

Date : April 08, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21C30-PTH02


Customer identification : Lime Steam Distilled - West Indies - LL01062011R

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 : Sarah-Eve Tremblay, M. Sc. A., Chimiste

Analysis date : April 08, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid

Refractive index: 1.4756 ± 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
4,5-Dihydrotoluene	0.10	Alkene
3-Methylenecyclohexadiene	0.02	Alkene
Octane	tr	Alkane
(3Z)-Hexenol	tr	Aliphatic alcohol
Cyclofenchene	0.01	Monoterpene
Heptanal	0.01	Aliphatic aldehyde
Nonane	0.02	Alkane
Tricyclene	0.02	Monoterpene
α -Thujene	0.02	Monoterpene
α -Pinene	1.09	Monoterpene
β -Fenchene?	tr	Monoterpene
Camphene	0.46	Monoterpene
α -Fenchene	0.18	Monoterpene
Thuja-2,4(10)-diene	tr	Monoterpene
1,4-Dimethyl-4-vinylcyclohexene?	0.01	Monoterpene
Geranic oxide	0.02	Monoterpenic ether
Sabinene	0.01	Monoterpene
β -Pinene	2.35	Monoterpene
3-Methyl-3-cyclohexenone	0.02	Aliphatic ketone
6-Methyl-5-hepten-2-one	tr	Aliphatic ketone
<i>trans</i> -Dehydroxylinool oxide	0.01	Monoterpenic ether
Myrcene	1.19	Monoterpene
α -Phellandrene	0.33	Monoterpene
Pseudolimonene	0.04	Monoterpene
Δ^3 -Carene	0.02	Monoterpene
α -Terpinene	2.77	Monoterpene
1,4-Cineole	1.69	Monoterpenic ether
ortho-Cymene	0.01	Monoterpene
para-Cymene	1.97	Monoterpene
β -Phellandrene	1.81*	Monoterpene
1,8-Cineole	[1.81]*	Monoterpenic ether
Limonene	47.57	Monoterpene
(Z?)-Citroside	0.02	Monoterpenic ether
(Z)- β -Ocimene	0.20	Monoterpene
(E?)-Citroside	0.24	Monoterpenic ether
(E)- β -Ocimene	0.43	Monoterpene
γ -Terpinene	12.45	Monoterpene
<i>cis</i> -Sabinene hydrate	tr	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Octanol	0.02	Aliphatic alcohol
Fenchone	0.17	Monoterpenic ketone
para-Cymenene	0.22	Monoterpene
Terpinolene	8.76	Monoterpene
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	0.13	Monoterpenic alcohol

Nonanal	0.04	Aliphatic aldehyde
endo-Fenchol	0.49	Monoterpenic alcohol
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
Myrcenol	0.03	Monoterpenic alcohol
Limona ketone	0.02	Normonoterpenic ketone
allo-Ocimene	0.01	Monoterpene
<i>cis</i> -Limonene oxide	0.01	Monoterpenic ether
1-Terpineol	0.56	Monoterpenic alcohol
<i>trans</i> -Limonene oxide	0.01	Monoterpenic ether
Cosmene isomer II	0.03	Monoterpene
Epoxyterpinolene	0.03	Monoterpenic ether
<i>cis</i> - β -Terpineol	0.55	Monoterpenic alcohol
Unknown	tr	Unknown
Isoborneol	0.04	Monoterpenic alcohol
(<i>Z</i>)-Ocimenol	0.05	Monoterpenic alcohol
Borneol	0.37	Monoterpenic alcohol
<i>trans</i> - β -Terpineol	0.08	Monoterpenic alcohol
α -Phellandren-8-ol	0.03	Monoterpenic alcohol
(<i>E</i>)-Ocimenol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.43	Monoterpenic alcohol
4-Methylacetophenone	0.01	Simple phenolic
para-Cymen-8-ol	0.06	Monoterpenic alcohol
α -Terpineol	6.73	Monoterpenic alcohol
<i>cis</i> -Piperitol	tr	Monoterpenic alcohol
γ -Terpineol	0.93	Monoterpenic alcohol
<i>trans</i> -Piperitol	tr	Monoterpenic alcohol
Decanal	0.07	Aliphatic aldehyde
<i>trans</i> -Carveol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	tr	Monoterpenic aldehyde
<i>cis</i> -Carveol	tr	Monoterpenic alcohol
Nerol	tr	Monoterpenic alcohol
2,3-Epoxygeranial?	0.01	Monoterpenic aldehyde
Unknown	0.02	Oxygenated monoterpene
Neral	0.09	Monoterpenic aldehyde
Geraniol	0.02	Monoterpenic alcohol
Unknown	0.01	Unknown
<i>trans</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Geranial	0.12	Monoterpenic aldehyde
Unknown	0.02	Unknown
Unknown	0.01	Oxygenated monoterpene
<i>cis</i> -Ascaridole glycol	tr	Monoterpenic alcohol
Unknown	tr	Unknown
Undecanal	tr	Aliphatic aldehyde
Unknown	0.01	Monoterpenic alcohol
δ -Elemene	0.05	Sesquiterpene
Neryl acetate	0.05	Monoterpenic ester
α -Copaene	tr	Sesquiterpene
7-Cubebene	tr	Sesquiterpene
7-Cubebene epimer?	0.02	Aliphatic alcohol
β -Bourbonene	0.01	Sesquiterpene
Geranyl acetate	0.06	Monoterpenic ester
β -Elemene	0.04	Sesquiterpene

Isocaryophyllene	tr	Sesquiterpene
Dodecanal	tr	Aliphatic aldehyde
<i>cis</i> - α -Bergamotene	0.06	Sesquiterpene
β -Caryophyllene	0.22	Sesquiterpene
α -Santalene	0.03	Sesquiterpene
γ -Elemene	0.03	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.49	Sesquiterpene
α -Humulene	0.07	Sesquiterpene
β -Santalene	0.02	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.05	Sesquiterpene
Selina-4,11-diene	0.09	Sesquiterpene
α -Amorphene	0.04	Sesquiterpene
β -Selinene	0.08	Sesquiterpene
Unknown	0.02	Sesquiterpene
δ -Selinene	0.10	Sesquiterpene
Valencene	0.01	Sesquiterpene
α -Selinene	0.06	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	0.02	Sesquiterpene
β -Bisabolene	0.89	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	0.46	Sesquiterpene
(<i>Z</i>)- γ -Bisabolene	0.04	Sesquiterpene
δ -Cadinene	0.03	Sesquiterpene
Selina-4(15),7(11)-diene	0.03	Sesquiterpene
Unknown	0.16	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.04	Sesquiterpene
Germacrene B	0.05	Sesquiterpene
Caryophyllenyl alcohol	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	tr	Sesquiterpenic ether
Globulol	tr	Sesquiterpenic alcohol
Junenol	0.02	Sesquiterpenic alcohol
10-epi- γ -Eudesmol	tr	Sesquiterpenic alcohol
Clovan-2 β -ol	0.02	Sesquiterpenic alcohol
γ -Eudesmol	0.03	Sesquiterpenic alcohol
β -Eudesmol	0.01	Sesquiterpenic alcohol
Unknown	0.01	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
(<i>E</i>)-Bisabol-11-ol	tr	Sesquiterpenic alcohol
epi- α -Bisabolol	0.02	Sesquiterpenic alcohol
α -Bisabolol	0.02	Sesquiterpenic alcohol
Juniper camphor	tr	Sesquiterpenic alcohol
Consolidated total	98.89%	

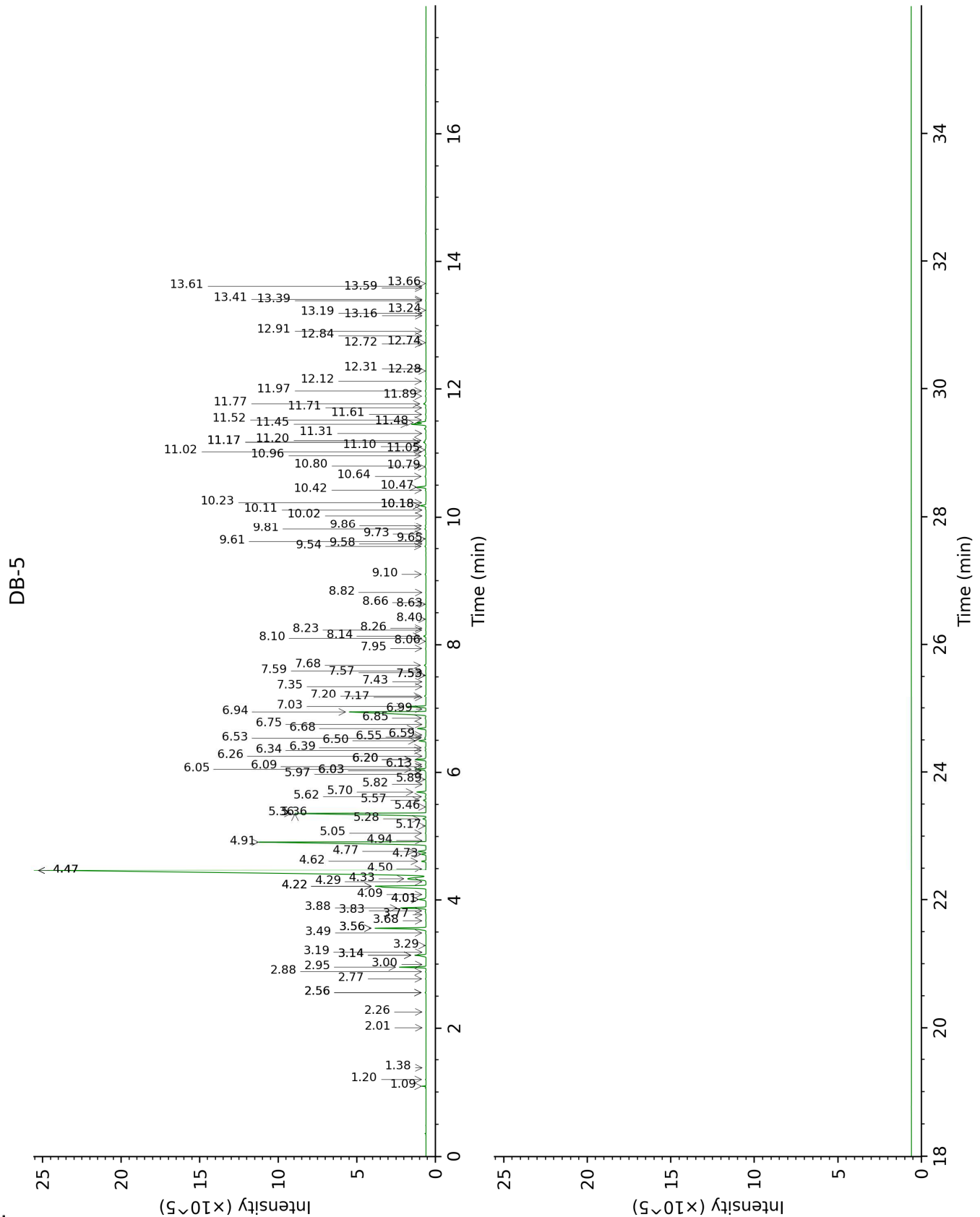
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

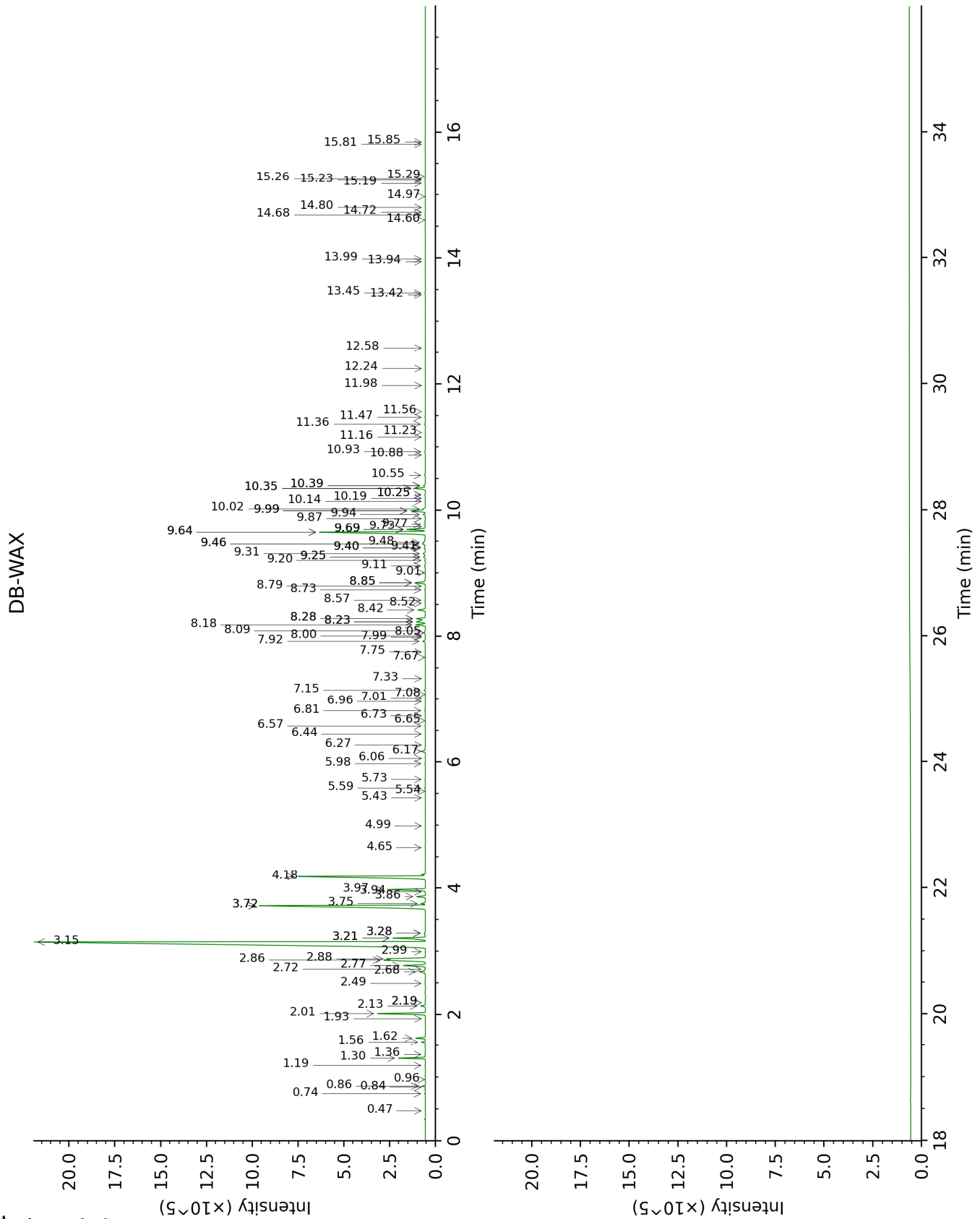
Note: no correction factor was applied

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	%
4,5-Dihydrotoluene	1.09	759	0.10	0.86	918	0.10
3-Methylenecyclohexadiene	1.20	774	0.02	0.96	935	0.01
Octane	1.38	802	tr	0.47	788	tr
(3Z)-Hexenol	2.01	858	tr	5.59	1344	0.04
Cyclofenchene	2.26	879	0.01	0.84	915	tr
Heptanal	2.56*	905	0.03	2.99	1152	0.01
Nonane	2.56*	905	[0.03]	0.74	895	0.02
Tricyclene	2.77	919	0.02	1.18	973	0.02
α -Thujene	2.88	927	0.02	1.36	1002	0.03
α -Pinene	2.95	932	1.09	1.30	993	1.09
β -Fenchene?	3.00	934	tr			
Camphene	3.14*	944	0.65	1.62	1029	0.46
α -Fenchene	3.14*	944	[0.65]	1.56	1022	0.18
Thuja-2,4(10)-diene	3.19	947	tr	2.19*	1085	0.02
1,4-Dimethyl-4-vinylcyclohexene?	3.29	954	0.01	1.93	1060	0.01
Geranic oxide	3.49	968	0.02	2.14	1080	0.23
Sabinene	3.56*	973	2.56	2.19*	1085	[0.02]
β -Pinene	3.56*	973	[2.56]	2.01	1068	2.35
3-Methyl-3-cyclohexenone	3.68	980	0.02	5.98	1372	0.04
6-Methyl-5-hepten-2-one	3.77	987	tr	4.99	1300	0.01
<i>trans</i> -Dehydroxylinalool oxide	3.83	991	0.01	3.28*	1174	0.07
Myrcene	3.88	994	1.19	2.77	1135	1.20
α -Phellandrene	4.01*	1003	0.44	2.68	1127	0.33
Pseudolimonene	4.01*	1003	[0.44]	2.72	1130	0.04
Δ^3 -Carene	4.09	1008	0.02	2.49	1112	0.03
α -Terpinene	4.22*	1016	4.49	2.86	1141	2.77
1,4-Cineole	4.22*	1016	[4.49]	2.88	1143	1.69
ortho-Cymene	4.29	1020	0.01	3.94	1224	0.01
para-Cymene	4.33	1023	1.97	3.97	1226	1.92
β -Phellandrene	4.47*	1032	49.38	3.21*	1169	1.80
1,8-Cineole	4.47*	1032	[49.38]	3.21*	1169	[1.80]
Limonene	4.47*	1032	[49.38]	3.15	1164	47.57
(Z)-Citroxide	4.50	1034	0.02	3.28*	1174	[0.07]
(Z)- β -Ocimene	4.62	1041	0.20	3.72*	1208	12.69
(E)-Citroxide	4.73	1048	0.24	3.75	1210	0.20
(E)- β -Ocimene	4.77	1051	0.43	3.86	1218	0.43
γ -Terpinene	4.91	1060	12.45	3.72*	1208	[12.69]
<i>cis</i> -Sabinene hydrate	4.94	1062	tr	6.73	1428	0.02
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.05	1069	0.03	4.65	1275	0.02
Octanol	5.17	1076	0.02	7.99	1523	0.01
Fenchone	5.28	1083	0.17	5.54	1341	tr
para-Cymenene	5.36*	1089	8.97	6.17	1387	0.22

Terpinolene	5.36*	1089	[8.97]	4.18	1241	8.76
<i>trans</i> -Sabinene hydrate	5.46	1095	0.01	7.75	1505	0.01
Linalool	5.57	1102	0.13	7.92	1518	0.14
Nonanal	5.62	1105	0.04	5.73	1354	0.02
endo-Fenchol	5.70	1110	0.49	8.23*†	1542	1.23
<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.82	1118	0.01	8.79	1586	0.01
Myrcenol	5.89	1122	0.03	8.73	1582	0.03
Limona ketone	5.97	1128	0.02	7.66	1498	tr
allo-Ocimene	6.03*	1131	0.03	5.43	1333	0.01
<i>cis</i> -Limonene oxide	6.03*	1131	[0.03]	6.27	1394	0.01
1-Terpineol	6.05	1133	0.56	8.18	1538	0.53
<i>trans</i> -Limonene oxide	6.09	1135	0.01	6.44	1406	0.01
Cosmene isomer II	6.13	1137	0.03	6.06	1378	tr
Epoxyterpinolene	6.20*	1142	0.59	6.57	1416	0.03
<i>cis</i> -β-Terpineol	6.20*	1142	[0.59]	8.85*	1590	0.58
Unknown [m/z 109, 124 (45), 119 (41), 43 (35), 91 (28), 95 (25)...]	6.26	1146	tr	6.65	1422	0.01
Isoborneol	6.34	1152	0.04	9.20	1619	0.04
(<i>Z</i>)-Ocimenol	6.39	1154	0.05	9.25*	1623	0.11
Borneol	6.50	1161	0.37	9.64*	1655	6.93
<i>trans</i> -β-Terpineol	6.53	1164	0.08	9.46*	1640	0.18
α-Phellandren-8-ol	6.55	1165	0.03	9.99*	1684	0.91
(<i>E</i>)-Ocimenol	6.59	1167	0.01	9.48	1642	0.12
Terpinen-4-ol	6.68	1173	0.43	8.42	1557	0.42
4-Methylacetophenone	6.75	1178	0.01	10.25*	1705	0.04
para-Cymen-8-ol	6.85	1184	0.06	11.36	1800	0.06
α-Terpineol	6.94	1190	6.73	9.64*	1655	[6.93]
<i>cis</i> -Piperitol	6.99	1193	tr	9.40*	1635	0.07
γ-Terpineol	7.03	1196	0.93	9.69*	1659	0.96
<i>trans</i> -Piperitol	7.17	1205	tr	10.19	1700	0.01
Decanal	7.20	1207	0.07	7.15	1459	0.07
<i>trans</i> -Carveol	7.35	1217	0.01	11.23	1789	0.01
2,3-Epoxyneral?	7.43	1222	tr			
<i>cis</i> -Carveol	7.53*	1228	0.01	11.56	1818	tr
Nerol	7.53*	1228	[0.01]	10.88	1758	tr
2,3-Epoxygeranial?	7.57	1231	0.01			
Unknown [m/z 137, 152 (28), 43 (25), 91 (24), 109 (23), 119 (19)]	7.59	1233	0.02	11.16	1782	0.01
Neral	7.68	1239	0.09	9.31	1627	0.17
Geraniol	7.95	1257	0.02	11.47	1810	0.02
Unknown [m/z 43, 128 (61), 79 (60), 127 (52), 58 (50)...]	8.06	1264	0.01	11.98	1854	tr
<i>trans</i> -Ascaridole glycol	8.10	1267	0.01	13.99	2041	0.01
Geranial	8.14	1270	0.12	9.94	1679	0.12
Unknown [m/z 43, 79 (78), 128 (46), 58 (42), 127 (42)...]	8.23	1276	0.02			

Unknown [m/z 95, 67 (45), 41 (42), 110 (42), 43 (41), 59 (36)]	8.26	1278	0.01	12.24	1878	0.01
<i>cis</i> -Ascaridole glycol	8.40	1287	tr	14.60	2100	0.01
Unknown [m/z 112, 97 (93), 83 (60), 43 (46), 41 (20), 69 (19)...]	8.64	1303	tr			
Undecanal	8.66	1305	tr	8.52	1565	0.02
Unknown [m/z 97, 112 (92), 83 (62), 43 (44), 41 (25)... 170? (4)]	8.82	1316	0.01	14.80	2121	0.01
δ -Elemene	9.10	1336	0.05	6.81	1434	0.04
Neryl acetate	9.54	1367	0.05	10.02	1686	0.11
α -Copaene	9.58	1370	tr	7.01	1449	tr
7-Cubebene	9.61	1372	tr	6.96	1445	0.01
7-Cubebene epimer?	9.65	1375	0.02	7.08	1454	tr
β -Bourbonene	9.73	1380	0.01	7.33	1473	0.01
Geranyl acetate	9.81	1386	0.06	10.39*	1717	0.11
β -Elemene	9.86	1390	0.04	8.28*†	1546	[1.23]
Isocaryophyllene	10.02	1401	tr	8.00	1524	tr
Dodecanal	10.11	1408	tr	9.87	1674	0.01
<i>cis</i> - α -Bergamotene	10.18*	1413	0.33	8.06	1528	0.06
β -Caryophyllene	10.18*	1413	[0.33]	8.28*†	1546	[1.23]
α -Santalene	10.23	1416	0.03	8.08	1531	0.02
γ -Elemene	10.42	1431	0.03	8.85*	1590	[0.58]
<i>trans</i> - α -Bergamotene	10.47	1435	0.49	8.23*†	1542	[1.23]
α -Humulene	10.64	1447	0.07	9.11	1612	0.07
β -Santalene	10.79	1458	0.02	9.00	1603	0.03
(<i>E</i>)- β -Farnesene	10.80	1459	0.05	9.40*	1635	[0.07]
Selina-4,11-diene	10.96	1471	0.09	9.25*	1623	[0.11]
α -Amorphene	11.02	1476	0.04	9.41	1636	0.03
β -Selinene	11.05	1478	0.08	9.69*	1659	[0.96]
Unknown [m/z 41, 69 (90), 79 (78), 93 (72), 91 (70)...204]	11.10	1482	0.02	8.57	1569	0.03
δ -Selinene	11.17*	1487	0.17	9.46*	1640	[0.18]
Valencene	11.17*	1487	[0.17]	9.74	1662	0.01
α -Selinene	11.20	1489	0.06	9.77	1665	0.07
(<i>Z</i>)- α -Bisabolene	11.31	1497	0.02	10.14	1696	0.01
β -Bisabolene	11.45†	1508	1.33	9.99*	1684	[0.91]
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	11.48†	1510	[1.33]	10.35*	1713	0.63
(<i>Z</i>)- γ -Bisabolene	11.52	1513	0.04	9.69*	1659	[0.96]
δ -Cadinene	11.60	1520	0.03	10.25*	1705	[0.04]
Selina-4(15),7(11)-diene	11.71	1528	0.03	10.39*	1717	[0.11]
Unknown [m/z 189, 204 (92), 161 (65), 133 (51), 105 (51), 91 (51), 119 (45)]	11.77	1533	0.16	10.35*	1713	[0.63]
(<i>E</i>)- α -Bisabolene	11.89	1542	0.04	10.56	1731	0.08
Germacrene B	11.97	1549	0.05	10.93	1763	0.05
Caryophyllenyl alcohol	12.12	1561	0.04	13.45	1989	0.04
Caryophyllene oxide	12.28	1574	tr	12.58	1908	0.01
Globulol	12.32	1576	tr			

Junenol	12.72	1608	0.02	13.42	1986	0.01
10-epi- γ -Eudesmol	12.74	1609	tr	13.94	2037	tr
Clovan-2 β -ol	12.84	1618	0.02			
γ -Eudesmol	12.92	1624	0.03	14.68	2108	0.03
β -Eudesmol	13.16	1644	0.01	15.24	2164	0.01
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109)40)... 204 (35), 222 (2)]	13.19	1647	0.01	14.97	2138	tr
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.24	1651	0.01	14.72	2113	tr
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.39	1664	0.02	15.81	2223	0.01
(<i>E</i>)-Bisabol-11-ol	13.41	1665	tr	15.18	2159	0.02
epi- α -Bisabolol	13.58	1680	0.02	15.29	2170	0.01
α -Bisabolol	13.61	1682	0.02	15.26	2166	0.02
Juniper camphor	13.66	1686	tr	15.85	2227	0.01
Total identified		98.99%			98.79%	
Total reported		99.31%			98.91%	

*: 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