

Date : June 12, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23F05-PTH01


Customer identification : Lime Steam Distilled - Mexico - LL0109R

Type : Essential oil

Source : *Citrus aurantifolia* ct. Distilled

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 : June 08, 2023

Checked and approved by :

Sylvain Mercier, M. Sc., Chimiste 2014-005

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid

Refractive index: 1.4763 ± 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	tr	Aliphatic alcohol
4,5-Dihydrotoluene	0.02	Alkene
1-Methylcyclohexa-1,3-diene	0.10	Alkene
3-Methylenecyclohexadiene	0.02	Alkene
Octane	0.01	Alkane
Cyclofenchene	0.01	Monoterpene
Bornylene	0.01	Monoterpene
Nonane	0.02	Alkane
Heptanal	0.02	Aliphatic aldehyde
Tricyclene	0.03	Monoterpene
α -Thujene	0.03	Monoterpene
α -Pinene	1.14	Monoterpene
β -Fenchene?	0.01	Monoterpene
α -Fenchene	0.17	Monoterpene
Camphene	0.44	Monoterpene
1,4-Dimethyl-4-vinylcyclohexene?	0.02	Monoterpene
Unknown	0.03	Monoterpene
Geranic oxide	0.22	Monoterpenic ether
β -Pinene	2.39	Monoterpene
Sabinene	tr	Monoterpene
3-Methyl-3-cyclohexenone	0.05	Aliphatic ketone
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.04	Monoterpenic ether
Myrcene	1.17	Monoterpene
α -Phellandrene	0.31	Monoterpene
Pseudolimonene	0.04	Monoterpene
Menthatriene isomer I	0.03	Monoterpene
Octanal	0.02	Aliphatic aldehyde
Δ^3 -Carene	0.03	Monoterpene
1,4-Cineole	1.93	Monoterpenic ether
α -Terpinene	2.13	Monoterpene
para-Cymene	2.88	Monoterpene
1,8-Cineole	1.69	Monoterpenic ether
Limonene	47.67	Monoterpene
(<i>Z</i> ?)-Citroside	0.04	Monoterpenic ether
(<i>Z</i>)- β -Ocimene	0.20	Monoterpene
(<i>E</i> ?)-Citroside	0.22	Monoterpenic ether
(<i>E</i>)- β -Ocimene	0.42	Monoterpene
γ -Terpinene	11.81	Monoterpene
<i>cis</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
para-Mentha-3,8-diene	0.02	Monoterpene
Octanol	0.02	Aliphatic alcohol
Terpinolene isomer	0.17	Monoterpene
para-Cymenene	0.23	Monoterpene

Terpinolene	8.52	Monoterpene
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	0.15	Monoterpenic alcohol
Nonanal	0.04	Aliphatic aldehyde
1,3,8- <i>para</i> -Menthatriene	0.04	Monoterpene
endo-Fenchol	0.39	Monoterpenic alcohol
<i>trans</i> - <i>para</i> -Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
Myrcenol	0.04	Monoterpenic alcohol
Limona ketone	0.03	Normonoterpenic ketone
<i>cis</i> -Limonene oxide	0.03	Monoterpenic ether
allo-Ocimene	0.02	Monoterpene
1-Terpineol	0.45	Monoterpenic alcohol
<i>trans</i> -Limonene oxide	0.01	Monoterpenic ether
Unknown	0.02	Unknown
Epoxyterpinolene	0.12	Monoterpenic ether
<i>cis</i> - β -Terpineol	0.49	Monoterpenic alcohol
Isoborneol	0.04	Monoterpenic alcohol
(<i>Z</i>)-Ocimenol	0.05	Monoterpenic alcohol
Borneol	0.20	Monoterpenic alcohol
α -Phellandren-8-ol	0.04	Monoterpenic alcohol
<i>trans</i> - β -Terpineol	0.11	Monoterpenic alcohol
(<i>E</i>)-Ocimenol	0.13	Monoterpenic alcohol
Terpinen-4-ol	0.37	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	0.12	Monoterpenic alcohol
α -Terpineol	6.73	Monoterpenic alcohol
γ -Terpineol	0.94	Monoterpenic alcohol
Decanal	0.05	Aliphatic aldehyde
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
<i>cis</i> -Carveol	0.02	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Neral	0.09	Monoterpenic aldehyde
Geraniol	0.04	Monoterpenic alcohol
Geranial	0.12	Monoterpenic aldehyde
<i>trans</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Unknown	0.06	Unknown
Unknown	0.02	Oxygenated monoterpene
<i>cis</i> -Ascaridole glycol	0.04	Monoterpenic alcohol
Unknown	0.03	Unknown
Undecanal	0.01	Aliphatic aldehyde
Unknown	0.06	Monoterpenic alcohol
δ -Elemene	0.05	Sesquiterpene
Unknown	0.02	Unknown
Neryl acetate	0.06	Monoterpenic ester
Geranyl acetate	0.06	Monoterpenic ester
β -Elemene	0.06	Sesquiterpene
Dodecanal	0.04	Aliphatic aldehyde
β -Caryophyllene	0.28	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.05	Sesquiterpene
α -Santalene	0.04	Sesquiterpene
γ -Elemene	0.05	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.44	Sesquiterpene

α-Humulene	0.08	Sesquiterpene
β-Santalene	0.03	Sesquiterpene
(E)-β-Farnesene	0.05	Sesquiterpene
Selina-4,11-diene	0.10	Sesquiterpene
Germacrene D	0.04	Sesquiterpene
β-Selinene	0.03	Sesquiterpene
δ-Selinene	0.12	Sesquiterpene
α-Selinene	0.07	Sesquiterpene
(Z)-α-Bisabolene	0.11	Sesquiterpene
β-Bisabolene	0.81	Sesquiterpene
(3E,6E)-α-Farnesene	0.52	Sesquiterpene
β-Curcumene	0.01	Sesquiterpene
γ-Cadinene	0.02	Sesquiterpene
(Z)-γ-Bisabolene	0.05	Sesquiterpene
δ-Cadinene	0.04	Sesquiterpene
Selina-4,7(11)-diene?	0.12	Sesquiterpene
(E)-α-Bisabolene	0.05	Sesquiterpene
Germacrene B	0.04	Sesquiterpene
Caryophyllenyl alcohol	0.05	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Junenol	0.03	Sesquiterpenic alcohol
10-epi-γ-Eudesmol	0.02	Sesquiterpenic alcohol
Clovan-2β-ol	0.02	Sesquiterpenic alcohol
γ-Eudesmol	0.03	Sesquiterpenic alcohol
Unknown	0.01	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
α-Bisabolol	0.02	Sesquiterpenic alcohol
epi-α-Bisabolol	0.03	Sesquiterpenic alcohol
Consolidated total	99.33%	

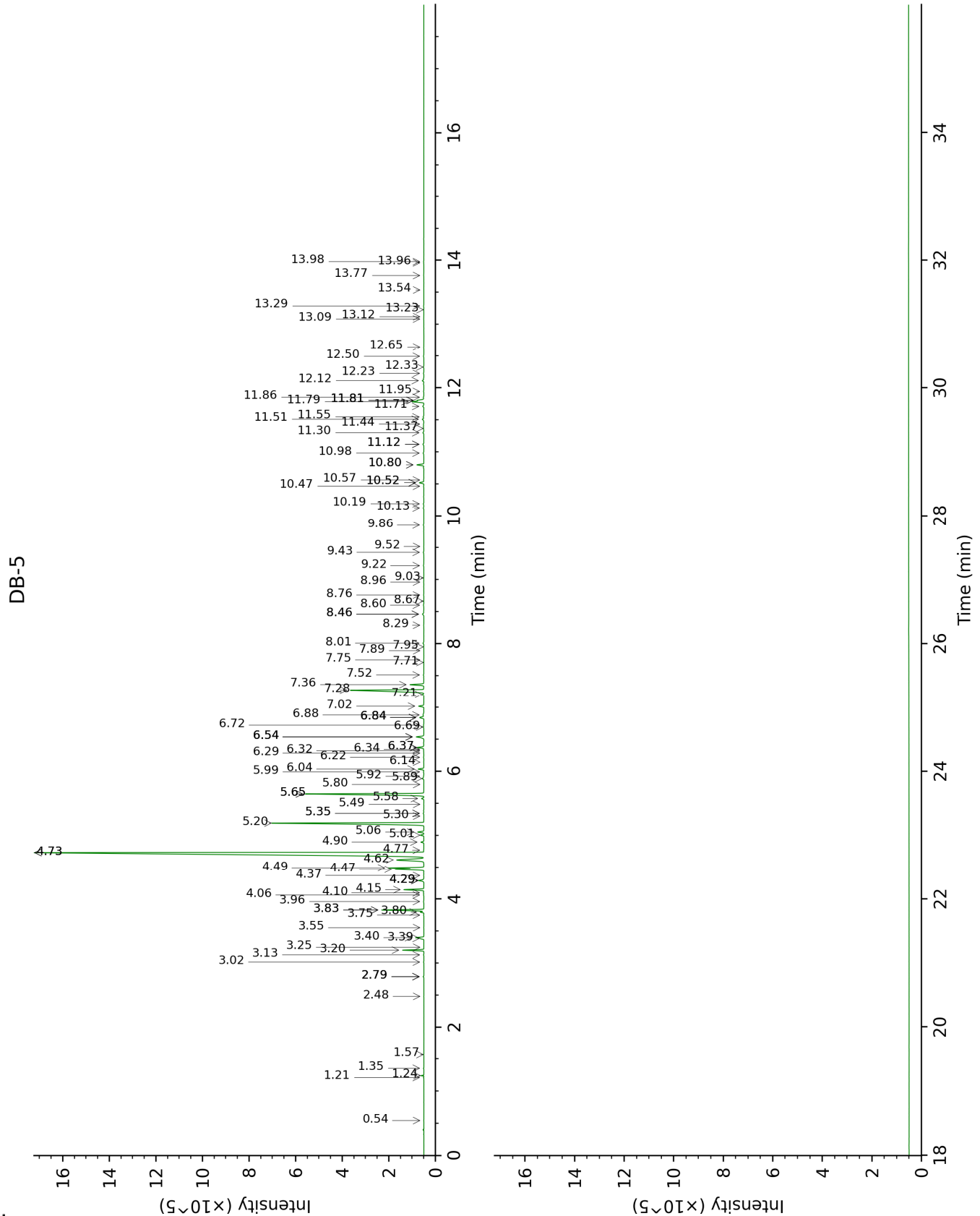
tr: The compound has been detected below 0.005% of total signal.

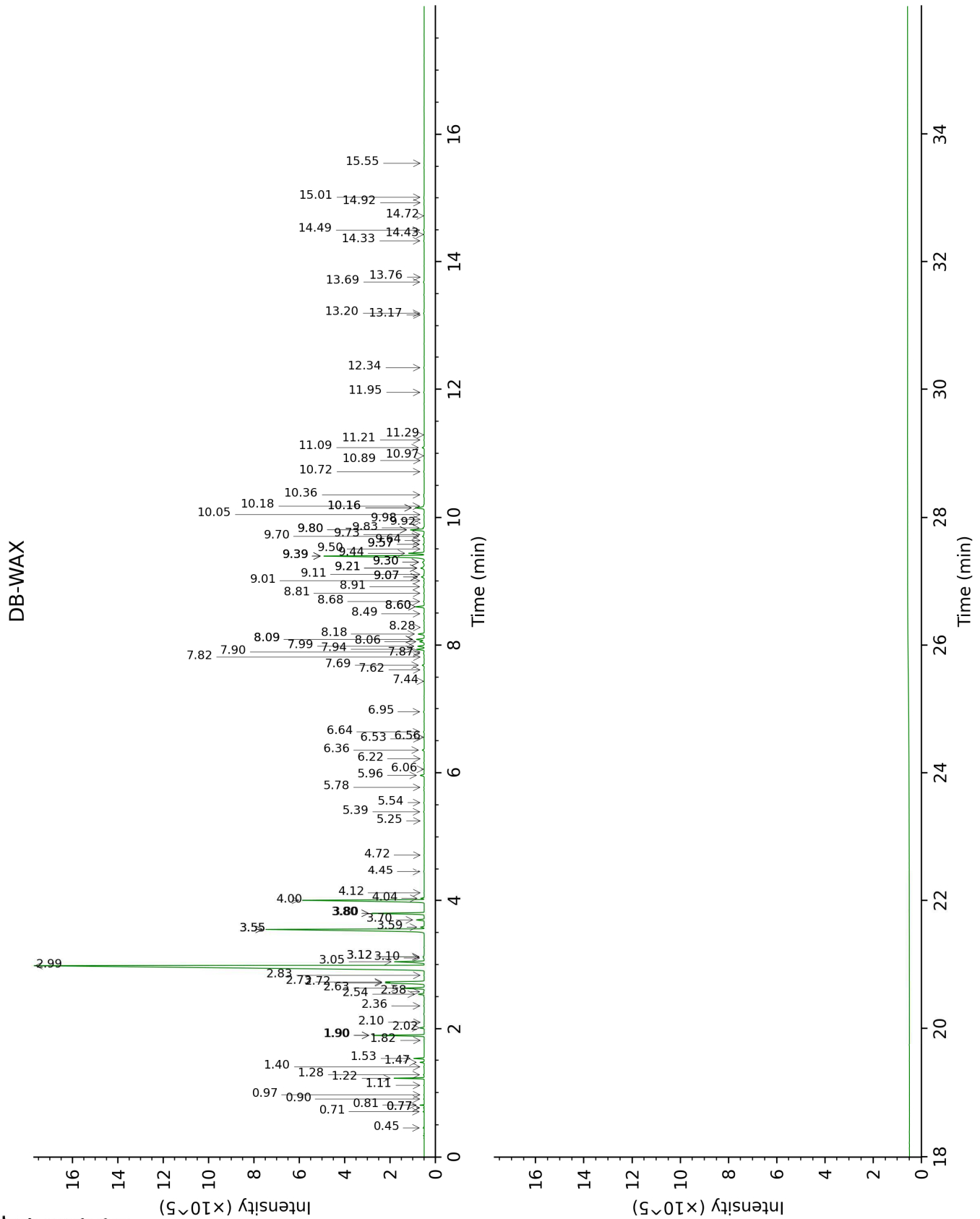
Note: no correction factor was applied

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	0.54	606	tr	1.40	1016	0.02
4,5-Dihydrotoluene	1.21	755	0.02	0.76*	914	0.02
1-Methylcyclohexa-1,3-diene	1.24	759	0.10	0.81	921	0.11
3-Methylenecyclohexadiene	1.35	774	0.02	0.90	937	0.02
Octane	1.57	803	0.01	0.45	784	0.02
Cyclofenchene	2.48	878	0.01	0.76*	914	[0.02]
Bornylene	2.79*	904	0.05	0.97	948	0.01
Nonane	2.79*	904	[0.05]	0.71	898	0.02
Heptanal	2.79*	904	[0.05]	2.84	1152	0.02
Tricyclene	3.02	919	0.03	1.11	973	0.02
α -Thujene	3.13	926	0.03	1.28	1002	0.03
α -Pinene	3.20	931	1.14	1.22	992	1.13
β -Fenchene?	3.25	934	0.01			
α -Fenchene	3.39†	943	0.64	1.47	1023	0.17
Camphene	3.40†	944	[0.64]	1.53	1029	0.44
1,4-Dimethyl-4-vinylcyclohexene?	3.55	954	0.02	1.82	1059	0.01
Unknown [m/z 93, 91 (60), 121 (55), 136 (42), 79 (40)]	3.75	967	0.03	1.90*	1067	2.42
Geranic oxide	3.80	970	0.22	2.02	1079	0.22
β -Pinene	3.83*	972	2.40	1.90*	1067	[2.42]
Sabinene	3.83*	972	[2.40]	2.10	1088	tr
3-Methyl-3-cyclohexenone	3.96	981	0.05	5.78	1372	0.03
6-Methyl-5-hepten-2-one	4.06	987	0.03	4.72	1301	0.01
<i>trans</i> -Dehydroxylinalool oxide	4.10	990	0.04	3.10	1174	0.04
Myrcene	4.15	993	1.17	2.63	1135	1.18
α -Phellandrene	4.29*	1002	0.43	2.54	1127	0.31
Pseudolimonene	4.29*	1002	[0.43]	2.58	1130	0.04
Menthatriene isomer I	4.29*	1002	[0.43]	3.12*	1175	0.06
Octanal	4.29*	1002	[0.43]	4.12	1255	0.02
Δ^3 -Carene	4.37	1007	0.03	2.36	1112	0.03
1,4-Cineole	4.47	1013	1.93	2.73†	1143	[4.05]
α -Terpinene	4.49	1015	2.13	2.72†	1142	4.05
para-Cymene	4.62	1023	2.88	3.80*	1230	2.84
1,8-Cineole	4.73*	1030	48.97	3.05	1169	1.69
Limonene	4.73*	1030	[48.97]	2.99	1164	47.67
(Z)-Citroxide	4.77	1032	0.04	3.12*	1175	[0.06]
(Z)- β -Ocimene	4.90	1040	0.20	3.55*	1211	12.13
(E)-Citroxide	5.01	1047	0.22	3.59	1213	0.18
(E)- β -Ocimene	5.06	1050	0.42	3.70	1222	0.41
γ -Terpinene	5.20	1059	11.81	3.55*	1211	[12.13]
<i>cis</i> -Sabinene hydrate	5.30	1066	0.02	6.56	1430	0.01

Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.35*	1068	0.06	4.45	1280	0.03
para-Mentha-3,8-diene	5.35*	1068	[0.06]	3.80*	1230	[2.84]
Octanol	5.49	1077	0.02	7.82	1526	0.01
Terpinolene isomer	5.58	1083	0.17	4.04	1248	0.15
para-Cymenene	5.65*	1087	8.68	5.96	1385	0.23
Terpinolene	5.65*	1087	[8.68]	4.00	1246	8.52
trans-Sabinene hydrate	5.80	1096	0.01	7.62	1510	0.03
Linalool	5.89	1102	0.15	7.69	1516	0.12
Nonanal	5.92	1104	0.04	5.54	1354	0.03
1,3,8-para-Menthatriene	5.99	1109	0.04	5.39	1344	0.04
endo-Fenchol	6.04	1112	0.39	7.99	1539	0.38
trans-para-Mentha-2,8-dien-1-ol	6.14	1118	0.03	8.60*	1588	0.52
Myrcenol	6.22	1123	0.04	8.49	1579	0.04
Limona ketone	6.29	1127	0.03	7.44	1496	0.01
cis-Limonene oxide	6.32	1130	0.03	6.06	1392	0.01
allo-Ocimene	6.34	1131	0.02	5.25	1333	0.01
1-Terpineol	6.37*	1133	0.48	7.94	1535	0.45
trans-Limonene oxide	6.37*	1133	[0.48]	6.22	1404	0.01
Unknown [m/z 109, 124 (45), 119 (41), 43 (35), 91 (28), 95 (25)...]	6.54*	1144	0.65	6.53	1428	0.02
Epoxyterpinolene	6.54*	1144	[0.65]	6.36	1414	0.12
cis-β-Terpineol	6.54*	1144	[0.65]	8.60*	1588	[0.52]
Isoborneol	6.69	1153	0.04	9.01	1620	0.04
(Z)-Ocimenol	6.72	1155	0.05	9.07*	1625	0.20
Borneol	6.84*	1163	0.35	9.39*	1652	6.96
α-Phellandren-8-ol	6.84*	1163	[0.35]	9.73	1680	0.04
trans-β-Terpineol	6.84*	1163	[0.35]	9.20*	1636	0.28
(E)-Ocimenol	6.88	1165	0.13	9.30*	1644	0.15
Terpinen-4-ol	7.02	1174	0.37	8.18	1554	0.36
para-Cymen-8-ol	7.21	1186	0.12	11.09	1796	0.12
α-Terpineol	7.28	1190	6.73	9.39*	1652	[6.96]
γ-Terpineol	7.36	1196	0.94	9.44	1655	0.93
Decanal	7.52	1206	0.05	6.95	1460	0.05
trans-Carveol	7.71	1219	0.02	10.97	1785	0.01
2,3-Epoxyneral?	7.75	1221	0.03			
cis-Carveol	7.89	1231	0.02	11.29	1813	0.01
Unknown [m/z 137, 152 (28), 43 (25), 91 (24), 109 (23), 119 (19)]	7.95	1235	0.03	10.89	1779	0.02
Neral	8.01	1239	0.09	9.11	1628	0.04
Geraniol	8.29	1257	0.04	11.21	1806	0.03
Geranial	8.46*	1269	0.14	9.70	1677	0.12
trans-Ascaridole glycol	8.46*	1269	[0.14]	13.76	2042	0.01
Unknown [m/z 43, 79 (78), 128 (46), 58 (42), 127 (42)...]	8.60	1278	0.06			

Unknown [m/z 95, 67 (45), 41 (42), 110 (42), 43 (41), 59 (36)]	8.67	1282	0.02	11.95	1873	0.03
<i>cis</i> -Ascaridole glycol	8.76	1289	0.04	14.33	2098	0.05
Unknown [m/z 112, 97 (93), 83 (60), 43 (46), 41 (20), 69 (19)...]	8.96	1302	0.03			
Undecanal	9.03	1307	0.01	8.28	1562	0.01
Unknown [m/z 97, 112 (92), 83 (62), 43 (44), 41 (25)... 170? (4)]	9.22	1320	0.06	14.50	2114	0.06
δ -Elemene	9.43	1335	0.05	6.64	1436	0.04
Unknown [m/z 133, 105 (45), 91 (38), 119 (36)... 150 (3)]	9.52	1341	0.02			
Neryl acetate	9.86	1365	0.06	9.83	1688	0.07
Geranyl acetate	10.13	1384	0.06	10.18	1717	0.05
β -Elemene	10.19	1389	0.06	8.06†	1545	0.82
Dodecanal	10.47	1408	0.04	9.64	1672	0.02
β -Caryophyllene	10.52*	1412	0.33	8.09*†	1547	[0.82]
<i>cis</i> - α -Bergamotene	10.52*	1412	[0.33]	7.87	1530	0.05
α -Santalene	10.57	1416	0.04	7.90	1532	0.02
γ -Elemene	10.80*	1433	0.50	8.68	1594	0.05
<i>trans</i> - α -Bergamotene	10.80*	1433	[0.50]	8.09*†	1547	[0.82]
α -Humulene	10.98	1447	0.08	8.92	1612	0.08
β -Santalene	11.12*	1457	0.09	8.81	1604	0.03
(<i>E</i>)- β -Farnesene	11.12*	1457	[0.09]	9.20*	1636	[0.28]
Selina-4,11-diene	11.30	1470	0.10	9.07*	1625	[0.20]
Germacrene D	11.37	1475	0.04	9.39*	1652	[6.96]
β -Selinene	11.44	1480	0.03	9.50	1661	0.04
δ -Selinene	11.51	1486	0.12	9.30*	1644	[0.15]
α -Selinene	11.55	1489	0.07	9.58*	1667	0.08
(<i>Z</i>)- α -Bisabolene	11.71	1501	0.11	9.80*	1686	0.92
β -Bisabolene	11.79†	1506	1.29	9.80*	1686	[0.92]
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	11.81*†	1508	[1.29]	10.16*	1715	0.64
β -Curcumene	11.81*†	1508	[1.29]	9.92	1695	0.01
γ -Cadinene	11.81*†	1508	[1.29]	9.98	1700	0.02
(<i>Z</i>)- γ -Bisabolene	11.86	1512	0.05	9.58*	1667	[0.08]
δ -Cadinene	11.95	1519	0.04	10.05	1706	0.04
Selina-4,7(11)-diene?	12.12	1532	0.12	10.16*	1715	[0.64]
(<i>E</i>)- α -Bisabolene	12.23	1541	0.05	10.36	1733	0.04
Germacrene B	12.33	1549	0.04	10.72	1764	0.04
Caryophyllenyl alcohol	12.50	1562	0.05	13.20	1988	0.04
Caryophyllene oxide	12.65	1574	0.02	12.34	1908	0.04
Junenol	13.09	1608	0.03	13.17	1986	0.01
10-epi- γ -Eudesmol	13.12	1612	0.02	13.69	2035	0.06
Clovan-2 β -ol	13.23	1621	0.02			
γ -Eudesmol	13.29	1625	0.03	14.43	2107	0.03
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.54	1646	0.01	14.72	2137	0.02

Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.76	1665	0.02	15.55	2222	0.02
α -Bisabolol	13.96	1681	0.02	14.92	2158	0.02
epi- α -Bisabolol	13.98	1682	0.03	15.01	2166	0.03
Total identified	98.62%			98.79%		
Total reported	98.90%			99.00%		

*: 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