

Date : January 24, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23A17-PTH03

Customer identification : Lemon - Italy - L60116R

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 : Amélie Simard, Analyste

Analysis date : January 23, 2023

Checked and approved by :

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.4745 ± 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
Hexanal	tr	Aliphatic aldehyde
Octane	tr	Alkane
Tricyclene	0.01	Monoterpene
α -Thujene	0.36	Monoterpene
α -Pinene	1.80	Monoterpene
α -Fenchene	0.01	Monoterpene
Camphene	0.06	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Sabinene	1.75	Monoterpene
β -Pinene	12.76	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.41	Monoterpene
Pseudolimonene	0.03	Monoterpene
α -Phellandrene	0.03	Monoterpene
Octanal	0.06	Aliphatic aldehyde
Δ^3 -Carene	0.01	Monoterpene
α -Terpinene	0.17	Monoterpene
para-Cymene	0.31	Monoterpene
Limonene	65.20	Monoterpene
β -Phellandrene	0.23	Monoterpene
1,8-Cineole	0.11	Monoterpenic ether
(Z)- β -Ocimene	0.04	Monoterpene
(E)- β -Ocimene	0.07	Monoterpene
γ -Terpinene	8.53	Monoterpene
cis-Sabinene hydrate	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.38	Monoterpene
trans-Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	0.16	Monoterpenic alcohol
Nonanal	0.14	Aliphatic aldehyde
endo-Fenchol	0.01	Monoterpenic alcohol
trans-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
cis-Limonene oxide	0.03	Monoterpenic ether
trans-Limonene oxide	0.04	Monoterpenic ether
Epoxyterpinolene	0.03	Monoterpenic ether
Citronellal	0.12	Monoterpenic aldehyde
Borneol	0.02	Monoterpenic alcohol
Unknown	0.02	Unknown
Terpinen-4-ol	0.04	Monoterpenic alcohol
Isogeranial	0.02	Monoterpenic aldehyde
α -Terpineol	0.17	Monoterpenic alcohol
Decanal	0.06	Aliphatic aldehyde
trans-Piperitol	0.01	Monoterpenic alcohol
trans-Carveol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	0.01	Monoterpenic aldehyde

Nerol	0.04	Monoterpenic alcohol
2,3-Epoxygeranial?	0.03	Monoterpenic aldehyde
Neral	1.23	Monoterpenic aldehyde
Carvone	tr	Monoterpenic ketone
Geraniol	0.05	Monoterpenic alcohol
Geranial	1.87	Monoterpenic aldehyde
Perillaldehyde	0.01	Monoterpenic aldehyde
Undecanal	0.01	Aliphatic aldehyde
Unknown	0.01	Unknown
Citronellyl acetate	0.04	Monoterpenic ester
Neryl acetate	0.38	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
Geranyl acetate	0.36	Monoterpenic ester
Dodecanal	0.02	Aliphatic aldehyde
β -Caryophyllene	0.22	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.01	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.22	Sesquiterpene
α -Humulene	0.02	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.03	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.02	Sesquiterpene
Valencene	0.03	Sesquiterpene
Bicyclogermacrene	0.02	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	0.03	Sesquiterpene
β -Bisabolene	0.35	Sesquiterpene
(<i>Z</i>)- γ -Bisabolene	0.01	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.01	Sesquiterpene
Spathulenol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
α -Bisabolol	0.02	Sesquiterpenic alcohol
meta-Camphorene	0.02	Diterpene
Citropten	0.04	Furanocoumarin
Bergapten	0.01	Furanocoumarin
Consolidated total	99.48%	

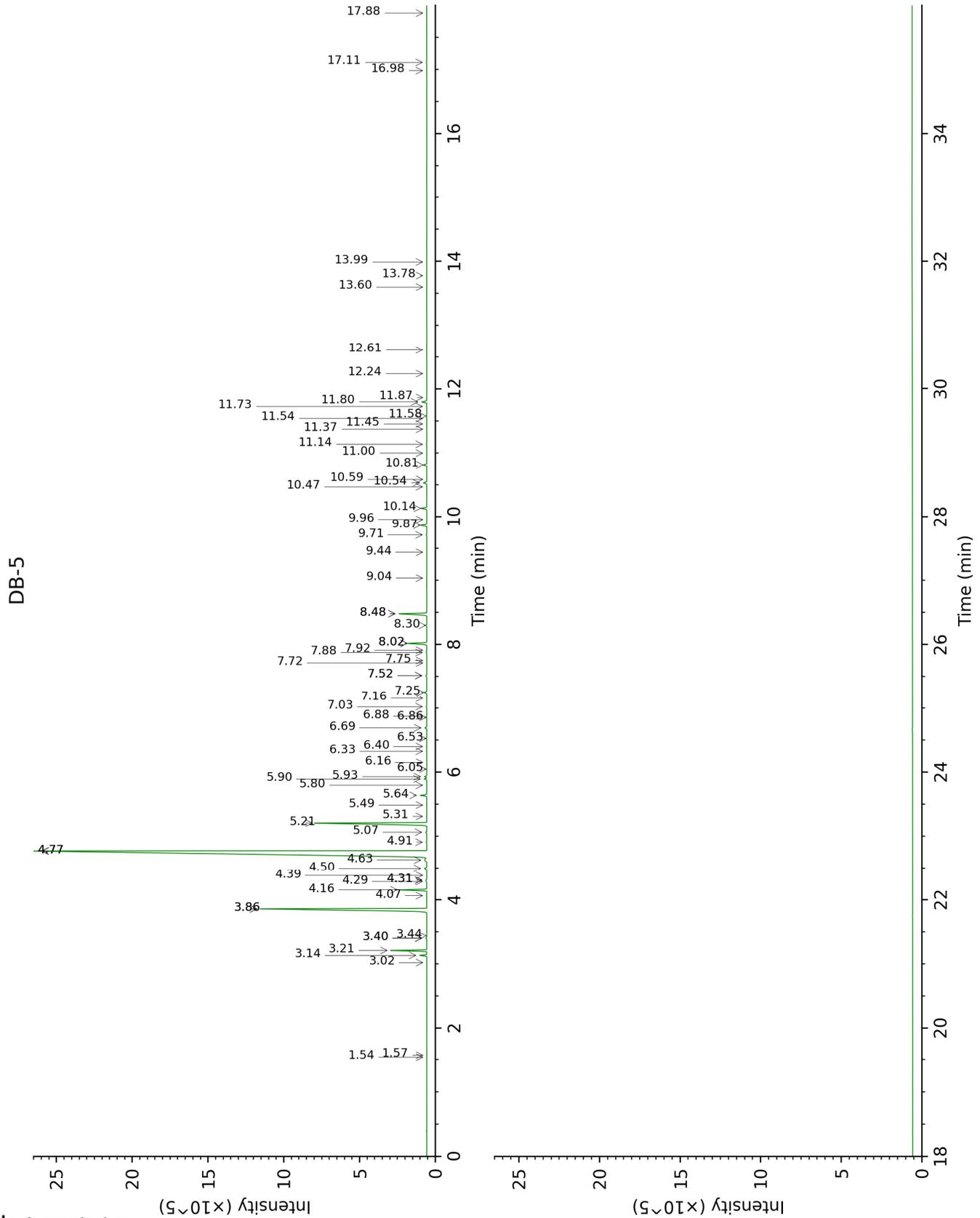
tr: The compound has been detected below 0.005% of total signal.

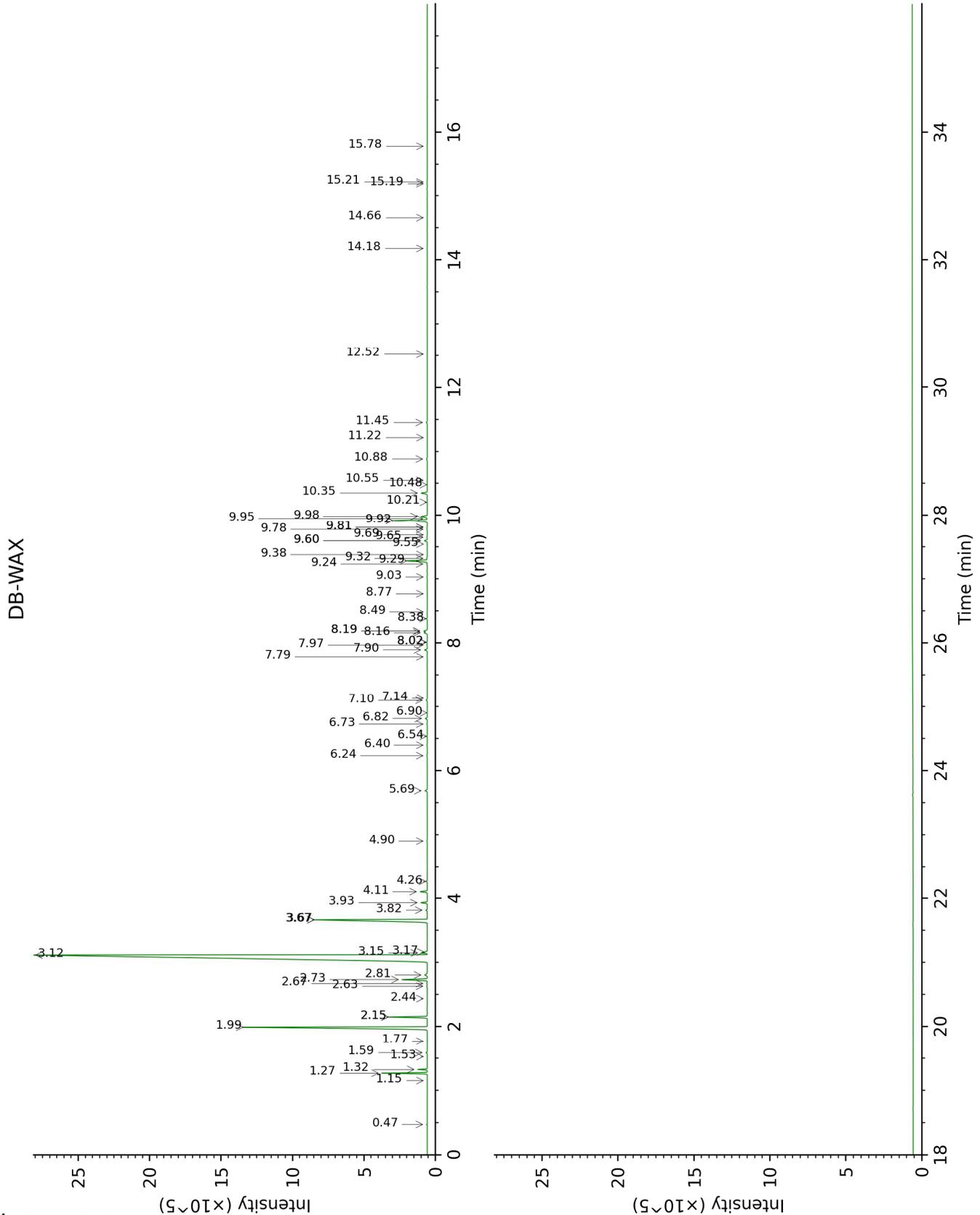
Note: no correction factor was applied

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	%
Hexanal	1.54	799	tr	1.77	1043	0.01
Octane	1.57	803	tr	0.47	782	0.01
Tricyclene	3.02	918	0.01	1.15	968	tr
α -Thujene	3.14	926	0.36	1.32	996	0.35
α -Pinene	3.21	931	1.80	1.27	989	1.79
α -Fenchene	3.40*	943	0.07	1.53	1017	0.01
Camphene	3.40*	943	[0.07]	1.59	1024	0.06
Thuja-2,4(10)-diene	3.44	946	0.01	2.15*	1083	1.78
Sabinene	3.86*	973	14.51	2.15*	1083	[1.78]
β -Pinene	3.86*	973	[14.51]	1.99	1066	12.76
6-Methyl-5-hepten-2-one	4.07	986	0.02	4.90	1297	0.02
Myrcene	4.16	992	1.41	2.73	1133	1.42
Pseudolimonene	4.29	1001	0.03	2.67	1128	0.03
α -Phellandrene	4.31*	1003	0.09	2.63	1124	0.03
Octanal	4.31*	1003	[0.09]	4.26	1253	0.06
Δ^3 -Carene	4.39	1007	0.01	2.44	1108	0.01
α -Terpinene	4.50	1014	0.17	2.81	1138	0.18
para-Cymene	4.63	1022	0.31	3.93	1228	0.33
Limonene	4.77*	1031	65.44	3.12	1164	65.20
β -Phellandrene	4.77*	1031	[65.44]	3.15	1167	0.23
1,8-Cineole	4.77*	1031	[65.44]	3.16	1168	0.11
(Z)- β -Ocimene	4.91	1040	0.04	3.67*	1208	8.58
(E)- β -Ocimene	5.07	1050	0.07	3.82	1219	0.07
γ -Terpinene	5.21	1059	8.53	3.67*	1208	[8.58]
cis-Sabinene hydrate	5.31	1065	0.02	6.73	1430	0.02
Octanol	5.49	1076	0.02	7.97	1524	0.03
Terpinolene	5.64	1086	0.38	4.10	1241	0.37
trans-Sabinene hydrate	5.80	1095	0.02	7.79	1510	0.02
Linalool	5.90	1102	0.16	7.90	1518	0.15
Nonanal	5.93	1104	0.14	5.69	1354	0.13
endo-Fenchol	6.05	1111	0.01	8.16†	1539	0.42
trans-para-Mentha-2,8-dien-1-ol	6.16	1118	0.02	8.77	1586	0.01
cis-Limonene oxide	6.33	1129	0.03	6.24	1393	0.03
trans-Limonene oxide	6.40	1134	0.04	6.40	1405	0.02
Epoxyterpinolene	6.53	1142	0.03	6.54	1416	0.01
Citronellal	6.69	1152	0.12	6.82	1436	0.11
Borneol	6.86	1162	0.02	9.60*	1653	0.17
Unknown [m/z 43, 109 (68), 67 (62),	6.88	1164	0.02	7.14	1460	0.01

81 (36), 41 (31), 137 (29), 79 (26)...						
Terpinen-4-ol	7.02	1173	0.04	8.38	1556	0.04
Isogeranial	7.16	1182	0.02	8.02*	1527	0.03
α -Terpineol	7.26	1188	0.17	9.60*	1653	[0.17]
Decanal	7.52*	1204	0.07	7.10	1458	0.06
<i>trans</i> -Piperitol	7.52*	1204	[0.07]	10.21	1702	0.01
<i>trans</i> -Carveol	7.72	1218	0.01	11.22	1788	0.01
2,3-Epoxyneral?	7.75	1220	0.01			
Nerol	7.88	1228	0.04	10.88	1760	0.05
2,3-Epoxygeranial?	7.92	1231	0.03			
Neral	8.02*	1238	1.23	9.28	1627	1.23
Carvone	8.02*	1238	[1.23]	9.81*	1670	0.02
Geraniol	8.30	1257	0.05	11.45	1808	0.06
Geranial	8.48*	1269	1.90	9.92*	1679	2.22
Perillaldehyde	8.48*	1269	[1.90]	10.48	1726	0.01
Undecanal	9.04	1306	0.01	8.49	1564	0.01
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...	9.44	1334	0.01	12.52	1903	0.01
Citronellyl acetate	9.71	1353	0.04	9.24	1623	0.03
Neryl acetate	9.87	1364	0.38	9.98	1684	0.39
α -Copaene	9.96	1371	0.01	6.90	1443	0.01
Geranyl acetate	10.14	1383	0.36	10.35	1714	0.38
Dodecanal	10.47	1407	0.02	9.78	1667	0.02
β -Caryophyllene	10.54	1412	0.22	8.19*†	1541	[0.42]
<i>cis</i> - α -Bergamotene	10.59	1416	0.01	8.02*	1527	[0.03]
<i>trans</i> - α - Bergamotene	10.81	1432	0.22	8.19*†	1541	[0.42]
α -Humulene	11.00	1446	0.02	9.03	1607	0.02
(<i>E</i>)- β -Farnesene	11.14	1456	0.03	9.32	1630	0.04
Germacrene D	11.37	1474	0.01	9.55	1648	0.01
<i>trans</i> - β - Bergamotene	11.45	1480	0.02	9.38	1635	0.01
Valencene	11.54	1486	0.03	9.65	1657	0.03
Bicyclogermacrene	11.58	1489	0.02	9.81*	1670	[0.02]
(<i>Z</i>)- α -Bisabolene	11.73	1500	0.03	9.95	1681	0.02
β -Bisabolene	11.80	1505	0.35	9.92*	1679	[2.22]
(<i>Z</i>)- γ -Bisabolene	11.86	1511	0.01	9.69	1660	0.01
(<i>E</i>)- α -Bisabolene	12.24	1540	0.01	10.55	1732	0.02
Spathulenol	12.61	1569	0.02	14.18	2058	0.02
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.60	1649	0.01	14.66	2105	0.01
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.78	1663	0.02	15.78	2218	0.01
α -Bisabolol	13.99	1681	0.02	15.21	2160	0.02
meta-Camphorene	16.98	1947	0.02	15.19	2158	0.01

Citropten	17.11	1959	0.04	
Bergapten	17.88	2034	0.01	
Total identified		99.33%		99.32%
Total reported		99.39%		99.35%

*: 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