

Date : 2025-02-20

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 25A16-PTH04

**Customer Identification** : Neroli - Egypt/Tunisia - N10113R

**Type** : Essential Oil

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

**Customer** : Plant Therapy

Checked and approved by:

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

*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 from the first version issued on 2025-01-30 to correct the customer identification.

## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

**\*ISO**

**Results :** See analysis summary (next page)

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

**Date :** 2025-01-27

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4701 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Dany Massé B. Sc. Chimiste

**Date :** 2025-01-17

## 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
Methacrolein	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Ethanol	tr	Aliphatic alcohol
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	1.16	Monoterpene
Camphene	0.04	Monoterpene
Sabinene	1.96	Monoterpene
$\beta$ -Pinene	7.90	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.05	Monoterpene
6-Methyl-5-hepten-2-ol	0.03	Aliphatic alcohol
$\alpha$ -Phellandrene	0.01	Monoterpene
Pseudolimonene	0.11	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.01	Monoterpene
(2E)-Hexenyl acetate	0.01	Aliphatic ester
<i>para</i> -Cymene	0.05	Monoterpene
Limonene	13.81	Monoterpene
$\beta$ -Phellandrene	0.05	Monoterpene
1,8-Cineole	0.12	Monoterpenic ether
Benzyl alcohol	0.01	Simple phenolic
(Z)- $\beta$ -Ocimene	1.16	Monoterpene
(E)- $\beta$ -Ocimene	3.19	Monoterpene
$\gamma$ -Terpinene	0.03	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.13	Monoterpenic alcohol
Terpinolene	0.25	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.13	Monoterpenic alcohol
<i>para</i> -Cymenene	tr	Monoterpene
$\alpha$ -Pinene oxide	0.02	Monoterpenic ether
Rosefuran	0.01	Monoterpenic ether
Linalool	43.07	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.01	Aliphatic ketone
Phenylethyl alcohol	0.09	Simple phenolic
<i>cis-para</i> -Menth-2-en-1-ol	0.02	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.02	Monoterpenic ether
allo-Ocimene	0.04	Monoterpene
(Z)-Myroxide	0.01	Monoterpenic ether
Benzeneacetonitrile	0.03	Simple phenolic

<i>trans</i> -Pinocarveol	0.02	Monoterpenic alcohol
neo-allo-Ocimene	0.02	Monoterpene
<i>trans-para</i> -Menth-2-en-1-ol	0.03	Monoterpenic alcohol
Camphor	0.09	Monoterpenic ketone
( <i>E</i> )-Myroxide	0.02	Monoterpenic ether
Epoxyterpinolene	0.02	Monoterpenic ether
Borneol	0.05	Monoterpenic alcohol
$\delta$ -Terpineol	0.03	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.10	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	6.49	Monoterpenic alcohol
Myrtenol	0.02	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.08	Monoterpenic alcohol
Lilac alcohol A	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
Linalyl formate	0.02	Monoterpenic ester
Nerol	0.91	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Phenylethyl acetate	0.09	Phenolic ester
Geraniol	1.92	Monoterpenic alcohol
Linalyl acetate	4.38	Monoterpenic ester
( <i>trans</i> ?) -Linalool oxide acetate (fur.)?	0.02	Monoterpenic ester
Geranial	0.04	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.03	Monoterpenic alcohol
Bornyl acetate	0.04	Monoterpenic ester
Indole	0.17	Indole
$\delta$ -Elemene isomer	0.01	Sesquiterpene
Methyl anthranilate	0.49	Phenolic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
$\alpha$ -Terpinyl acetate	0.04	Monoterpenic ester
Eugenol	0.01	Phenylpropanoid
Neryl acetate	1.76	Monoterpenic ester
$\alpha$ -Copaene	0.01	Sesquiterpene
Geranyl acetate	3.11	Monoterpenic ester
$\beta$ -Elemene	0.02	Sesquiterpene
$\beta$ -Caryophyllene	0.53	Sesquiterpene
$\alpha$ -Humulene	0.05	Sesquiterpene
Geranylacetone	0.01	Monoterpenic ketone
( <i>E</i> )- $\beta$ -Farnesene	0.09	Sesquiterpene
Germacrene D	0.03	Sesquiterpene
Bicyclogermacrene	0.06	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	0.01	Sesquiterpene

(3E,6E)- $\alpha$ -Farnesene	0.02	Sesquiterpene
$\gamma$ -Cadinene	0.01	Sesquiterpene
$\delta$ -Cadinene	0.01	Sesquiterpene
$\alpha$ -Elemol	0.02	Sesquiterpenic alcohol
(E)-Nerolidol	1.51	Sesquiterpenic alcohol
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.06	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Viridiflorol	0.01	Sesquiterpenic alcohol
Humulene epoxide II	0.01	Sesquiterpenic ether
$\alpha$ -Cadinol	0.01	Sesquiterpenic alcohol
$\alpha$ -Bisabolol	0.02	Sesquiterpenic alcohol
2,3-Dihydrofarnesol	0.02	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.02	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	1.39	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.07	Sesquiterpenic aldehyde
Octadecane	0.01	Alkane
(2E,6E)-Farnesyl acetate	0.02	Sesquiterpenic ester
Unknown	0.06	Unknown
<i>meta</i> -Camphorene	0.02	Diterpene
Unknown	0.01	Unknown
Tricosane	0.02	Alkane
Pentacosane	0.02	Alkane
Heptacosane	0.01	Alkane
<b>Consolidated total</b>	<b>99.01</b>	

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

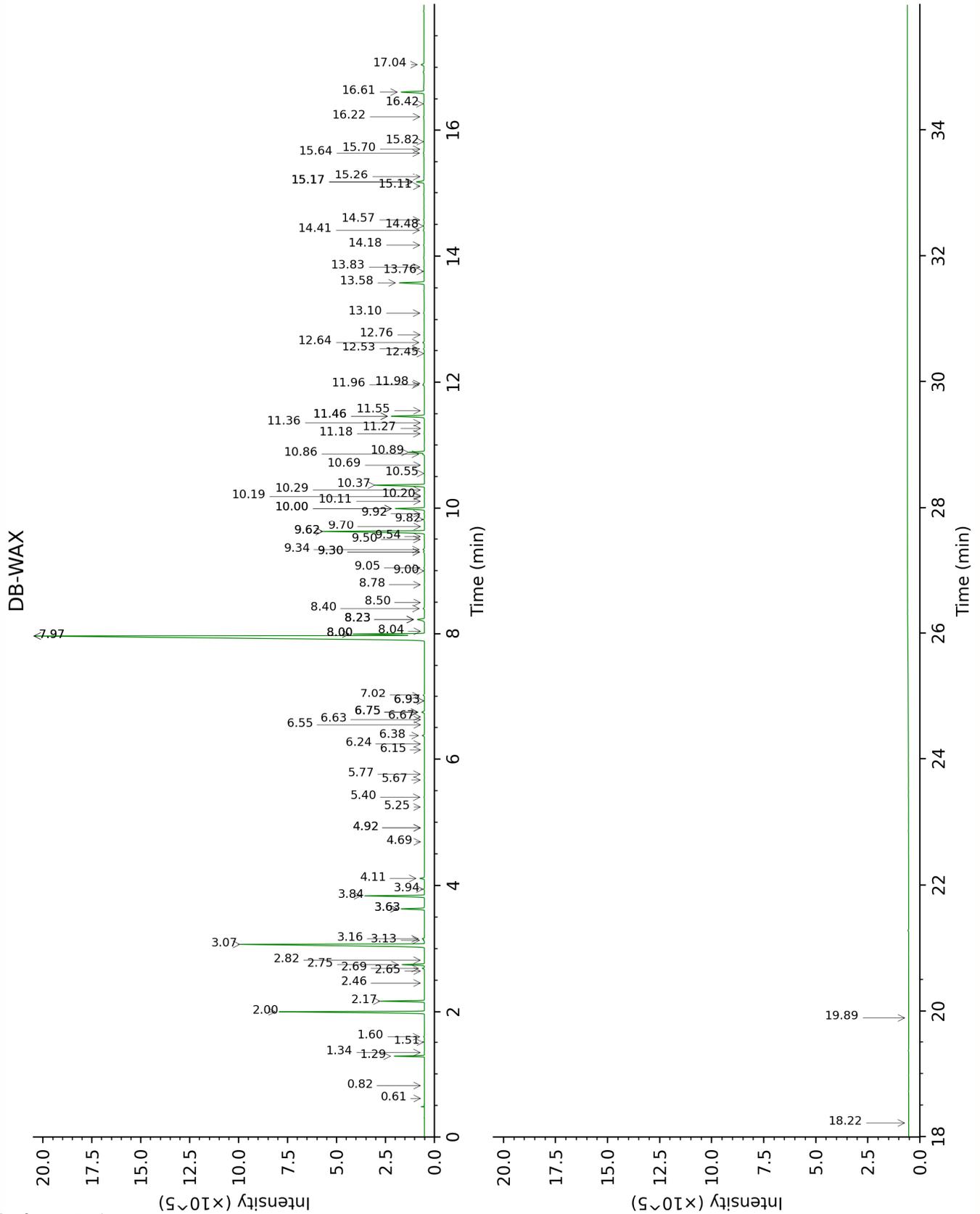
Note: no correction factor was applied

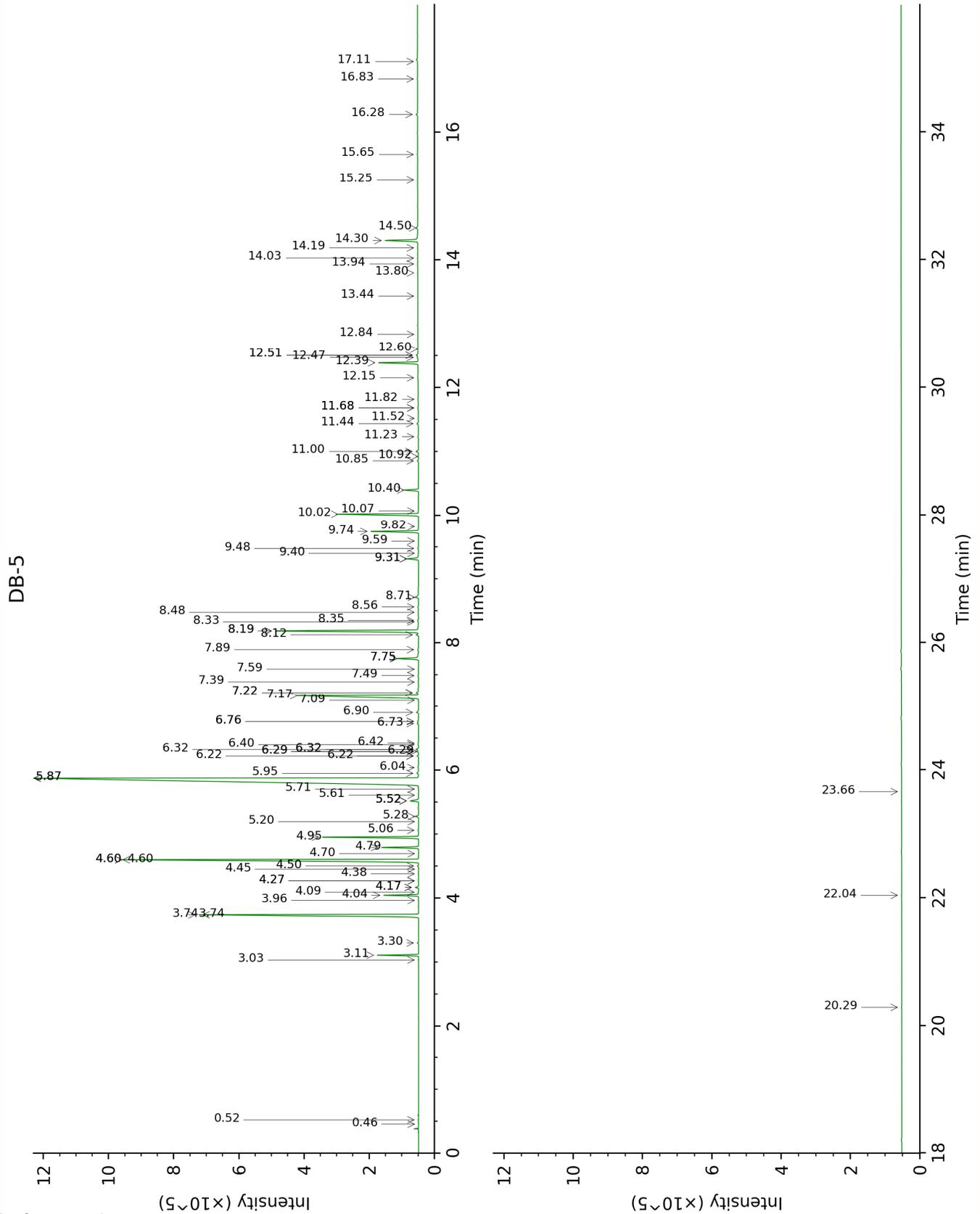
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

**Bracketed value ((xx)):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Methacrolein	Column DB-WAX			Column DB-5		
	0.62	843.8	tr	0.46	550.3	tr
2-Methyl-3-buten-2-ol	1.51	1016.6	0.01	0.52	605.3	0.01
Ethanol	0.82	909.6	tr			
$\alpha$ -Thujene	1.34	999.6	0.01	3.03	926.2	0.01
$\alpha$ -Pinene	1.29	990.2	1.16	3.11	931.1	1.16
Camphene	1.60	1026.3	0.04	3.30	943.9	0.04
Sabinene	2.17	1084.0	1.96	3.74*	973.1	[9.86]
$\beta$ -Pinene	2.00	1066.7	7.90	3.74*	973.1	[9.86]
6-Methyl-5-hepten-2-one	4.92*	1299.2	[0.01]	3.96	988.0	0.02
Myrcene	2.75	1133.6	1.05	4.04	993.4	1.05
6-Methyl-5-hepten-2-ol	6.75*	1432.7	[0.17]	4.09	996.6	0.03
$\alpha$ -Phellandrene	2.65	1125.5	0.01	4.17*	1001.5	[0.11]
Pseudolimonene	2.69	1128.8	0.11	4.17*	1001.5	[0.11]
(3Z)-Hexenyl acetate	4.69	1282.7	0.01	4.27*	1008.0	[0.02]
$\Delta^3$ -Carene	2.46	1110.3	0.01	4.27*	1008.0	[0.02]
$\alpha$ -Terpinene	2.82	1139.2	0.02	4.38	1015.0	0.01
(2E)-Hexenyl acetate	4.92*	1299.2	[0.01]	4.45	1019.6	0.01
<i>para</i> -Cymene	3.94	1227.1	0.05	4.50	1022.7	0.05
Limonene	3.07	1159.3	13.81	4.60*	1028.8	[13.99]
$\beta$ -Phellandrene	3.13	1164.4	0.05	4.60*	1028.8	[13.99]
1,8-Cineole	3.16	1166.3	0.12	4.60*	1028.8	[13.99]
Benzyl alcohol	11.55	1816.9	0.02	4.70	1034.8	0.01
(Z)- $\beta$ -Ocimene	3.63*	1204.0	[1.18]	4.79	1040.8	1.16
(E)- $\beta$ -Ocimene	3.84	1219.3	3.20	4.95	1051.0	3.19
$\gamma$ -Terpinene	3.63*	1204.0	[1.18]	5.06	1057.7	0.03
<i>cis</i> -Sabinene hydrate	6.75*	1432.7	[0.17]	5.20	1066.2	0.01
<i>cis</i> -Linalool oxide (fur.)	6.38	1405.2	0.12	5.28	1071.3	0.13
Terpinolene	4.11	1239.7	0.25	5.52*	1086.6	[0.39]
<i>trans</i> -Linalool oxide (fur.)	6.75*	1432.7	[0.17]	5.52*	1086.6	[0.39]
<i>para</i> -Cymenene	6.15	1388.8	tr	5.52*	1086.6	[0.39]
$\alpha$ -Pinene oxide	5.24	1323.9	0.02	5.61	1092.1	0.02
Rosefuran	5.77	1361.2	0.02	5.70	1098.2	0.01
Linalool	7.97*†	1524.0	[43.59]	5.87*	1108.9	[43.08]
(Z)-6-Methyl-3,5-heptadien-2-one	8.04	1529.8	0.01	5.87*	1108.9	[43.08]

Phenylethyl alcohol	11.96	1853.2	0.10	5.95	1113.8	0.09
<i>cis-para</i> -Menth-2-en-1-ol	7.97*†	1524.0	[43.59]	6.04	1119.5	0.02
<i>cis</i> -Limonene oxide	6.24	1395.6	0.02	6.22*	1131.0	[0.06]
allo-Ocimene	5.40	1335.1	0.04	6.22*	1131.0	[0.06]
( <i>Z</i> )-Myroxide	6.67	1427.2	0.01	6.29*	1135.5	[0.06]
Benzeneacetonitrile	11.98	1855.4	0.03	6.29*	1135.5	[0.06]
<i>trans</i> -Pinocarveol	9.00	1604.0	0.02	6.29*	1135.5	[0.06]
neo-allo-Ocimene	5.67	1354.6	0.02	6.32*	1137.7	[0.11]
<i>trans-para</i> -Menth-2-en-1-ol	8.78	1586.9	0.03	6.32*	1137.7	[0.11]
Camphor	7.02	1452.8	0.09	6.32*	1137.7	[0.11]
( <i>E</i> )-Myroxide	6.93*	1446.0	[0.02]	6.40	1142.4	0.02
Epoxyterpinolene	6.55	1417.8	tr	6.42	1143.8	0.02
Borneol	9.62*	1654.8	[6.51]	6.73	1163.4	0.05
δ-Terpineol	9.30*	1628.3	[0.08]	6.76*	1165.6	[0.05]
<i>cis</i> -Linalool oxide (pyr.)	10.11	1694.4	0.02	6.76*	1165.6	[0.05]
Terpinen-4-ol	8.40	1557.6	0.09	6.90	1174.6	0.10
<i>para</i> -Cymen-8-ol	11.36	1800.0	0.02	7.09	1186.8	0.01
α-Terpineol	9.62*	1654.8	[6.51]	7.17	1191.5	6.49
Myrtenol	10.68	1742.8	0.02	7.22*	1194.7	[0.11]
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	12.64	1914.6	0.08	7.22*	1194.7	[0.11]
Lilac alcohol A	9.70	1661.1	0.01	7.39	1205.6	0.03
(3 <i>E</i> ,5 <i>E</i> )-2,6-Dimethylocta-3,5,7-trien-2-ol	11.18	1785.2	0.03	7.49	1212.5	0.03
Linalyl formate	8.23*	1544.2	[0.56]	7.59	1219.2	0.02
Nerol	10.89	1760.1	0.91	7.75*	1230.3	[0.91]
Citronellol	10.55	1731.7	0.02	7.75*	1230.3	[0.91]
Neral	9.30*	1628.3	[0.08]	7.89	1239.6	0.04
Phenylethyl acetate	10.86	1757.6	0.10	8.12	1255.1	0.09
Geraniol	11.46*	1809.2	[1.93]	8.19*	1259.2	[6.31]
Linalyl acetate	8.00*†	1526.4	[3.68]	8.19*	1259.2	[6.31]
( <i>trans</i> ?) -Linalool oxide acetate (fur.)?	8.50	1565.0	0.02	8.33	1268.6	0.02
Geranial	9.92	1678.5	0.03	8.35	1270.2	0.04
2,6-Dimethyl-1,7-octadiene-3,6-diol	14.48	2088.9	0.04	8.48	1278.7	0.03
Bornyl acetate	8.00*†	1526.4	[3.68]	8.56	1284.4	0.04
Indole	17.04	2355.1	0.19	8.71	1294.4	0.17
δ-Elemene isomer	6.63	1423.9	0.01	9.31*	1336.3	[0.50]
Methyl anthranilate	15.17*	2158.6	[0.51]	9.31*	1336.3	[0.50]

Hodiendiol derivative	12.76	1925.9	0.02	9.40	1342.5	0.02
$\alpha$ -Terpinyl acetate	9.50	1644.5	0.03	9.48	1347.8	0.04
Eugenol	14.57	2098.2	0.03	9.59	1356.0	0.01
Neryl acetate	10.00*	1685.0	[1.74]	9.74	1366.6	1.76
$\alpha$ -Copaene	6.93*	1446.0	[0.02]	9.82	1372.1	0.01
Geranyl acetate	10.37	1715.9	3.09	10.02	1386.2	3.11
$\beta$ -Elemene	8.23*	1544.2	[0.56]	10.07	1389.8	0.02
$\beta$ -Caryophyllene	8.23*	1544.2	[0.56]	10.40	1413.4	0.53
$\alpha$ -Humulene	9.05	1608.2	0.04	10.85	1447.4	0.05
Geranylacetone	11.46*	1809.2	[1.93]	10.92	1452.6	0.01
(E)- $\beta$ -Farnesene	9.34	1631.5	0.10	11.00	1458.4	0.09
Germacrene D	9.54	1648.3	0.03	11.23	1475.5	0.03
Bicyclogermacrene	9.82	1671.1	0.05	11.44	1490.8	0.06
(3Z,6E)- $\alpha$ -Farnesene	10.00*	1685.0	[1.74]	11.52	1497.0	0.01
(3E,6E)- $\alpha$ -Farnesene	10.29	1709.4	0.02	11.68*	1509.3	[0.03]
$\gamma$ -Cadinene	10.19	1700.5	0.01	11.68*	1509.3	[0.03]
$\delta$ -Cadinene	10.20	1701.9	0.02	11.82	1519.9	0.01
$\alpha$ -Elemol	13.83	2026.3	0.02	12.15	1546.3	0.02
(E)-Nerolidol	13.58	2002.3	1.51	12.39	1564.8	1.51
Spathulenol	14.18	2059.7	0.03	12.47	1571.3	0.03
Caryophyllene oxide	12.53	1904.6	0.06	12.51*	1574.2	[0.08]
Caryophyllene oxide isomer	12.45	1897.4	0.01	12.51*	1574.2	[0.08]
Viridiflorol	13.76	2019.7	0.01	12.60	1581.8	0.01
Humulene epoxide II	13.10	1957.7	0.04	12.84	1600.4	0.01
$\alpha$ -Cadinol	15.26	2167.0	0.02	13.44	1649.4	0.01
$\alpha$ -Bisabolol	15.17*	2158.6	[0.51]	13.80	1679.2	0.02
2,3-Dihydrofarnesol	15.82	2225.0	0.01	13.94	1690.7	0.02
(2E,6Z)-Farnesol	16.22	2266.2	0.03	14.03	1698.2	0.02
(2E,6Z)-Farnesal	15.11	2151.9	0.01	14.19	1711.7	0.01
(2E,6E)-Farnesol	16.61	2307.8	1.42	14.30	1721.7	1.39
(2E,6E)-Farnesal	15.64	2206.1	0.06	14.50	1738.7	0.07
Octadecane	11.27	1792.2	0.01	15.25	1803.6	0.01
(2E,6E)-Farnesyl acetate	15.70	2212.5	0.02	15.65	1840.7	0.02
Unknown COGU XXIII [m/z 93, 69 (93), 109 (84), 135 (82), 203 (74), 41 (49)...]	14.41	2082.4	0.05	16.28	1897.6	0.06
<i>meta</i> -Camphorene	15.17*	2158.6	[0.51]	16.83	1950.0	0.02
Unknown CIAU IX				17.11	1976.0	0.01

[m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]						
Tricosane	16.42	2287.8	0.02	20.28	2302.7	0.02
Pentacosane	18.22	2486.3	0.02	22.04	2502.9	0.02
Heptacosane	19.90	2685.0	0.01	23.66	2702.2	0.01
Total reported		98.73%			98.96%	

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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