

Date : May 04, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 21D20-ORA02

**Customer identification** : Lemon - Italy - 3 years - 044365A

**Type** : Essential oil

**Source** : *Citrus x limon*

**Customer** : Organic Aromas Inc.

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

**Analysis date** : May 03, 2021

Checked and approved by :

\_\_\_\_\_  
Alexis St-Gelais, M. Sc., chimiste 2013-174

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4748 \pm 0.0003$  (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
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Octane	0.01	Alkane
Nonane	tr	Alkane
Heptanal	0.01	Aliphatic aldehyde
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.36	Monoterpene
$\alpha$ -Pinene	1.68	Monoterpene
Camphene	0.06	Monoterpene
Sabinene	1.80	Monoterpene
$\beta$ -Pinene	10.83	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	1.22	Monoterpene
$\alpha$ -Phellandrene	0.03	Monoterpene
Octanal	0.02	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.10	Monoterpene
para-Cymene	1.43	Monoterpene
Limonene	68.40	Monoterpene
$\beta$ -Phellandrene	0.25	Monoterpene
(Z)- $\beta$ -Ocimene	0.04	Monoterpene
(E)- $\beta$ -Ocimene	0.11	Monoterpene
$\gamma$ -Terpinene	6.82	Monoterpene
cis-Sabinene hydrate	0.03	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.29	Monoterpene
trans-Sabinene hydrate	0.03	Monoterpenic alcohol
Linalool	0.08	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
cis-Limonene oxide	0.04	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.04	Monoterpenic alcohol
trans-Limonene oxide	0.05	Monoterpenic ether
Epoxyterpinolene	0.02	Monoterpenic ether
Citronellal	0.03	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.04	Monoterpenic alcohol
Isogeranial	0.01	Monoterpenic aldehyde
para-Cymen-8-ol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	0.11	Monoterpenic alcohol
trans-Isopiperitenol	0.01	Monoterpenic alcohol
trans-Piperitol	0.01	Monoterpenic alcohol
Decanal	0.01	Aliphatic aldehyde
trans-Carveol	0.03	Monoterpenic alcohol
2,3-Epoxyneral?	0.01	Monoterpenic aldehyde
Nerol	0.05	Monoterpenic alcohol

2,3-Epoxygeranial?	0.02	Monoterpenic aldehyde
Neral	0.67	Monoterpenic aldehyde
Geraniol	0.02	Monoterpenic alcohol
Geranial	1.08	Monoterpenic aldehyde
Limonen-10-ol	0.01	Monoterpenic alcohol
Undecanal	0.01	Aliphatic aldehyde
<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	0.01	Monoterpenic peroxide
Unknown	0.01	Unknown
para-Mentha-1,8-diene-4-hydroperoxide	0.04	Monoterpenic peroxide
Citronellyl acetate	0.03	Monoterpenic ester
Neryl acetate	0.50	Monoterpenic ester
$\alpha$ -Copaene	0.01	Sesquiterpene
Geranyl acetate	0.28	Monoterpenic ester
Dodecanal	0.01	Aliphatic aldehyde
$\beta$ -Caryophyllene	0.24	Sesquiterpene
<i>cis</i> - $\alpha$ -Bergamotene	0.01	Sesquiterpene
$\alpha$ -Santalene	0.02	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.45	Sesquiterpene
$\alpha$ -Humulene	0.02	Sesquiterpene
Neryl propionate	0.02	Monoterpenic ester
$\beta$ -Santalene	0.02	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.05	Sesquiterpene
Geranyl propionate	0.02	Monoterpenic ester
<i>trans</i> - $\beta$ -Bergamotene	0.03	Sesquiterpene
Valencene	0.02	Sesquiterpene
Bicyclogermacrene	0.01	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.01	Sesquiterpene
$\beta$ -Bisabolene	0.68	Sesquiterpene
$\delta$ -Cadinene	0.01	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.03	Sesquiterpene
Spathulenol	0.11	Sesquiterpenic alcohol
Caryophyllene oxide	0.05	Sesquiterpenic ether
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.04	Sesquiterpenic alcohol
Myristic acid	0.01	Aliphatic acid
Pentadecylic acid	0.05	Aliphatic acid
meta-Camphorene	0.01	Diterpene
Citropten	0.05	Furanocoumarin
Palmitic acid	0.10	Aliphatic acid
Linoleic acid	0.09	Aliphatic acid
Oleic acid	0.08	Aliphatic acid
Stearic acid	0.02	Aliphatic acid
<b>Consolidated total</b>	<b>99.17%</b>	

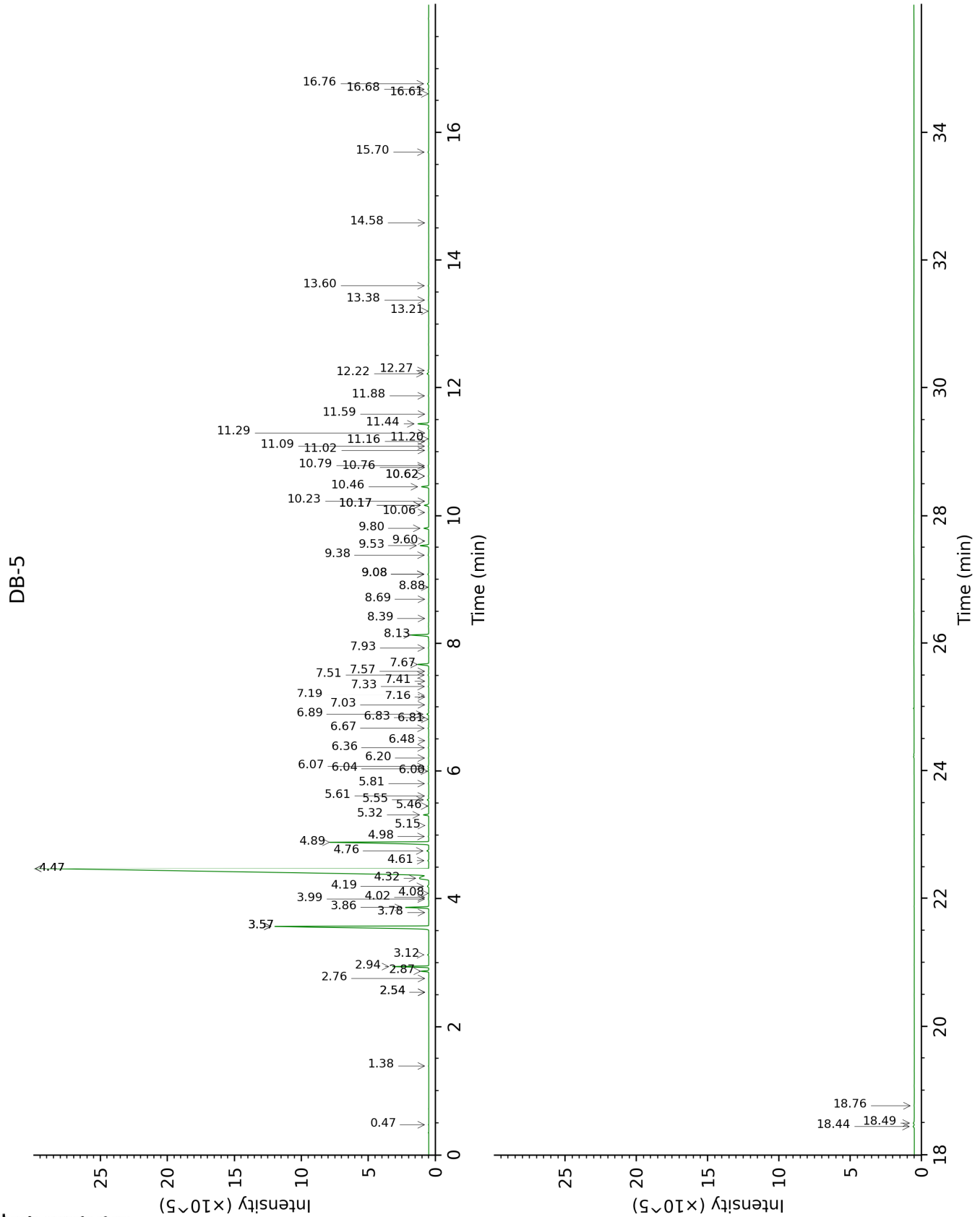
tr: The compound has been detected below 0.005% of total signal.

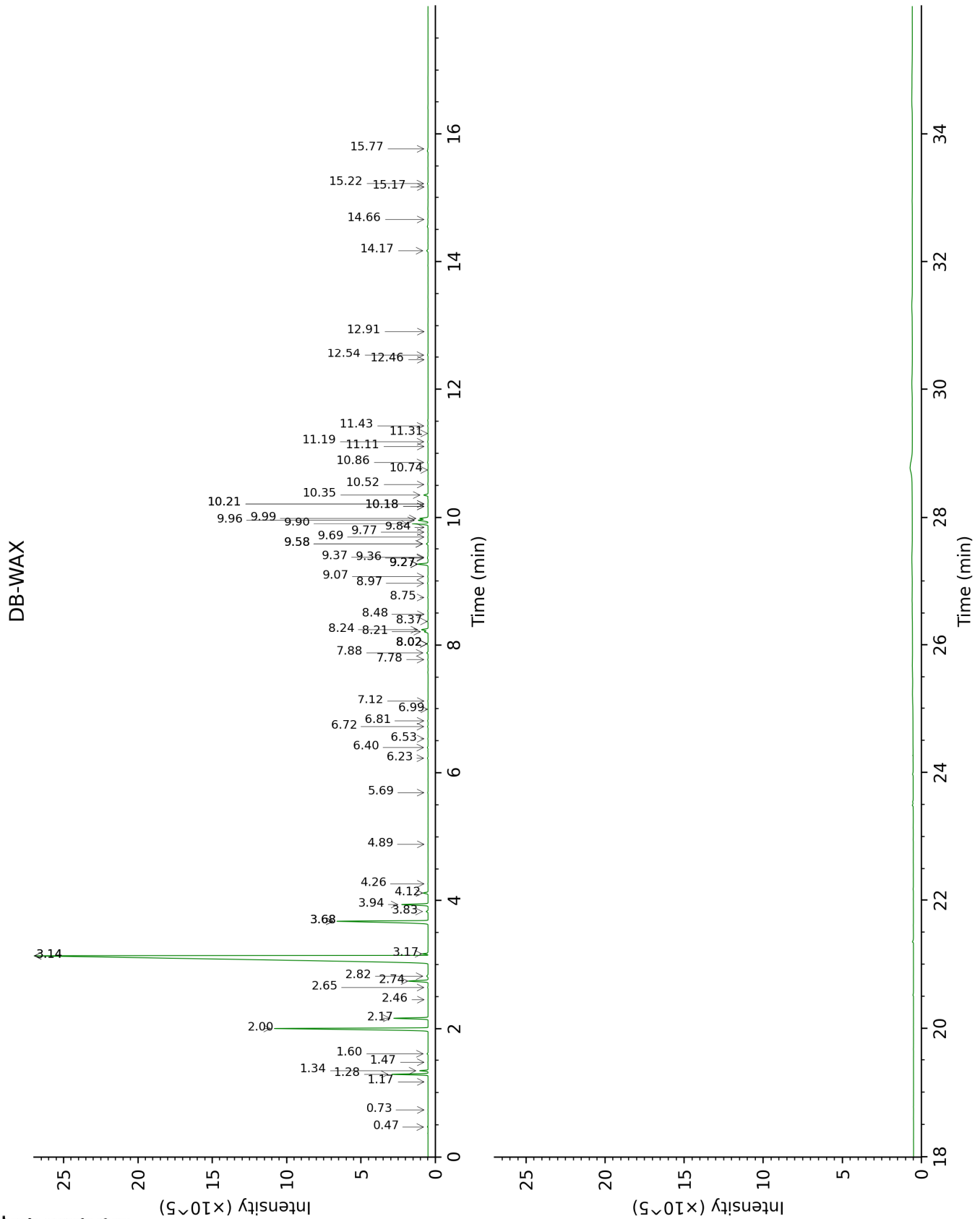
Note: no correction factor was applied

**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	%
2-Methyl-3-buten-2-ol	0.47	600	0.01	1.47	1014	0.01
Octane	1.38	804	0.01	0.47	784	0.01
Nonane	2.54*	905	0.01	0.73	896	tr
Heptanal	2.54*	905	[0.01]	3.14*	1165	68.51
Tricyclene	2.76	919	0.01	1.17	972	0.01
$\alpha$ -Thujene	2.87	927	0.36	1.34	1001	0.37
$\alpha$ -Pinene	2.94	932	1.68	1.28	992	1.68
Camphene	3.12	944	0.06	1.60	1027	0.06
Sabinene	3.57*	974	12.58	2.16	1084	1.80
$\beta$ -Pinene	3.57*	974	[12.58]	2.00	1068	10.83
6-Methyl-5-hepten-2-one	3.78	989	0.01	4.89	1298	0.01
Myrcene	3.86	994	1.22	2.74	1134	1.22
$\alpha$ -Phellandrene	3.99	1003	0.03	2.64	1126	0.03
Octanal	4.02	1005	0.02	4.26	1251	0.01
$\Delta^3$ -Carene	4.08	1009	0.01	2.46	1111	0.01
$\alpha$ -Terpinene	4.19	1016	0.10	2.82	1140	0.10
para-Cymene	4.32	1024	1.43	3.94	1227	1.55
Limonene	4.47*	1034	68.65	3.14*	1165	[68.51]
$\beta$ -Phellandrene	4.47*	1034	[68.65]	3.17	1168	0.25
(Z)- $\beta$ -Ocimene	4.60	1042	0.04	3.68*	1208	6.88
(E)- $\beta$ -Ocimene	4.76	1052	0.11	3.83	1219	0.11
$\gamma$ -Terpinene	4.89	1060	6.82	3.68*	1208	[6.88]
cis-Sabinene hydrate	4.98	1066	0.03	6.72	1429	0.03
Octanol	5.15	1076	0.01	8.02*	1528	0.05
Terpinolene	5.32	1087	0.29	4.12	1241	0.29
trans-Sabinene hydrate	5.46	1096	0.03	7.78	1508	0.02
Linalool	5.55	1102	0.08	7.88	1517	0.08
Nonanal	5.61	1106	0.02	5.69	1354	0.02
trans-para-Mentha-2,8-dien-1-ol	5.81	1118	0.03	8.75	1584	0.02
cis-Limonene oxide	6.00	1130	0.04	6.23	1392	0.04
cis-para-Mentha-2,8-dien-1-ol	6.04	1133	0.04	9.27*	1626	0.70
trans-Limonene oxide	6.07	1135	0.05	6.40	1405	0.04
Epoxyterpinolene	6.20	1144	0.02	6.53	1415	0.02
Citronellal	6.36	1154	0.03	6.81	1436	0.03
Borneol	6.48	1161	0.01	9.58*	1652	0.11
Terpinen-4-ol	6.67	1174	0.04	8.37	1555	0.03
Isogeranial	6.81	1183	0.01	8.02*	1528	[0.05]
para-Cymen-8-ol	6.84	1184	0.01	11.31	1798	0.01
$\alpha$ -Terpineol	6.89	1188	0.11	9.58*	1652	[0.11]

<i>trans</i> -Isopiperitenol	7.03	1197	0.01	10.18*	1700	0.02
<i>trans</i> -Piperitol	7.16	1205	0.01	10.22*	1703	0.01
Decanal	7.19	1207	0.01	7.12	1459	0.02
<i>trans</i> -Carveol	7.33	1217	0.03	11.18	1786	0.03
2,3-Epoxyneral?	7.41	1222	0.01			
Nerol	7.51	1229	0.05	10.86	1759	0.04
2,3-Epoxygeranial?	7.57	1233	0.02			
Neral	7.68	1240	0.67	9.27*	1626	[0.70]
Geraniol	7.93	1257	0.02	11.43	1808	0.03
Geranial	8.13	1271	1.08	9.90	1678	1.06
Limonen-10-ol	8.39	1288	0.01	12.91	1942	0.01
Undecanal	8.69	1308	0.01	8.48	1564	tr
<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	8.88	1322	0.01			
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.08*	1336	0.05	12.46	1900	0.01
para-Mentha-1,8-diene-4-hydroperoxide	9.08*	1336	[0.05]			
Citronellyl acetate	9.38	1357	0.03	9.27*	1626	[0.70]
Neryl acetate	9.53	1368	0.50	9.99	1685	0.54
$\alpha$ -Copaene	9.60	1373	0.01	6.99	1449	0.01
Geranyl acetate	9.80	1387	0.28	10.35	1715	0.28
Dodecanal	10.06	1405	0.01	9.76	1667	0.02
$\beta$ -Caryophyllene	10.17*	1413	0.29	8.21†	1542	0.69
<i>cis</i> - $\alpha$ -Bergamotene	10.17*	1413	[0.29]	8.02*	1528	[0.05]
$\alpha$ -Santalene	10.23	1418	0.02	8.02*	1528	[0.05]
<i>trans</i> - $\alpha$ -Bergamotene	10.46	1435	0.45	8.24†	1545	[0.69]
$\alpha$ -Humulene	10.62*	1447	0.03	9.07	1610	0.02
Neryl propionate	10.62*	1447	[0.03]	10.74	1749	0.02
$\beta$ -Santalene	10.76	1457	0.02	8.97	1601	0.03
( <i>E</i> )- $\beta$ -Farnesene	10.79	1459	0.05	9.36	1634	0.04
Geranyl propionate	11.02	1477	0.02	11.11	1780	0.01
<i>trans</i> - $\beta$ -Bergamotene	11.09	1482	0.03	9.37	1635	0.02
Valencene	11.16	1488	0.02	9.69	1660	0.02
Bicyclogermacrene	11.20	1491	0.01	9.84	1673	0.02
( <i>Z</i> )- $\alpha$ -Bisabolene	11.30	1497	0.01	10.18*	1700	[0.02]
$\beta$ -Bisabolene	11.44	1508	0.68	9.96	1683	0.68
$\delta$ -Cadinene	11.59	1520	0.01	10.22*	1703	[0.01]
( <i>E</i> )- $\alpha$ -Bisabolene	11.88	1543	0.03	10.52	1729	0.03
Spathulenol	12.22	1570	0.11	14.17	2061	0.10
Caryophyllene oxide	12.27	1574	0.05	12.54	1906	0.04
Unknown [m/z 94, 43 (89), 41 (67),	13.21	1650	0.03	14.66	2109	0.02

122 (46), 69 (41)...222]						
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.38	1664	0.02	15.77	2222	0.02
α-Bisabolol	13.60	1682	0.04	15.22	2165	0.04
Myristic acid	14.58	1767	0.01			
Pentadecylic acid	15.70	1866	0.05			
meta-Camphorene	16.61	1951	0.01	15.17	2160	0.01
Citropten	16.68	1958	0.05			
Palmitic acid	16.76	1966	0.10			
Linoleic acid	18.44	2132	0.09			
Oleic acid	18.49	2138	0.08			
Stearic acid	18.76	2166	0.02			
<b>Total identified</b>		<b>99.11%</b>			<b>98.80%</b>	
<b>Total reported</b>		<b>99.16%</b>			<b>98.86%</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