

Date : 2023-07-07

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 23F29-PTH01

**Customer Identification :** Organic Lemon - Mexico - L70113R

**Type :** Essential Oil

**Source :** *Citrus x limon*

**Customer :** Plant Therapy

Checked and approved by:

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

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## 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 :** Amélie Simard, Analyste

**Date :** 2023-07-06

## PHYSICOCHEMICAL DATA

**Physical aspect :** Bright yellow liquid

**Analyst :** Cindy Caron B. Sc.

**Date :** 2023-06-29

**Refractive index :**  $1.4743 \pm 0.0003$  (20 °C)

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

**Analyst :** Cindy Caron B. Sc.

**Date :** 2023-07-06

## 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
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Hexanal	tr	Aliphatic aldehyde
Octane	tr	Alkane
Nonane	tr	Alkane
Heptanal	tr	Aliphatic aldehyde
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.34	Monoterpene
$\alpha$ -Pinene	1.57	Monoterpene
Camphene	0.05	Monoterpene
$\alpha$ -Fenchene	tr	Monoterpene
Sabinene	1.59	Monoterpene
$\beta$ -Pinene	8.23	Monoterpene
6-Methyl-5-hepten-2-one	0.04	Aliphatic ketone
Myrcene	1.56	Monoterpene
$\alpha$ -Phellandrene	0.04	Monoterpene
Octanal	0.07	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.16	Monoterpene
<i>para</i> -Cymene	0.12	Monoterpene
$\beta$ -Phellandrene	0.29	Monoterpene
Limonene	71.64	Monoterpene
( <i>Z</i> )- $\beta$ -Ocimene	0.07	Monoterpene
( <i>E</i> )- $\beta$ -Ocimene	0.12	Monoterpene
$\gamma$ -Terpinene	7.35	Monoterpene
<i>cis</i> -Sabinene hydrate	0.06	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.35	Monoterpene
<i>trans</i> -Sabinene hydrate	0.06	Monoterpenic alcohol
Linalool	0.11	Monoterpenic alcohol
Nonanal	0.11	Aliphatic aldehyde
<i>trans-para</i> -Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.02	Monoterpenic ether
Camphor	0.01	Monoterpenic ketone
Epoxyterpinolene	0.01	Monoterpenic ether
Citronellal	0.10	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
Isoneral	tr	Monoterpenic aldehyde
Terpinen-4-ol	0.03	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene

Isogeranial	0.01	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.23	Monoterpenic alcohol
Decanal	0.05	Aliphatic aldehyde
<i>trans</i> -Piperitol	tr	Monoterpenic alcohol
<i>trans</i> -Carveol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	0.01	Monoterpenic aldehyde
Nerol	0.08	Monoterpenic alcohol
Citronellol	0.01	Monoterpenic alcohol
2,3-Epoxygeranial?	0.02	Monoterpenic aldehyde
Neral	0.80	Monoterpenic aldehyde
Geraniol	0.02	Monoterpenic alcohol
Geranial	1.30	Monoterpenic aldehyde
Geranyl formate	0.01	Monoterpenic ester
Undecanal	0.03	Aliphatic aldehyde
<i>trans-para</i> -Mentha-2,8-diene-1-hydroperoxide	0.01	Monoterpenic peroxide
Citronellyl acetate	0.03	Monoterpenic ester
Neryl acetate	0.45	Monoterpenic ester
Geranyl acetate	0.15	Monoterpenic ester
Dodecanal	0.01	Aliphatic aldehyde
$\beta$ -Caryophyllene	0.20	Sesquiterpene
<i>cis</i> - $\alpha$ -Bergamotene	0.03	Sesquiterpene
$\alpha$ -Santalene	0.02	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.44	Sesquiterpene
$\alpha$ -Humulene	0.02	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.03	Sesquiterpene
$\beta$ -Santalene	0.02	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Geranyl propionate	0.01	Monoterpenic ester
<i>trans</i> - $\beta$ -Bergamotene	0.03	Sesquiterpene
Valencene	0.02	Sesquiterpene
Bicyclogermacrene	0.04	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.06	Sesquiterpene
$\beta$ -Bisabolene	0.64	Sesquiterpene
$\delta$ -Cadinene	tr	Sesquiterpene
( <i>E</i> )- $\gamma$ -Bisabolene	0.01	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.02	Sesquiterpene
Spathulenol	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	tr	Sesquiterpenic ether
Globulol	0.01	Sesquiterpenic alcohol
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.05	Sesquiterpenic alcohol
Myristic acid	tr	Aliphatic acid
<i>meta</i> -Camphorene	0.01	Diterpene

Citropten	0.08	Furanocoumarin
Palmitic acid	0.01	Aliphatic acid
Ethyl palmitate	0.01	Aliphatic ester
Linoleic acid	0.02	Aliphatic acid
Byakangelicol	0.02	Furanocoumarin
$\alpha$ -Tocopherol	0.01	Tocopherol
$\gamma$ -Sitosterol?	0.01	Sterol
<b>Consolidated total</b>	<b>99.35</b>	

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

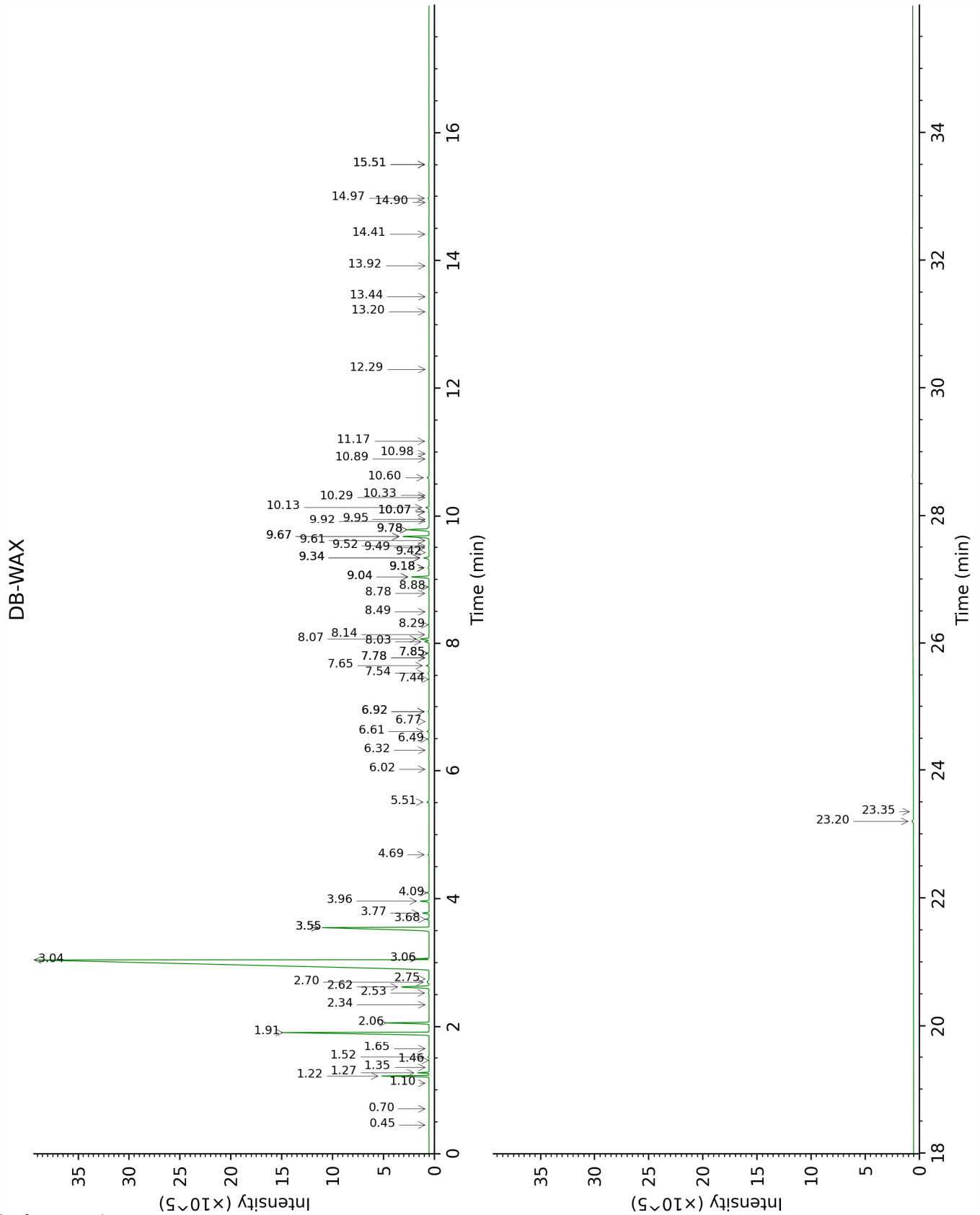
Note: no correction factor was applied

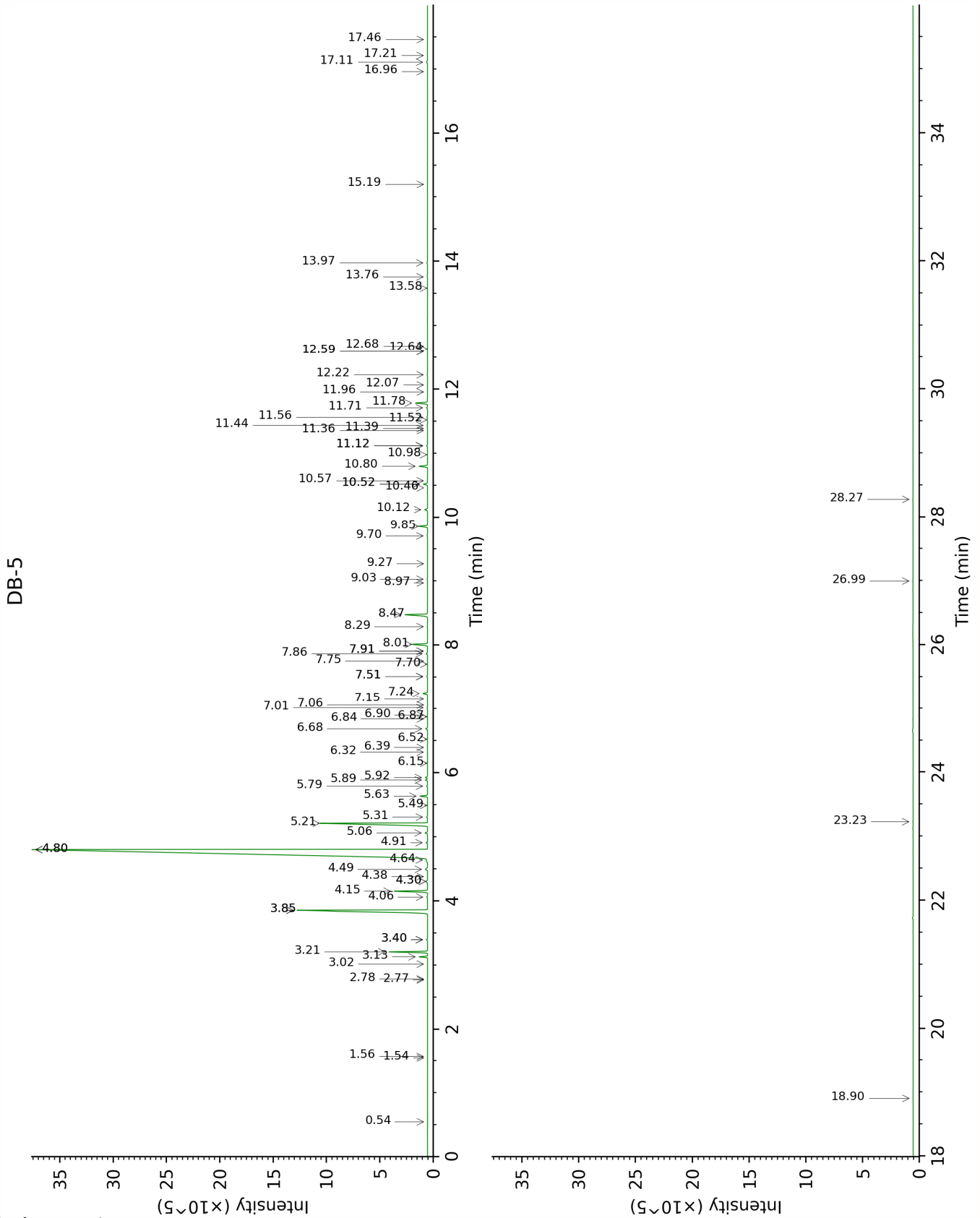
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

2-Methyl-3-buten-2-ol	Column DB-WAX			Column DB-5		
	1.35	1012.2	tr	0.54	606.2	tr
Hexanal	1.65	1042.3	tr	1.54	800.0	tr
Octane	0.45	783.7	tr	1.56	803.2	tr
Nonane	0.70	899.0	tr	2.77	902.1	tr
Heptanal	2.75	1145.4	tr	2.78	903.4	tr
Tricyclene	1.10	973.6	tr	3.02	918.9	0.01
$\alpha$ -Thujene	1.27	1002.0	0.35	3.13	926.3	0.34
$\alpha$ -Pinene	1.22	993.1	1.57	3.21	931.4	1.57
Camphene	1.52	1029.0	0.05	3.40*	943.9	[0.05]
$\alpha$ -Fenchene	1.46	1023.4	tr	3.40*	943.9	[0.05]
Sabinene	2.06	1085.0	1.59	3.86*	974.0	[9.78]
$\beta$ -Pinene	1.91	1069.2	8.23	3.86*	974.0	[9.78]
6-Methyl-5-hepten-2-one	4.69	1299.1	0.04	4.06	987.4	0.05
Myrcene	2.62	1135.1	1.57	4.15	993.5	1.56
$\alpha$ -Phellandrene	2.53	1127.5	0.04	4.30*	1003.5	[0.11]
Octanal	4.09	1252.9	0.07	4.30*	1003.5	[0.11]
$\Delta$ 3-Carene	2.34	1112.5	0.01	4.38	1008.3	0.01
$\alpha$ -Terpinene	2.70	1141.2	0.16	4.49	1015.4	0.16
<i>para</i> -Cymene	3.78	1228.5	0.25	4.64	1024.5	0.11
$\beta$ -Phellandrene	3.06	1171.2	0.29	4.80*	1034.6	[71.70]
Limonene	3.04	1169.6	71.64	4.80*	1034.6	[71.70]
(Z)- $\beta$ -Ocimene	3.55*	1211.1	[7.44]	4.91	1041.3	0.07
(E)- $\beta$ -Ocimene	3.68	1221.2	0.12	5.06	1050.8	0.12
$\gamma$ -Terpinene	3.55*	1211.1	[7.44]	5.21	1060.2	7.35
<i>cis</i> -Sabinene hydrate	6.49	1426.5	0.06	5.31	1066.3	0.06
Octanol	7.78*	1523.6	[0.02]	5.49	1077.7	0.01
Terpinolene	3.96	1242.9	0.35	5.63	1086.6	0.35
<i>trans</i> -Sabinene hydrate	7.54	1504.8	0.06	5.79	1096.4	0.06
Linalool	7.65	1514.0	0.12	5.89	1102.4	0.11
Nonanal	5.51	1354.2	0.10	5.92	1104.8	0.11
<i>trans-para</i> -Mentha-2,8-dien-1-ol	8.50	1580.1	0.01	6.15	1119.0	0.01
<i>cis</i> -Limonene oxide	6.02	1391.6	0.01	6.32	1130.0	0.02
Camphor	6.77	1447.1	0.01	6.39	1134.7	0.01
Epoxyterpinolene	6.32	1413.4	tr	6.52	1142.8	0.01
Citronellal	6.61	1435.5	0.09	6.68	1153.2	0.10
Borneol	9.34*	1648.1	[0.26]	6.84	1163.0	0.01
Unknown UNKN	6.92*	1458.8	[0.04]	6.87	1165.2	0.01

XXV [m/z 43, 109 (68), 67 (62), 81 (36), 41 (31), 137 (29), 79 (26)...]						
Isoneral	7.44	1497.7	0.01	6.90	1166.7	tr
Terpinen-4-ol	8.14	1552.1	0.03	7.01	1174.2	0.03
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.18*	1635.4	[0.07]	7.06	1176.9	0.01
Isogeranial	7.78*	1523.6	[0.02]	7.15	1182.9	0.01
$\alpha$ -Terpineol	9.34*	1648.1	[0.26]	7.24	1188.8	0.23
Decanal	6.92*	1458.8	[0.04]	7.51*	1205.7	[0.05]
<i>trans</i> -Piperitol	9.95	1698.9	tr	7.51*	1205.7	[0.05]
<i>trans</i> -Carveol	10.98	1786.8	0.01	7.70	1218.6	0.01
2,3-Epoxyneral?				7.75	1221.7	0.01
Nerol	10.60	1754.4	0.09	7.86	1229.4	0.08
Citronellol	10.29	1727.6	0.01	7.90*	1232.2	[0.03]
2,3-Epoxygeranial?				7.90*	1232.2	[0.03]
Neral	9.04*	1623.7	[0.83]	8.01	1239.2	0.80
Geraniol	11.17	1803.5	0.03	8.29	1257.6	0.02
Geranial	9.67*	1675.8	[1.32]	8.47	1270.2	1.30
Geranyl formate	9.49	1661.1	0.03	8.97	1303.2	0.01
Undecanal	8.29	1564.1	0.02	9.03	1307.2	0.03
<i>trans-para</i> -Mentha-2,8-diene-1-hydroperoxide				9.27	1324.1	0.01
Citronellyl acetate	9.04*	1623.7	[0.83]	9.70	1354.8	0.03
Neryl acetate	9.78*	1684.5	[1.10]	9.85	1365.4	0.45
Geranyl acetate	10.14	1714.2	0.15	10.12	1384.4	0.15
Dodecanal	9.61	1670.5	0.01	10.46	1408.5	0.01
$\beta$ -Caryophyllene	8.03	1543.4	0.20	10.52*	1412.8	[0.23]
<i>cis</i> - $\alpha$ -Bergamotene	7.85*	1529.2	[0.04]	10.52*	1412.8	[0.23]
$\alpha$ -Santalene	7.85*	1529.2	[0.04]	10.57	1416.7	0.02
<i>trans</i> - $\alpha$ -Bergamotene	8.07	1546.7	0.42	10.80	1433.5	0.44
$\alpha$ -Humulene	8.88	1610.8	0.02	10.98	1446.9	0.02
( <i>E</i> )- $\beta$ -Farnesene	9.18*	1635.4	[0.07]	11.12*	1457.3	[0.06]
$\beta$ -Santalene	8.78	1602.8	0.02	11.12*	1457.3	[0.06]
Germacrene D	9.42	1655.1	0.01	11.36	1475.0	0.01
Geranyl propionate	10.89	1779.6	0.01	11.39	1477.3	0.01
<i>trans</i> - $\beta$ -Bergamotene	9.18*	1635.4	[0.07]	11.44	1480.9	0.03

Valencene	9.52	1663.6	0.01	11.52	1487.3	0.03
Bicyclogermacrene	9.67*	1675.8	[1.32]	11.56	1490.2	0.04
(Z)- $\alpha$ -Bisabolene	9.92	1696.0	tr	11.71	1501.3	0.06
$\beta$ -Bisabolene	9.78*	1684.5	[1.10]	11.78	1506.9	0.64
$\delta$ -Cadinene	10.07*	1708.5	[0.03]	11.96	1520.5	tr
(E)- $\gamma$ -Bisabolene	10.07*	1708.5	[0.03]	12.07	1529.1	0.01
(E)- $\alpha$ -Bisabolene	10.33	1730.6	0.02	12.22	1541.6	0.02
Spathulenol	13.92	2059.5	0.01	12.59*	1570.4	[0.02]
Germacrene D-4-ol	13.20	1990.2	0.01	12.59*	1570.4	[0.02]
Caryophyllene oxide	12.29	1904.5	tr	12.64	1573.8	tr
Globulol	13.44	2012.3	tr	12.68	1577.2	0.01
Unknown CILI I [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	14.41	2107.9	0.02	13.58	1650.2	0.03
Unknown CILI II [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	15.51*	2220.6	[0.03]	13.76	1664.7	0.04
$\alpha$ -Bisabolol	14.97	2165.1	0.04	13.97	1682.7	0.05
Myristic acid				15.19	1787.1	tr
<i>meta</i> -Camphorene	14.90	2158.6	0.01	16.96	1948.8	0.01
Citropten	23.20	3175.4	0.10	17.11	1962.7	0.08
Palmitic acid				17.21	1972.6	0.01
Ethyl palmitate	15.51*	2220.6	[0.03]	17.46	1996.4	0.01
Linoleic acid	23.35	3197.6	0.01	18.90	2140.4	0.02
Byakangelicol				23.23	2629.0	0.02
$\alpha$ -Tocopherol				26.99	3115.6	0.01
$\gamma$ -Sitosterol?				28.27	3236.7	0.01
Total reported		99.29%			99.08%	

\*: 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