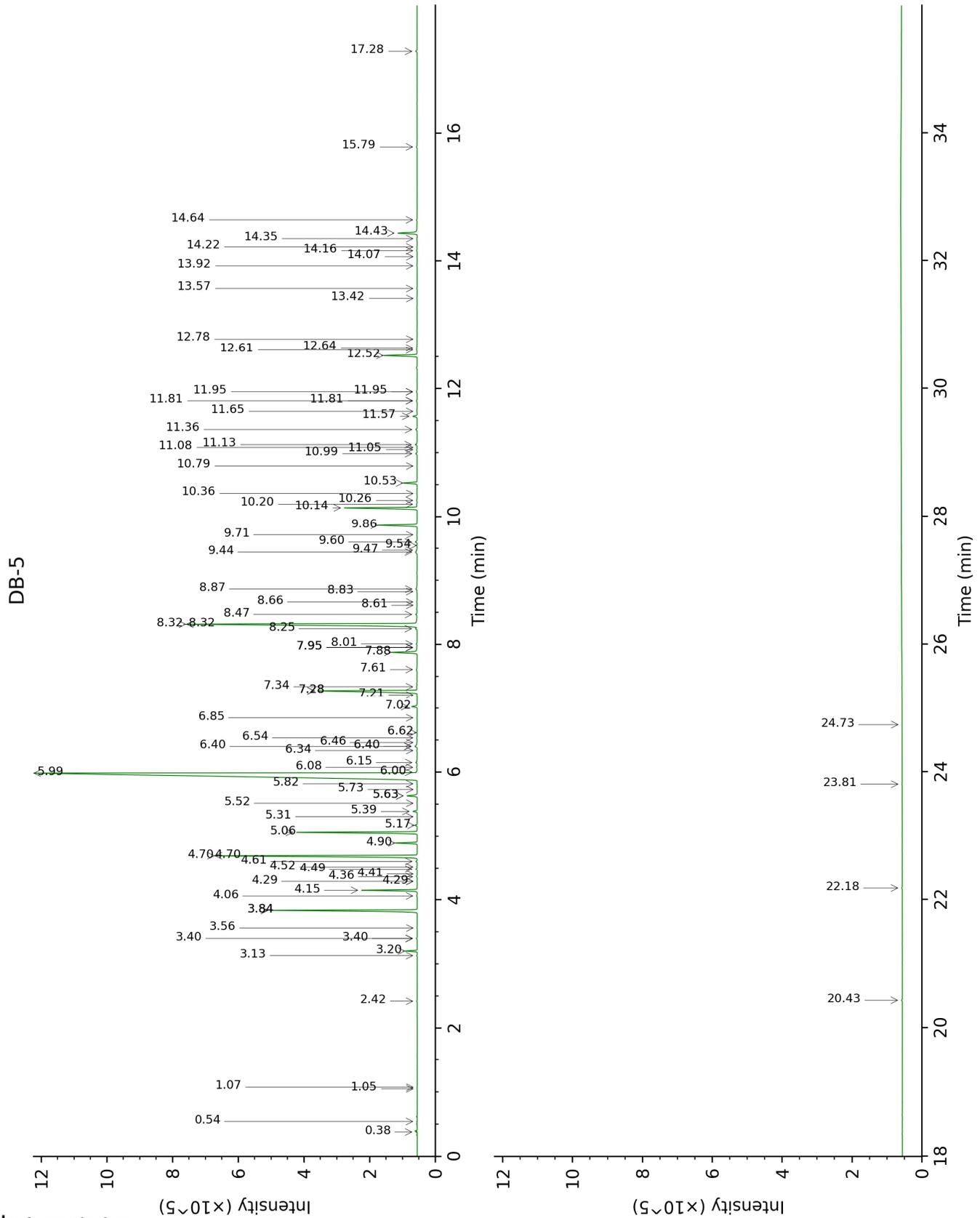
tr: The compound has been detected below 0.005% of total signal.

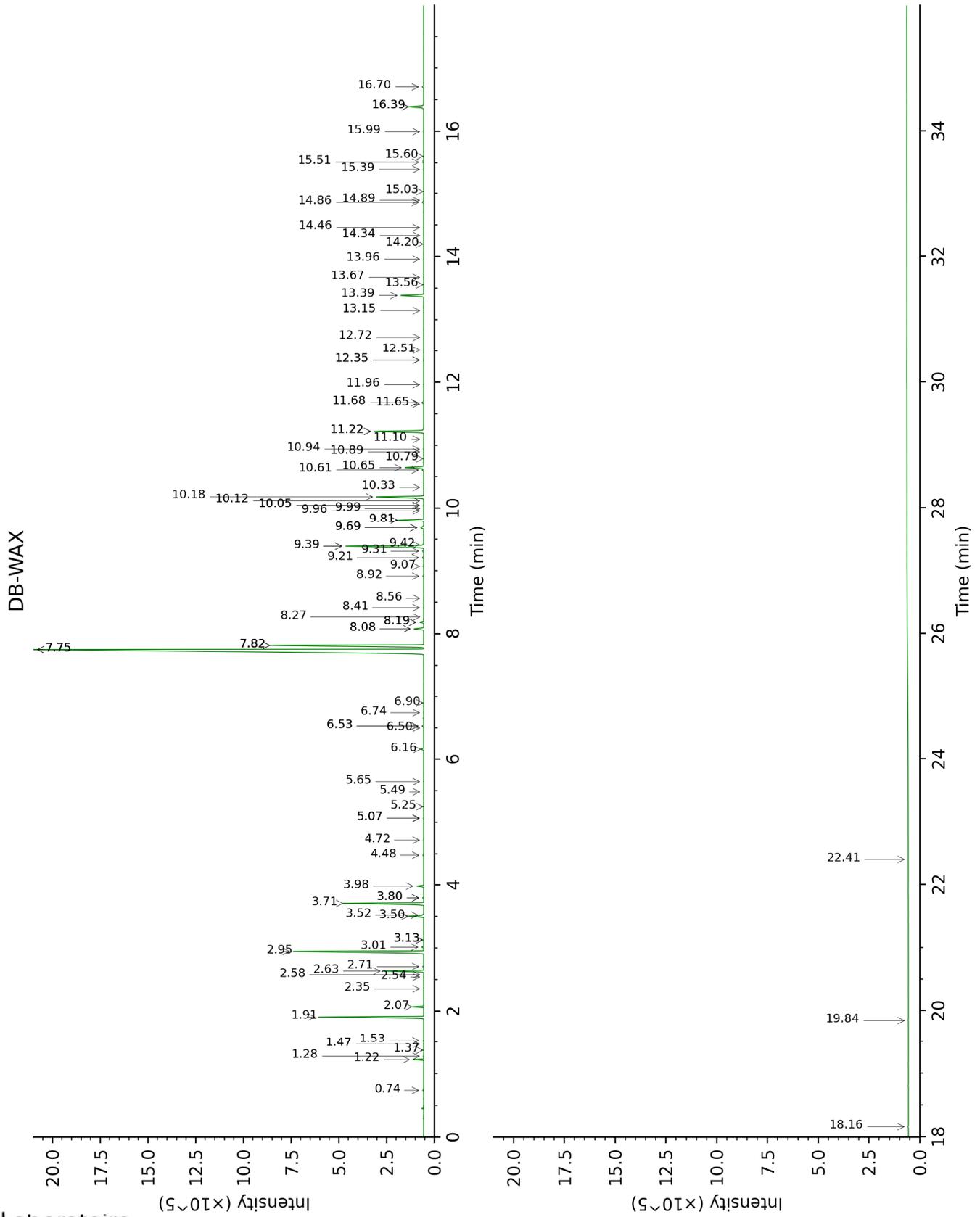
Note: no correction factor was applied

**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	%
Ethanol	0.38	499	0.02	0.74	909	0.02
2-Methyl-3-buten-2-ol	0.54	606	0.01	1.37	1013	0.01
Isoamyl alcohol	1.05	733	0.01	3.13*	1176	0.04
2-Methylbutanol	1.07	736	tr	3.13*	1176	[0.04]
Hexanol	2.42	873	0.03	5.07*	1320	0.03
$\alpha$ -Thujene	3.13	926	0.02	1.28	1002	0.02
$\alpha$ -Pinene	3.20	931	0.39	1.22	992	0.38
Camphene	3.40*	944	0.04	1.53	1029	0.02
$\alpha$ -Fenchene	3.40*	944	[0.04]	1.47	1023	tr
Benzaldehyde	3.56	954	0.01	6.90	1455	0.02
Sabinene	3.84*	972	5.84	2.07	1084	0.50
$\beta$ -Pinene	3.84*	972	[5.84]	1.91	1068	5.31
6-Methyl-5-hepten-2-one	4.06	987	0.02	4.72	1302	0.03
Myrcene	4.15	993	1.91	2.64	1135	1.90
$\alpha$ -Phellandrene	4.29*	1002	0.02	2.54	1127	0.01
Pseudolimonene	4.29*	1002	[0.02]	2.58	1130	0.01
$\Delta^3$ -Carene	4.36	1007	0.03	2.35	1112	0.01
(3Z)-Hexenyl acetate	4.40	1009	0.01	4.48	1283	0.05
$\alpha$ -Terpinene	4.49	1014	0.05	2.71	1141	0.05
meta-Cymene	4.52	1017	0.02	3.80*	1229	0.05
para-Cymene	4.61	1022	0.05	3.80*	1229	[0.05]
Limonene	4.70*	1028	8.98	2.95	1161	8.86
$\beta$ -Phellandrene	4.70*	1028	[8.98]	3.01	1166	0.11
(Z)- $\beta$ -Ocimene	4.90	1040	0.78	3.50†	1207	0.89
(E)- $\beta$ -Ocimene	5.06	1051	4.69	3.71	1223	4.70
$\gamma$ -Terpinene	5.17	1057	0.10	3.52†	1208	[0.89]
cis-Sabinene hydrate	5.31	1066	0.01	6.53*	1428	0.10
cis-Linalool oxide (fur.)	5.39	1071	0.17	6.16	1400	0.17
$\alpha$ -Pinene oxide analog	5.52	1079	0.01	5.07*	1320	[0.03]
Terpinolene	5.63*	1086	0.45	3.98	1244	0.37
trans-Linalool oxide (fur.)	5.63*	1086	[0.45]	6.53*	1428	[0.10]
$\alpha$ -Pinene oxide	5.73	1092	0.01	5.07*	1320	[0.03]
Rosefuran	5.82	1098	0.01	5.65	1362	0.02
Linalool	5.99	1108	46.24	7.75*†	1520	55.90
(Z)-6-Methyl-3,5-heptadien-2-one	6.00	1109	0.05	7.82*†	1526	[55.90]
Phenylethyl alcohol	6.08	1114	0.04	11.65	1846	0.02
cis-para-Menth-2-en-1-ol	6.15	1119	0.05	7.75*†	1520	[55.90]
allo-Ocimene	6.34	1131	0.02	5.25	1333	0.01
(Z)-Myroxide	6.40*	1135	0.15	6.50	1425	0.01

Benzeneacetonitrile	6.40*	1135	[0.15]	11.68	1848	0.14
neo-allo-Ocimene	6.46	1138	0.02	5.49	1350	0.01
(E)-Myroxide	6.54	1143	0.02	6.74	1444	0.02
Lilac aldehyde A	6.62	1148	0.02			
Borneol	6.85	1163	0.01	9.39*†	1652	5.20
Terpinen-4-ol	7.02	1174	0.23	8.19*	1555	0.24
para-Cymen-8-ol	7.21	1186	0.01	11.10	1796	0.02
α-Terpineol	7.28*	1190	5.15	9.39*†	1652	[5.20]
Myrtenal	7.28*	1190	[5.15]	8.27	1561	0.01
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	7.34	1194	0.04	12.35*	1909	0.06
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.61	1212	0.04	10.94	1783	0.04
Nerol	7.88	1230	1.13	10.65	1758	1.16
Unknown [m/z 137, 152 (28), 43 (25), 91 (24), 109 (23), 119 (19)]	7.95*	1235	0.03	10.90	1779	0.02
Citronellol	7.95*	1235	[0.03]	10.33	1730	0.01
6,7-Dihydro-7-hydroxylinalool	7.95*	1235	[0.03]	12.72	1943	0.01
Neral	8.01	1239	0.04	9.07	1625	0.05
Phenylethyl acetate	8.25	1254	0.08	10.61	1754	0.09
Linalyl acetate	8.32*	1259	13.08	7.82*†	1526	[55.90]
Geraniol	8.32*	1259	[13.08]	11.22*	1807	3.15
Geranial	8.47	1269	0.06	9.68*	1676	0.24
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.61	1279	0.01	14.20	2085	0.01
Bornyl acetate	8.66	1282	0.02	7.82*†	1526	[55.90]
1-Nitro-2-phenylethane	8.83	1293	0.01	13.67	2034	0.02
Indole	8.87	1296	0.08	16.70	2345	0.09
Methyl anthranilate	9.44	1336	0.12	14.86	2152	0.10
Linalyl propionate	9.47	1338	0.03	8.42	1573	0.03
Hodiendiol derivative	9.54	1343	0.01	12.51	1924	0.01
α-Terpinyl acetate	9.60	1347	0.08	9.31	1645	0.09
Eugenol	9.71	1355	0.02	14.34	2098	0.01
Neryl acetate	9.86	1365	1.60	9.81*	1686	1.60
Geranyl acetate	10.14	1385	3.09	10.18	1718	3.10
β-Elemene	10.20	1389	0.03	8.08*	1546	0.61
(Z)-Jasmone	10.26	1393	0.03	11.96	1874	0.02
Dimethyl anthranilate	10.36	1401	0.01	13.15	1983	0.01
β-Caryophyllene	10.53	1413	0.59	8.08*	1546	[0.61]
Aromadendrene	10.79	1432	0.01	8.19*	1555	[0.24]
α-Humulene	10.99	1447	0.07	8.92	1612	0.06
Geranylacetone	11.05	1452	0.03	11.22*	1807	[3.15]
allo-Aromadendrene	11.08	1454	0.01	8.56	1585	0.01

(E)-β-Farnesene	11.13	1457	0.08	9.21	1637	0.09
Germacrene D	11.36	1475	0.07	9.42†	1654	[5.20]
Bicyclogermacrene	11.57	1490	0.20	9.68*	1676	[0.24]
(3Z,6E)-α-Farnesene	11.65	1496	0.02	9.81*	1686	[1.60]
γ-Cadinene	11.81*	1508	0.04	9.96	1699	0.01
(3E,6E)-α-Farnesene	11.81*	1508	[0.04]	10.12	1712	0.01
δ-Cadinene	11.95*	1519	0.04	10.05*	1706	0.04
<i>trans</i> -Calamenene	11.95*	1519	[0.04]	10.79	1770	0.01
(E)-Nerolidol	12.52	1564	1.47	13.39	2006	1.45
Spathulenol	12.61	1571	0.03	13.96	2062	0.02
Caryophyllene oxide	12.64	1574	0.03	12.35*	1909	[0.06]
Viridiflorol	12.78	1584	0.02	13.56	2022	0.01
τ-Cadinol	13.42	1636	0.02	14.46	2111	0.02
α-Cadinol	13.57	1649	0.02	15.03	2169	0.02
(8Z)-Heptadecene	13.92	1678	0.03	10.05*	1706	[0.04]
2,3-Dihydrofarnesol	14.07	1690	0.01	15.60	2228	0.02
(2E,6Z)-Farnesol	14.16	1697	0.03	15.99	2269	0.03
Heptadecane	14.22	1702	0.01	10.00	1702	0.01
(2E,6Z)-Farnesal	14.35	1713	0.02	14.89	2155	0.02
(2E,6E)-Farnesol	14.43	1720	0.95	16.39*	2311	1.04
(2E,6E)-Farnesal	14.64	1738	0.02	15.40	2206	0.03
(2E,6E)-Farnesyl acetate	15.79	1839	0.03	15.51	2218	0.10
Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	17.28	1978	0.07			
Tricosane	20.43	2301	0.05	16.39*	2311	[1.04]
Pentacosane	22.18	2500	0.03	18.16	2509	0.03
Heptacosane	23.81	2700	0.02	19.84	2710	0.02
Squalene	24.74	2820	0.01	22.41	3045	0.01
<b>Total identified</b>		<b>99.31%</b>			<b>98.86%</b>	
<b>Total reported</b>		<b>99.38%</b>			<b>98.87%</b>	

\*: 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