

**Date :** December 19, 2022

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 22L12-PTH01

**Customer identification :** Lemon ORGANIC - Mexico - L70112R

**Type :** Essential oil

**Source :** *Citrus x limon*

**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 :** December 19, 2022

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright yellow liquid

**Refractive index:**  $1.4744 \pm 0.0003$  (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
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.40	Monoterpene
$\alpha$ -Pinene	1.74	Monoterpene
Camphene	0.06	Monoterpene
$\beta$ -Pinene	10.12	Monoterpene
Sabinene	1.76	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	1.58	Monoterpene
$\alpha$ -Phellandrene	0.03	Monoterpene
Pseudolimonene	tr	Monoterpene
Octanal	0.07	Aliphatic aldehyde
$\alpha$ -Terpinene	0.16	Monoterpene
para-Cymene	0.25	Monoterpene
1,8-Cineole	0.02	Monoterpenic ether
$\beta$ -Phellandrene	0.30	Monoterpene
Limonene	68.02	Monoterpene
(Z)- $\beta$ -Ocimene	0.05	Monoterpene
(E)- $\beta$ -Ocimene	0.10	Monoterpene
$\gamma$ -Terpinene	8.44	Monoterpene
cis-Sabinene hydrate	0.03	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.36	Monoterpene
trans-Sabinene hydrate	0.03	Monoterpenic alcohol
Linalool	0.11	Monoterpenic alcohol
Nonanal	0.10	Aliphatic aldehyde
cis-Limonene oxide	0.01	Monoterpenic ether
trans-Limonene oxide	0.01	Monoterpenic ether
Camphor	0.01	Monoterpenic ketone
Epoxyterpinolene	0.01	Monoterpenic ether
Citronellal	0.11	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Isoneral	0.01	Monoterpenic aldehyde
Terpinen-4-ol	0.05	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene
Isogeranial	0.01	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.16	Monoterpenic alcohol
Decanal	0.06	Aliphatic aldehyde
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.05	Monoterpenic alcohol
2,3-Epoxygeranial?	0.04	Monoterpenic aldehyde
Neral	0.68	Monoterpenic aldehyde
Geraniol	0.02	Monoterpenic alcohol
Geranial	1.12	Monoterpenic aldehyde
Geranyl formate	0.01	Monoterpenic ester
Undecanal	0.03	Aliphatic aldehyde

<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	0.01	Monoterpenic peroxide
para-Mentha-1,8-diene-4-hydroperoxide	0.01	Monoterpenic peroxide
Citronellyl acetate	0.04	Monoterpenic ester
Neryl acetate	0.44	Monoterpenic ester
Geranyl acetate	0.28	Monoterpenic ester
Dodecanal	0.01	Aliphatic aldehyde
<i>cis</i> - $\alpha$ -Bergamotene	0.02	Sesquiterpene
$\beta$ -Caryophyllene	0.19	Sesquiterpene
$\alpha$ -Santalene	0.01	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.41	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	0.02	Sesquiterpene
Valencene	0.04	Sesquiterpene
Bicyclogermacrene	0.05	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.05	Sesquiterpene
$\beta$ -Bisabolene	0.60	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.02	Sesquiterpene
Germacrene D-4-ol	0.01	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.03	Sesquiterpenic alcohol
Myristic acid	0.06	Aliphatic acid
Pentadecylic acid	0.01	Aliphatic acid
Citropten	0.06	Furanocoumarin
Palmitic acid	0.06	Aliphatic acid
Ethyl palmitate	0.01	Aliphatic ester
Linoleic acid	0.02	Aliphatic acid
Stearic acid	0.02	Aliphatic acid
Byakangelicol	0.02	Furanocoumarin
<b>Consolidated total</b>	<b>98.83%</b>	

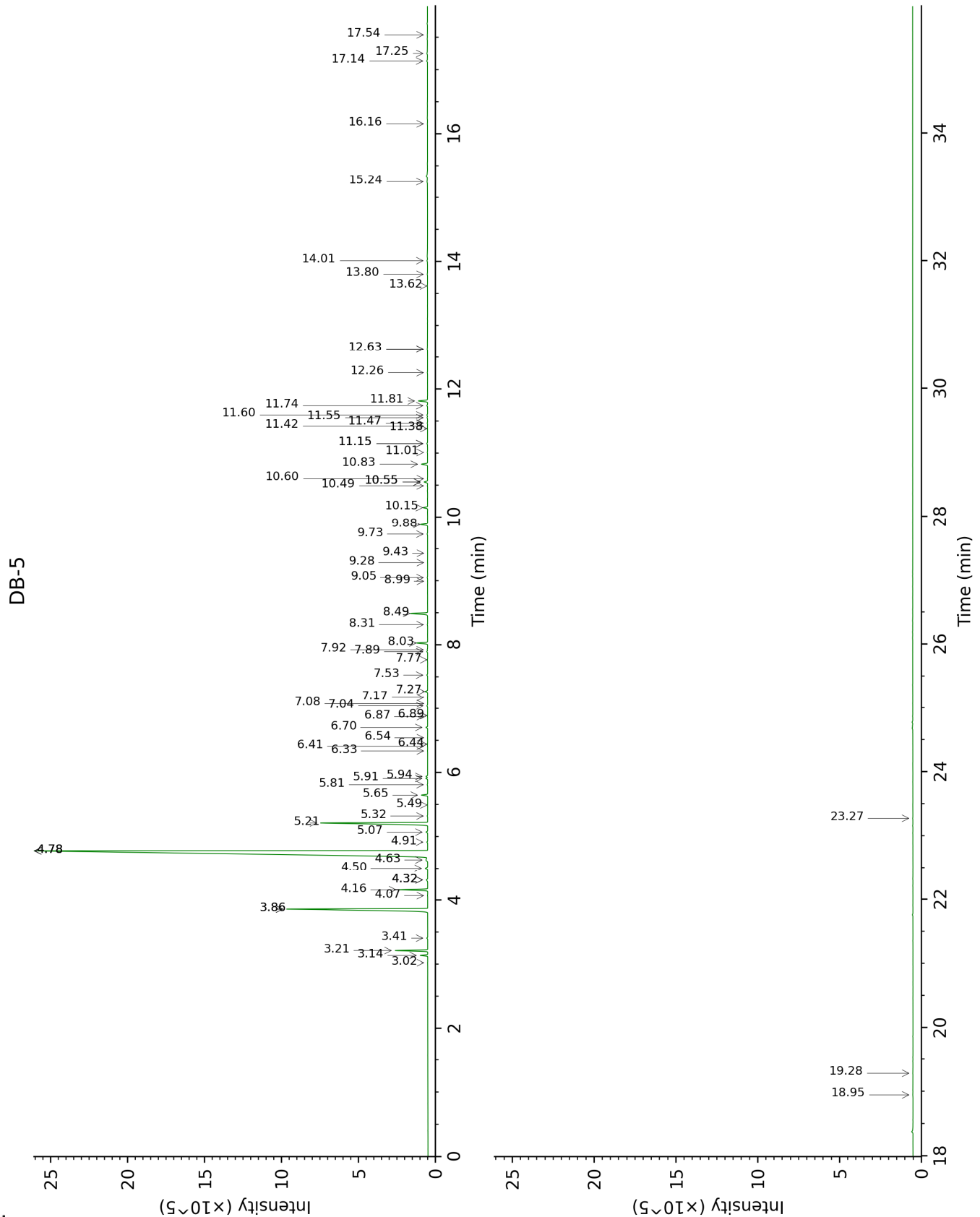
tr: The compound has been detected below 0.005% of total signal.

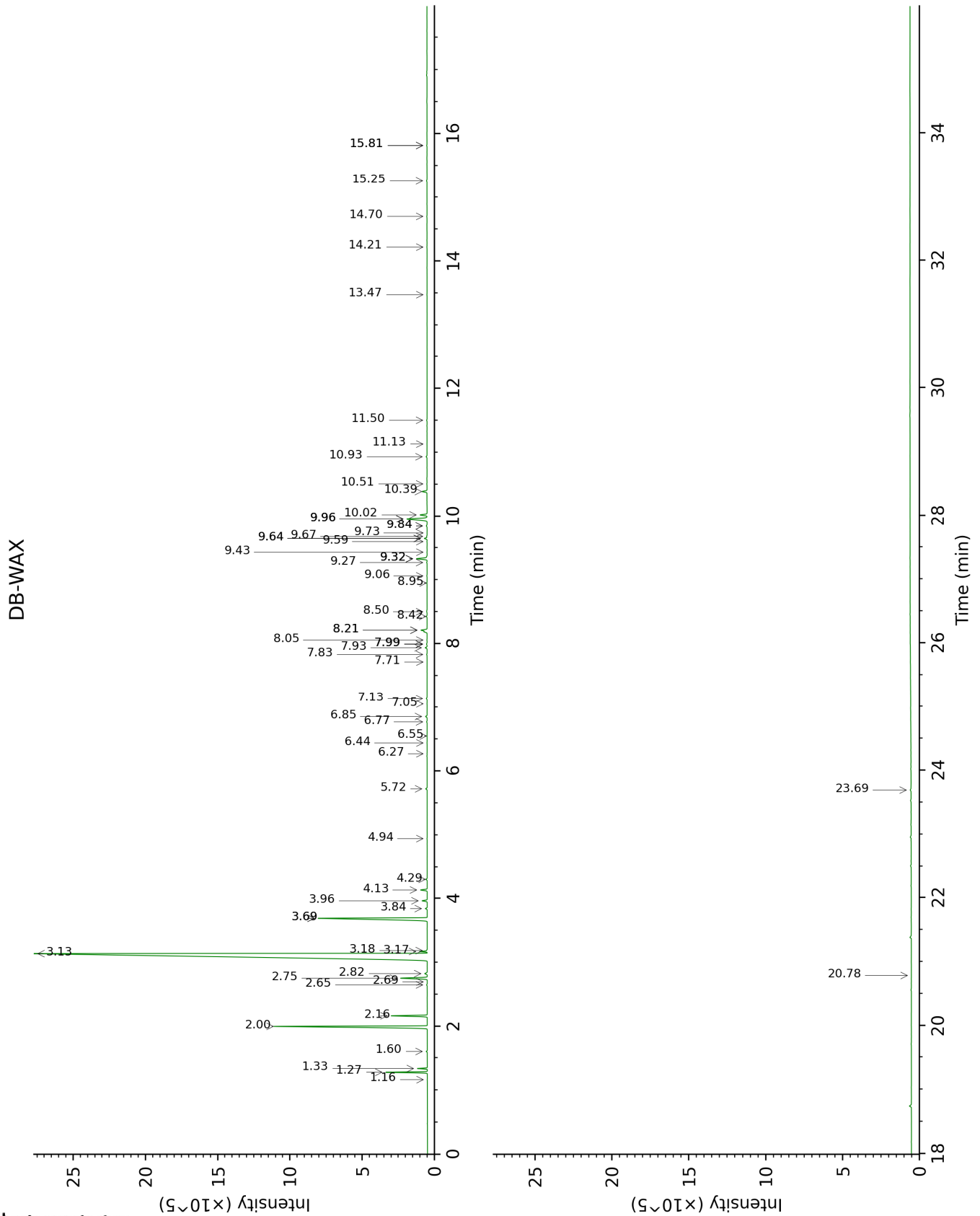
Note: no correction factor was applied

**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	%
Tricyclene	3.02	918	0.01	1.16	969	0.01
$\alpha$ -Thujene	3.14	925	0.40	1.33	997	0.39
$\alpha$ -Pinene	3.21	930	1.74	1.27	989	1.74
Camphene	3.41	943	0.06	1.60	1024	0.05
$\beta$ -Pinene	3.86*	973	11.87	2.00	1066	10.12
Sabinene	3.86*	973	[11.87]	2.16	1083	1.76
6-Methyl-5-hepten-2-one	4.07	986	0.01	4.94	1299	0.01
Myrcene	4.16	992	1.58	2.75	1133	1.58
$\alpha$ -Phellandrene	4.32*	1002	0.11	2.65	1125	0.03
Pseudolimonene	4.32*	1002	[0.11]	2.69	1128	tr
Octanal	4.32*	1002	[0.11]	4.30	1254	0.07
$\alpha$ -Terpinene	4.50	1014	0.16	2.82	1139	0.16
para-Cymene	4.64	1022	0.25	3.96	1228	0.28
1,8-Cineole	4.78*	1031	68.35	3.18	1168	0.02
$\beta$ -Phellandrene	4.78*	1031	[68.35]	3.17	1167	0.30
Limonene	4.78*	1031	[68.35]	3.13	1164	68.02
(Z)- $\beta$ -Ocimene	4.91	1040	0.05	3.69*	1208	8.48
(E)- $\beta$ -Ocimene	5.07	1050	0.10	3.84	1219	0.10
$\gamma$ -Terpinene	5.21	1058	8.44	3.69*	1208	[8.48]
cis-Sabinene hydrate	5.32	1065	0.03	6.77	1432	0.03
Octanol	5.49	1076	0.01	8.06	1529	0.02
Terpinolene	5.65	1086	0.36	4.13	1241	0.36
trans-Sabinene hydrate	5.81	1096	0.03	7.83	1512	0.03
Linalool	5.91	1102	0.11	7.94	1520	0.11
Nonanal	5.94	1104	0.10	5.72	1355	0.09
cis-Limonene oxide	6.34	1129	0.01	6.27	1395	0.01
trans-Limonene oxide	6.41	1134	0.01	6.44	1407	0.01
Camphor	6.44	1136	0.01	7.05	1453	0.01
Epoxyterpinolene	6.54	1142	0.01	6.55	1415	0.01
Citronellal	6.70	1152	0.11	6.85	1438	0.09
Borneol	6.87	1163	0.01	9.64*	1655	0.17
Isoneral	6.89	1164	0.01	7.71	1502	0.01
Terpinen-4-ol	7.04	1174	0.05	8.42	1558	0.05
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	7.08	1176	0.01	9.43	1637	0.01
Isogeranial	7.17	1182	0.01	7.99*	1524	0.04
$\alpha$ -Terpineol	7.27	1188	0.16	9.64*	1655	[0.17]
Decanal	7.53	1205	0.06	7.13	1459	0.05
2,3-Epoxyneral?	7.77	1221	0.02			
Nerol	7.89	1229	0.05	10.93	1762	0.06
2,3-Epoxygeranial?	7.92	1231	0.04			



Neral	8.03	1238	0.68	9.32*	1629	0.73
Geraniol	8.32	1257	0.02	11.50	1811	0.03
Geranial	8.49	1269	1.12	9.96*	1680	1.73
Geranyl formate	8.99	1302	0.01	9.73	1662	0.01
Undecanal	9.05	1306	0.03	8.50	1563	0.04
<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	9.28	1322	0.01			
para-Mentha-1,8-diene-4-hydroperoxide	9.43	1333	0.01			
Citronellyl acetate	9.73	1354	0.04	9.27	1624	0.03
Neryl acetate	9.88	1364	0.44	10.02	1685	0.44
Geranyl acetate	10.15	1383	0.28	10.39	1716	0.30
Dodecanal	10.49	1408	0.01	9.84*	1671	0.06
<i>cis</i> - $\alpha$ -Bergamotene	10.55*	1412	0.24	7.99*	1524	[0.04]
$\beta$ -Caryophyllene	10.55*	1412	[0.24]	8.21*†	1541	0.60
$\alpha$ -Santalene	10.60	1416	0.01	7.99*	1524	[0.04]
<i>trans</i> - $\alpha$ -Bergamotene	10.83	1433	0.41	8.21*†	1541	[0.60]
$\alpha$ -Humulene	11.01	1446	0.02	9.06	1607	0.03
( <i>E</i> )- $\beta$ -Farnesene	11.15*	1456	0.05	9.32*	1629	[0.73]
$\beta$ -Santalene	11.15*	1456	[0.05]	8.95	1598	0.02
Germacrene D	11.38	1474	0.01	9.59	1651	0.02
Geranyl propionate	11.42	1477	0.01	11.13	1778	0.01
<i>trans</i> - $\beta$ -Bergamotene	11.47	1480	0.02	9.32*	1629	[0.73]
Valencene	11.55	1486	0.04	9.67	1657	0.03
Bicyclogermacrene	11.60	1490	0.05	9.84*	1671	[0.06]
( <i>Z</i> )- $\alpha$ -Bisabolene	11.74	1500	0.05	9.96*	1680	[1.73]
$\beta$ -Bisabolene	11.81	1506	0.60	9.96*	1680	[1.73]
( <i>E</i> )- $\alpha$ -Bisabolene	12.26	1540	0.02	10.50	1726	0.01
Germacrene D-4-ol	12.63*	1570	0.03	13.47	1989	0.01
Spathulenol	12.63*	1570	[0.03]	14.22	2060	0.01
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.62	1649	0.02	14.70	2106	0.02
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.80	1664	0.02	15.81*	2219	0.02
$\alpha$ -Bisabolol	14.01	1682	0.03	15.25	2162	0.03
Myristic acid	15.24	1787	0.06			
Pentadecylic acid	16.16	1869	0.01	20.78	2779	0.01
Citropten	17.14	1961	0.06	23.69	3161	0.06
Palmitic acid	17.25	1972	0.06			
Ethyl palmitate	17.54	1999	0.01	15.81*	2219	[0.02]
Linoleic acid	18.95	2140	0.02			
Stearic acid	19.28	2174	0.02			
Byakangelicol	23.28	2628	0.02			

<b>Total identified</b>	<b>98.81%</b>	<b>98.49%</b>
<b>Total reported</b>	<b>98.86%</b>	<b>98.53%</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