

Date : April 4, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23C13-NPA07

Customer identification : NPS00044 - Lavandula angustifolia - Bulgaria - Lot # NP0069

Type : Essential oil

Source : Lavandula angustifolia

Customer : Nature Packaged

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 : March 21, 2023

Checked and approved by :

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

Notes: 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.

This report is an update from the first version issued on March 27, 2023, to format it for online publication.

*P*HYSICO*C*HEMICAL *D*ATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4613 ± 0.0003 (20 °C; method PC-MAT-016)

*C*ONCLUSION

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
Acetone	0.07	Aliphatic ketone
Isobutyral	0.01	Aliphatic aldehyde
Methacrolein	0.01	Aliphatic aldehyde
3-Buten-2-one	0.02	Aliphatic ketone
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
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
Prenal	0.01	Aliphatic aldehyde
Hexanal	0.01	Aliphatic aldehyde
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.08	Aliphatic ether
(3Z)-Hexenol	0.04	Aliphatic alcohol
Hexanol	0.12	Aliphatic alcohol
Unknown	0.02	Unknown
Tricyclene	0.02	Monoterpene
α-Thujene	0.10	Monoterpene
α-Pinene	0.19	Monoterpene
Camphepane	0.14	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Butyl isobutyrate	0.02	Aliphatic ester
Sabinene	0.04	Monoterpene
β-Pinene	0.04	Monoterpene
Octen-3-ol	0.24	Aliphatic alcohol
Octan-3-one	1.23	Aliphatic ketone
Dehydro-1,8-cineole	0.02	Monoterpenic ether
Myrcene	0.60	Monoterpene
Butyl butyrate	0.09	Aliphatic ester
Pseudolimonene	0.01	Monoterpene
Octan-3-ol	0.25	Aliphatic alcohol
α-Phellandrene	0.04	Monoterpene
cis-Dehydroxylinalool oxide	0.02	Monoterpenic ether
Δ3-Carene	0.09	Monoterpene
α-Terpinene	0.04	Monoterpene
Hexyl acetate	0.47	Aliphatic ester
meta-Cymene	0.04	Monoterpene
para-Cymene	0.19	Monoterpene
Limonene	0.33	Monoterpene
1,8-Cineole	0.66	Monoterpenic ether
β-Phellandrene	0.25	Monoterpene
Lavender lactone	0.02	Aliphatic lactone
(Z)-β-Ocimene	3.82	Monoterpene
(E)-β-Ocimene	2.30	Monoterpene

γ -Terpinene	0.13	Monoterpene
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.13	Monoterpenic alcohol
Octanol	0.03	Aliphatic alcohol
α -Pinene oxide analog	0.05	Monoterpenic ether
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.08	Monoterpene
trans-Linalool oxide (fur.)	0.07	Monoterpenic alcohol
α -Pinene oxide	0.01	Monoterpenic ether
Rosefuran	0.03	Monoterpenic ether
trans-Sabinene hydrate	0.05	Monoterpenic alcohol
Linalool	31.72	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
β -Thujone	0.03	Monoterpenic ketone
Octen-3-yl acetate	0.77	Aliphatic ester
Unknown	0.04	Unknown
α -Campholenal	0.04	Monoterpenic aldehyde
Octan-3-yl acetate	0.12	Aliphatic ester
allo-Ocimene	0.07	Monoterpene
(Z)-Myroxide	0.06	Monoterpenic ether
Camphor	0.23	Monoterpenic ketone
trans-Verbenol	0.03	Monoterpenic alcohol
(E)-Myroxide	tr	Monoterpenic ether
Hexyl isobutyrate	0.08	Aliphatic ester
Nerol oxide	0.02	Aliphatic ether
Borneol	0.59	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.03	Monoterpenic alcohol
Lavandulol	1.20	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	0.07	Alkene
Terpinen-4-ol	4.41	Monoterpenic alcohol
Cryptone	0.24	Normonoterpenic ketone
meta-Cymen-8-ol	0.10	Monoterpenic alcohol
para-Cymen-8-ol	0.08	Monoterpenic alcohol
α -Terpineol	1.05	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Hexyl butyrate	0.28	Aliphatic ester
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.03	Monoterpenic alcohol
Verbenone	0.03	Monoterpenic ketone
Unknown	0.04	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.07	Monoterpenic alcohol
Octyl acetate	0.02	Aliphatic ester
trans-Carveol	0.03	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
Nerol	0.20	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.03	Aliphatic ester
Cuminal	0.09	Monoterpenic aldehyde
Carvone	0.04	Monoterpenic ketone
Neral	0.04	Monoterpenic aldehyde
Hexyl isovalerate	0.02	Aliphatic ester
Geraniol	0.44	Monoterpenic alcohol
Linalyl acetate	29.81	Monoterpenic ester

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Geranial	0.05	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.01	Monoterpenic alcohol
Bornyl acetate	0.11	Monoterpenic ester
Lavandulyl acetate	3.12	Monoterpenic ester
Hexyl tiglate	0.04	Aliphatic ester
Hodiendiol derivative	0.01	Oxygenated monoterpane
Unknown	0.02	Oxygenated monoterpane
Unknown	0.02	Oxygenated monoterpane
Hodiendiol derivative III	0.02	Oxygenated monoterpane
Neryl acetate	0.28	Monoterpenic ester
α -Copaene	0.02	Sesquiterpene
β -Bourbonene	0.03	Sesquiterpene
Geranyl acetate	0.48	Monoterpenic ester
7-epi-Sesquithujene	0.09	Sesquiterpene
Hexyl hexanoate	0.09	Aliphatic ester
Isocaryophyllene	0.02	Sesquiterpene
Sesquithujene	0.04	Sesquiterpene
β -Caryophyllene	3.68	Sesquiterpene
α -Santalene	0.40	Sesquiterpene
Coumarin	0.05	Coumarin
Lavandulyl isobutyrate	0.01	Monoterpenic ester
<i>trans</i> - α -Bergamotene	0.14	Sesquiterpene
Sesquisabinene A	0.06	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.02	Sesquiterpene
α -Humulene	0.14	Sesquiterpene
Lavandulyl butyrate?	0.13	Monoterpenic ester
β -Santalene	0.02	Sesquiterpene
(<i>E</i>)- β -Farnesene	3.64	Sesquiterpene
Germacrene D	0.48	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.06	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	0.04	Sesquiterpene
γ -Cadinene	0.12	Sesquiterpene
δ -Cadinene	0.03	Sesquiterpene
β -Sesquiphellandrene	0.03	Sesquiterpene
Isocaryophyllene epoxide B	0.03	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.22	Sesquiterpenic ether
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
τ -Cadinol	0.06	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
<i>cis</i> -14-nor-Muurol-5-en-4-one?	0.01	Norsesquiterpenic ketone
Consolidated total	98.56%	

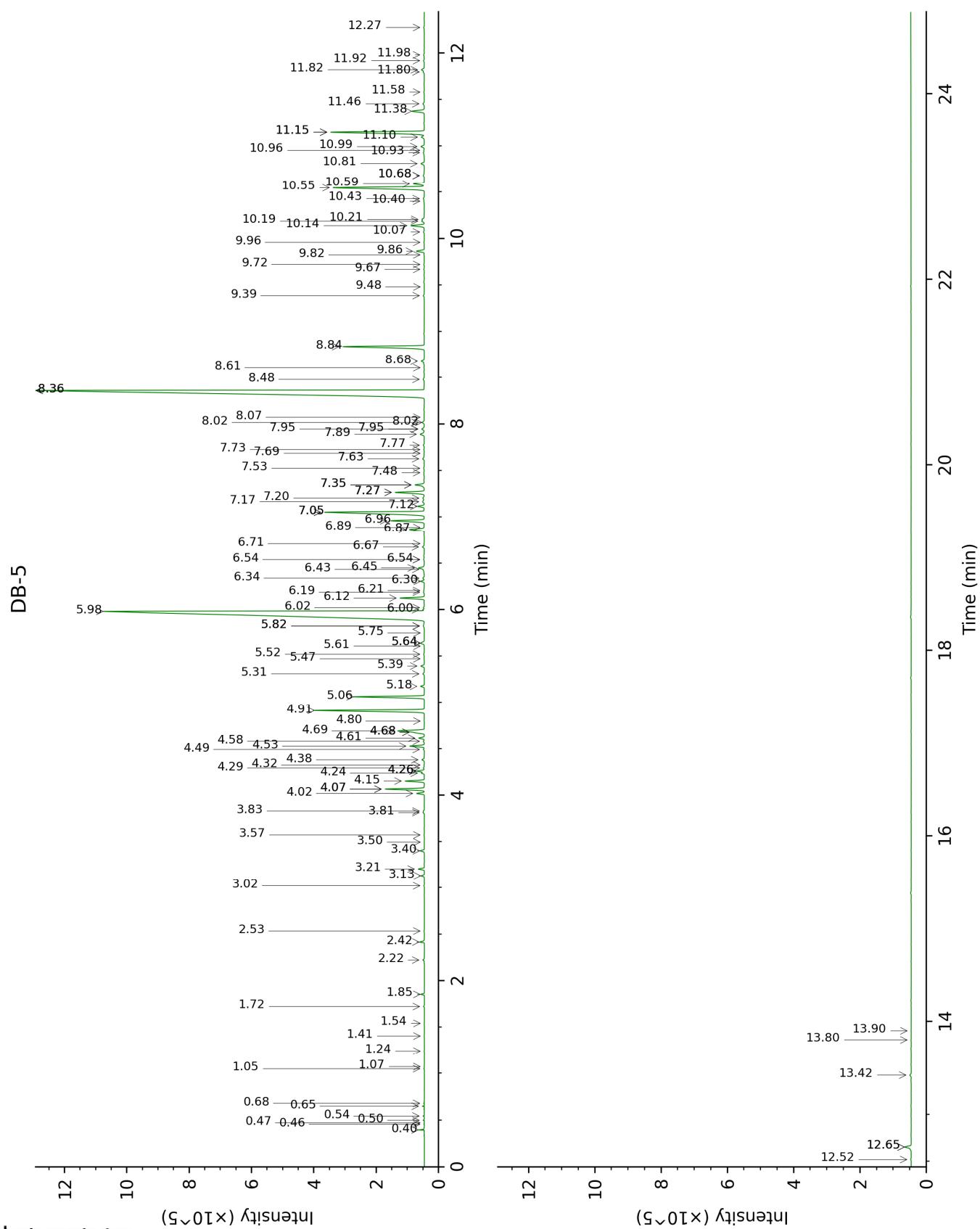
tr: The compound has been detected below 0.005% of total signal.

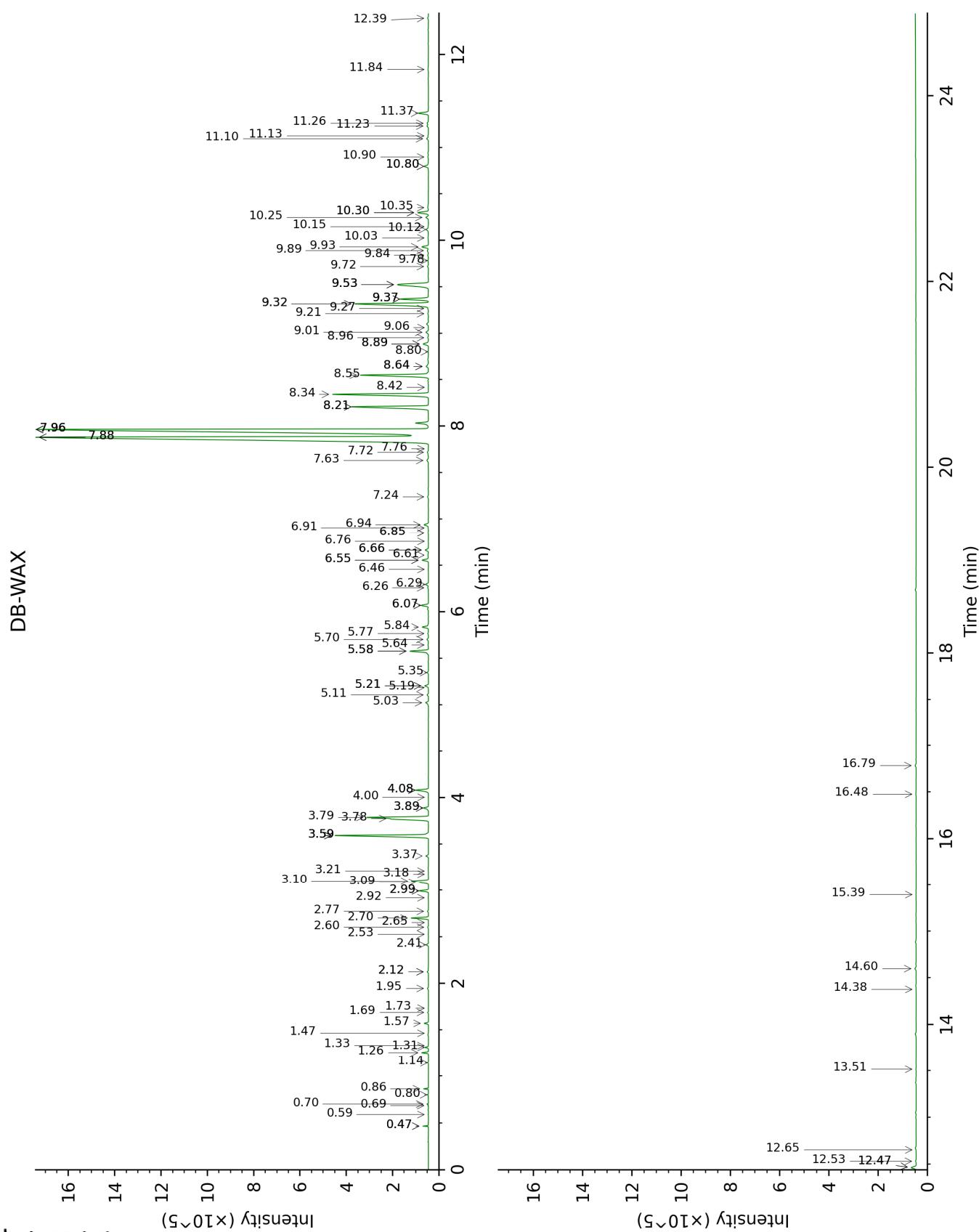
Note: no correction factor was applied

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	%
Acetone	0.40	500	0.07	0.47*	784	0.08
Isobutyral	0.46	538	0.01	0.47*	784	[0.08]
Methacrolein	0.47	551	0.01	0.59	843	tr
3-Buten-2-one	0.50	572	0.02	0.80	911	0.02
2-Methyl-3-buten-2-ol	0.54	606	0.01	1.46	1015	0.01
Isovaleral	0.65	641	0.02	0.70	888	0.02
2-Methylbutyral	0.68	651	0.01	0.69	881	0.01
Isoamyl alcohol	1.05	733	0.01	3.21	1176	0.01
2-Methylbutanol	1.07	736	0.01	3.18	1173	0.01
Toluene	1.24	759	0.01	1.33	1002	0.01
Prenal	1.40	781	0.01	2.99*	1158	0.34
Hexanal	1.54	800	0.01	1.73	1043	tr
Butyl acetate	1.72	816	0.02	1.69	1038	0.02
Methyl hexyl ether	1.85	827	0.08	0.86	922	0.09
(3Z)-Hexenol	2.22	857	0.04	5.58*	1350	0.79
Hexanol	2.42	873	0.12	5.21*	1323	0.15
Unknown [m/z 59, 85 (88), 41 (57), 43 (43)...]	2.53	882	0.02	5.64	1355	0.03
Tricyclene	3.02	919	0.02	1.14	971	0.02
α-Thujene	3.13	926	0.10	1.31	1000	0.09
α-Pinene	3.21	931	0.19	1.26	991	0.18
Camphepane	3.40	944	0.14	1.57	1026	0.12
Thuja-2,4(10)-diene	3.50	950	0.01	2.12*	1084	0.05
Butyl isobutyrate	3.57	955	0.02	2.53	1120	0.01
Sabinene	3.81†	971	0.08	2.12*	1084	[0.05]
β-Pinene	3.83†	972	[0.08]	1.95	1065	0.04
Octen-3-ol	4.02	984	0.24	6.55*	1421	0.26
Octan-3-one	4.06*	987	1.24	3.78†	1221	3.54
Dehydro-1,8-cineole	4.06*	987	[1.24]	2.92	1152	0.02
Myrcene	4.15	993	0.60	2.70	1134	0.59
Butyl butyrate	4.24	999	0.09	3.37	1190	0.09
Pseudolimonene	4.26*	1000	0.25	2.65	1130	0.01
Octan-3-ol	4.26*	1000	[0.25]	5.84	1368	0.25
α-Phellandrene	4.29	1002	0.04	2.60	1126	0.03
cis-Dehydroxylinalool oxide	4.32	1004	0.02	3.59*	1207	3.96
Δ3-Carene	4.38	1008	0.09	2.41	1111	0.08
α-Terpinene	4.49	1015	0.04	2.77	1140	0.04
Hexyl acetate	4.53	1017	0.47	4.08*	1245	0.55
meta-Cymene	4.58	1020	0.04	3.89*	1230	0.22
para-Cymene	4.61	1022	0.19	3.89*	1230	[0.22]
Limonene	4.68*†	1026	1.25	2.99*	1158	[0.34]
1,8-Cineole	4.68*†	1026	[1.25]	3.10	1167	0.66
β-Phellandrene	4.69†	1027	[1.25]	3.09	1166	0.25

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Lavender lactone	4.80	1034	0.02	8.96	1606	0.03
(Z)- β -Ocimene	4.91	1041	3.82	3.59*	1207	[3.96]
(E)- β -Ocimene	5.06	1050	2.30	3.79†	1222	[3.54]
γ -Terpinene	5.18	1058	0.13	3.59*	1207	[3.96]
cis-Sabinene hydrate	5.31	1066	0.06	6.66*	1430	0.14
cis-Linalool oxide (fur.)	5.39	1071	0.13	6.29	1402	0.13
Octanol	5.47	1076	0.03	7.96*†	1528	[62.42]
α -Pinene oxide analog	5.52	1079	0.05	5.21*	1323	[0.15]
Isoterpinolene	5.61	1084	0.01	4.00	1239	0.01
Terpinolene	5.64*	1086	0.17	4.08*	1245	[0.55]
trans-Linalool oxide (fur.)	5.64*	1086	[0.17]	6.66*	1430	[0.14]
α -Pinene oxide	5.75	1093	0.01	5.19	1321	0.01
Rosefuran	5.82*	1098	0.07	5.77	1364	0.03
trans-Sabinene hydrate	5.82*	1098	[0.07]	7.72	1509	0.05
Linalool	5.98	1108	31.72	7.88*†	1522	62.42
(Z)-6-Methyl-3,5-heptadien-2-one	6.00	1109	0.03	7.96*†	1528	[62.42]
β -Thujone	6.02	1110	0.03	6.07*	1386	0.31
Octen-3-yl acetate	6.12	1117	0.77	5.58*	1350	[0.79]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	6.19	1121	0.04	9.37*	1640	1.20
α -Campholenal	6.20	1122	0.04	6.76	1437	0.01
Octan-3-yl acetate	6.30	1128	0.12	5.03	1309	0.11
allo-Ocimene	6.34	1131	0.07	5.35	1333	0.05
(Z)-Myroxide	6.43	1137	0.06	6.61	1426	0.04
Camphor	6.45	1138	0.23	6.94	1450	0.20
trans-Verbenol	6.54*	1143	0.05	9.27	1632	0.03
(E)-Myroxide	6.54*	1143	[0.05]	6.85*	1444	0.02
Hexyl isobutyrate	6.67	1152	0.08	5.11	1316	0.06
Nerol oxide	6.71	1154	0.02	6.55*	1421	[0.26]
Borneol	6.86	1164	0.59	9.52*	1653	2.11
cis-Linalool oxide (pyr.)	6.89	1166	0.03	10.03	1694	0.04
Lavandulol	6.96	1170	1.20	9.37*	1640	[1.20]
(3E,5Z)-Undeca-1,3,5-triene	7.05*	1176	4.50	5.70	1359	0.07
Terpinen-4-ol	7.05*	1176	[4.50]	8.34	1558	4.41
Cryptone	7.12	1180	0.24	8.89*	1601	0.27
meta-Cymen-8-ol	7.17	1183	0.10	11.23	1796	0.07
para-Cymen-8-ol	7.20	1186	0.08	11.26	1799	0.07
α -Terpineol	7.27*	1190	1.07	9.52*	1653	[2.11]
Myrtenal	7.27*	1190	[1.07]	8.42	1564	0.01
Hexyl butyrate	7.35*	1195	0.38	6.07*	1386	[0.31]
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	7.35*	1195	[0.38]	12.53	1913	0.03

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Verbenone	7.48	1203	0.03	9.37*	1640	[1.20]
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.52	1206	0.04			
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.63	1213	0.07	11.10	1785	0.08
Octyl acetate	7.69	1217	0.02	6.85*	1444	[0.02]
trans-Carveol	7.73	1220	0.03	11.13	1787	0.03
Bornyl formate	7.77	1223	0.05	7.76	1512	0.01
Nerol	7.89	1231	0.20	10.80*	1760	0.20
Hexyl 2-methylbutyrate	7.95*	1234	0.13	6.26	1399	0.03
Cuminal	7.95*	1234	[0.13]	10.30*	1717	0.48
Carvone	8.02*	1239	0.09	9.72	1668	0.04
Neral	8.02*	1239	[0.09]	9.21	1627	0.04
Hexyl isovalerate	8.07	1243	0.02	6.46	1414	0.02
Geraniol	8.36*	1262	30.25	11.37	1809	0.44
Linalyl acetate	8.36*	1262	[30.25]	7.96*†	1528	[62.42]
Geranial	8.48	1270	0.05	9.84	1678	0.04
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.61	1278	0.01	14.38	2087	0.01
Bornyl acetate	8.68	1283	0.11	7.96*†	1528	[62.42]
Lavandulyl acetate	8.84	1294	3.12	8.55	1574	3.16
Hexyl tiglate	9.39	1332	0.04	8.64*	1581	0.13
Hodiendiol derivative	9.48	1338	0.01	12.66	1924	0.01
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.67	1352	0.02	10.80*	1760	[0.20]
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.72	1355	0.02	10.90	1768	0.04
Hodiendiol derivative III	9.82	1363	0.02	12.47*	1906	0.23
Neryl acetate	9.86	1366	0.28	9.93	1686	0.29
α-Copaene	9.96	1372	0.02	6.91	1448	0.02
β-Bourbonene	10.07	1380	0.03	7.24	1473	0.04
Geranyl acetate	10.14	1385	0.48	10.30*	1717	[0.48]
7-epi-Sesquithujene	10.19	1388	0.09	7.63	1502	0.09
Hexyl hexanoate	10.21	1390	0.09	8.64*	1581	[0.13]
Isocaryophyllene	10.40	1403	0.02	7.96*†	1528	[62.42]
Sesquithujene	10.43	1405	0.04	7.88*†	1522	[62.42]
β-Caryophyllene	10.55	1414	3.68	8.21*	1547	3.77
α-Santalene	10.59	1417	0.40	7.96*†	1528	[62.42]
Coumarin	10.68*	1424	0.07	16.78	2336	0.05
Lavandulyl isobutyrate	10.68*	1424	[0.07]	9.06	1615	0.01

<i>trans</i> - α -Bergamotene	10.81	1434	0.14	8.21*	1547	[3.77]
Sesquabinene A	10.93	1443	0.06	8.89*	1601	[0.27]
<i>cis</i> - β -Bergamotene?	10.96	1444	0.02			
α -Humulene	11.00	1447	0.14	9.01	1611	0.12
Lavandulyl butyrate?	11.10	1455	0.13	10.25	1712	0.12
β -Santalene	11.15*	1459	3.66	8.80	1594	0.02
(<i>E</i>)- β -Farnesene	11.15*	1459	[3.66]	9.32*	1636	3.73
Germacrene D	11.38	1476	0.48	9.52*	1653	[2.11]
<i>trans</i> - β -Bergamotene	11.46	1482	0.06	9.32*	1636	[3.73]
Isodaucene	11.58	1491	0.02	9.78	1674	0.03
β -Bisabolene	11.80	1507	0.04	9.89	1682	0.06
γ -Cadinene	11.82	1509	0.12	10.12	1701	0.12
δ -Cadinene	11.92	1517	0.03	10.15	1704	0.02
β -Sesquiphellandrene	11.98	1522	0.03	10.35	1721	0.04
Isocaryophyllene epoxide B	12.27	1545	0.03	11.84	1850	0.04
(<i>E</i>)-Nerolidol	12.52	1564	0.02	13.51	2004	0.01
Caryophyllene oxide	12.65*	1574	0.29	12.47*	1906	[0.23]
Caryophyllene oxide isomer	12.65*	1574	[0.29]	12.39	1900	0.04
τ -Cadinol	13.42	1636	0.06	14.60	2109	0.06
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	13.80	1668	0.02	16.48	2302	0.03
<i>cis</i> -14-nor-Muurol-5-en-4-one?	13.90	1676	0.01	15.39	2189	0.01
Total identified		98.59%			98.23%	
Total reported		98.74%			98.29%	

*: 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