

**Date :** November 16, 2021

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 21K11-PTH05


**Customer identification :** Neroli - Egypt - N10109213R

**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 :** Seydou Ka, Ph. D.

**Analysis date :** November 15, 2021

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4673 \pm 0.0003$  (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
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	tr	Aliphatic alcohol
Octane	tr	Alkane
(2E)-Hexenol	tr	Aliphatic alcohol
Hexanol	0.02	Aliphatic alcohol
$\alpha$ -Thujene	0.02	Monoterpene
$\alpha$ -Pinene	0.37	Monoterpene
Camphene	0.03	Monoterpene
Benzaldehyde	0.03	Simple phenolic
$\beta$ -Pinene	4.85	Monoterpene
Sabinene	0.57	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
Myrcene	1.88	Monoterpene
$\alpha$ -Phellandrene	0.01	Monoterpene
$\Delta^3$ -Carene	0.03	Monoterpene
(3Z)-Hexenyl acetate	tr	Aliphatic ester
$\alpha$ -Terpinene	0.06	Monoterpene
para-Cymene	0.03	Monoterpene
Limonene	8.88	Monoterpene
$\beta$ -Phellandrene	0.10	Monoterpene
(Z)- $\beta$ -Ocimene	0.78	Monoterpene
(E)- $\beta$ -Ocimene	4.73	Monoterpene
$\gamma$ -Terpinene	0.10	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.16	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.38	Monoterpene
trans-Linalool oxide (fur.)	0.09	Monoterpenic alcohol
$\alpha$ -Pinene oxide	0.01	Monoterpenic ether
trans-Sabinene hydrate	tr	Monoterpenic alcohol
Linalool	41.46	Monoterpenic alcohol
Phenylethyl alcohol	0.03	Simple phenolic
cis-para-Menth-2-en-1-ol	0.06	Monoterpenic alcohol
allo-Ocimene	0.02	Monoterpene
Benzeneacetonitrile	0.19	Simple phenolic
neo-allo-Ocimene	0.01	Monoterpene
(E)-Myroxide	0.02	Monoterpenic ether
Lilac aldehyde A	0.03	Monoterpenic aldehyde
Borneol	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.21	Monoterpenic alcohol
$\alpha$ -Terpineol	4.86	Monoterpenic alcohol
Hodiendiol	0.01	Monoterpenic alcohol
Safranal	0.01	Monoterpenic aldehyde
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.04	Monoterpenic alcohol

Linalyl formate	0.02	Monoterpenic ester
Nerol	1.10	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Phenylethyl acetate	0.15	Phenolic ester
Geraniol	2.76	Monoterpenic alcohol
Linalyl acetate	12.77	Monoterpenic ester
Geranial	0.06	Monoterpenic aldehyde
Bornyl acetate	0.01	Monoterpenic ester
1-Nitro-2-phenylethane	0.03	Simple phenolic
Indole	0.18	Indole
4-Vinylguaiaicol	0.02	Simple phenolic
$\delta$ -Elemene	0.05	Sesquiterpene
Methyl anthranilate	0.15	Phenolic ester
Linalyl propionate	0.02	Monoterpenic ester
$\alpha$ -Terpinyl acetate	0.08	Monoterpenic ester
Eugenol	0.02	Phenylpropanoid
Neryl acetate	1.51	Monoterpenic ester
Geranyl acetate	2.89	Monoterpenic ester
$\beta$ -Elemene	0.06	Sesquiterpene
(Z)-Jasmone	0.03	Jasmonate
$\beta$ -Caryophyllene	0.68	Sesquiterpene
$\alpha$ -Humulene	0.01	Sesquiterpene
Geranylacetone	0.04	Monoterpenic ketone
allo-Aromadendrene	0.01	Sesquiterpene
(E)- $\beta$ -Farnesene	0.12	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
Bicyclogermacrene	0.24	Sesquiterpene
(3Z,6E)- $\alpha$ -Farnesene	0.03	Sesquiterpene
$\gamma$ -Cadinene	0.07	Sesquiterpene
$\delta$ -Cadinene	0.03	Sesquiterpene
(E)-Nerolidol	3.20	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
Viridiflorol	tr	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.01	Sesquiterpenic alcohol
(8Z)-Heptadecene	0.04	Alkene
2,3-Dihydrofarnesol	0.03	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.06	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	0.05	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	1.80	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.04	Sesquiterpenic aldehyde
(2E,6E)-Farnesyl acetate	0.03	Sesquiterpenic ester
meta-Camphorene	0.01	Diterpene
Unknown	0.24	Unknown
Tricosane	0.05	Alkane
Tetracosane	0.01	Alkane
Pentacosane	0.04	Alkane
Heptacosane	0.02	Alkane
Squalene	0.02	Triterpene
<b>Consolidated total</b>	<b>99.11%</b>	

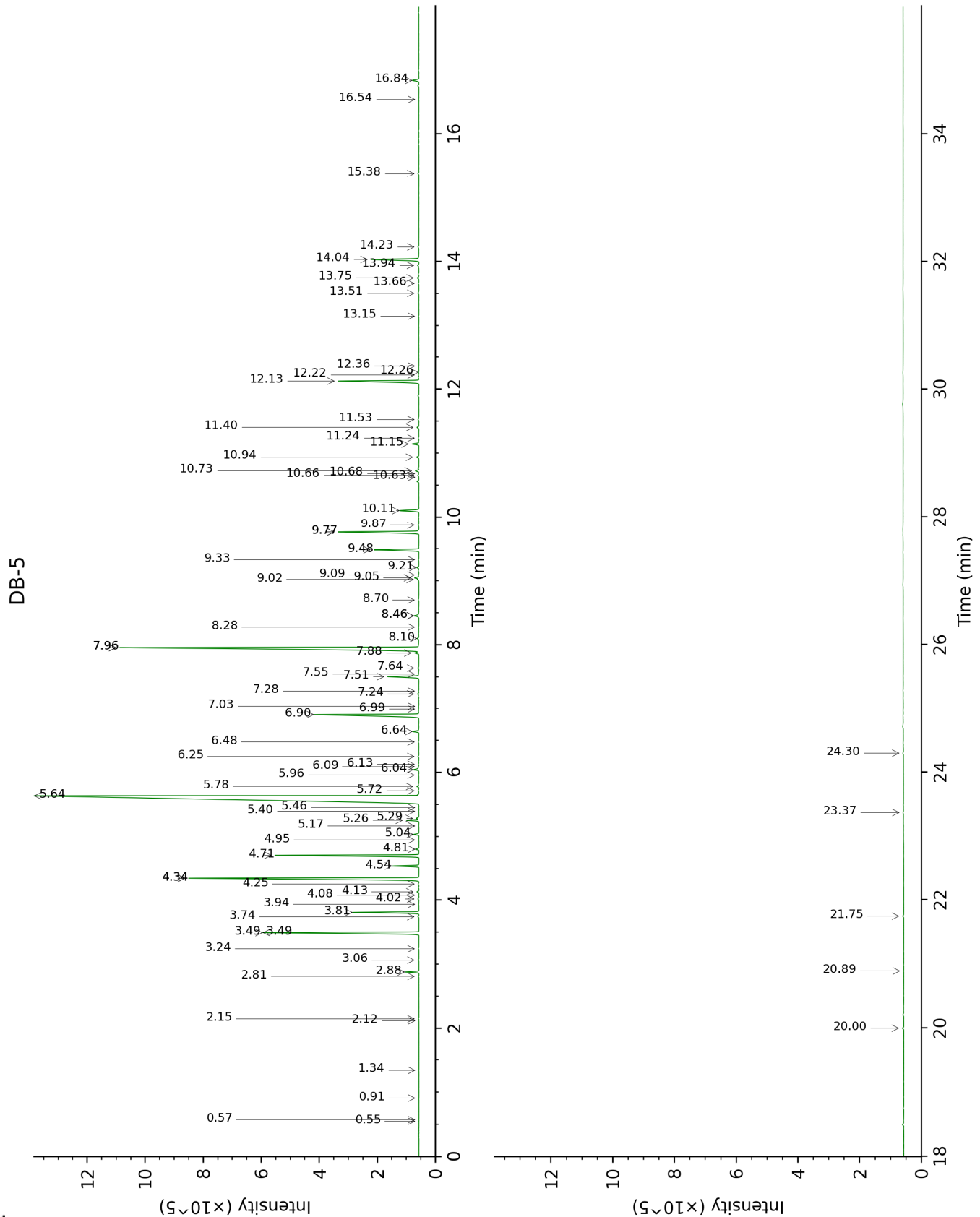
tr: The compound has been detected below 0.005% of total signal.

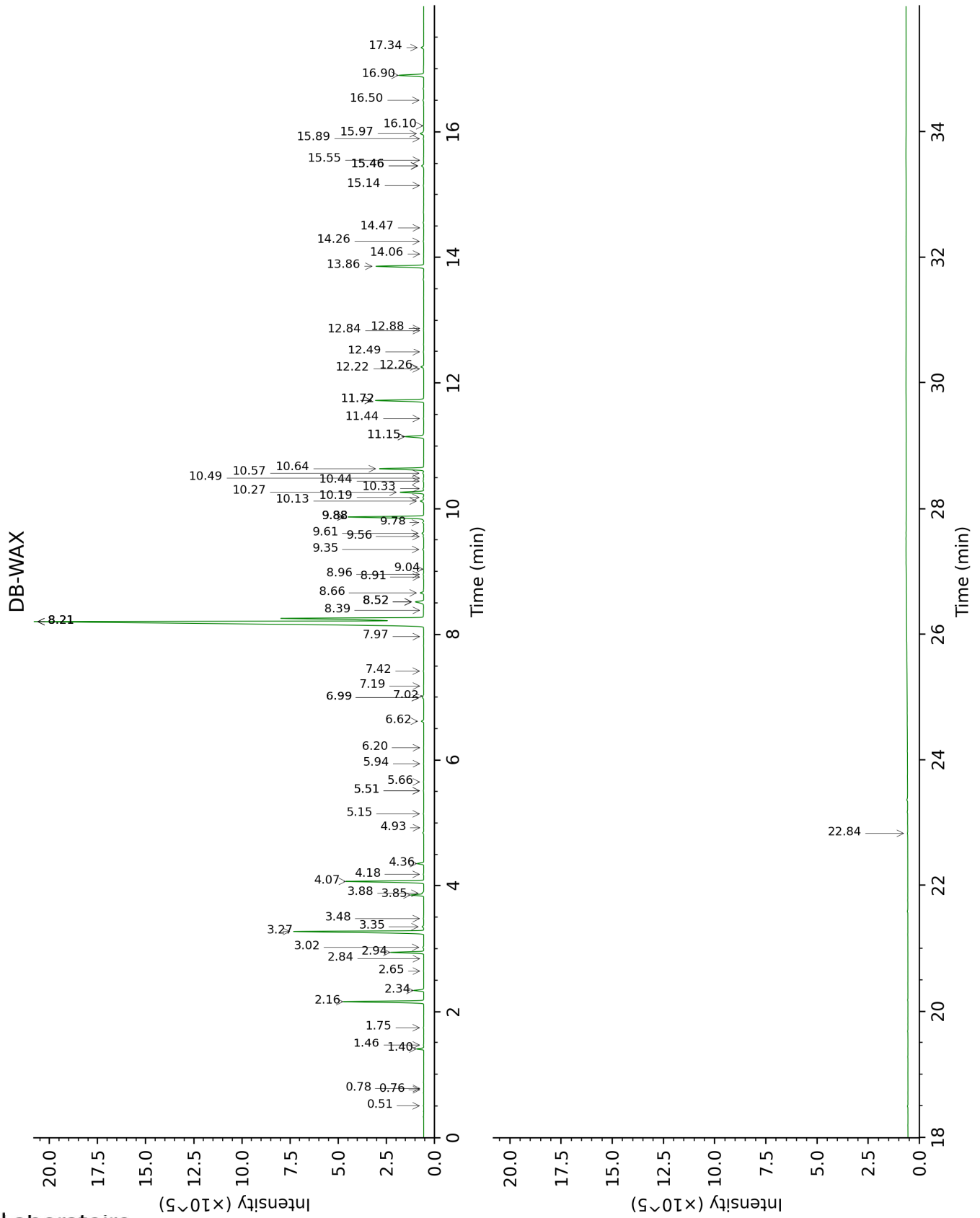
Note: no correction factor was applied

**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	%
Isovaleral	0.55	640	tr	0.78	889	tr
2-Methylbutyral	0.57	650	tr	0.76	881	tr
Isoamyl alcohol	0.91	734	tr	3.48	1176	0.03
Octane	1.34	801	tr	0.51	786	0.01
(2E)-Hexenol	2.12	870	tr	6.20	1373	0.01
Hexanol	2.15	872	0.02	5.52*	1325	0.02
$\alpha$ -Thujene	2.81	924	0.02	1.46	998	0.02
$\alpha$ -Pinene	2.88	929	0.37	1.40	992	0.38
Camphene	3.06	942	0.03	1.75	1026	0.03
Benzaldehyde	3.24	954	0.03	7.42	1463	0.03
$\beta$ -Pinene	3.49*	970	5.39	2.16	1067	4.85
Sabinene	3.49*	970	[5.39]	2.34	1085	0.57
6-Methyl-5-hepten-2-one	3.74	987	0.03	5.15	1299	0.03
Myrcene	3.81	992	1.88	2.94	1134	1.84
$\alpha$ -Phellandrene	3.94	1000	0.01	2.84	1126	0.01
$\Delta^3$ -Carene	4.02	1006	0.03	2.65	1111	0.01
(3Z)-Hexenyl acetate	4.08	1010	tr	4.93	1285	0.01
$\alpha$ -Terpinene	4.13	1013	0.06	3.02	1140	0.06
para-Cymene	4.25	1021	0.03	4.18	1230	0.03
Limonene	4.34*	1026	8.95	3.27	1160	8.88
$\beta$ -Phellandrene	4.34*	1026	[8.95]	3.35	1166	0.10
(Z)- $\beta$ -Ocimene	4.54	1039	0.78	3.85	1205	0.77
(E)- $\beta$ -Ocimene	4.71	1050	4.73	4.07	1221	4.70
$\gamma$ -Terpinene	4.81	1056	0.10	3.88	1207	0.10
cis-Sabinene hydrate	4.95	1065	0.01	6.99*	1431	0.09
cis-Linalool oxide (fur.)	5.04	1070	0.16	6.62	1404	0.15
Octanol	5.17	1079	0.01	8.21*	1522	54.30
Terpinolene	5.26	1084	0.38	4.36	1243	0.39
trans-Linalool oxide (fur.)	5.29	1086	0.09	6.99*	1431	[0.09]
$\alpha$ -Pinene oxide	5.40	1093	0.01	5.52*	1325	[0.02]
trans-Sabinene hydrate	5.46	1097	tr	7.97	1504	0.02
Linalool	5.64	1109	41.46	8.21*	1522	[54.30]
Phenylethyl alcohol	5.72	1114	0.03	12.22	1853	0.01
cis-para-Menth-2-en-1-ol	5.78	1118	0.06	8.21*	1522	[54.30]
allo-Ocimene	5.96	1130	0.02	5.66	1335	0.01
Benzeneacetonitrile	6.04	1135	0.19	12.26	1855	0.18
neo-allo-Ocimene	6.09	1138	0.01	5.94	1355	0.01
(E)-Myroxide	6.13	1140	0.02	7.19	1446	0.02
Lilac aldehyde A	6.25	1148	0.03			
Borneol	6.48	1163	0.02	9.88*	1654	5.02
Terpinen-4-ol	6.64	1173	0.21	8.66	1557	0.21

α-Terpineol	6.90	1190	4.86	9.88*	1654	[5.02]
Hodiendiol	6.99	1196	0.01	12.88	1911	0.01
Safranal	7.03	1198	0.01	8.96	1580	0.03
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.24	1212	0.04	11.44	1783	0.03
Linalyl formate	7.28	1215	0.02	8.52*	1546	0.69
Nerol	7.51	1230	1.10	11.15*	1759	1.31
Citronellol	7.55	1233	0.02			
Neral	7.64	1239	0.04	9.56	1628	0.04
Phenylethyl acetate	7.88	1255	0.15	11.15*	1759	[1.31]
Geraniol	7.96*	1260	15.53	11.72*	1808	3.11
Linalyl acetate	7.96*	1260	[15.53]	8.21*	1522	[54.30]
Geranial	8.10	1270	0.06	10.19	1678	0.05
Bornyl acetate	8.28	1282	0.01	8.39	1536	0.02
1-Nitro-2-phenylethane	8.46*	1294	0.19	14.26	2040	0.03
Indole	8.46*	1294	[0.19]	17.34	2355	0.18
4-Vinylguaiacol	8.70	1311	0.02	15.14	2127	0.03
δ-Elemene	9.02	1333	0.05	7.02	1433	0.06
Methyl anthranilate	9.05	1335	0.15	15.46*	2159	0.15
Linalyl propionate	9.09	1338	0.02	8.91	1577	0.02
α-Terpinyl acetate	9.21	1347	0.08	9.78	1646	0.07
Eugenol	9.33	1355	0.02			
Neryl acetate	9.48	1366	1.51	10.27	1685	1.51
Geranyl acetate	9.76*	1386	2.96	10.64	1716	2.89
β-Elemene	9.76*	1386	[2.96]	8.52*	1546	[0.69]
(Z)-Jasmone	9.87	1394	0.03	12.49	1876	0.02
β-Caryophyllene	10.11	1410	0.68	8.52*	1546	[0.69]
α-Humulene	10.63	1449	0.01	9.35	1611	0.07
Geranylacetone	10.66	1452	0.04	11.72*	1808	[3.11]
allo-Aromadendrene	10.68	1454	0.01	9.04	1586	0.01
(E)-β-Farnesene	10.73	1457	0.12	9.61	1632	0.12
Germacrene D	10.94	1473	0.08	9.88*	1654	[5.02]
Bicyclogermacrene	11.15	1488	0.24	10.13	1674	0.26
(3Z,6E)-α-Farnesene	11.24	1495	0.03	10.33	1690	0.04
γ-Cadinene	11.40	1508	0.07	10.44	1700	0.05
δ-Cadinene	11.53	1517	0.03	10.49	1704	0.03
(E)-Nerolidol	12.13	1565	3.20	13.86	2002	3.16
Spathulenol	12.22	1572	0.02	14.47	2061	0.01
Caryophyllene oxide	12.26	1575	0.01	12.84	1908	0.01
Viridiflorol	12.36	1583	tr	14.06	2021	0.01
α-Cadinol	13.15	1647	0.01	15.55	2168	0.01
(8Z)-Heptadecene	13.51	1677	0.04	10.57	1710	0.06
2,3-Dihydrofarnesol	13.66	1690	0.03	16.10	2224	0.02
(2E,6Z)-Farnesol	13.75	1697	0.06	16.50	2266	0.06
(2E,6Z)-Farnesal	13.94	1713	0.05	15.46*	2159	[0.15]
(2E,6E)-Farnesol	14.04	1722	1.80	16.90	2308	1.77
(2E,6E)-Farnesal	14.23	1738	0.04	15.90	2203	0.02

(2E,6E)-Farnesyl acetate	15.38	1840	0.03	15.98	2211	0.28
meta-Camphorene	16.54	1948	0.01	15.46*	2159	[0.15]
Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	16.84	1976	0.24			
Tricosane	20.00	2301	0.05			
Tetracosane	20.89	2402	0.01			
Pentacosane	21.74	2501	0.04			
Heptacosane	23.37	2701	0.02			
Squalene	24.30	2822	0.02	22.84	3024	0.02
<b>Total identified</b>		<b>98.80%</b>			<b>99.12%</b>	
<b>Total reported</b>		<b>99.04%</b>			<b>99.12%</b>	

\*: 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