

**Date :** June 09, 2023

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 23E26-NPA01


**Customer identification :** Neroli - Egypt - NPS00051 - Lot # NP0019

**Type :** Essential oil

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

**Customer :** Nature Packaged

**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

*Notes: 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 from the first version issued on June 9, 2023, to format it for online publication.*

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4672 \pm 0.0003$  (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
Ethyl acetate	tr	Aliphatic ester
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Hexanol	0.02	Aliphatic alcohol
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.03	Monoterpene
$\alpha$ -Pinene	0.41	Monoterpene
$\alpha$ -Fenchene	tr	Monoterpene
Camphene	0.03	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.59	Monoterpene
$\beta$ -Pinene	6.32	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
Myrcene	2.19	Monoterpene
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
$\alpha$ -Phellandrene	0.02	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.02	Monoterpenic ether
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.07	Monoterpene
para-Cymene	0.06	Monoterpene
Limonene	7.29	Monoterpene
$\beta$ -Phellandrene	0.12	Monoterpene
( <i>Z</i> )- $\beta$ -Ocimene	0.87	Monoterpene
( <i>E</i> )- $\beta$ -Ocimene	5.11	Monoterpene
$\gamma$ -Terpinene	0.12	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.11	Monoterpenic alcohol
Terpinolene	0.43	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.04	Monoterpenic alcohol
$\alpha$ -Pinene oxide	0.02	Monoterpenic ether
Rosefuran	0.01	Monoterpenic ether
Linalool	48.03	Monoterpenic alcohol
Phenylethyl alcohol	0.05	Simple phenolic
<i>cis</i> -para-Menth-2-en-1-ol	0.05	Monoterpenic alcohol
allo-Ocimene	0.02	Monoterpene
Benzeneacetonitrile	0.16	Simple phenolic
<i>trans</i> -para-Menth-2-en-1-ol	0.02	Monoterpenic alcohol
( <i>E</i> )-Myroxide	0.02	Monoterpenic ether
Terpinen-4-ol	0.26	Monoterpenic alcohol
$\alpha$ -Terpineol	5.18	Monoterpenic alcohol
Myrtenal	tr	Monoterpenic aldehyde
Safranal	0.02	Monoterpenic aldehyde
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.03	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>E</i> )-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol

Nerol	1.17	Monoterpenic alcohol
Citronellol	0.01	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene
Neral	0.04	Monoterpenic aldehyde
Geraniol	3.20	Monoterpenic alcohol
Linalyl acetate	8.49	Monoterpenic ester
Geranial	0.07	Monoterpenic aldehyde
Bornyl acetate	0.01	Monoterpenic ester
1-Nitro-2-phenylethane	0.01	Simple phenolic
Indole	0.11	Indole
Methyl anthranilate	0.15	Phenolic ester
Linalyl propionate	0.03	Monoterpenic ester
Hodiendiol derivative	0.01	Oxygenated monoterpene
$\alpha$ -Terpinyl acetate	0.09	Monoterpenic ester
Neryl acetate	1.65	Monoterpenic ester
Geranyl acetate	3.12	Monoterpenic ester
$\beta$ -Elemene	0.03	Sesquiterpene
(Z)-Jasmone	0.03	Jasmonate
Dimethyl anthranilate	0.03	Phenolic ester
$\beta$ -Caryophyllene	0.40	Sesquiterpene
$\alpha$ -Humulene	0.05	Sesquiterpene
Geranylacetone	0.02	Monoterpenic ketone
(E)- $\beta$ -Farnesene	0.05	Sesquiterpene
Germacrene D	0.06	Sesquiterpene
Bicyclogermacrene	0.09	Sesquiterpene
Valencene	0.01	Sesquiterpene
$\alpha$ -Muurolene	0.01	Sesquiterpene
(3Z,6E)- $\alpha$ -Farnesene	0.01	Sesquiterpene
$\gamma$ -Cadinene	tr	Sesquiterpene
(3E,6E)- $\alpha$ -Farnesene	0.01	Sesquiterpene
$\delta$ -Cadinene	0.01	Sesquiterpene
<i>trans</i> -Calamenene	tr	Sesquiterpene
Methyl N-formylanthranilate	0.03	Phenolic ester
(E)-Nerolidol	1.44	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
$\alpha$ -Cadinol	0.01	Sesquiterpenic alcohol
(8Z)-Heptadecene	0.01	Alkene
$\alpha$ -Bisabolol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.02	Sesquiterpenic alcohol
Heptadecane	0.01	Alkane
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.65	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.03	Sesquiterpenic aldehyde
(2E,6E)-Farnesyl acetate	0.02	Sesquiterpenic ester
Unknown	0.07	Unknown
Tricosane	0.03	Alkane
Pentacosane	0.04	Alkane
Heptacosane	0.02	Alkane
Squalene	0.02	Triterpene
<b>Consolidated total</b>	<b>99.33%</b>	

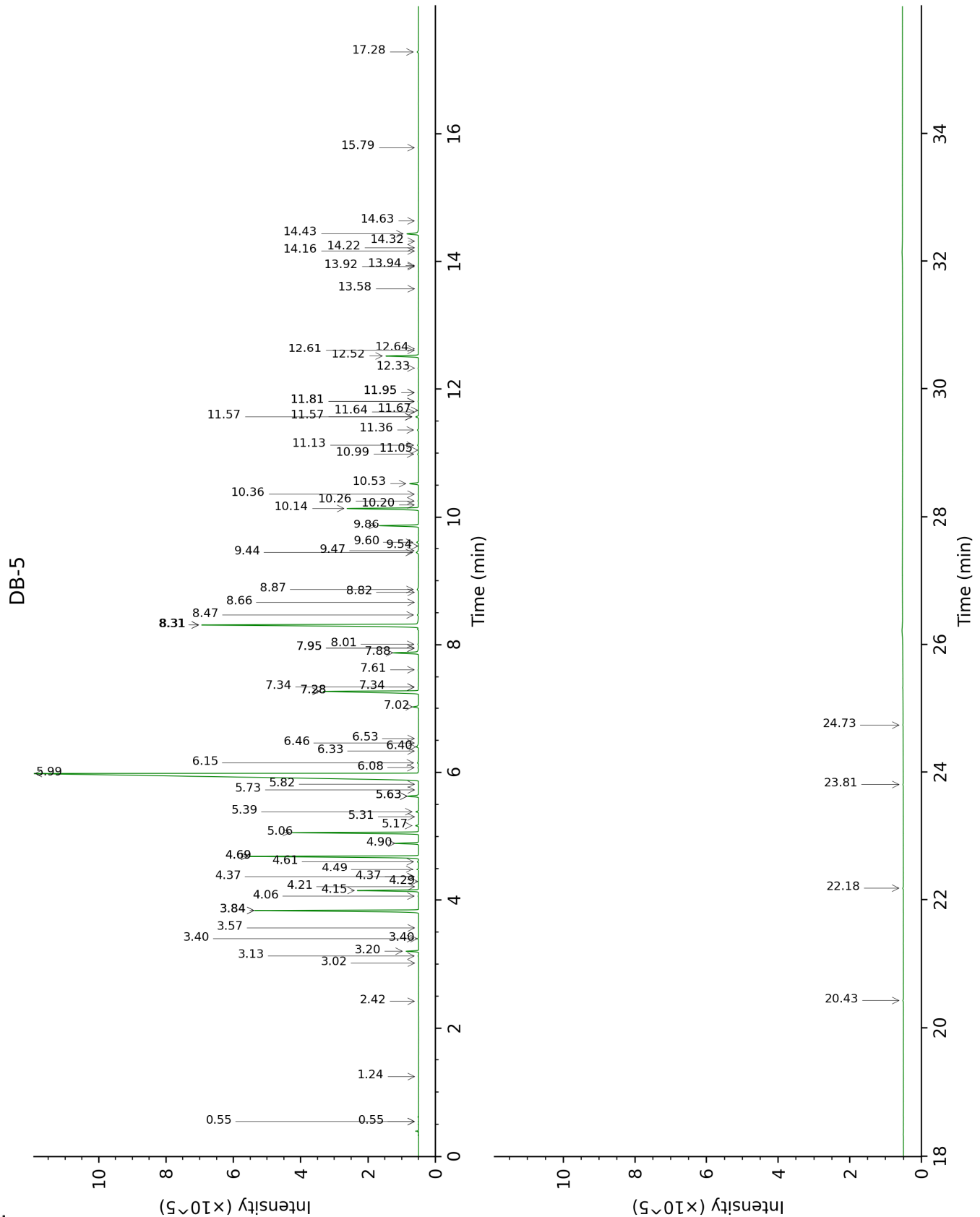
tr: The compound has been detected below 0.005% of total signal.

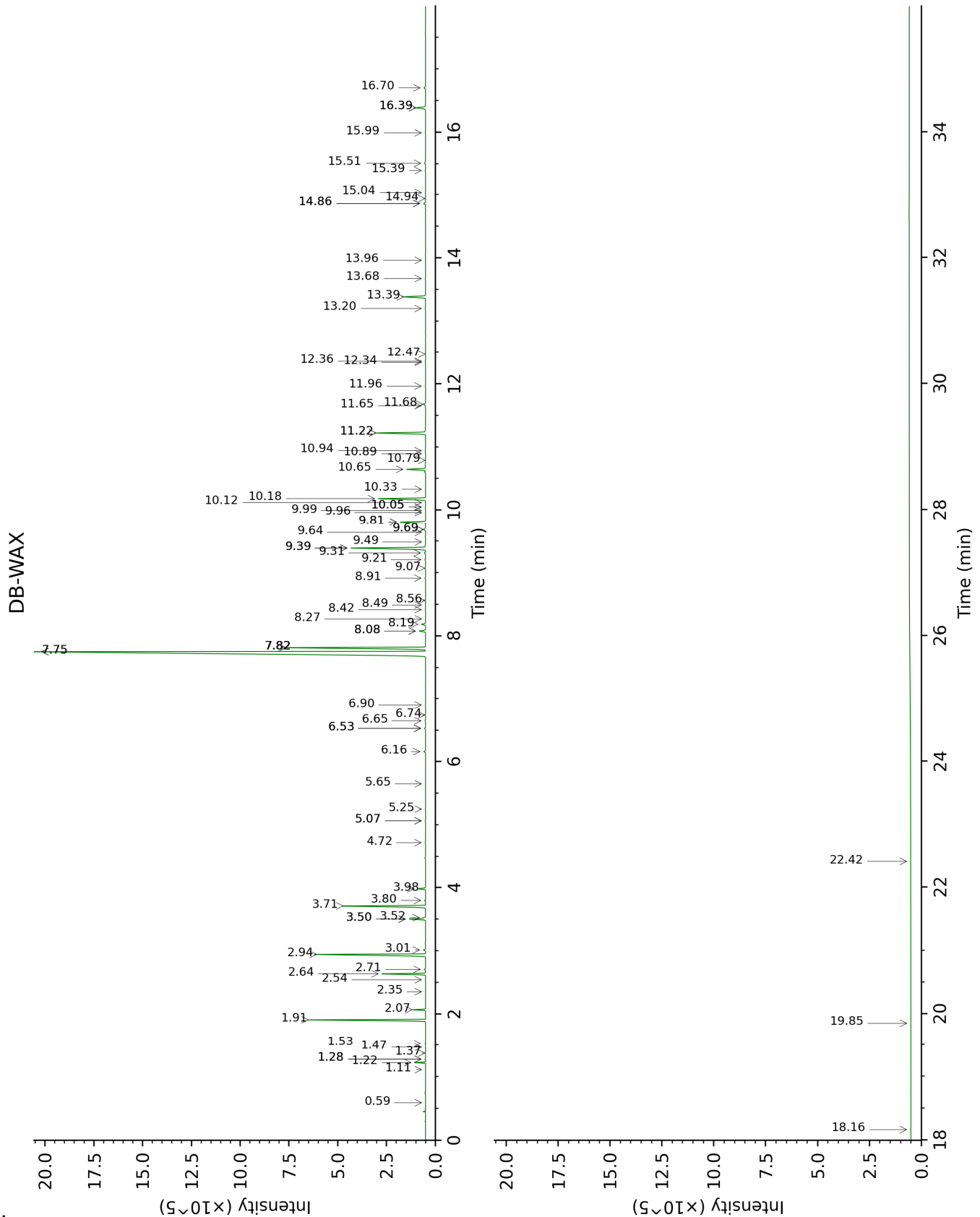
Note: no correction factor was applied

**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	%
Ethyl acetate	0.54*	606	0.01	0.59	854	tr
2-Methyl-3-buten-2-ol	0.54*	606	[0.01]	1.37	1013	tr
Toluene	1.24	759	tr	1.28*	1002	0.02
Hexanol	2.42	874	0.02	5.07*	1320	0.03
Tricyclene	3.02	919	0.01	1.11	973	tr
$\alpha$ -Thujene	3.13	926	0.03	1.28*	1002	[0.02]
$\alpha$ -Pinene	3.20	931	0.41	1.22	992	0.41
$\alpha$ -Fenchene	3.40*	944	0.04	1.47	1022	tr
Camphene	3.40*	944	[0.04]	1.53	1029	0.03
Benzaldehyde	3.57	955	0.01	6.90	1455	0.02
Sabinene	3.84*	972	6.91	2.07	1084	0.59
$\beta$ -Pinene	3.84*	972	[6.91]	1.91	1068	6.32
6-Methyl-5-hepten-2-one	4.06	987	0.03	4.72	1302	0.04
Myrcene	4.15	993	2.19	2.64	1135	2.18
6-Methyl-5-hepten-2-ol	4.21	997	0.01	6.65	1436	0.04
$\alpha$ -Phellandrene	4.29	1002	0.02	2.54	1128	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.37*	1007	0.03	3.50*†	1207	0.98
$\Delta^3$ -Carene	4.37*	1007	[0.03]	2.35	1112	0.01
$\alpha$ -Terpinene	4.49	1015	0.07	2.71	1141	0.07
para-Cymene	4.61	1022	0.06	3.80	1229	0.05
Limonene	4.69*	1028	7.40	2.94	1160	7.29
$\beta$ -Phellandrene	4.69*	1028	[7.40]	3.01	1166	0.12
( <i>Z</i> )- $\beta$ -Ocimene	4.90	1040	0.87	3.50*†	1207	[0.98]
( <i>E</i> )- $\beta$ -Ocimene	5.06	1051	5.11	3.71	1223	5.13
$\gamma$ -Terpinene	5.17	1057	0.12	3.52†	1208	[0.98]
<i>cis</i> -Sabinene hydrate	5.31	1066	0.01	6.53*	1428	0.06
<i>cis</i> -Linalool oxide (fur.)	5.39	1071	0.11	6.16	1400	0.11
Terpinolene	5.63*	1086	0.47	3.98	1244	0.43
<i>trans</i> -Linalool oxide (fur.)	5.63*	1086	[0.47]	6.53*	1428	[0.06]
$\alpha$ -Pinene oxide	5.73	1092	0.02	5.07*	1320	[0.03]
Rosefuran	5.82	1098	0.01	5.65	1362	0.01
Linalool	5.98	1108	48.03	7.75*†	1520	56.58
Phenylethyl alcohol	6.08	1114	0.05	11.65	1846	0.03
<i>cis</i> -para-Menth-2-en-1-ol	6.15	1119	0.05	7.75*†	1520	[56.58]
allo-Ocimene	6.34	1130	0.02	5.25	1333	0.01
Benzeneacetonitrile	6.40	1135	0.16	11.68	1848	0.15
<i>trans</i> -para-Menth-2-en-1-ol	6.46	1138	0.02	8.56	1584	0.02
( <i>E</i> )-Myroxide	6.53	1143	0.02	6.74	1444	0.02

Terpinen-4-ol	7.02	1174	0.26	8.19	1555	0.26
$\alpha$ -Terpineol	7.28*	1190	5.18	9.39*	1652	5.24
Myrtenal	7.28*	1190	[5.18]	8.27	1561	tr
Safranal	7.34*	1195	0.04	8.49	1579	0.02
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	7.34*	1195	[0.04]	12.36	1909	0.03
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.61	1212	0.03	10.94	1783	0.03
Nerol	7.88	1230	1.17	10.65	1758	1.22
Citronellol	7.95*	1235	0.03	10.33	1730	0.01
Unknown [m/z 137, 152 (28), 43 (25), 91 (24), 109 (23), 119 (19)]	7.95*	1235	[0.03]	10.89	1779	0.01
Neral	8.01	1239	0.04	9.07	1625	0.04
Geraniol	8.31*	1259	11.84	11.22*	1807	3.23
Linalyl acetate	8.31*	1259	[11.84]	7.82*†	1526	[56.58]
Geranial	8.47	1269	0.07	9.69*	1676	0.16
Bornyl acetate	8.66	1282	0.01	7.82*†	1526	[56.58]
1-Nitro-2-phenylethane	8.82	1293	0.01	13.68	2034	0.02
Indole	8.87	1296	0.11	16.70	2345	0.11
Methyl anthranilate	9.44	1336	0.15	14.86*	2152	0.14
Linalyl propionate	9.47	1338	0.03	8.42	1573	0.02
Hodiendiol derivative	9.54	1343	0.01	12.47	1920	0.02
$\alpha$ -Terpinyl acetate	9.60	1347	0.09	9.32	1646	0.09
Neryl acetate	9.86	1365	1.65	9.81*	1686	1.65
Geranyl acetate	10.14	1385	3.12	10.18	1718	3.15
$\beta$ -Elemene	10.20	1389	0.03	8.08*	1546	0.41
(Z)-Jasmone	10.26	1393	0.03	11.96	1874	0.03
Dimethyl anthranilate	10.36	1401	0.03	13.20	1988	0.04
$\beta$ -Caryophyllene	10.53	1413	0.40	8.08*	1546	[0.41]
$\alpha$ -Humulene	10.99	1447	0.05	8.92	1612	0.05
Geranylacetone	11.05	1452	0.02	11.22*	1807	[3.23]
(E)- $\beta$ -Farnesene	11.13	1457	0.05	9.21	1637	0.06
Germacrene D	11.36	1475	0.06	9.39*	1652	[5.24]
Bicyclogermacrene	11.57*	1490	0.13	9.69*	1676	[0.16]
Valencene	11.57*	1490	[0.13]	9.49	1660	0.01
$\alpha$ -Muurolene	11.64	1496	0.01	9.64	1672	tr
(3Z,6E)- $\alpha$ -Farnesene	11.67	1498	0.01	9.81*	1686	[1.65]
$\gamma$ -Cadinene	11.81*	1508	0.03	9.96	1699	tr
(3E,6E)- $\alpha$ -Farnesene	11.81*	1508	[0.03]	10.12	1712	0.01
$\delta$ -Cadinene	11.95*	1519	0.03	10.05*	1706	0.02
<i>trans</i> -Calamenene	11.95*	1519	[0.03]	10.79	1770	tr
Methyl N-formylanthranilate	12.33	1549	0.03			
(E)-Nerolidol	12.52	1564	1.44	13.39	2006	1.44
Spathulenol	12.61	1571	0.02	13.96	2062	0.01

Caryophyllene oxide	12.64	1573	0.02	12.34	1908	0.01
$\alpha$ -Cadinol	13.58	1649	0.01	15.04	2169	0.01
(8Z)-Heptadecene	13.92	1678	0.01	10.05*	1706	[0.02]
$\alpha$ -Bisabolol	13.94	1679	0.01	14.94	2160	0.01
(2E,6Z)-Farnesol	14.16	1698	0.02	15.99	2269	0.02
Heptadecane	14.22	1702	0.01	9.99	1702	0.01
(2E,6Z)-Farnesal	14.32	1710	0.01	14.86*	2152	[0.14]
(2E,6E)-Farnesol	14.43	1720	0.65	16.39*	2311	0.72
(2E,6E)-Farnesal	14.64	1738	0.03	15.40	2206	0.02
(2E,6E)-Farnesyl acetate	15.79	1839	0.02	15.51	2218	0.09
Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	17.28	1978	0.07			
Tricosane	20.43	2301	0.03	16.39*	2311	[0.72]
Pentacosane	22.18	2501	0.04	18.16	2509	0.03
Heptacosane	23.81	2700	0.02	19.85	2711	0.02
Squalene	24.73	2820	0.02	22.42	3047	0.01
<b>Total identified</b>		<b>99.46%</b>			<b>99.28%</b>	
<b>Total reported</b>		<b>99.53%</b>			<b>99.29%</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