

Date : September 15, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20114-PTH02


Customer identification : Lavender - L40115207R

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

Analysis date : September 15, 2020

Checked and approved by :



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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4606 ± 0.0003 (20 °C; method PC-MAT-016)

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

Compound	Min. %	Max. %	Observed %	Complies?
α-Terpineol		2.0	1.0	Yes
Lavandulyl acetate		8	3	Yes
Terpinen-4-ol		8	3	Yes
Lavandulol		3.0	1.0	Yes
Linalyl acetate	25	47	33	Yes
Linalool	20	43	32	Yes
Camphor		1.5	0.3	Yes
Octan-3-one		3.0	1.3	Yes
(E)-β-Ocimene	tr	6	2	Yes
(Z)-β-Ocimene	1	10	4	Yes
β-Phellandrene		1.0	0.3	Yes
1,8-Cineole		3.0	0.9	Yes
Limonene		1.0	0.4	Yes
Refractive index	1.4600	1.4660	1.4606	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	tr	Aliphatic aldehyde
3-Buten-2-one	tr	Aliphatic ketone
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.13	Aliphatic ether
(3Z)-Hexenol	0.02	Aliphatic alcohol
Hexanol	0.09	Aliphatic alcohol
Tricyclene	0.02	Monoterpene
α -Thujene	0.10	Monoterpene
α -Pinene	0.20	Monoterpene
Camphene	0.16	Monoterpene
α -Fenchene	tr	Monoterpene
5,5-Dimethyl-2(5H)-furanone	0.01	Aliphatic lactone
Butyl isobutyrate	0.02	Aliphatic ester
endo-Isocamphane	tr	Monoterpene
β -Pinene	0.05	Monoterpene
Sabinene	0.05	Monoterpene
Octen-3-ol	0.24	Aliphatic alcohol
Octan-3-one	1.29	Aliphatic ketone
Myrcene	0.60	Monoterpene
Butyl butyrate	0.10	Aliphatic ester
Octan-3-ol	0.27	Aliphatic alcohol
α -Phellandrene	0.04	Monoterpene
Pseudolimonene	0.01	Monoterpene
Δ^3 -Carene	0.14	Monoterpene
α -Terpinene	0.04	Monoterpene
Hexyl acetate	0.61	Aliphatic ester
ortho-Cymene	0.04	Monoterpene
para-Cymene	0.16	Monoterpene
Limonene	0.36	Monoterpene
β -Phellandrene	0.30	Monoterpene
1,8-Cineole	0.88	Monoterpenic ether
(Z)- β -Ocimene	3.75	Monoterpene
(E)- β -Ocimene	2.15	Monoterpene
γ -Terpinene	0.14	Monoterpene
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.12	Monoterpenic alcohol
Octanol	0.04	Aliphatic alcohol
Isoterpinolene	0.01	Monoterpene
trans-Linalool oxide (fur.)	0.08	Monoterpenic alcohol

Terpinolene	0.11	Monoterpene
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Rosefuran	0.02	Monoterpenic ether
Linalool	31.78	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
Octen-3-yl acetate	0.65	Aliphatic ester
Unknown	0.02	Unknown
Octan-3-yl acetate	0.10	Aliphatic ester
allo-Ocimene	0.05	Monoterpene
(<i>Z</i>)-Myroxide	0.02	Monoterpenic ether
Camphor	0.26	Monoterpenic ketone
<i>trans</i> -Verbenol	0.03	Monoterpenic alcohol
(<i>E</i>)-Myroxide	tr	Monoterpenic ether
Unknown	0.03	Oxygenated monoterpene
Hexyl isobutyrate	0.07	Aliphatic ester
Nerol oxide	0.02	Aliphatic ether
Borneol	0.58	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.02	Monoterpenic alcohol
Lavandulol	0.99	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	0.07	Alkene
Terpinen-4-ol	3.15	Monoterpenic alcohol
Cryptone	0.23	Normonoterpenic ketone
meta-Cymen-8-ol	0.07	Monoterpenic alcohol
para-Cymen-8-ol	0.06	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
α -Terpineol	0.96	Monoterpenic alcohol
Hexyl butyrate	0.43	Aliphatic ester
Verbenone	0.02	Monoterpenic ketone
Unknown	0.01	Unknown
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
exo-2-Hydroxycineole	0.01	Monoterpenic alcohol
Bornyl formate	0.03	Monoterpenic ester
Nerol	0.17	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.11	Aliphatic ester
Carvone	0.01	Monoterpenic ketone
Neral	0.02	Monoterpenic aldehyde
Hexyl isovalerate	0.01	Aliphatic ester
Linalyl acetate	32.96	Monoterpenic ester
Geraniol	0.40	Monoterpenic alcohol
Phellandral	0.04	Monoterpenic aldehyde
(<i>trans</i> ?) -Linalool oxide acetate (fur.)?	0.03	Monoterpenic ester
Geranial	0.02	Monoterpenic aldehyde
iso-Isopulegyl acetate	0.03	Monoterpenic ester
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Bornyl acetate	0.12	Monoterpenic ester
Lavandulyl acetate	2.91	Monoterpenic ester
Hexyl tiglate	0.05	Aliphatic ester
Hodiendiol derivative	0.02	Oxygenated monoterpene
Unknown	0.03	Oxygenated monoterpene
Neryl acetate	0.32	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
β -Bourbonene	0.03	Sesquiterpene

Geranyl acetate	0.45	Monoterpenic ester
Hexyl hexanoate	0.10	Aliphatic ester
7-epi-Sesquithujene	0.10	Sesquiterpene
α -Cedrene	0.05	Sesquiterpene
β -Caryophyllene	3.18	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.02	Sesquiterpene
α -Santalene	0.36	Sesquiterpene
Lavandulyl isobutyrate	0.01	Monoterpenic ester
Coumarin	0.03	Coumarin
<i>trans</i> - α -Bergamotene	0.13	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.08	Sesquiterpene
α -Humulene	0.11	Sesquiterpene
Lavandulyl butyrate?	0.11	Monoterpenic ester
(<i>E</i>)- β -Farnesene	3.57	Sesquiterpene
Germacrene D	0.40	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.05	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
Lavandulyl isovalerate	0.01	Monoterpenic ester
γ -Cadinene	0.16	Sesquiterpene
β -Bisabolene	0.01	Sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
δ -Cadinene	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.31	Sesquiterpenic ether
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
Dendrolasin	0.02	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
Consolidated total	99.04%	

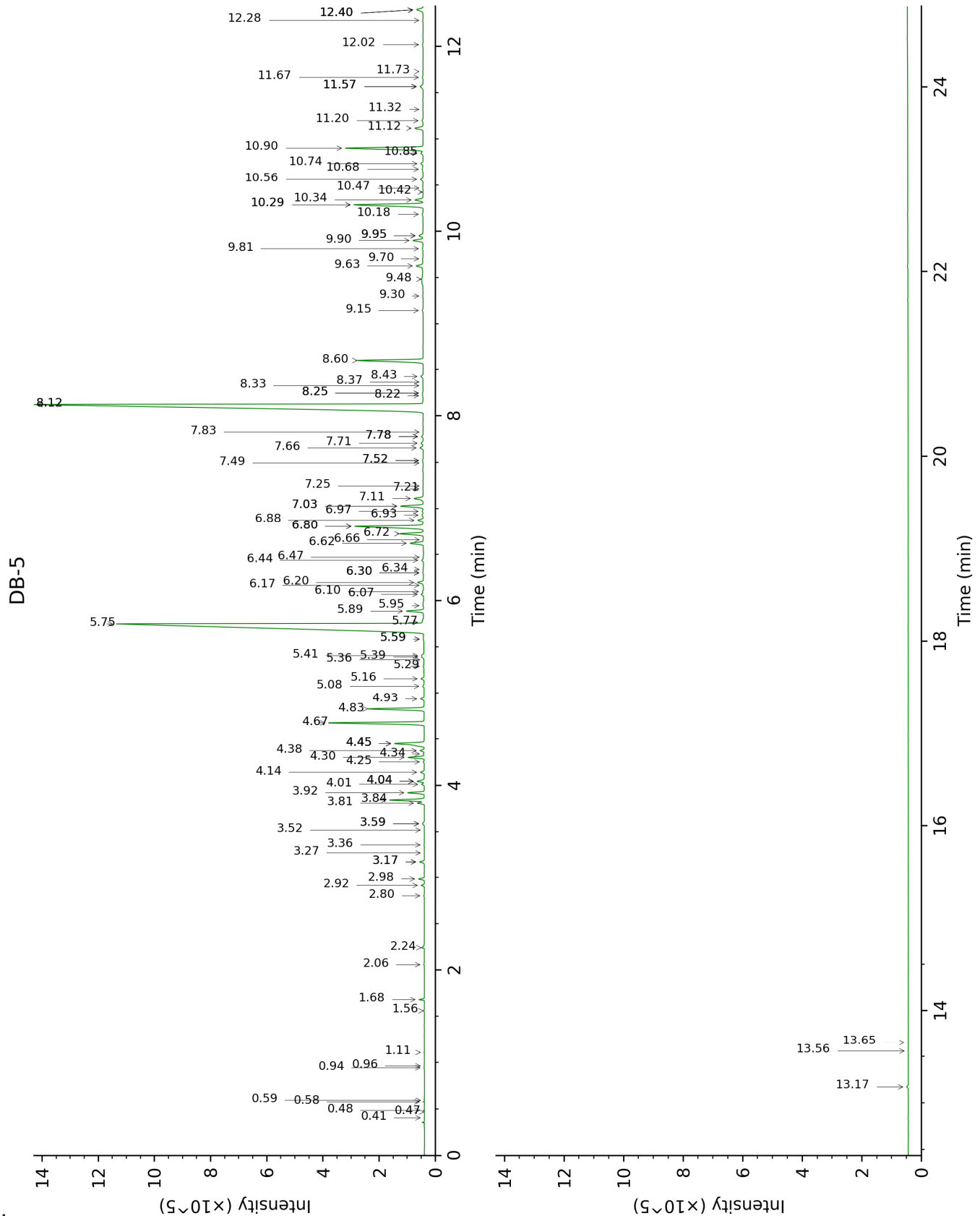
tr: The compound has been detected below 0.005% of total signal.

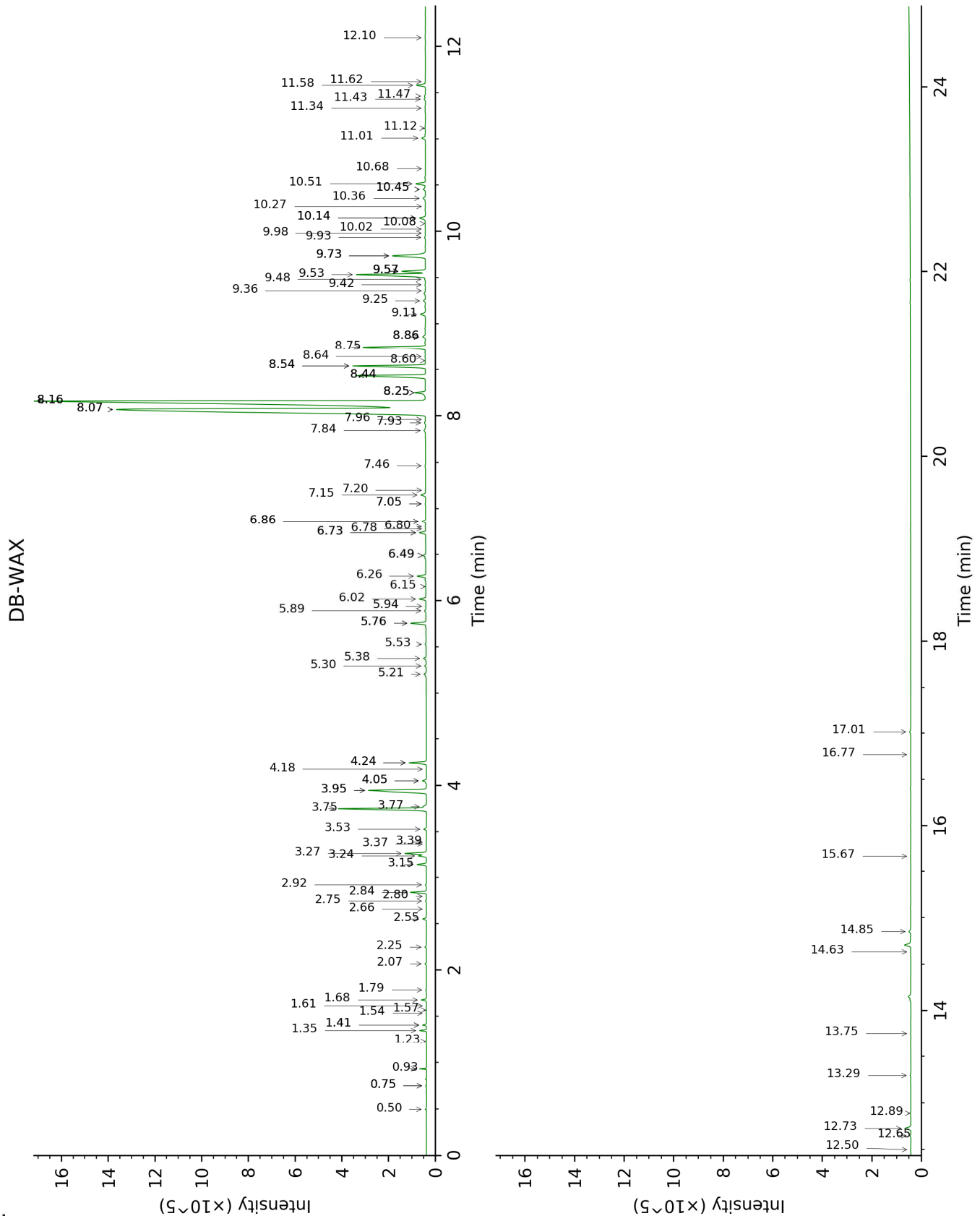
Note: no correction factor was applied

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.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutyral	0.41	533	tr	0.50	780	0.02
3-Buten-2-one	0.47	588	tr			
2-Methyl-3-buten-2-ol	0.48	603	0.01	1.54	1012	0.01
Isovaleral	0.58	639	0.02	0.75*	883	0.02
2-Methylbutyral	0.59	646	tr	0.75*	883	[0.02]
Isoamyl alcohol	0.94	733	0.01	3.39	1174	0.01
2-Methylbutanol	0.96	736	tr	3.37	1173	0.01
Toluene	1.11	758	0.01	1.41*	999	0.10
Butyl acetate	1.56	816	0.02	1.79	1037	0.02
Methyl hexyl ether	1.68	826	0.13	0.93	922	0.13
(3Z)-Hexenol	2.06	858	0.02	5.76*	1345	0.64
Hexanol	2.24	874	0.09	5.38	1317	0.12
Tricyclene	2.80	918	0.02	1.23	971	0.02
α-Thujene	2.92	925	0.10	1.41*	999	[0.10]
α-Pinene	2.98	930	0.20	1.35	990	0.19
Camphene	3.18*	942	0.17	1.68	1026	0.16
α-Fenchene	3.18*	942	[0.17]	1.61	1020	tr
5,5-Dimethyl-2(5H)-furanone	3.27	949	0.01	8.54*	1553	3.15
Butyl isobutyrate	3.36	955	0.02	2.66	1118	0.01
endo-Isocamphane	3.52	965	tr	1.57	1015	tr
β-Pinene	3.59*	970	0.11	2.07	1064	0.05
Sabinene	3.59*	970	[0.11]	2.25	1082	0.05
Octen-3-ol	3.81	985	0.24	6.73*	1416	0.26
Octan-3-one	3.84	987	1.29	3.95*	1216	3.39
Myrcene	3.92	992	0.60	2.84	1132	0.58
Butyl butyrate	4.01	998	0.10	3.53	1185	0.10
Octan-3-ol	4.04*	1000	0.31	6.02	1364	0.27
α-Phellandrene	4.04*	1000	[0.31]	2.75	1124	0.04
Pseudolimonene	4.04*	1000	[0.31]	2.80	1128	0.01
Δ3-Carene	4.14	1007	0.14	2.55	1109	0.14
α-Terpinene	4.25	1014	0.04	2.92	1138	0.04
Hexyl acetate	4.30	1017	0.61	4.24*	1238	0.72
ortho-Cymene	4.34	1019	0.04	4.05*	1224	0.19
para-Cymene	4.38	1021	0.16	4.05*	1224	[0.19]
Limonene	4.45*	1026	1.55	3.15	1156	0.36
β-Phellandrene	4.45*	1026	[1.55]	3.24	1163	0.30
1,8-Cineole	4.45*	1026	[1.55]	3.27	1165	0.88
(Z)-β-Ocimene	4.68	1040	3.75	3.75	1202	3.70
(E)-β-Ocimene	4.83	1050	2.15	3.95*	1216	[3.39]
γ-Terpinene	4.94	1056	0.14	3.77	1204	0.13
cis-Sabinene hydrate	5.08	1065	0.06	6.86*	1426	0.15
cis-Linalool oxide (fur.)	5.16	1070	0.12	6.49*†	1398	0.16

Octanol	5.29	1079	0.04	8.16*†	1524	[64.59]
Isoterpinolene	5.36	1083	0.01	4.18	1233	0.01
<i>trans</i> -Linalool oxide (fur.)	5.39†	1085	0.19	6.86*	1426	[0.15]
Terpinolene	5.41†	1086	[0.19]	4.24*	1238	[0.72]
<i>trans</i> -Sabinene hydrate	5.59*	1097	0.02	7.96	1508	0.01
Rosefuran	5.59*	1097	[0.02]	5.94	1358	0.02
Linalool	5.75	1108	31.78	8.07*†	1517	64.59
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	5.77	1108	0.04	8.16*†	1524	[64.59]
Octen-3-yl acetate	5.89	1116	0.65	5.76*	1345	[0.64]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.95	1120	0.02	9.57*†	1635	[4.59]
Octan-3-yl acetate	6.07	1128	0.10	5.21	1305	0.10
allo-Ocimene	6.10	1130	0.05	5.53	1328	0.04
(<i>Z</i>)-Myroxide	6.17	1134	0.02	6.78	1419	0.01
Camphor	6.20	1136	0.26	7.15	1447	0.24
<i>trans</i> -Verbenol	6.30*	1142	0.04	9.48	1628	0.03
(<i>E</i>)-Myroxide	6.30*	1142	[0.04]	7.05*	1440	0.03
Unknown [m/z 95, 43 (74), 109 (72), 82 (62), 110 (50)... 152 (14)]	6.34	1145	0.03	7.05*	1440	[0.03]
Hexyl isobutyrate	6.44	1151	0.07	5.30	1312	0.06
Nerol oxide	6.47	1153	0.02	6.80	1421	0.02
Borneol	6.62	1163	0.58	9.74*	1648	1.95
<i>cis</i> -Linalool oxide (pyr.)	6.66	1165	0.02	10.27	1692	0.01
Lavandulol	6.72	1169	0.99	9.57*†	1635	[4.59]
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	6.80*	1174	3.26	5.89	1355	0.07
Terpinen-4-ol	6.80*	1174	[3.26]	8.54*	1553	[3.15]
Cryptone	6.88	1179	0.23	9.10	1597	0.26
meta-Cymen-8-ol	6.93	1182	0.07	11.43	1790	0.06
para-Cymen-8-ol	6.97	1185	0.06	11.47	1793	0.05
Myrtenal	7.03*	1189	0.99	8.60	1558	0.01
α-Terpineol	7.03*	1189	[0.99]	9.74*	1648	[1.95]
Hexyl butyrate	7.11	1194	0.43	6.26	1382	0.38
Verbenone	7.21	1201	0.02	9.57*†	1635	[4.59]
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.25	1203	0.01	6.15	1374	0.01
<i>trans</i> -Carveol	7.49	1219	0.02	11.34	1782	0.03
exo-2-	7.52*	1221	0.04	11.62	1807	0.01

Hydroxycineole						
Bornyl formate	7.52*	1221	[0.04]	8.07*†	1517	[64.59]
Nerol	7.66	1230	0.17	11.01	1755	0.17
Hexyl 2-methylbutyrate	7.71	1233	0.11	6.49*†	1398	[0.16]
Carvone	7.78*	1238	0.08	9.98	1668	0.01
Neral	7.78*	1238	[0.08]	9.42	1623	0.02
Hexyl isovalerate	7.83	1241	0.01	6.73*	1416	[0.26]
Linalyl acetate	8.12*	1261	33.36	8.16*†	1524	[64.59]
Geraniol	8.12*	1261	[33.36]	11.58	1803	0.40
Phellandral	8.22	1268	0.04	9.93	1664	0.04
(<i>trans</i> ?) <i>-</i> Linalool oxide acetate (fur.)?	8.25*	1269	0.04	8.64	1561	0.03
Geranial	8.25*	1269	[0.04]	10.08	1677	0.02
iso-Isopulegyl acetate	8.33	1275	0.03			
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.37	1277	0.02	14.63	2084	0.01
Bornyl acetate	8.43	1281	0.12	8.25*	1531	0.51
Lavandulyl acetate	8.60	1293	2.91	8.75	1569	2.86
Hexyl tiglate	9.15	1330	0.05	8.86*	1578	0.15
Hodiendiol derivative	9.30	1341	0.02	12.89	1920	0.02
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.48	1354	0.03	11.12	1764	0.02
Neryl acetate	9.63	1364	0.32	10.14*	1682	0.31
α -Copaene	9.70	1369	0.01	7.20	1451	0.01
β -Bourbonene	9.81	1377	0.03	7.46	1471	0.04
Geranyl acetate	9.90	1383	0.45	10.51	1712	0.45
Hexyl hexanoate	9.95*	1387	0.20	8.86*	1578	[0.15]
7-epi-Sesquithujene	9.95*	1387	[0.20]	7.84	1499	0.10
α -Cedrene	10.18	1403	0.05	7.93	1506	0.05
β -Caryophyllene	10.29*	1411	3.25	8.44*	1545	3.31
<i>cis</i> - α -Bergamotene	10.29*	1411	[3.25]	8.25*	1531	[0.51]
α -Santalene	10.34	1415	0.36	8.25*	1531	[0.51]
Lavandulyl isobutyrate	10.42	1421	0.01	9.36	1618	0.01
Coumarin	10.47	1424	0.03	17.01	2327	0.06
<i>trans</i> - α -Bergamotene	10.56	1431	0.13	8.44*	1545	[3.31]
<i>cis</i> - β -Bergamotene?	10.68	1440	0.08			
α -Humulene	10.74	1444	0.11	9.25	1609	0.10
Lavandulyl	10.85	1453	0.11	10.45*	1707	0.13

butyrate?						
(E)-β-Farnesene	10.90	1457	3.57	9.53†	1632	4.59
Germacrene D	11.12	1473	0.40	9.74*	1648	[1.95]
trans-β-Bergamotene	11.20	1479	0.05	9.57*†	1635	[4.59]
Isodaucene	11.32	1488	0.02	10.02	1672	0.01
Lavandulyl isovalerate	11.57*	1507	0.18	10.68	1727	0.01
γ-Cadinene	11.57*	1507	[0.18]	10.36	1699	0.16
β-Bisabolene	11.57*	1507	[0.18]	10.14*	1682	[0.31]
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.67	1514	0.04	13.30	1957	0.04
δ-Cadinene	11.73	1519	0.02	10.45*	1707	[0.13]
Isocaryophyllene epoxide B	12.02	1542	0.04	12.10	1849	0.03
(E)-Nerolidol	12.28	1563	0.02	13.75	2000	0.01
Caryophyllene oxide	12.40*	1572	0.36	12.73	1905	0.31
Caryophyllene oxide isomer	12.40*	1572	[0.36]	12.65	1898	0.04
Dendrolasin	12.40*	1572	[0.36]	12.50	1884	0.02
τ-Cadinol	13.17	1634	0.08	14.85	2106	0.09
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	13.56	1666	0.01	16.77	2301	0.01
cis-14-nor-Muurool-5-en-4-one?	13.65	1674	0.01	15.67	2187	0.01
Total identified		99.08%			98.23%	
Total reported		99.22%			98.30%	

*: 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