

Date : March 31, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21C23-PTH01


Customer identification : Lavender - L40117206R

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 : Seydou Ka, M. Sc.

Analysis date : March 30, 2021

Checked and approved by :



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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

Refractive index: 1.4608 ± 0.0003 (20 °C; method PC-MAT-016)

ISO 3515:2004 - OIL OF CLONAL LAVENDER - "OTHER ORIGINS"

Compound	Min. %	Max. %	Observed %	Complies?
Limonene		1.0	0.4	Yes
1,8-Cineole		3.0	1.7	Yes
β-Phellandrene		1.0	0	Yes
(Z)-β-Ocimene	1	10	4	Yes
(E)-β-Ocimene	tr	6	2	Yes
Octan-3-one		3.0	1.7	Yes
Linalool	20	43	33	Yes
Linalyl acetate	25	47	27	Yes
Lavandulol		3.0	1.0	Yes
Terpinen-4-ol		8	3	Yes
Lavandulyl acetate		8	3	Yes
α-Terpineol		2.0	1.1	Yes
Camphor		1.5	0.2	Yes
Refractive index	1.4600	1.4660	1.4608	Yes

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
Isobutyral	0.01	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
Ethyl acetate	0.02	Aliphatic ester
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Hexanal	0.01	Aliphatic aldehyde
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.19	Aliphatic ether
(3Z)-Hexenol	0.04	Aliphatic alcohol
Hexanol	0.13	Aliphatic alcohol
Hashishene	0.01	Monoterpene
Tricyclene	0.03	Monoterpene
α -Thujene	0.11	Monoterpene
α -Pinene	0.19	Monoterpene
Camphene	0.22	Monoterpene
α -Fenchene	0.01	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Benzaldehyde	tr	Simple phenolic
Butyl isobutyrate	0.01	Aliphatic ester
exo-Isocamphane	0.01	Monoterpene
β -Pinene	0.07	Monoterpene
Sabinene	0.06	Monoterpene
Octen-3-ol	0.29	Aliphatic alcohol
Octan-3-one	1.70	Aliphatic ketone
Myrcene	0.67	Monoterpene
Pseudolimonene	0.02	Monoterpene
Octan-3-ol	0.40	Aliphatic alcohol
Butyl butyrate	0.12	Aliphatic ester
α -Phellandrene	0.05	Monoterpene
cis-Dehydroxylinalool oxide	0.06	Monoterpenic ether
Δ^3 -Carene	0.17	Monoterpene
(3Z)-Hexenyl acetate	0.02	Aliphatic ester
α -Terpinene	0.05	Monoterpene
Hexyl acetate	0.73	Aliphatic ester
ortho-Cymene	0.07	Monoterpene
para-Cymene	0.21	Monoterpene
Limonene	0.40	Monoterpene
1,8-Cineole	1.72	Monoterpenic ether
Lavender lactone	0.01	Aliphatic lactone
Benzyl alcohol	0.01	Simple phenolic
(Z)- β -Ocimene	3.93	Monoterpene
(E)- β -Ocimene	2.46	Monoterpene

γ-Terpinene	0.16	Monoterpene
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.14	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
α-Pinene oxide analog	0.02	Monoterpenic ether
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.09	Monoterpene
trans-Linalool oxide (fur.)	0.11	Monoterpenic alcohol
Rosefuran	0.05	Monoterpenic ether
Linalool	32.53	Monoterpenic alcohol
Hotrienol	0.07	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.01	Aliphatic ketone
Octen-3-yl acetate	0.81	Aliphatic ester
Unknown	0.05	Unknown
Octan-3-yl acetate	0.16	Aliphatic ester
allo-Ocimene	0.05	Monoterpene
trans-Pinocarveol	0.05	Monoterpenic alcohol
(Z)-Myroxide	0.02	Monoterpenic ether
Camphor	0.24	Monoterpenic ketone
(E)-Myroxide	0.02	Monoterpenic ether
trans-Verbenol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
Nerol oxide	0.02	Aliphatic ether
Hexyl isobutyrate	0.09	Aliphatic ester
Borneol	0.78	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.03	Monoterpenic alcohol
Lavandulol	1.02	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	0.09	Alkene
Terpinen-4-ol	3.14	Monoterpenic alcohol
Cryptone	0.28	Normonoterpenic ketone
meta-Cymen-8-ol	0.08	Monoterpenic alcohol
Unknown	0.07	Unknown
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α-Terpineol	1.05	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Hexyl butyrate	0.46	Aliphatic ester
Hodiendiol	0.02	Monoterpenic alcohol
Verbenone	0.02	Monoterpenic ketone
Unknown	0.03	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.02	Monoterpenic alcohol
Octyl acetate	0.01	Aliphatic ester
trans-Carveol	0.05	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
cis-Carveol	0.01	Monoterpenic alcohol
Nerol	0.14	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.15	Aliphatic ester
Neral	0.01	Monoterpenic aldehyde
Carvone	0.05	Monoterpenic ketone
Hexyl isovalerate	0.07	Aliphatic ester
Linalyl acetate	27.44	Monoterpenic ester
Geraniol	0.44	Monoterpenic alcohol
Geranial	0.04	Monoterpenic aldehyde

2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Bornyl acetate	0.14	Monoterpenic ester
Cuminol	0.05	Monoterpenic alcohol
Lavandulyl acetate	2.73	Monoterpenic ester
Unknown	0.01	Oxygenated monoterpene
Hexyl tiglate	0.04	Aliphatic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
Unknown	0.07	Oxygenated monoterpene
Unknown	0.16	Oxygenated monoterpene
Neryl acetate	0.31	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
7-Cubebene	0.02	Sesquiterpene
Daucene	0.01	Sesquiterpene
β -Bourbonene	0.06	Sesquiterpene
7-epi-Sesquithujene?	0.01	Sesquiterpene
Geranyl acetate	0.51	Monoterpenic ester
Hexyl hexanoate	0.16	Aliphatic ester
7-epi-Sesquithujene	0.09	Sesquiterpene
Isocaryophyllene	0.01	Sesquiterpene
Sesquithujene	0.01	Sesquiterpene
β -Caryophyllene	3.57	Sesquiterpene
α -Santalene	0.41	Sesquiterpene
Lavandulyl isobutyrate	0.05	Monoterpenic ester
<i>trans</i> - α -Bergamotene	0.14	Sesquiterpene
Sesquisabinene A	0.07	Sesquiterpene
α -Humulene	0.09	Sesquiterpene
Lavandulyl butyrate?	0.12	Monoterpenic ester
(<i>E</i>)- β -Farnesene	4.31	Sesquiterpene
β -Santalene	tr	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.02	Sesquiterpene
Germacrene D	0.55	Sesquiterpene
α -Curcumene	0.02	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.04	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
Lavandulyl isovalerate	0.03	Monoterpenic ester
γ -Cadinene	0.18	Sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.01	Sesquiterpene
Isocaryophyllene epoxide B	0.01	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.25	Sesquiterpenic ether
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Humulene epoxide II	tr	Sesquiterpenic ether
τ -Cadinol	0.08	Sesquiterpenic alcohol
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.01	Sesquiterpenic alcohol
<i>cis</i> -14-nor-Muurool-5-en-4-one?	0.01	Norsesquiterpenic ketone
Herniarin	0.01	Coumarin
9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	0.01	Homoditerpene
Consolidated total	99.15%	

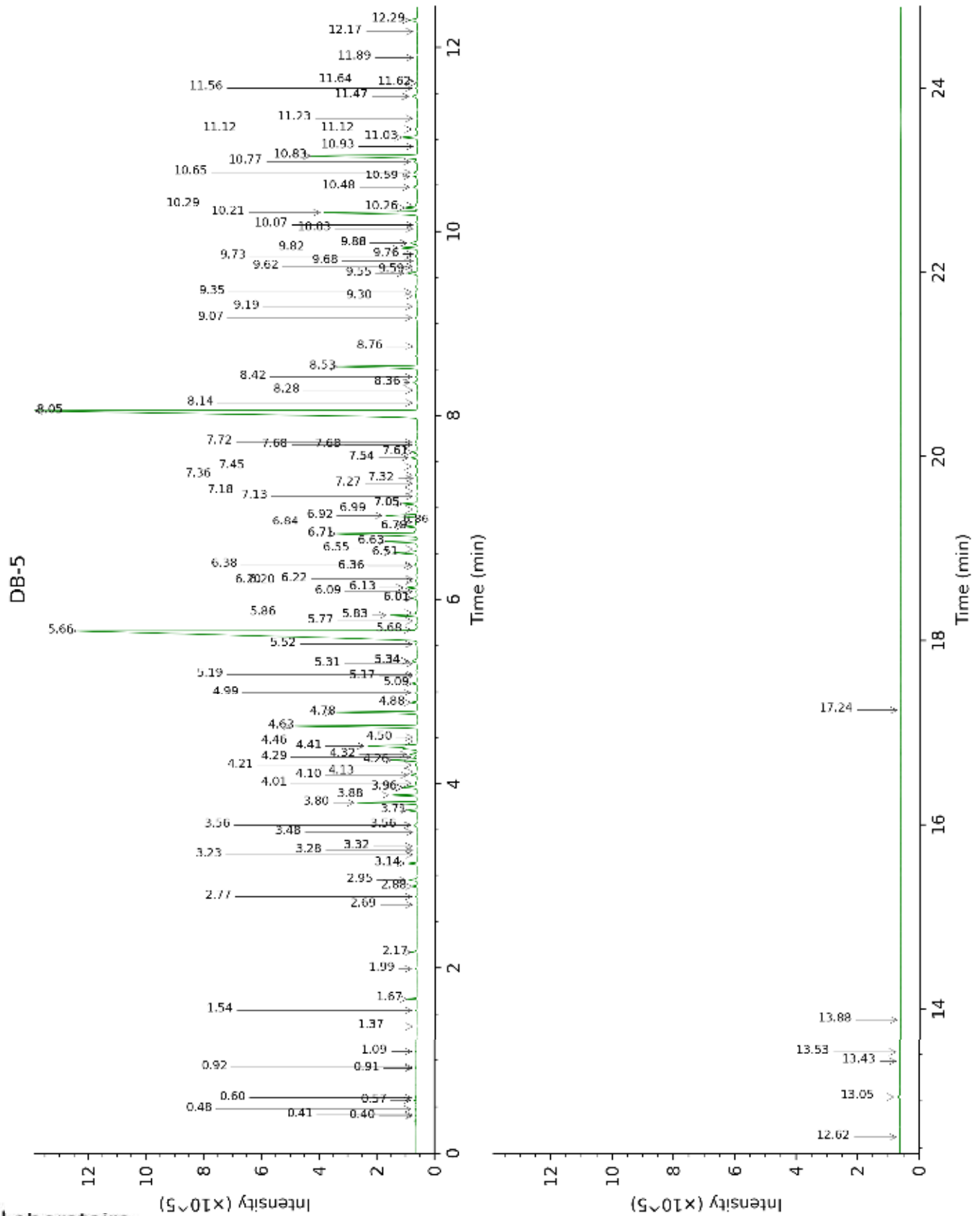
tr: The compound has been detected below 0.005% of total signal.

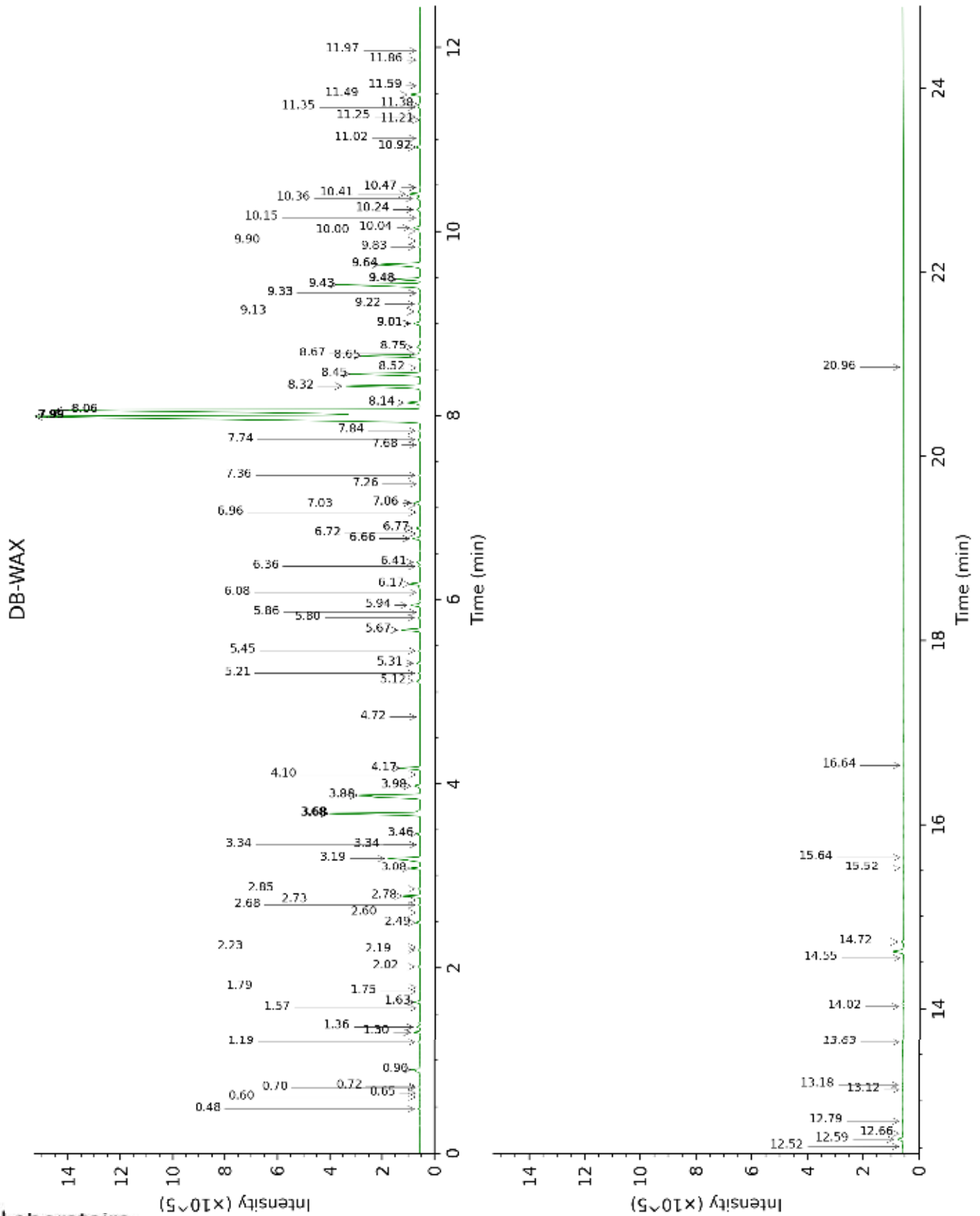
Note: no correction factor was applied

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	%
Isobutylal	0.40	536	0.01	0.48	784	0.02
Methacrolein	0.41	548	tr	0.60	841	tr
Ethyl acetate	0.48	605	0.02	0.65	857	tr
Isovaleral	0.57	640	0.02	0.72	885	0.01
2-Methylbutylal	0.60	651	0.01	0.70	879	tr
Isoamyl alcohol	0.91	731	0.01	3.34*	1178	0.01
2-Methylbutanol	0.92	732	0.01	3.34*	1178	[0.01]
Toluene	1.09	758	0.01	1.36*	1001	0.12
Hexanal	1.37	800	0.01	1.79	1044	0.01
Butyl acetate	1.54	817	0.02	1.74	1040	0.02
Methyl hexyl ether	1.66	827	0.19	0.90	922	0.34
(3Z)-Hexenol	1.99	856	0.04	5.67*	1349	0.81
Hexanol	2.17	871	0.13	5.31*	1323	0.13
Hashishene	2.68	913	0.01	1.30*	992	0.20
Tricyclene	2.77	919	0.03	1.19	972	0.04
α -Thujene	2.88	926	0.11	1.36*	1001	[0.12]
α -Pinene	2.95	931	0.19	1.30*	992	[0.20]
Camphene	3.14*	944	0.23	1.63*	1028	0.22
α -Fenchene	3.14*	944	[0.23]	1.57	1022	0.01
Thuja-2,4(10)-diene	3.23	950	0.01	2.22	1088	0.03
Benzaldehyde	3.28	953	tr	7.26	1466	0.01
Butyl isobutyrate	3.32	956	0.01	2.60	1120	0.02
exo-Isocamphane	3.48	967	0.01	1.63*	1028	[0.22]
β -Pinene	3.56*	972	0.11	2.02	1067	0.07
Sabinene	3.56*	972	[0.11]	2.19	1085	0.06
Octen-3-ol	3.71	983	0.29	6.66*	1422	0.29
Octan-3-one	3.80	988	1.70	3.88*	1219	4.02
Myrcene	3.88	994	0.67	2.78	1134	0.67
Pseudolimonene	3.96*	999	0.50	2.74	1131	0.02
Octan-3-ol	3.96*	999	[0.50]	5.94	1369	0.40
Butyl butyrate	3.96*	999	[0.50]	3.46	1188	0.12
α -Phellandrene	3.96*	999	[0.50]	2.68	1127	0.05
<i>cis</i> -Dehydroxylinalool oxide	4.01	1002	0.06	3.68*	1205	4.02
Δ^3 -Carene	4.10	1008	0.17	2.49	1112	0.16
(3Z)-Hexenyl acetate	4.13	1010	0.02	4.72	1280	0.01
α -Terpinene	4.20	1015	0.05	2.86	1140	0.06
Hexyl acetate	4.26	1018	0.73	4.17*	1240	0.82
ortho-Cymene	4.29	1020	0.07	3.98*	1226	0.27
para-Cymene	4.32	1022	0.21	3.98*	1226	[0.27]
Limonene	4.41*†	1028	2.16	3.08	1158	0.40
1,8-Cineole	4.41*†	1028	[2.16]	3.19	1167	1.72
Lavender lactone	4.46	1031	0.01	9.00*	1601	0.33
Benzyl alcohol	4.50	1034	0.01	11.58*	1818	0.02
(Z)- β -Ocimene	4.63	1042	3.93	3.68*	1205	[4.02]
(E)- β -Ocimene	4.78	1051	2.46	3.88*	1219	[4.02]

γ-Terpinene	4.88	1058	0.16	3.68*	1205	[4.02]
<i>cis</i> -Sabinene hydrate	4.99	1065	0.06	6.77*	1430	0.17
<i>cis</i> -Linalool oxide (fur.)	5.10	1071	0.14	6.40	1402	0.15
Octanol	5.17	1076	0.02	8.06*†	1528	[59.42]
α-Pinene oxide analog	5.19	1078	0.02	5.31*	1323	[0.13]
Isoterpinolene	5.31	1085	0.01	4.10	1235	0.01
Terpinolene	5.34*	1087	0.21	4.17*	1240	[0.82]
<i>trans</i> -Linalool oxide (fur.)	5.34*	1087	[0.21]	6.77*	1430	[0.17]
Rosefuran	5.52	1098	0.05	5.86	1363	0.01
Linalool	5.66†	1108	32.59	7.99*†	1522	59.42
Hotrienol	5.68†	1108	[32.59]	8.67	1575	0.07
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	5.77	1114	0.01	8.06*†	1528	[59.42]
Octen-3-yl acetate	5.83	1118	0.81	5.67*	1349	[0.81]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.86	1120	0.05	9.48*	1640	1.00
Octan-3-yl acetate	6.02*	1130	0.19	5.12	1309	0.16
allo-Ocimene	6.02*	1130	[0.19]	5.45	1333	0.05
<i>trans</i> -Pinocarveol	6.09	1135	0.05	9.00*	1601	[0.33]
(<i>Z</i>)-Myroxide	6.13*	1138	0.32	6.72*	1426	0.04
Camphor	6.13*	1138	[0.32]	7.06*	1451	0.28
(<i>E</i>)-Myroxide	6.20*	1142	0.05	6.96*	1444	0.03
<i>trans</i> -Verbenol	6.20*	1142	[0.05]	9.33*	1628	0.02
Unknown [m/z 81, 138 (33), 96 (27), 67 (20), 79 (19), 95 (16)...]	6.22	1144	0.01			
Nerol oxide	6.36	1152	0.02	6.72*	1426	[0.04]
Hexyl isobutyrate	6.38	1154	0.09	5.21	1315	0.07
Borneol	6.51	1162	0.78	9.64*	1653	2.32
<i>cis</i> -Linalool oxide (pyr.)	6.55	1164	0.03	10.15	1695	0.04
Lavandulol	6.63	1170	1.02	9.48*	1640	[1.00]
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	6.71*†	1175	3.28	5.80	1359	0.09
Terpinen-4-ol	6.71*†	1175	[3.28]	8.45	1558	3.14
Cryptone	6.79*	1180	0.37	9.00*	1601	[0.33]
meta-Cymen-8-ol	6.79*	1180	[0.37]	11.35	1797	0.08
Unknown [m/z 43, 135 (73), 59 (46), 93 (39), 91 (35), 81 (32)...]	6.84	1183	0.07			
para-Cymen-8-ol	6.86	1185	0.02	11.38	1800	0.07
α-Terpineol	6.92	1188	1.05	9.64*	1653	[2.32]
Myrtenal	6.99	1193	0.02	8.52	1563	0.02
Hexyl butyrate	7.05*	1197	0.49	6.17	1385	0.46
Hodiendiol	7.05*	1197	[0.49]	12.66	1914	0.02

Verbenone	7.13	1202	0.02	9.48*	1640	[1.00]
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.18	1205	0.03	6.08	1379	0.01
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.27	1211	0.02	11.22	1786	0.02
Octyl acetate	7.32	1214	0.01	6.96*	1444	[0.03]
trans-Carveol	7.36	1217	0.05	11.25	1788	0.03
Bornyl formate	7.45	1223	0.05	7.84	1510	0.06
cis-Carveol	7.54*	1230	0.19	11.58*	1818	[0.02]
Nerol	7.54*	1230	[0.19]	10.92*	1760	0.21
Hexyl 2-methylbutyrate	7.60	1234	0.15	6.36	1399	0.05
Neral	7.68*	1239	0.06	9.33*	1628	[0.02]
Carvone	7.68*	1239	[0.06]	9.83	1669	0.05
Hexyl isovalerate	7.72	1241	0.07	6.66*	1422	[0.29]
Linalyl acetate	8.05*	1264	27.88	8.06*†	1528	[59.42]
Geraniol	8.05*	1264	[27.88]	11.49	1809	0.44
Geranial	8.14	1270	0.04	10.00	1683	0.05
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.28	1279	0.02	14.55	2094	0.02
Bornyl acetate	8.36	1284	0.14	8.14*	1534	0.58
Cuminol	8.42	1288	0.05	14.02	2043	0.07
Lavandulyl acetate	8.53	1296	2.73	8.65	1573	2.71
Unknown [m/z 150, 107 (98), 91 (79), 108 (61)]	8.76	1311	0.01	11.86	1843	0.02
Hexyl tiglate	9.07	1333	0.04	8.75*	1581	0.21
Hodiendiol derivative	9.19	1342	0.02	12.79	1926	0.02
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.30	1350	0.07	10.92*	1760	[0.21]
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.35	1353	0.16	11.02	1768	0.03
Neryl acetate	9.55	1367	0.31	10.04	1686	0.31
α-Copaene	9.59	1370	0.01	7.03	1450	0.02
7-Cubebene	9.62	1373	0.02	7.06*	1451	[0.28]
Daucene	9.68	1377	0.01	7.06*	1451	[0.28]
β-Bourbonene	9.73	1380	0.06	7.36	1474	0.06
7-epi-Sesquithujene?	9.76	1382	0.01	7.68	1498	tr
Geranyl acetate	9.82	1387	0.51	10.41	1716	0.49
Hexyl hexanoate	9.88*	1390	0.25	8.75*	1581	[0.21]
7-epi-Sesquithujene	9.88*	1390	[0.25]	7.74	1502	0.09
Isocaryophyllene	10.03	1402	0.01	7.99*†	1522	[59.42]
Sesquithujene	10.07	1404	0.01	7.99*†	1522	[59.42]

β-Caryophyllene	10.20	1414	3.57	8.32*	1548	3.63
α-Santalene	10.26	1418	0.41	8.14*	1534	[0.58]
Lavandulyl isobutyrate	10.29	1421	0.05	9.22	1619	0.09
<i>trans</i> -α-Bergamotene	10.48	1435	0.14	8.32*	1548	[3.63]
Sesquisabinene A	10.59	1444	0.07	9.00*	1601	[0.33]
α-Humulene	10.65	1448	0.09	9.14*	1612	0.11
Lavandulyl butyrate?	10.76	1456	0.12	10.36	1712	0.17
(<i>E</i>)-β-Farnesene	10.83*	1461	4.23	9.43*	1636	4.24
β-Santalene	10.83*	1461	[4.23]	9.00*	1601	[0.33]
<i>trans</i> -Cadina-1(6),4-diene	10.93	1468	0.02	9.14*	1612	[0.11]
Germacrene D	11.03	1476	0.55	9.64*	1653	[2.32]
α-Curcumene	11.12*	1482	0.06	10.47*	1722	0.06
<i>trans</i> -β-Bergamotene	11.12*	1482	[0.06]	9.43*	1636	[4.24]
Isodaucene	11.23	1491	0.02	9.90	1674	0.03
Lavandulyl isovalerate	11.47*	1509	0.21	10.47*	1722	[0.06]
γ-Cadinene	11.47*	1509	[0.21]	10.24*	1702	0.19
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.56	1516	0.04	13.18	1962	0.04
δ-Cadinene	11.62	1521	0.01	10.24*	1702	[0.19]
β-Sesquiphellandrene	11.64	1523	0.01	10.47*	1722	[0.06]
Isocaryophyllene epoxide B	11.89	1542	0.01	11.97	1852	0.03
(<i>E</i>)-Nerolidol	12.17	1564	0.01	13.63	2004	0.01
Caryophyllene oxide	12.30*	1574	0.30	12.59	1908	0.25
Caryophyllene oxide isomer	12.30*	1574	[0.30]	12.52	1901	0.03
Humulene epoxide II	12.62	1600	tr	13.12	1957	0.01
τ-Cadinol	13.05	1635	0.08	14.72	2111	0.15
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5β-ol	13.43	1666	0.01	16.64	2308	0.01
<i>cis</i> -14-nor-Muurolo-5-en-4-one?	13.53	1675	0.01	15.52	2191	0.01
Herniarin	13.88	1704	0.01	20.96	2810	0.01
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	17.24	2010	0.01	15.64	2203	0.02
Total identified		98.76%			97.76%	
Total reported		99.20%			97.86%	

*: 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