

Date : December 09, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20L08-PTH10

Customer identification : Lavender - Bulgaria - L40116203R

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 : Alexis St-Gelais, M. Sc., chimiste

Analysis date : December 09, 2020

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)

ISO 3515:2004 - OIL OF CLONAL LAVENDER - BULGARIA

Compound	Min. %	Max. %	Observed %	Complies?
α-Terpineol	0.8	2.0	1.0	Yes
Lavandulyl acetate	2	5	3	Yes
Terpinen-4-ol	2	5	4	Yes
Lavandulol	0.3		1.1	Yes
Linalyl acetate	30	42	30	Yes
Linalool	22	34	28	Yes
Camphor		0.6	0.3	Yes
Octan-3-one	0.2	1.6	1.2	Yes
(E)-β-Ocimene	2	5	3	Yes
(Z)-β-Ocimene	3	9	6	Yes
β-Phellandrene		0.6		
1,8-Cineole		2.0	1.1*	Yes
Limonene		0.6	0.3	Yes
Refractive index	1.4590	1.4630	1.4621	Yes

*Coeluted on both columns considered

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	0.02	Aliphatic alcohol
Isobutyral	0.01	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
Ethyl acetate	tr	Aliphatic ester
Isovaleral	0.04	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.02	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Hexanal	0.01	Aliphatic aldehyde
Butyl acetate	0.01	Aliphatic ester
Methyl hexyl ether	0.09	Aliphatic ether
(3Z)-Hexenol	0.02	Aliphatic alcohol
Hexanol	0.12	Aliphatic alcohol
Tricyclene	0.02	Monoterpene
α-Thujene	0.12	Monoterpene
α-Pinene	0.24	Monoterpene
α-Fenchene	tr	Monoterpene
Camphepane	0.17	Monoterpene
5,5-Dimethyl-2(5H)-furanone	0.01	Aliphatic lactone
Butyl isobutyrate	0.01	Aliphatic ester
β-Pinene	0.05	Monoterpene
Sabinene	0.06	Monoterpene
Octen-3-ol	0.27	Aliphatic alcohol
Octan-3-one	1.21	Aliphatic ketone
Myrcene	0.62	Monoterpene
trans-Dehydroxylinalool oxide	0.03	Monoterpenic ether
Butyl butyrate	0.08	Aliphatic ester
Octan-3-ol	0.27	Aliphatic alcohol
α-Phellandrene	0.05	Monoterpene
Pseudolimonene	0.01	Monoterpene
cis-Dehydroxylinalool oxide	0.02	Monoterpenic ether
Δ3-Carene	0.17	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
α-Terpinene	0.07	Monoterpene
Hexyl acetate	0.50	Aliphatic ester
ortho-Cymene	0.05	Monoterpene
para-Cymene	0.16	Monoterpene
Limonene	0.35	Monoterpene
β-Phellandrene	1.11*	Monoterpene
1,8-Cineole	[1.11]*	Monoterpenic ether
Lavender lactone	0.01	Aliphatic lactone
(Z)-β-Ocimene	5.65	Monoterpene
(E)-β-Ocimene	2.88	Monoterpene
γ-Terpinene	0.20	Monoterpene

<i>cis</i> -Sabinene hydrate	0.06	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.12	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
α -Pinene oxide analog	0.03	Monoterpenic ether
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.10	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.09	Monoterpenic alcohol
Rosefuran	0.02	Monoterpenic ether
<i>trans</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	27.73	Monoterpenic alcohol
Hotrienol	0.06	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
Octen-3-yl acetate	0.91	Aliphatic ester
Octan-3-yl acetate	0.10	Aliphatic ester
allo-Ocimene	0.06	Monoterpene
<i>cis</i> -Limonene oxide	tr	Monoterpenic ether
<i>trans</i> -Pinocarveol	0.02	Monoterpenic alcohol
<i>trans</i> -Limonene oxide	0.01	Monoterpenic ether
Camphor	0.25	Monoterpenic ketone
(Z)-Myroxide	0.04	Monoterpenic ether
Unknown	0.01	Oxygenated monoterpene
(E)-Myroxide	0.03	Monoterpenic ether
Hexyl isobutyrate	0.08	Aliphatic ester
Nerol oxide	0.02	Aliphatic ether
Borneol	0.74	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.02	Monoterpenic alcohol
Lavandulol	1.07	Monoterpenic alcohol
Terpinen-4-ol	4.30	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	0.09	Alkene
Cryptone	0.22	Normonoterpenic ketone
Butyl hexanoate	0.01	Aliphatic ester
meta-Cymen-8-ol	0.08	Monoterpenic alcohol
para-Cymen-8-ol	0.09	Monoterpenic alcohol
α -Terpineol	0.98	Monoterpenic alcohol
Hexyl butyrate	0.34	Aliphatic ester
Hodiendiol	0.01	Monoterpenic alcohol
Verbenone	0.01	Monoterpenic ketone
Unknown	0.04	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol
Octyl acetate	0.02	Aliphatic ester
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
Nerol	0.16	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.05	Aliphatic ester
Carvone	0.04	Monoterpenic ketone
Cuminal	0.03	Monoterpenic aldehyde
Neral	0.08	Monoterpenic aldehyde
Hexyl isovalerate	0.02	Aliphatic ester
Linalyl acetate	29.70	Monoterpenic ester
Geraniol	0.44	Monoterpenic alcohol
Geranal	0.04	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.01	Monoterpenic alcohol

Bornyl acetate	0.18	Monoterpenic ester
Lavandulyl acetate	3.03	Monoterpenic ester
Hexyl tiglate	0.07	Aliphatic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
Unknown	0.02	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.33	Monoterpenic ester
α -Copaene	0.05	Sesquiterpene
β -Bourbonene	0.03	Sesquiterpene
1,5-diepi- β -Bourbonene	0.01	Sesquiterpene
Geranyl acetate	0.46	Monoterpenic ester
7-epi-Sesquithujene	0.10	Sesquiterpene
Hexyl hexanoate	0.11	Aliphatic ester
Isocaryophyllene	0.06	Sesquiterpene
β -Caryophyllene	3.93	Sesquiterpene
α -Santalene	0.51	Sesquiterpene
Coumarin	0.07	Coumarin
<i>trans</i> - α -Bergamotene	0.16	Sesquiterpene
Sesquisabinene A	0.03	Sesquiterpene
α -Humulene	0.14	Sesquiterpene
Lavandulyl butyrate?	0.14	Monoterpenic ester
(<i>E</i>)- β -Farnesene	3.98	Sesquiterpene
β -Santalene	0.04	Sesquiterpene
Germacrene D	0.59	Sesquiterpene
ar-Curcumene	0.01	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.06	Sesquiterpene
Isodaucene	0.03	Sesquiterpene
β -Bisabolene	0.04	Sesquiterpene
γ -Cadinene	0.18	Sesquiterpene
Lavandulyl isovalerate	0.02	Monoterpenic ester
Unknown	0.06	Oxygenated sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.03	Sesquiterpene
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Caryophyllene oxide	0.31	Sesquiterpenic ether
Cubenol	0.01	Sesquiterpenic alcohol
τ -Cadinol	0.11	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
α -Bisabolol	0.01	Sesquiterpenic alcohol
Consolidated total	98.41%	

*: 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

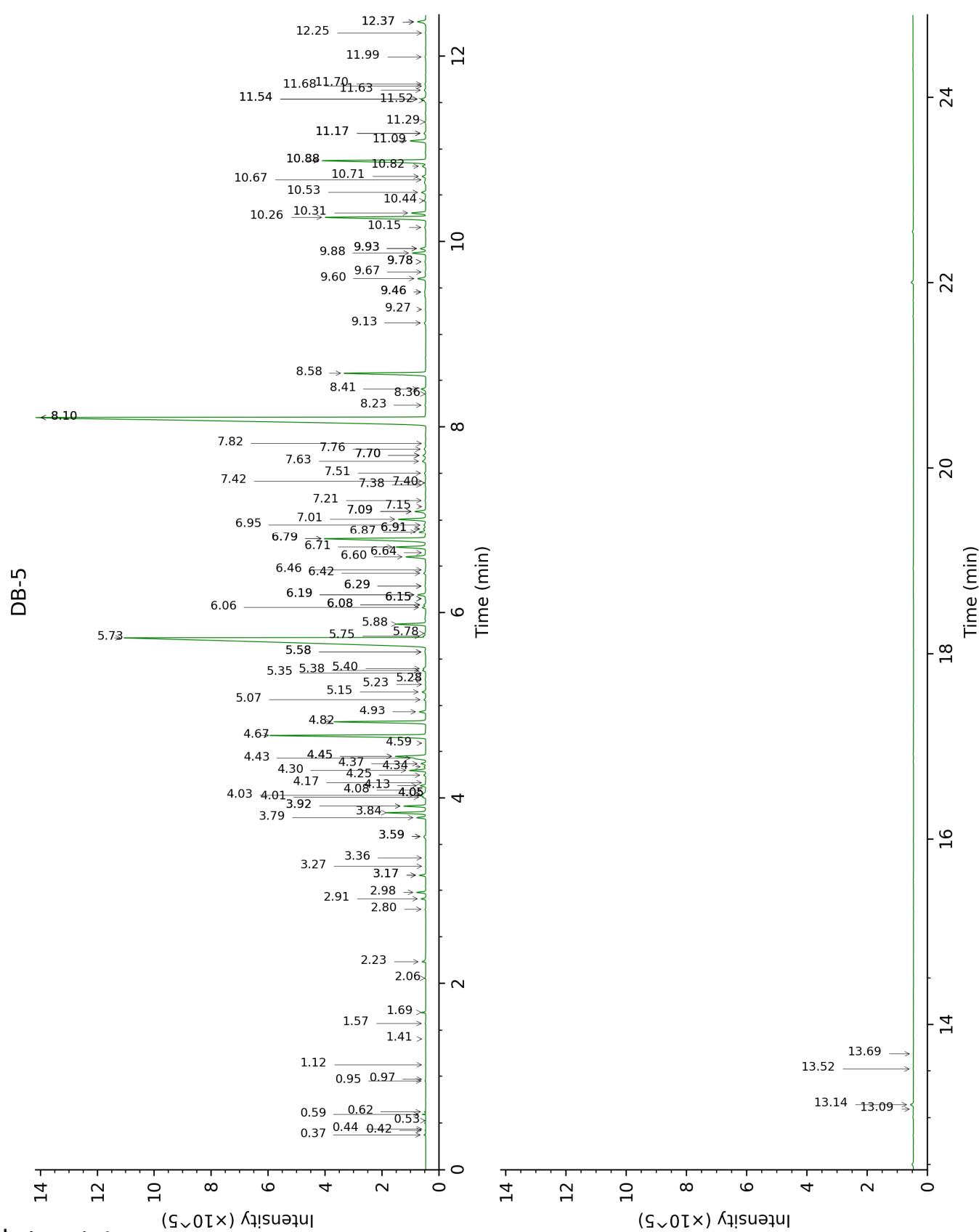
tr: The compound has been detected below 0.005% of total signal.

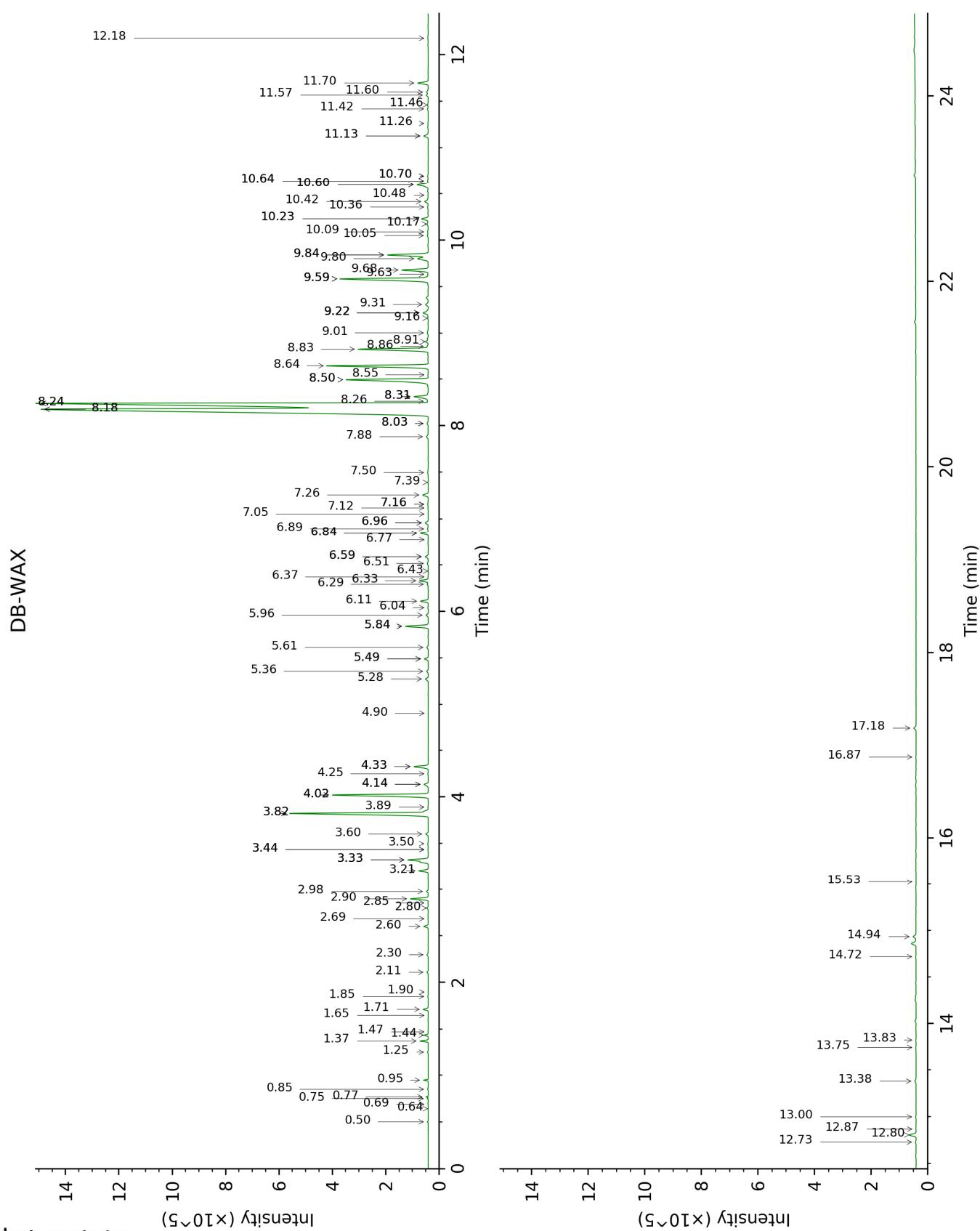
Note: no correction factor was applied

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	%
Ethanol	0.37	520	0.02	0.85	903	0.01
Isobutyral	0.42	540	0.01	0.50	780	0.01
Methacrolein	0.44	549	tr	0.64	839	tr
Ethyl acetate	0.53	605	tr	0.69	857	0.01
Isovaleral	0.59	638	0.04	0.77	886	0.04
2-Methylbutyral	0.62	650	0.01	0.75	879	0.01
Isoamyl alcohol	0.95	739	0.02	3.44*	1175	0.02
2-Methylbutanol	0.97	742	0.01	3.44*	1175	[0.02]
Toluene	1.12	764	0.01	1.47	1000	0.01
Hexanal	1.41	805	0.01	1.90	1043	tr
Butyl acetate	1.57	820	0.01	1.85	1038	0.02
Methyl hexyl ether	1.69	830	0.09	0.95	919	0.10
(3Z)-Hexenol	2.06	860	0.02	5.84*	1349	0.91
Hexanol	2.24	875	0.12	5.49*	1324	0.14
Tricyclene	2.80	918	0.02	1.25	970	0.02
α -Thujene	2.91	926	0.12	1.44	997	0.12
α -Pinene	2.98	930	0.24	1.37	990	0.24
α -Fenchene	3.17*	943	0.18	1.65	1018	tr
Camphene	3.17*	943	[0.18]	1.71	1025	0.17
5,5-Dimethyl-2(5H)-furanone	3.27	949	0.01	8.55	1550	0.02
Butyl isobutyrate	3.36	955	0.01	2.68	1116	0.01
β -Pinene	3.59*	970	0.09	2.11	1064	0.05
Sabinene	3.59*	970	[0.09]	2.30	1083	0.06
Octen-3-ol	3.79	984	0.27	6.84*	1422	0.30
Octan-3-one	3.84	987	1.21	4.02*	1218	4.09
Myrcene	3.92*	992	0.65	2.90	1132	0.62
<i>trans</i> -Dehydroxylinalool oxide	3.92*	992	[0.65]	3.50	1180	0.03
Butyl butyrate	4.01	998	0.08	3.60	1188	0.10
Octan-3-ol	4.03	1000	0.27	6.11	1368	0.30
α -Phellandrene	4.05*	1001	0.06	2.80	1125	0.05
Pseudolimonene	4.05*	1001	[0.06]	2.86	1129	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.08	1003	0.02	3.89	1209	0.01
Δ^3 -Carene	4.13	1006	0.17	2.60	1109	0.16
(3Z)-Hexenyl acetate	4.16	1008	0.01	4.90	1282	0.01
α -Terpinene	4.25	1014	0.07	2.98	1139	0.07
Hexyl acetate	4.30	1017	0.50	4.33*	1241	0.61
ortho-Cymene	4.34	1019	0.05	4.14*	1227	0.19
para-Cymene	4.37	1021	0.16	4.14*	1227	[0.19]
Limonene	4.43†	1025	1.46	3.21	1157	0.35
β -Phellandrene	4.45*†	1026	[1.46]	3.32*	1166	1.09
1,8-Cineole	4.45*†	1026	[1.46]	3.32*	1166	[1.09]
Lavender lactone	4.59	1035	0.01	9.22*	1603	0.29

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(Z)- β -Ocimene	4.67	1040	5.65	3.82*	1204	5.87
(E)- β -Ocimene	4.82	1050	2.88	4.02*	1218	[4.09]
γ -Terpinene	4.93	1056	0.20	3.82*	1204	[5.87]
<i>cis</i> -Sabinene hydrate	5.06	1065	0.06	6.96*	1430	0.15
<i>cis</i> -Linalool oxide (fur.)	5.15	1070	0.12	6.59*	1403	0.13
Octanol	5.23	1075	0.01	8.26	1528	0.03
α -Pinene oxide analog	5.28	1079	0.03	5.49*	1324	[0.14]
Isoterpinolene	5.35	1083	0.01	4.25	1235	0.02
Terpinolene	5.38	1085	0.10	4.33*	1241	[0.61]
<i>trans</i> -Linalool oxide (fur.)	5.40	1086	0.09	6.96*	1430	[0.15]
Rosefuran	5.58*	1097	0.06	6.04	1363	0.02
<i>trans</i> -Sabinene hydrate	5.58*	1097	[0.06]	8.02*	1510	0.07
Linalool	5.73	1107	27.73	8.18*†	1522	57.53
Hotrienol	5.75	1108	0.06	8.86	1574	0.04
(Z)-6-Methyl-3,5- heptadien-2-one	5.78	1110	0.04	8.24*†	1527	[57.53]
Octen-3-yl acetate	5.88	1116	0.91	5.84*	1349	[0.91]
Octan-3-yl acetate	6.06	1128	0.10	5.28	1308	0.13
allo-Ocimene	6.08*	1130	0.07	5.61	1332	0.06
<i>cis</i> -Limonene oxide	6.08*	1130	[0.07]	6.43	1391	tr
<i>trans</i> -Pinocarveol	6.15*	1134	0.03	9.22*	1603	[0.29]
<i>trans</i> -Limonene oxide	6.15*	1134	[0.03]	6.59*	1403	[0.13]
Camphor	6.19*	1137	0.30	7.26	1452	0.25
(Z)-Myroxide	6.19*	1137	[0.30]	6.89	1426	0.04
Unknown [m/z 95, 43 (74), 109 (72), 82 (62), 110 (50)... 152 (14)]	6.28*	1143	0.04	7.05	1437	0.01
(E)-Myroxide	6.28*	1143	[0.04]	7.16*	1445	0.04
Hexyl isobutyrate	6.42	1152	0.08	5.36	1314	0.07
Nerol oxide	6.46	1154	0.02	6.84*	1422	[0.30]
Borneol	6.60	1163	0.74	9.84*	1653	1.72
<i>cis</i> -Linalool oxide (pyr.)	6.64	1166	0.02	10.36	1694	0.04
Lavandulol	6.70	1170	1.07	9.68	1640	1.10
Terpinen-4-ol	6.80*	1176	4.45	8.64	1558	4.30
(3E,5Z)-Undeca- 1,3,5-triene	6.80*	1176	[4.45]	5.96	1357	0.09
Cryptone	6.87	1181	0.22	9.22*	1603	[0.29]
Butyl hexanoate	6.91*	1183	0.10	6.37	1387	0.01
meta-Cymen-8-ol	6.91*	1183	[0.10]	11.57	1796	0.08
para-Cymen-8-ol	6.95	1186	0.09	11.60	1799	0.09
α -Terpineol	7.01	1190	0.98	9.84*	1653	[1.72]
Hexyl butyrate	7.09*	1195	0.40	6.33	1384	0.34
Hodiendiol	7.09*	1195	[0.40]	12.87	1912	0.01
Verbenone	7.15	1199	0.01	9.64	1636	0.02

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Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.21	1203	0.04	6.29	1381	0.05
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.38	1214	0.03	11.42	1784	0.04
Octyl acetate	7.40	1216	0.02	7.12	1442	0.02
trans-Carveol	7.42	1217	0.02	11.46	1787	0.03
Bornyl formate	7.51	1223	0.05	8.02*†	1510	[0.07]
Nerol	7.63	1232	0.16	11.13*†	1759	0.21
Hexyl 2-methylbutyrate	7.70*†	1236	0.12	6.52	1398	0.05
Carvone	7.70*†	1236	[0.12]	10.05	1670	0.04
Cuminal	7.70*†	1236	[0.12]	10.64*†	1718	0.03
Neral	7.76	1241	0.08	9.59*†	1632	4.12
Hexyl isovalerate	7.82	1245	0.02	6.77	1416	0.01
Linalyl acetate	8.10*†	1264	30.53	8.18*†	1522	[57.53]
Geraniol	8.10*†	1264	[30.53]	11.70	1808	0.44
Geranial	8.24	1273	0.04	10.17	1679	0.06
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.36	1281	0.01	14.72	2086	0.02
Bornyl acetate	8.41	1285	0.18	8.31*†	1532	0.66
Lavandulyl acetate	8.58	1297	3.03	8.83	1572	2.99
Hexyl tiglate	9.13	1330	0.07	9.01	1586	0.06
Hodiendiol derivative	9.27	1341	0.02	13.00	1924	0.03
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.46*†	1354	0.12	11.26	1771	0.02
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.46*†	1354	[0.12]	11.13*†	1759	[0.21]
Neryl acetate	9.60	1364	0.33	10.23*†	1684	0.29
α-Copaene	9.67	1369	0.05	7.16*†	1445	[0.04]
β-Bourbonene	9.78*†	1377	0.04	7.50	1470	0.03
1,5-diepi-β-Bourbonene	9.78*†	1377	[0.04]	7.39	1462	0.01
Geranyl acetate	9.88	1384	0.46	10.60*†	1715	0.57
7-epi-Sesquithujene	9.93*†	1387	0.19	7.88	1499	0.10
Hexyl hexanoate	9.93*†	1387	[0.19]	8.91	1578	0.11
Isocaryophyllene	10.15	1404	0.06	8.24*†	1527	[57.53]
β-Caryophyllene	10.26	1412	3.93	8.50*†	1546	3.99
α-Santalene	10.31	1415	0.51	8.31*†	1532	[0.66]
Coumarin	10.44	1425	0.07	17.18	2337	0.11
trans-α-Bergamotene	10.53	1432	0.16	8.50*†	1546	[3.99]
Sesquisabinene A	10.67	1443	0.03	9.16	1598	0.02
α-Humulene	10.71	1445	0.14	9.31	1610	0.12

Lavandulyl butyrate?	10.82	1454	0.14	10.60*	1715	[0.57]
(E)-β-Farnesene	10.88*	1458	4.02	9.59*	1632	[4.12]
β-Santalene	10.88*	1458	[4.02]	9.22*	1603	[0.29]
Germacrene D	11.09	1474	0.59	9.80	1650	0.56
α-Curcumene	11.17*	1480	0.07	10.70*	1723	0.02
trans-β-Bergamotene	11.17*	1480	[0.07]	9.59*	1632	[4.12]
Isodaucene	11.29	1489	0.03	10.09	1673	0.03
β-Bisabolene	11.52	1507	0.04	10.23*	1684	[0.29]
γ-Cadinene	11.54*	1508	0.20	10.42	1699	0.18
Lavandulyl isovalerate	11.54*	1508	[0.20]	10.70*	1723	[0.02]
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.63	1515	0.06	13.38	1959	0.07
δ-Cadinene	11.68	1519	0.01	10.48	1705	0.01
β-Sesquiphellandrene	11.70	1520	0.03	10.64*	1718	[0.03]
Isocaryophyllene epoxide B	11.99	1544	0.04	12.18	1850	0.05
(E)-Nerolidol	12.25	1564	0.02	13.83	2000	0.02
Caryophyllene oxide isomer	12.37*	1573	0.36	12.73	1899	0.03
Caryophyllene oxide	12.37*	1573	[0.36]	12.80	1906	0.31
Cubenol	13.09	1632	0.01	13.75	1992	0.03
τ-Cadinol	13.14	1636	0.11	14.94	2107	0.15
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	13.52	1667	0.02	16.87	2304	0.01
α-Bisabolol	13.69	1681	0.01	15.53	2165	0.01
Total identified	98.88%			98.06%		
Total reported	98.98%			98.21%		

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

t: 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