

Date : May 25, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23E18-PTH01


Customer identification : Lavender ORGANIC - Greece - L50117R

Type : Essential oil

Source : *Lavandula angustifolia*

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 : May 24, 2023

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4627 ± 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
Ethanol	tr	Aliphatic alcohol
Methacrolein	tr	Aliphatic aldehyde
3-Buten-2-one	0.01	Aliphatic ketone
2-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	tr	Simple phenolic
Prenal	0.01	Aliphatic aldehyde
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.10	Aliphatic ether
(3Z)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.08	Aliphatic alcohol
Tricyclene	0.02	Monoterpene
α -Thujene	0.13	Monoterpene
Camphene	0.14	Monoterpene
α -Fenchene	0.01	Monoterpene
5,5-Dimethyl-2(5H)-furanone	0.01	Aliphatic lactone
Thuja-2,4(10)-diene	0.01	Monoterpene
Butyl isobutyrate	0.02	Aliphatic ester
Sabinene	0.04	Monoterpene
β -Pinene	0.05	Monoterpene
Octen-3-ol	0.22	Aliphatic alcohol
Octan-3-one	1.08	Aliphatic ketone
Myrcene	0.75	Monoterpene
Butyl butyrate	0.11	Aliphatic ester
Octan-3-ol	0.20	Aliphatic alcohol
α -Phellandrene	0.04	Monoterpene
Δ^3 -Carene	0.11	Monoterpene
α -Terpinene	0.06	Monoterpene
Hexyl acetate	0.55	Aliphatic ester
meta-Cymene	0.05	Monoterpene
para-Cymene	0.26	Monoterpene
1,8-Cineole	0.82	Monoterpenic ether
Limonene	0.33	Monoterpene
Lavender lactone	0.02	Aliphatic lactone
(Z)- β -Ocimene	4.97	Monoterpene
(E)- β -Ocimene	3.02	Monoterpene
γ -Terpinene	0.17	Monoterpene
cis-Sabinene hydrate	0.05	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.23	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
α -Pinene oxide analog	0.07	Monoterpenic ether

Isoterpinolene	0.01	Monoterpene
Terpinolene	0.12	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.16	Monoterpenic alcohol
Rosefuran	0.07	Monoterpenic ether
Linalool	32.67	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.10	Aliphatic ketone
β -Thujone	0.05	Monoterpenic ketone
Octen-3-yl acetate	0.80	Aliphatic ester
Unknown	0.03	Unknown
Octan-3-yl acetate	0.10	Aliphatic ester
allo-Ocimene	0.08	Monoterpene
(<i>Z</i>)-Myroxide	0.03	Monoterpenic ether
Camphor	0.33	Monoterpenic ketone
(<i>E</i>)-Myroxide	0.06	Monoterpenic ether
Hexyl isobutyrate	0.09	Aliphatic ester
Nerol oxide	0.04	Aliphatic ether
Borneol	0.61	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Lavandulol	1.02	Monoterpenic alcohol
Terpinen-4-ol	5.34	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	0.03	Alkene
Cryptone	0.12	Normonoterpenic ketone
para-Cymen-8-ol	0.07	Monoterpenic alcohol
Unknown	0.07	Unknown
α -Terpineol	1.49	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Hexyl butyrate	0.44	Aliphatic ester
Verbenone	0.02	Monoterpenic ketone
Unknown	0.02	Unknown
(3 <i>E</i> ,5 <i>E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.02	Monoterpenic alcohol
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
Nerol	0.26	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.07	Aliphatic ester
Carvone	0.03	Monoterpenic ketone
Neral	0.03	Monoterpenic aldehyde
Geraniol	0.65	Monoterpenic alcohol
Linalyl acetate	25.64	Monoterpenic ester
Geranial	0.05	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.01	Monoterpenic alcohol
Bornyl acetate	0.15	Monoterpenic ester
Lavandulyl acetate	4.05	Monoterpenic ester
Hexyl tiglate	0.07	Aliphatic ester
Hodiendiol derivative	0.04	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.45	Monoterpenic ester
α -Copaene	0.02	Sesquiterpene
β -Bourbonene	0.04	Sesquiterpene
Geranyl acetate	0.75	Monoterpenic ester
7-epi-Sesquithujene	0.09	Sesquiterpene
Hexyl hexanoate	0.10	Aliphatic ester

Isocaryophyllene	0.02	Sesquiterpene
Sesquithujene	0.05	Sesquiterpene
β -Caryophyllene	3.01	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.02	Sesquiterpene
α -Santalene	0.39	Sesquiterpene
Lavandulyl isobutyrate	0.01	Monoterpenic ester
Coumarin	0.01	Coumarin
<i>trans</i> - α -Bergamotene	0.14	Sesquiterpene
Sesquisabinene A	0.02	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.04	Sesquiterpene
α -Humulene	0.11	Sesquiterpene
Lavandulyl butyrate?	0.11	Monoterpenic ester
(<i>E</i>)- β -Farnesene	2.76	Sesquiterpene
β -Santalene	0.01	Sesquiterpene
Germacrene D	0.24	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.07	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	0.03	Sesquiterpene
γ -Cadinene	0.11	Sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.35	Sesquiterpenic ether
Caryophyllene oxide isomer	0.05	Sesquiterpenic ether
τ -Cadinol	0.05	Sesquiterpenic alcohol
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
<i>cis</i> -14-nor-Muurool-5-en-4-one?	0.01	Norsesquiterpenic ketone
α -Pinene	0.28	Monoterpene
Consolidated total	98.64%	

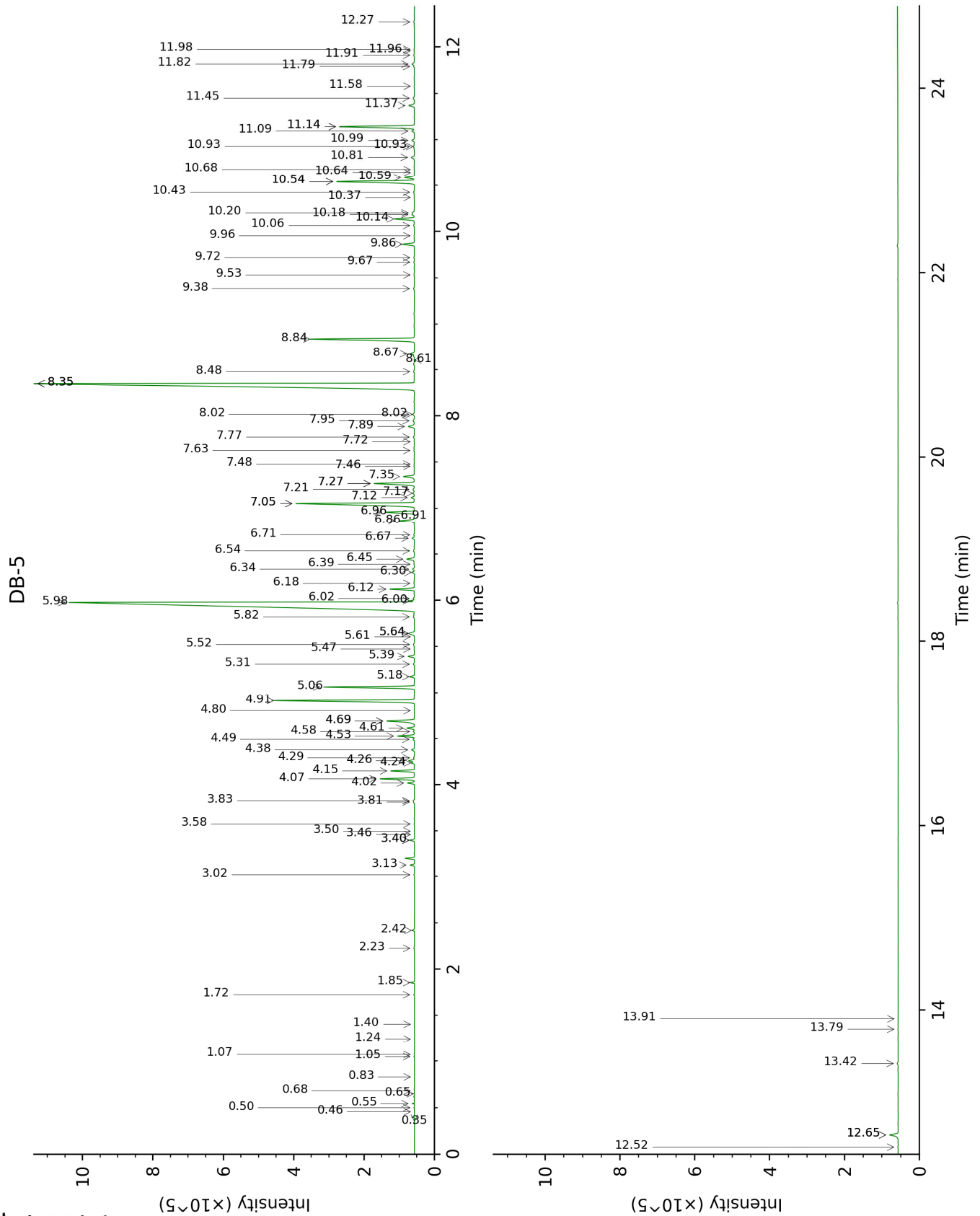
tr: The compound has been detected below 0.005% of total signal.

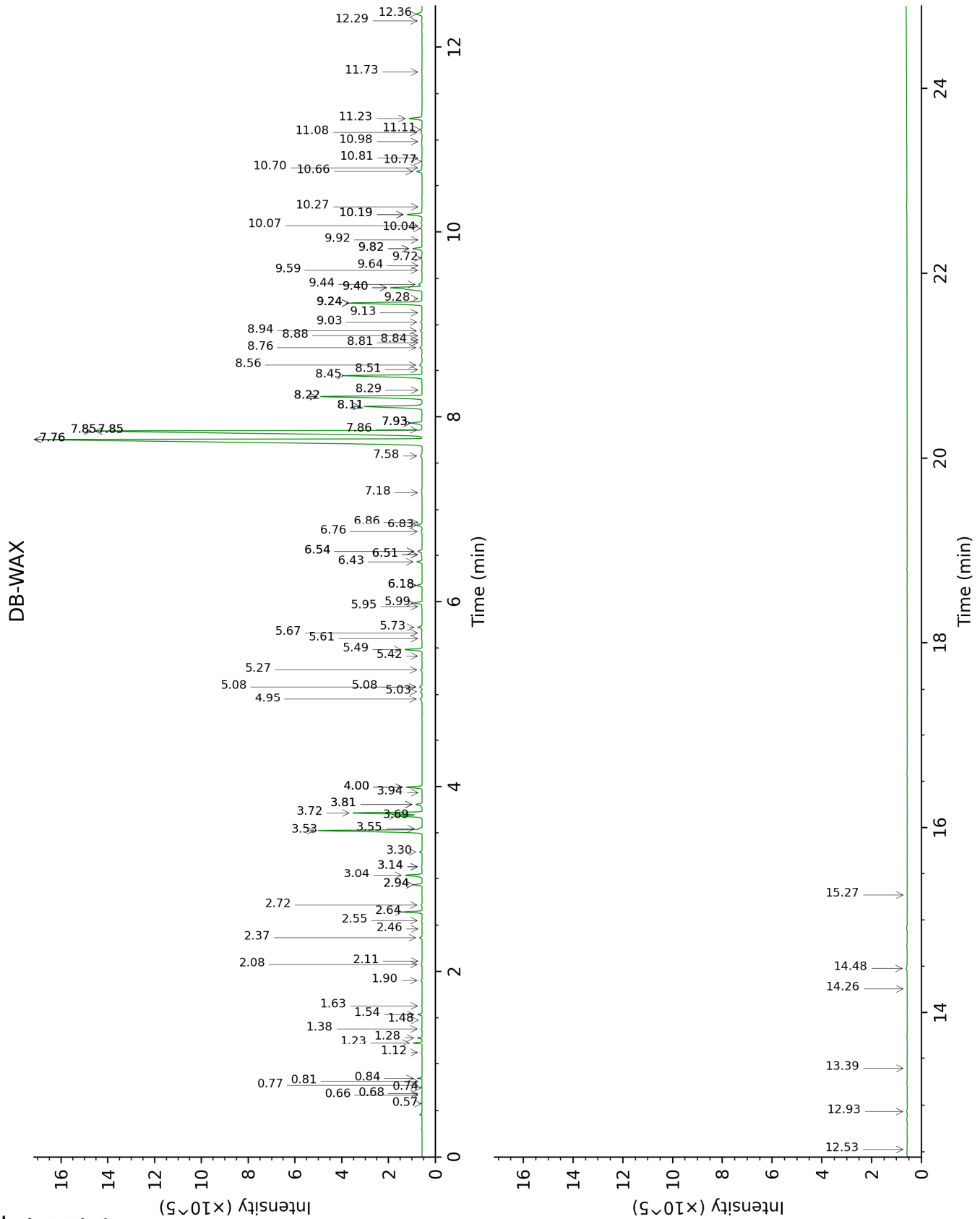
Note: no correction factor was applied

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	%
Ethanol	0.35	500	tr	0.74	906	tr
Methacrolein	0.46	540	tr	0.58	843	tr
3-Buten-2-one	0.50	574	0.01	0.77	910	0.01
2-Methyl-3-buten-2-ol	0.54	607	0.03	1.38	1010	0.02
Isovaleral	0.65	642	0.01	0.68	884	0.01
2-Methylbutyral	0.68	652	tr	0.66	877	tr
2-Ethylfuran	0.83	702	tr	0.81	918	tr
Isoamyl alcohol	1.05	733	0.01	3.14*	1173	0.04
2-Methylbutanol	1.07	736	0.01	3.14*	1173	[0.04]
Toluene	1.24	759	tr			
Prenal	1.40	781	0.01	2.94*	1156	0.34
Butyl acetate	1.72	817	0.02	1.63	1035	0.02
Methyl hexyl ether	1.86	827	0.10	0.84	923	0.10
(3Z)-Hexenol	2.23	858	0.03	5.42	1341	0.03
Hexanol	2.42	874	0.08	5.08*	1316	0.12
Tricyclene	3.02	919	0.02	1.12	971	0.02
α -Thujene	3.13	926	0.13	1.28	999	0.13
Camphene	3.40*	944	0.16	1.54	1026	0.14
α -Fenchene	3.40*	944	[0.16]	1.48	1020	0.01
5,5-Dimethyl-2(5H)-furanone	3.46	948	0.01	8.22*	1552	5.35
Thuja-2,4(10)-diene	3.50	950	0.01	2.11	1086	tr
Butyl isobutyrate	3.58	956	0.02	2.46	1117	0.01
Sabinene	3.81†	971	0.09	2.08	1082	0.04
β -Pinene	3.83†	972	[0.09]	1.90	1064	0.05
Octen-3-ol	4.02	985	0.22	6.43	1415	0.24
Octan-3-one	4.06	988	1.08	3.68	1217	1.10
Myrcene	4.15	993	0.75	2.64	1132	0.74
Butyl butyrate	4.24	999	0.11	3.30	1186	0.11
Octan-3-ol	4.26	1000	0.20	5.73	1363	0.21
α -Phellandrene	4.29	1002	0.04	2.55	1125	0.03
Δ 3-Carene	4.38	1008	0.11	2.37	1110	0.11
α -Terpinene	4.49	1015	0.06	2.72	1138	0.05
Hexyl acetate	4.53	1017	0.55	4.00*	1241	0.68
meta-Cymene	4.58	1020	0.05	3.81*	1227	0.29
para-Cymene	4.61	1023	0.26	3.81*	1227	[0.29]
1,8-Cineole	4.69*	1027	1.16	3.04	1165	0.82
Limonene	4.69*	1027	[1.16]	2.94*	1156	[0.34]
Lavender lactone	4.80	1034	0.02	8.88	1604	0.03
(Z)- β -Ocimene	4.91	1041	4.97	3.53†	1205	5.24
(E)- β -Ocimene	5.06	1051	3.02	3.72	1220	3.05
γ -Terpinene	5.18	1058	0.17	3.55†	1207	[5.24]
cis-Sabinene hydrate	5.31	1066	0.05	6.54*	1424	0.21
cis-Linalool oxide (fur.)	5.40	1071	0.23	6.18*	1396	0.25
Octanol	5.48	1076	0.02	7.86	1524	0.03

α-Pinene oxide analog	5.52	1080	0.07	5.08*	1316	[0.12]
Isoterpinolene	5.61	1085	0.01	3.94	1237	0.01
Terpinolene	5.64*	1087	0.29	4.00*	1241	[0.68]
<i>trans</i> -Linalool oxide (fur.)	5.64*	1087	[0.29]	6.54*	1424	[0.21]
Rosefuran	5.82	1098	0.07	5.66	1359	0.04
Linalool	5.98	1108	32.67	7.76*†	1516	58.58
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	6.00	1109	0.10	7.85*†	1523	[58.58]
β-Thujone	6.02	1111	0.05	5.95	1380	0.03
Octen-3-yl acetate	6.12	1117	0.80	5.49	1346	0.78
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	6.18	1121	0.03	9.28	1637	0.02
Octan-3-yl acetate	6.30	1128	0.10	4.95	1306	0.09
allo-Ocimene	6.34	1131	0.08	5.27	1330	0.06
(<i>Z</i>)-Myroxide	6.39	1134	0.03	6.51*	1421	0.05
Camphor	6.45	1138	0.33	6.83	1445	0.27
(<i>E</i>)-Myroxide	6.54	1143	0.06	6.76	1440	0.05
Hexyl isobutyrate	6.67	1152	0.09	5.03	1312	0.08
Nerol oxide	6.71	1154	0.04	6.51*	1421	[0.05]
Borneol	6.86	1164	0.61	9.40*	1647	2.13
<i>cis</i> -Linalool oxide (pyr.)	6.91	1167	0.01	9.92	1689	0.02
Lavandulol	6.96	1170	1.02	9.24*	1633	3.87
Terpinen-4-ol	7.05*	1176	5.40	8.22*	1552	[5.35]
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	7.05*	1176	[5.40]	5.60	1354	0.03
Cryptone	7.12	1180	0.12	8.76	1594	0.12
para-Cymen-8-ol	7.17	1183	0.07	11.11	1791	0.06
Unknown [m/z 43, 135 (73), 59 (46), 93 (39), 91 (35), 81 (32)...]	7.21	1186	0.07			
α-Terpineol	7.27*	1190	1.51	9.40*	1647	[2.13]
Myrtenal	7.27*	1190	[1.51]	8.29	1557	0.02
Hexyl butyrate	7.35	1195	0.44	5.99	1382	0.38
Verbenone	7.46	1202	0.02	9.24*	1633	[3.87]
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.48	1204	0.02	10.77	1762	0.03
(3 <i>E</i> ,5 <i>E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.63	1213	0.02	10.98	1780	0.03
<i>trans</i> -Carveol	7.72	1220	0.02	11.08	1788	0.07
Bornyl formate	7.77	1223	0.05	7.76*†	1516	[58.58]
Nerol	7.89	1230	0.26	10.66	1752	0.27
Hexyl 2-methylbutyrate	7.95	1235	0.07	6.18*	1396	[0.25]
Carvone	8.02*	1239	0.07	9.59	1662	0.03
Neral	8.02*	1239	[0.07]	9.13	1624	0.03

Geraniol	8.35*	1261	26.29	11.23	1801	0.65
Linalyl acetate	8.35*	1261	[26.29]	7.85*†	1523	[58.58]
Geranial	8.48	1270	0.05	9.72	1673	0.02
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.61	1278	0.01	14.26	2082	0.01
Bornyl acetate	8.67	1283	0.15	7.94*	1530	0.55
Lavandulyl acetate	8.84	1294	4.05	8.45	1570	4.11
Hexyl tiglate	9.38	1332	0.07	8.56	1579	0.14
Hodiendiol derivative	9.53	1342	0.04	12.53	1918	0.02
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.67	1352	0.04	10.70	1756	0.03
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.72	1355	0.04	10.81	1765	0.02
Neryl acetate	9.86	1366	0.45	9.82*	1681	0.47
α-Copaene	9.96	1372	0.02	6.86	1448	0.01
β-Bourbonene	10.06	1380	0.04	7.18	1472	0.03
Geranyl acetate	10.14	1385	0.75	10.19*	1712	0.77
7-epi-Sesquithujene	10.18	1388	0.09	7.58	1502	0.12
Hexyl hexanoate	10.20	1389	0.10	8.51	1575	0.04
Isocaryophyllene	10.37	1401	0.02	7.85*†	1523	[58.58]
Sesquithujene	10.43	1405	0.05	7.85*†	1523	[58.58]
β-Caryophyllene	10.54*	1414	3.09	8.11*	1544	3.16
cis-α-Bergamotene	10.54*	1414	[3.09]	7.94*	1530	[0.55]
α-Santalene	10.59	1417	0.39	7.94*	1530	[0.55]
Lavandulyl isobutyrate	10.64	1421	0.01	9.03	1616	0.08
Coumarin	10.68	1424	0.01			
trans-α-Bergamotene	10.81	1434	0.14	8.11*	1544	[3.16]
Sesquisabinene A	10.93*	1442	0.06	8.81	1598	0.02
cis-β-Bergamotene?	10.93*	1442	[0.06]			
α-Humulene	10.99	1447	0.11	8.94	1608	0.11
Lavandulyl butyrate?	11.09	1455	0.11	10.19*	1712	[0.77]
(E)-β-Farnesene	11.14*	1458	2.83	9.24*	1633	[3.87]
β-Santalene	11.14*	1458	[2.83]	8.84	1600	0.01
Germacrene D	11.37	1475	0.24	9.44	1650	0.21
trans-β-Bergamotene	11.45	1481	0.07	9.24*	1633	[3.87]
Isodaucene	11.58	1491	0.02	9.64	1666	0.01
β-Bisabolene	11.79	1507	0.03	9.82*	1681	[0.47]
γ-Cadinene	11.82	1509	0.11	10.04	1699	0.08
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.91	1516	0.04	12.93	1956	0.03
δ-Cadinene	11.96	1520	0.01	10.07	1702	0.01

β-Sesquiphellandrene	11.98	1521	0.02	10.27	1719	0.01
Isocaryophyllene epoxide B	12.27	1544	0.04	11.73	1846	0.04
(E)-Nerolidol	12.52	1564	0.02	13.40	1999	0.01
Caryophyllene oxide	12.65*	1574	0.39	12.36	1902	0.35
Caryophyllene oxide isomer	12.65*	1574	[0.39]	12.28	1895	0.05
τ-Cadinol	13.42	1636	0.05	14.48	2104	0.11
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	13.80	1667	0.02			
cis-14-nor-Muurool-5-en-4-one?	13.91	1676	0.01	15.27	2184	0.01
α-Pinene				1.23	990	0.28
Total identified		98.31%			98.24%	
Total reported		98.55%			98.38%	

*: 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