

Date : August 23, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21H20-PTH05


Customer identification : Lavender - Bulgaria - L40118209R

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

Analysis date : August 23, 2021

Checked and approved by :


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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4621 ± 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
Isobutyral	tr	Aliphatic aldehyde
Ethyl acetate	0.01	Aliphatic ester
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Hexanal	tr	Aliphatic aldehyde
Butyl acetate	0.01	Aliphatic ester
Methyl hexyl ether	0.08	Aliphatic ether
(3Z)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.09	Aliphatic alcohol
Hashishene	tr	Monoterpene
Tricyclene	0.02	Monoterpene
α -Thujene	0.12	Monoterpene
α -Pinene	0.25	Monoterpene
Camphene	0.17	Monoterpene
α -Fenchene	0.01	Monoterpene
5,5-Dimethyl-2(5H)-furanone	0.01	Aliphatic lactone
Butyl isobutyrate	0.02	Aliphatic ester
Sabinene	0.05	Monoterpene
β -Pinene	0.05	Monoterpene
Octen-3-ol	0.29	Aliphatic alcohol
Octan-3-one	1.04	Aliphatic ketone
Myrcene	0.60	Monoterpene
<i>trans</i> -Dehydroxylinalool oxide	0.02	Monoterpenic ether
Butyl butyrate	0.10	Aliphatic ester
Octan-3-ol	0.25	Aliphatic alcohol
Pseudolimonene	0.02	Monoterpene
α -Phellandrene	0.05	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
Δ^3 -Carene	0.20	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
α -Terpinene	0.07	Monoterpene
Hexyl acetate	0.48	Aliphatic ester
ortho-Cymene	0.05	Monoterpene
para-Cymene	0.17	Monoterpene
Limonene	0.35	Monoterpene
β -Phellandrene	0.21	Monoterpene
1,8-Cineole	0.95	Monoterpenic ether
Lavender lactone	0.01	Aliphatic lactone
(Z)- β -Ocimene	5.79	Monoterpene
(E)- β -Ocimene	2.79	Monoterpene
γ -Terpinene	0.20	Monoterpene

<i>cis</i> -Sabinene hydrate	0.09	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.14	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
α -Pinene oxide analog	0.04	Monoterpenic ether
Isoterpinolene	0.02	Monoterpene
Terpinolene	0.12	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.09	Monoterpenic alcohol
<i>trans</i> -Sabinene hydrate	0.04	Monoterpenic alcohol
Rosefuran	0.04	Monoterpenic ether
Linalool	27.98	Monoterpenic alcohol
Hotrienol	0.06	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
Octen-3-yl acetate	0.95	Aliphatic ester
Unknown	0.04	Unknown
Octan-3-yl acetate	0.12	Aliphatic ester
<i>cis</i> -Limonene oxide	0.01	Monoterpenic ether
allo-Ocimene	0.07	Monoterpene
(<i>Z</i>)-Myroxide	0.04	Monoterpenic ether
Camphor	0.30	Monoterpenic ketone
(<i>E</i>)-Myroxide	0.01	Monoterpenic ether
Unknown	0.05	Oxygenated monoterpene
Hexyl isobutyrate	0.09	Aliphatic ester
Nerol oxide	0.02	Aliphatic ether
Borneol	0.75	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.03	Monoterpenic alcohol
Lavandulol	0.98	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	0.08	Alkene
Terpinen-4-ol	4.92	Monoterpenic alcohol
Cryptone	0.12	Normonoterpenic ketone
meta-Cymen-8-ol	0.08	Monoterpenic alcohol
para-Cymen-8-ol	0.07	Monoterpenic alcohol
Butyl hexanoate	0.08	Aliphatic ester
α -Terpineol	0.95	Monoterpenic alcohol
Hexyl butyrate	0.40	Aliphatic ester
Verbenone	0.03	Monoterpenic ketone
Unknown	0.01	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	0.17	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.04	Aliphatic ester
Cuminal	0.03	Monoterpenic aldehyde
Neral	0.02	Monoterpenic aldehyde
Carvone	0.04	Monoterpenic ketone
Hexyl isovalerate	0.02	Aliphatic ester
Linalyl acetate	30.22	Monoterpenic ester
Geraniol	0.40	Monoterpenic alcohol
Geranial	0.04	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Bornyl acetate	0.18	Monoterpenic ester
Lavandulyl acetate	2.99	Monoterpenic ester
Hexyl tiglate	0.06	Aliphatic ester

Hodiendiol derivative	0.03	Oxygenated monoterpene
Unknown	0.03	Oxygenated monoterpene
Unknown	0.03	Oxygenated monoterpene
Neryl acetate	0.28	Monoterpenic ester
α -Copaene	0.03	Sesquiterpene
β -Bourbonene	0.04	Sesquiterpene
Geranyl acetate	0.46	Monoterpenic ester
Hexyl hexanoate	0.15	Aliphatic ester
7-epi-Sesquithujene	0.09	Sesquiterpene
Isocaryophyllene	0.01	Sesquiterpene
β -Caryophyllene	3.79	Sesquiterpene
α -Santalene	0.49	Sesquiterpene
Coumarin	0.05	Coumarin
<i>trans</i> - α -Bergamotene	0.16	Sesquiterpene
Sesquisabinene A	0.07	Sesquiterpene
α -Humulene	0.12	Sesquiterpene
β -Santalene	0.02	Sesquiterpene
Lavandulyl butyrate?	0.12	Monoterpenic ester
(<i>E</i>)- β -Farnesene	3.70	Sesquiterpene
Germacrene D	0.50	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.07	Sesquiterpene
<i>ar</i> -Curcumene	0.01	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	0.02	Sesquiterpene
γ -Cadinene	0.18	Sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.03	Sesquiterpene
Isocaryophyllene epoxide B	0.03	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	0.33	Sesquiterpenic ether
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Humulene epoxide I	0.01	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
τ -Cadinol	0.11	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 -Bisabolol	0.01	Sesquiterpenic alcohol
Phytone	0.01	Terpenic ketone
Consolidated total	98.98%	

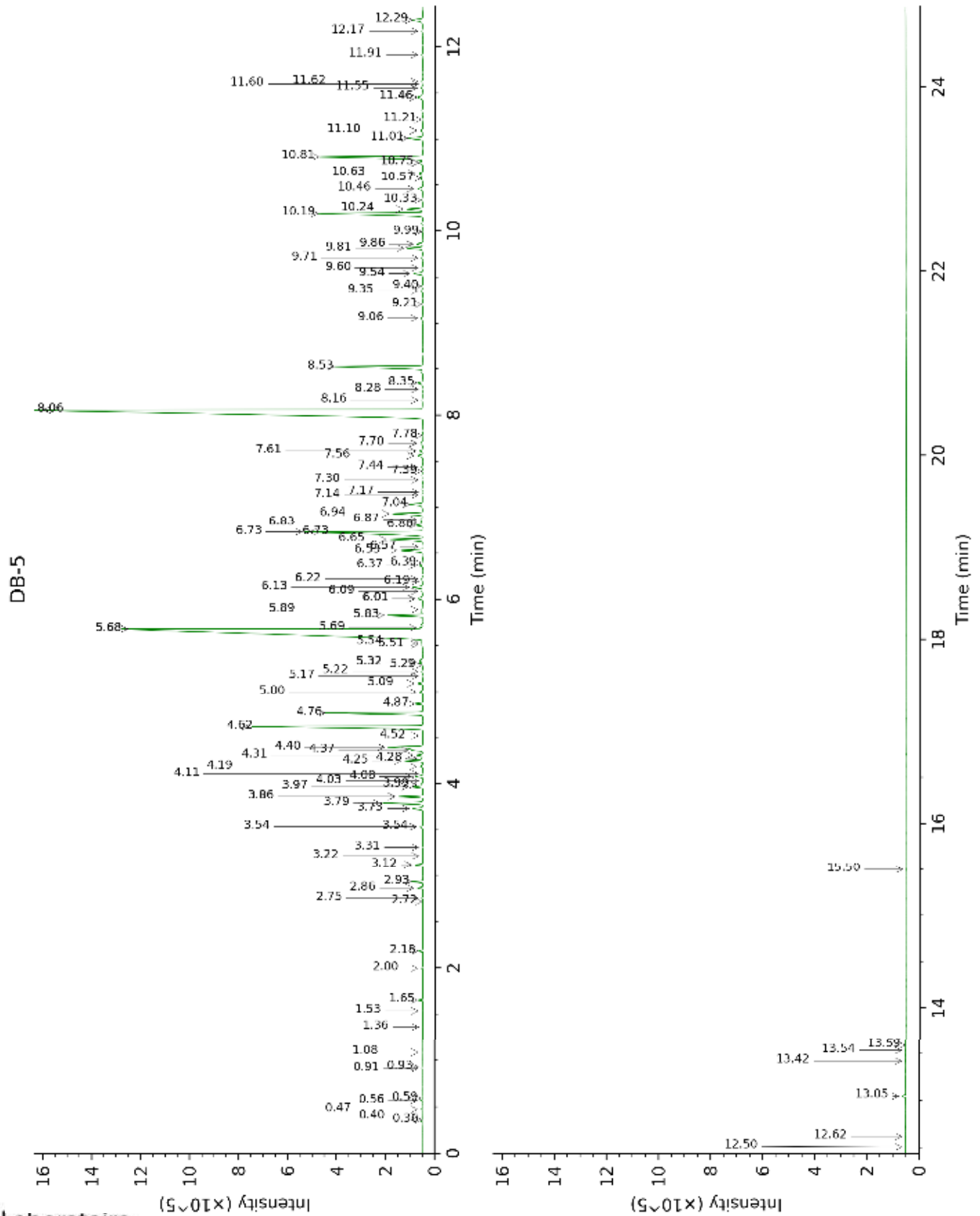
tr: The compound has been detected below 0.005% of total signal.

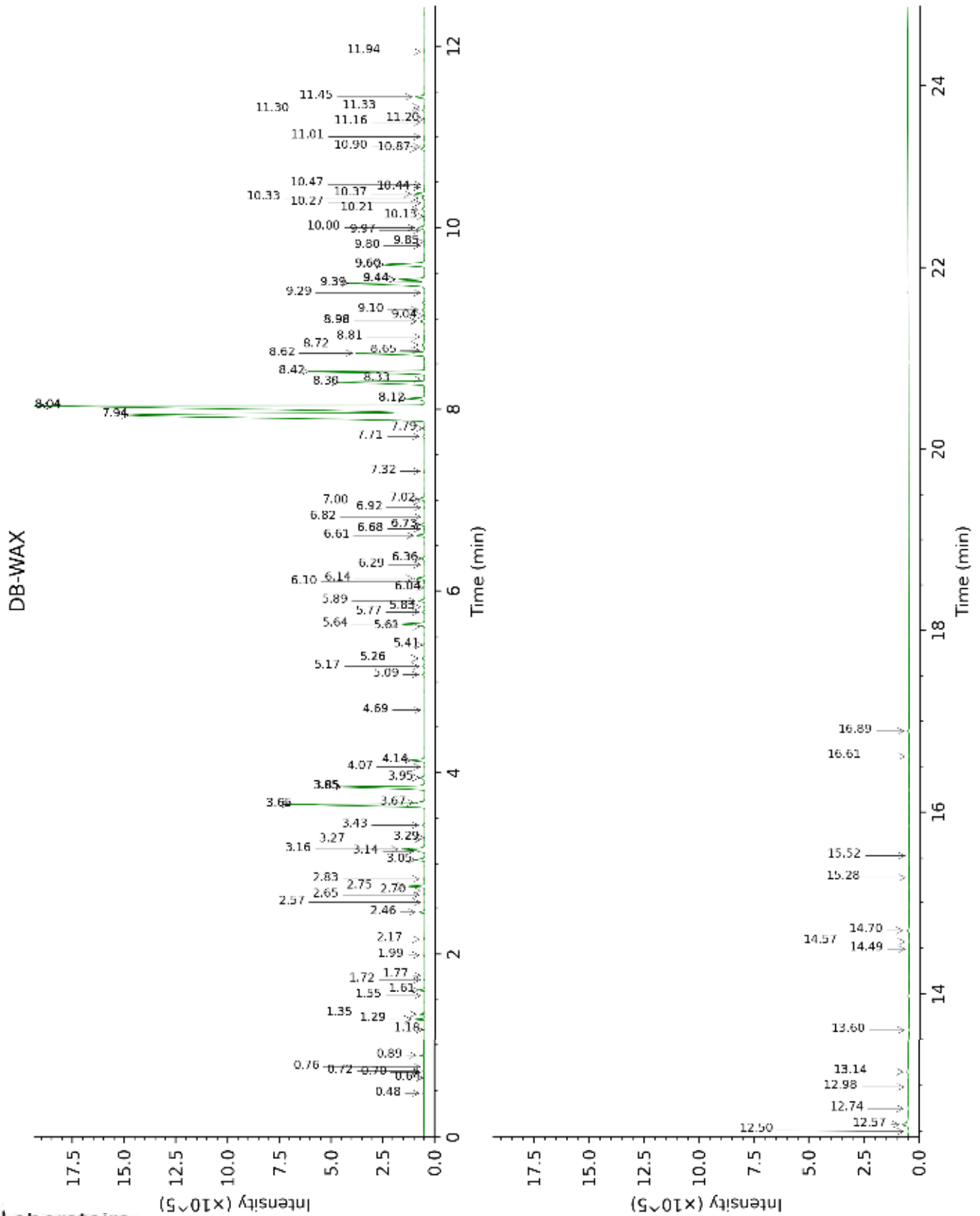
Note: no correction factor was applied

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	0.36	499	tr	0.76	901	tr
Isobutyral	0.40	536	tr	0.48	783	0.02
Ethyl acetate	0.47	607	0.01	0.64	857	tr
Isovaleral	0.56	642	0.02	0.72	886	0.02
2-Methylbutyral	0.59	652	0.01	0.70	880	0.01
Isoamyl alcohol	0.91	732	0.01	3.29*	1177	0.01
2-Methylbutanol	0.93	734	tr	3.29*	1177	[0.01]
Toluene	1.08	758	0.01	1.35*	999	0.13
Hexanal	1.36	800	tr	1.77	1042	0.01
Butyl acetate	1.53	817	0.01	1.72	1037	0.01
Methyl hexyl ether	1.65	827	0.08	0.89	922	0.08
(3Z)-Hexenol	2.00	857	0.03	5.61	1345	0.02
Hexanol	2.18	873	0.09	5.26*	1320	0.11
Hashishene	2.72	916	tr	1.29*	991	0.25
Tricyclene	2.75	918	0.02	1.18	971	0.02
α-Thujene	2.86	926	0.12	1.35*	999	[0.13]
α-Pinene	2.93	930	0.25	1.29*	991	[0.25]
Camphene	3.12*	943	0.18	1.61	1026	0.17
α-Fenchene	3.12*	943	[0.18]	1.55	1020	0.01
5,5-Dimethyl-2(5H)-furanone	3.22	950	0.01	8.33	1549	0.02
Butyl isobutyrate	3.31	956	0.02	2.57	1118	0.01
Sabinene	3.54*	971	0.10	2.17	1083	0.05
β-Pinene	3.54*	971	[0.10]	1.99	1065	0.05
Octen-3-ol	3.73	984	0.29	6.61*	1418	0.30
Octan-3-one	3.79	988	1.04	3.85*	1220	3.84
Myrcene	3.86*	993	0.60	2.75	1133	0.60
<i>trans</i> -Dehydroxylinalool oxide	3.86*	993	[0.60]	3.27	1175	0.02
Butyl butyrate	3.97*	1000	0.32	3.43	1188	0.10
Octan-3-ol	3.97*	1000	[0.32]	5.89	1366	0.25
Pseudolimonene	3.99*	1002	0.06	2.70	1129	0.02
α-Phellandrene	3.99*	1002	[0.06]	2.65	1125	0.05
<i>cis</i> -Dehydroxylinalool oxide	4.03	1004	0.01	3.67†	1207	6.01
Δ3-Carene	4.08	1008	0.20	2.46	1110	0.19
(3Z)-Hexenyl acetate	4.11	1010	0.01	4.69	1284	0.01
α-Terpinene	4.19	1014	0.07	2.82	1139	0.07
Hexyl acetate	4.25	1018	0.48	4.14*	1242	0.59
ortho-Cymene	4.28	1020	0.05	3.95*	1228	0.22
para-Cymene	4.31	1022	0.17	3.95*	1228	[0.22]
Limonene	4.36†	1026	1.49	3.05	1157	0.35
β-Phellandrene	4.40*†	1028	[1.49]	3.14	1164	0.21
1,8-Cineole	4.40*†	1028	[1.49]	3.16	1166	0.95
Lavender lactone	4.52	1036	0.01	9.04	1604	0.04

(Z)-β-Ocimene	4.62	1042	5.79	3.66*†	1206	[6.01]
(E)-β-Ocimene	4.76	1051	2.79	3.85*	1220	[3.84]
γ-Terpinene	4.86	1057	0.20	3.66*†	1206	[6.01]
cis-Sabinene hydrate	5.00	1066	0.09	6.73*	1427	0.18
cis-Linalool oxide (fur.)	5.09	1072	0.14	6.36*†	1399	0.18
Octanol	5.17	1077	0.02	8.04*†	1526	[58.39]
α-Pinene oxide analog	5.22	1080	0.04	5.26*	1320	[0.11]
Isoterpinolene	5.29	1084	0.02	4.06	1236	0.02
Terpinolene	5.32*†	1086	0.21	4.14*	1242	[0.59]
trans-Linalool oxide (fur.)	5.32*†	1086	[0.21]	6.73*	1427	[0.18]
trans-Sabinene hydrate	5.51	1098	0.04	7.80	1507	0.07
Rosefuran	5.54	1100	0.04	5.83	1361	0.02
Linalool	5.68*	1109	28.04	7.94*†	1518	58.39
Hotrienol	5.68*	1109	[28.04]	8.65	1574	0.06
(Z)-6-Methyl-3,5-heptadien-2-one	5.69	1110	0.04	8.04*†	1526	[58.39]
Octen-3-yl acetate	5.83	1119	0.95	5.64	1347	0.95
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.89	1122	0.04	9.44*	1636	1.05
Octan-3-yl acetate	6.01*	1130	0.19	5.09	1307	0.12
cis-Limonene oxide	6.01*	1130	[0.19]	6.29	1394	0.01
allo-Ocimene	6.01*	1130	[0.19]	5.41	1331	0.07
(Z)-Myroxide	6.09	1135	0.04	6.68*	1424	0.04
Camphor	6.13	1138	0.30	7.02	1449	0.27
(E)-Myroxide	6.19	1142	0.01	6.92	1442	0.02
Unknown [m/z 95, 43 (74), 109 (72), 82 (62), 110 (50)... 152 (14)]	6.22	1144	0.05	6.82	1434	0.01
Hexyl isobutyrate	6.37	1153	0.09	5.18	1314	0.07
Nerol oxide	6.40	1155	0.02	6.68*	1424	[0.04]
Borneol	6.53	1164	0.75	9.60*	1650	2.15
cis-Linalool oxide (pyr.)	6.57	1166	0.03	10.13	1693	0.02
Lavandulol	6.65	1171	0.98	9.44*	1636	[1.05]
(3E,5Z)-Undeca-1,3,5-triene	6.73*	1176	4.98	5.77	1357	0.08
Terpinen-4-ol	6.73*	1176	[4.98]	8.42	1556	4.92
Cryptone	6.80†	1181	0.27	8.98*	1599	0.23
meta-Cymen-8-ol	6.83*†	1183	[0.27]	11.30	1792	0.08
para-Cymen-8-ol	6.83*†	1183	[0.27]	11.33	1795	0.07
Butyl hexanoate	6.87	1185	0.08	6.10	1381	0.04
α-Terpineol	6.94	1190	0.95	9.60*	1650	[2.15]
Hexyl butyrate	7.04	1196	0.40	6.14	1384	0.35
Verbenone	7.14	1202	0.03	9.44*	1636	[1.05]

Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...] (3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.17	1205	0.01	6.04	1376	0.01
<i>trans</i> -Carveol	7.40	1220	0.02	11.20	1784	0.03
Bornyl formate	7.44	1223	0.05	7.94*†	1518	[58.39]
Nerol	7.56	1231	0.17	10.87	1756	0.17
Hexyl 2-methylbutyrate	7.61*	1234	0.10	6.36*†	1399	[0.18]
Cuminal	7.61*	1234	[0.10]	10.44*	1719	0.06
Neral	7.70*	1240	0.08	9.29	1625	0.02
Carvone	7.70*	1240	[0.08]	9.80	1667	0.04
Hexyl isovalerate	7.78	1246	0.02	6.61*	1418	[0.30]
Linalyl acetate	8.06*	1264	30.62	8.04*†	1526	[58.39]
Geraniol	8.06*	1264	[30.62]	11.44	1805	0.40
Geranial	8.16	1272	0.04	9.97	1680	0.07
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.28	1279	0.02	14.49	2086	0.01
Bornyl acetate	8.35	1284	0.18	8.12*	1532	0.76
Lavandulyl acetate	8.53	1296	2.99	8.62	1571	3.00
Hexyl tiglate	9.06	1333	0.06	8.81	1586	0.07
Hodiendiol derivative	9.21	1344	0.03	12.74	1921	0.04
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.35	1354	0.03	10.90	1758	0.03
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.40	1357	0.03	11.01	1768	0.02
Neryl acetate	9.54	1367	0.28	10.00*	1683	0.30
α-Copaene	9.60	1371	0.03	7.00	1447	0.02
β-Bourbonene	9.71	1379	0.04	7.32	1472	0.04
Geranyl acetate	9.82	1386	0.46	10.37	1714	0.46
Hexyl hexanoate	9.86*	1390	0.18	8.72	1579	0.15
7-epi-Sesquithujene	9.86*	1390	[0.18]	7.70	1500	0.09
Isocaryophyllene	9.99	1399	0.01	8.04*†	1526	[58.39]
β-Caryophyllene	10.19	1414	3.79	8.30*	1547	3.85
α-Santalene	10.24	1417	0.49	8.12*	1532	[0.76]
Coumarin	10.33	1424	0.05	16.89	2333	0.07
<i>trans</i> -α-Bergamotene	10.46	1434	0.16	8.30*	1547	[3.85]
Sesquisabinene A	10.57	1442	0.07	8.98*	1599	[0.23]
α-Humulene	10.63	1446	0.12	9.10	1609	0.12
β-Santalene	10.75*	1455	0.13	8.98*	1599	[0.23]
Lavandulyl butyrate?	10.75*	1455	[0.13]	10.33	1710	0.12
(E)-β-Farnesene	10.81	1460	3.70	9.39	1633	3.72

Germacrene D	11.01	1475	0.50	9.60*	1650	[2.15]
<i>trans</i> - β - Bergamotene	11.10*	1481	0.08	9.44*	1636	[1.05]
<i>ar</i> -Curcumene	11.10*	1481	[0.08]	10.48	1722	0.01
Isodaucene	11.21	1490	0.02	9.85	1670	0.02
β -Bisabolene	11.46*	1508	0.24	10.00*	1683	[0.30]
γ -Cadinene	11.46*	1508	[0.24]	10.20	1699	0.18
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.55	1516	0.05	13.14*	1958	0.06
δ -Cadinene	11.60	1519	0.01	10.27	1705	0.01
β - Sesquiphellandrene	11.62	1521	0.03	10.44*	1719	[0.06]
Isocaryophyllene epoxide B	11.91	1544	0.03	11.94	1849	0.04
(<i>E</i>)-Nerolidol	12.17	1564	0.04	13.60	2001	0.04
Caryophyllene oxide	12.29*	1574	0.38	12.57	1905	0.33
Caryophyllene oxide isomer	12.29*	1574	[0.38]	12.50	1898	0.03
Humulene epoxide I	12.50	1591	0.01	12.98	1943	0.01
Humulene epoxide II	12.62	1600	0.01	13.14*	1958	[0.06]
τ -Cadinol	13.05	1635	0.11	14.70	2107	0.13
(3 <i>Z</i>)-Caryophylla- 3,8(13)-dien-5 β -ol	13.42	1666	0.02	16.61	2303	0.01
<i>cis</i> -14-nor-Muurool- 5-en-4-one?	13.54	1675	0.01	15.52	2189	0.02
α -Bisabolol	13.59	1680	0.01	15.28	2164	0.01
Phytone	15.50	1847	0.01	14.57	2094	0.03
Total identified		98.70%			98.81%	
Total reported		98.92%			98.88%	

*: 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