

Date : September 21, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22I15-PTH01

Customer identification : Lavender - Bulgaria - L40119R

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 : Amélie Simard, Analyste

Analysis date : September 20, 2022

Checked and approved by :

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

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

Physical aspect: Clear liquid

Refractive index: 1.4618 ± 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
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	tr	Simple phenolic
Prenal	0.01	Aliphatic aldehyde
Hexanal	0.01	Aliphatic aldehyde
Butyl acetate	0.01	Aliphatic ester
Methyl hexyl ether	0.17	Aliphatic ether
(3Z)-Hexenol	0.02	Aliphatic alcohol
Hexanol	0.11	Aliphatic alcohol
Tricyclene	0.03	Monoterpene
α-Thujene	0.13	Monoterpene
α-Pinene	0.26	Monoterpene
α-Fenchene	0.01	Monoterpene
Camphepane	0.18	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Butyl isobutyrate	0.02	Aliphatic ester
Sabinene	0.07	Monoterpene
β-Pinene	0.06	Monoterpene
Octen-3-ol	0.43	Aliphatic alcohol
Octan-3-one	1.81	Aliphatic ketone
Myrcene	0.70	Monoterpene
trans-Dehydroxylinalool oxide	0.03	Monoterpenic ether
Butyl butyrate	0.11	Aliphatic ester
Octan-3-ol	0.46	Aliphatic alcohol
α-Phellandrene	0.05	Monoterpene
Pseudolimonene	0.01	Monoterpene
cis-Dehydroxylinalool oxide	0.01	Monoterpenic ether
Δ3-Carene	0.17	Monoterpene
(3Z)-Hexenyl acetate	0.02	Aliphatic ester
α-Terpinene	0.07	Monoterpene
Hexyl acetate	0.58	Aliphatic ester
meta-Cymene	0.05	Monoterpene
para-Cymene	0.22	Monoterpene
Limonene	0.44	Monoterpene
β-Phellandrene	0.47	Monoterpene
1,8-Cineole	0.79	Monoterpenic ether
Lavender lactone	0.01	Aliphatic lactone
(Z)-β-Ocimene	4.20	Monoterpene
(E)-β-Ocimene	2.32	Monoterpene
γ-Terpinene	0.20	Monoterpene
cis-Sabinene hydrate	0.09	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.21	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol

α-Pinene oxide analog	0.02	Monoterpenic ether
trans-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.12	Monoterpene
para-Cymenene	0.02	Monoterpene
α-Pinene oxide	0.01	Monoterpenic ether
trans-Sabinene hydrate	0.02	Monoterpenic alcohol
Rosefuran	0.10	Monoterpenic ether
Linalool	30.19	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.07	Aliphatic ketone
β-Thujone	0.05	Monoterpenic ketone
Octen-3-yl acetate	1.13	Aliphatic ester
Unknown	0.07	Unknown
Octan-3-yl acetate	0.12	Aliphatic ester
allo-Ocimene	0.08	Monoterpene
(Z)-Myroxide	0.07	Monoterpenic ether
Camphor	0.18	Monoterpenic ketone
cis-Verbenol	0.04	Monoterpenic alcohol
(E)-Myroxide	0.01	Monoterpenic ether
Hexyl isobutyrate	0.10	Aliphatic ester
Borneol	0.63	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.03	Monoterpenic alcohol
Lavandulol	1.29	Monoterpenic alcohol
Terpinen-4-ol	4.61	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	0.08	Alkene
Cryptone	0.22	Normonoterpenic ketone
meta-Cymen-8-ol	0.06	Monoterpenic alcohol
para-Cymen-8-ol	0.08	Monoterpenic alcohol
Butyl hexanoate	0.02	Aliphatic ester
α-Terpineol	1.12	Monoterpenic alcohol
Hodiendiol	0.06	Monoterpenic alcohol
Hexyl butyrate	0.43	Aliphatic ester
Verbenone	0.03	Monoterpenic ketone
Unknown	0.03	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.05	Monoterpenic alcohol
trans-Carveol	0.03	Monoterpenic alcohol
Bornyl formate	0.01	Monoterpenic ester
exo-2-Hydroxycineole	0.03	Monoterpenic alcohol
Nerol	0.21	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.12	Aliphatic ester
Neral	0.03	Monoterpenic aldehyde
Carvone	0.04	Monoterpenic ketone
Hexyl isovalerate	0.02	Aliphatic ester
Linalyl acetate	25.90	Monoterpenic ester
Geraniol	0.45	Monoterpenic alcohol
Geranal	0.05	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Bornyl acetate	0.14	Monoterpenic ester
Cuminol	0.04	Monoterpenic alcohol
Lavandulyl acetate	3.20	Monoterpenic ester
Unknown	0.02	Oxygenated monoterpenes
Hexyl tiglate	0.05	Aliphatic ester
Hodiendiol derivative	0.03	Oxygenated monoterpenes

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Unknown	0.05	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.33	Monoterpenic ester
α -Copaene	0.03	Sesquiterpene
Daucene	0.01	Sesquiterpene
β -Bourbonene	0.08	Sesquiterpene
1,5-diepi- β -Bourbonene	0.01	Sesquiterpene
Geranyl acetate	0.55	Monoterpenic ester
7-epi-Sesquithujene	0.11	Sesquiterpene
β -Elemene	0.04	Sesquiterpene
Hexyl hexanoate	0.11	Aliphatic ester
α -Funebrene	0.01	Sesquiterpene
Isocaryophyllene	0.02	Sesquiterpene
β -Caryophyllene	4.01	Sesquiterpene
α -Santalene	0.53	Sesquiterpene
Lavandulyl isobutyrate	0.04	Monoterpenic ester
Coumarin	0.03	Coumarin
<i>trans</i> - α -Bergamotene	0.17	Sesquiterpene
Sesquisabinene A	0.03	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.05	Sesquiterpene
α -Humulene	0.14	Sesquiterpene
Lavandulyl butyrate?	0.14	Monoterpenic ester
(<i>E</i>)- β -Farnesene	4.26	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.01	Sesquiterpene
Germacrene D	0.52	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	0.04	Sesquiterpene
γ -Cadinene	0.16	Sesquiterpene
Lavandulyl isovalerate	0.04	Monoterpenic ester
Unknown	0.05	Oxygenated sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.05	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.03	Sesquiterpenic alcohol
Dendrolasin	0.05	Sesquiterpenic ether
Caryophyllene oxide	0.40	Sesquiterpenic ether
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Humulene epoxide II	0.02	Sesquiterpenic ether
τ -Cadinol	0.09	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
Phytone	0.01	Terpenic ketone
9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	0.01	Homoditerpene
Consolidated total	98.55%	

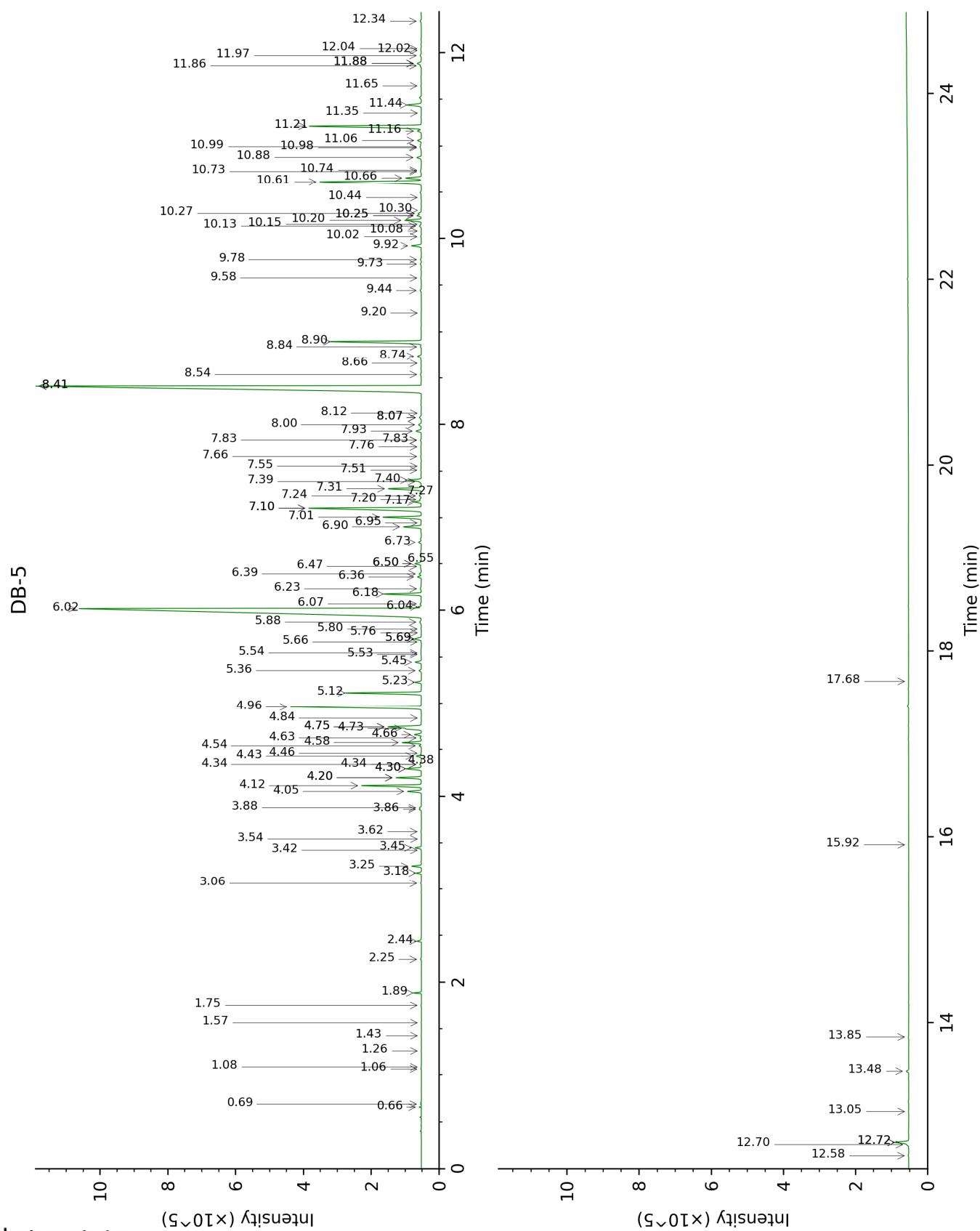
tr: The compound has been detected below 0.005% of total signal.

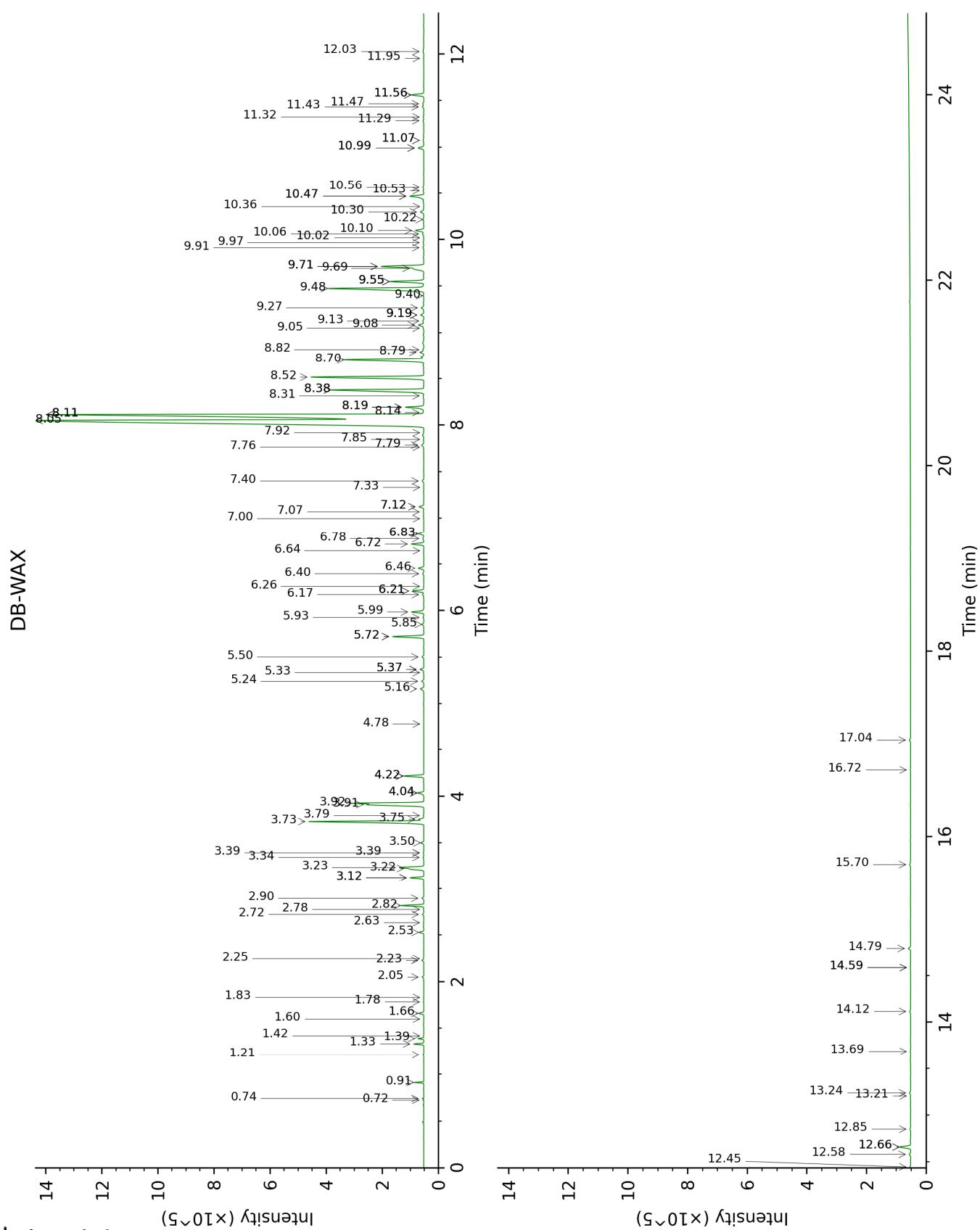
Note: no correction factor was applied

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	%
Isovaleral	0.66	642	0.02	0.74	888	0.02
2-Methylbutyral	0.69	652	0.01	0.72	881	0.01
Isoamyl alcohol	1.06	731	0.01	3.39*	1178	0.03
2-Methylbutanol	1.08	734	0.01	3.39*	1178	[0.03]
Toluene	1.26	758	tr	1.42	1002	0.01
Prenal	1.43	780	0.01	3.12*	1157	0.45
Hexanal	1.57	799	0.01	1.83	1044	tr
Butyl acetate	1.75	816	0.01	1.78	1039	0.01
Methyl hexyl ether	1.88	826	0.17	0.91	921	0.17
(3Z)-Hexenol	2.25	856	0.02	5.72*	1349	1.14
Hexanol	2.44	872	0.11	5.37*	1323	0.13
Tricyclene	3.06	919	0.03	1.21	973	0.02
α -Thujene	3.18	926	0.13	1.39	1000	0.14
α -Pinene	3.25	931	0.26	1.33	993	0.26
α -Fenchene	3.42†	942	0.19	1.60	1021	0.01
Camphepane	3.45†	944	[0.19]	1.66	1027	0.18
Thuja-2,4(10)-diene	3.54	950	0.01	2.25	1086	0.01
Butyl isobutyrate	3.62	955	0.02	2.64	1119	0.01
Sabinene	3.86†	971	0.12	2.23	1084	0.07
β -Pinene	3.88†	972	[0.12]	2.05	1066	0.06
Octen-3-ol	4.05	984	0.43	6.72	1421	0.45
Octan-3-one	4.12	988	1.81	3.91†	1217	4.10
Myrcene	4.20*	993	0.73	2.82	1133	0.70
<i>trans</i> -Dehydroxylinalool oxide	4.20*	993	[0.73]	3.34	1174	0.03
Butyl butyrate	4.30*	1000	0.52	3.50	1187	0.11
Octan-3-ol	4.30*	1000	[0.52]	5.99	1368	0.46
α -Phellandrene	4.34*	1003	0.06	2.72	1126	0.05
Pseudolimonene	4.34*	1003	[0.06]	2.78	1130	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.38	1005	0.01	3.79	1209	0.02
Δ 3-Carene	4.43	1008	0.17	2.53	1110	0.16
(3Z)-Hexenyl acetate	4.46	1010	0.02	4.78	1280	0.01
α -Terpinene	4.54	1015	0.07	2.90	1139	0.07
Hexyl acetate	4.58	1017	0.58	4.22*	1240	0.69
meta-Cymene	4.63	1020	0.05	4.04*	1226	0.26
para-Cymene	4.66	1023	0.22	4.04*	1226	[0.26]
Limonene	4.73†	1027	1.70	3.12*	1157	[0.45]
β -Phellandrene	4.74*†	1028	[1.70]	3.22	1165	0.47
1,8-Cineole	4.74*†	1028	[1.70]	3.23	1166	0.79
Lavender lactone	4.84	1034	0.01	9.13	1606	0.05
(Z)- β -Ocimene	4.96	1042	4.20	3.73†	1204	4.43
(E)- β -Ocimene	5.12	1051	2.32	3.92†	1218	[4.10]
γ -Terpinene	5.23	1058	0.20	3.75†	1206	[4.43]

<i>cis</i> -Sabinene hydrate	5.36	1066	0.09	6.83*	1430	0.23
<i>cis</i> -Linalool oxide (fur.)	5.45	1072	0.21	6.46	1402	0.21
Octanol	5.53	1077	0.02	8.11*†	1527	[56.13]
α -Pinene oxide analog	5.54	1078	0.02	5.34	1320	0.02
<i>trans</i> -Linalool oxide (fur.)	5.66	1085	0.01	6.83*	1430	[0.23]
Terpinolene	5.69*	1087	0.27	4.22*	1240	[0.69]
para-Cymenene	5.69*	1087	[0.27]	6.26	1388	0.02
α -Pinene oxide	5.76	1091	0.01	5.37*	1323	[0.13]
<i>trans</i> -Sabinene hydrate	5.80	1094	0.02	7.85	1506	0.02
Rosefuran	5.88	1099	0.10	5.93	1363	0.03
Linalool	6.02	1108	30.19	8.05†	1522	56.13
(Z)-6-Methyl-3,5-heptadien-2-one	6.04	1109	0.07	8.14	1528	0.02
β -Thujone	6.07	1111	0.05	6.21*	1384	0.42
Octen-3-yl acetate	6.18	1118	1.13	5.72*	1349	[1.14]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	6.23	1121	0.07	9.55*	1640	1.28
Octan-3-yl acetate	6.36	1129	0.12	5.16	1308	0.16
allo-Ocimene	6.39	1132	0.08	5.50	1333	0.07
(Z)-Myroxide	6.47	1137	0.07	6.78	1426	0.06
Camphor	6.50*	1138	0.22	7.12*	1452	0.20
<i>cis</i> -Verbenol	6.50*	1138	[0.22]	9.19*	1611	0.13
(E)-Myroxide	6.55	1141	0.01	7.00	1442	0.01
Hexyl isobutyrate	6.73	1153	0.10	5.24	1314	0.08
Borneol	6.90	1164	0.63	9.71*	1654	1.83
<i>cis</i> -Linalool oxide (pyr.)	6.95	1167	0.03	10.22	1694	0.04
Lavandulol	7.01	1171	1.29	9.55*	1640	[1.28]
Terpinen-4-ol	7.10*	1177	4.69	8.52	1558	4.61
(3E,5Z)-Undeca-1,3,5-triene	7.10*	1177	[4.69]	5.85	1358	0.08
Cryptone	7.17	1181	0.22	9.08	1602	0.24
meta-Cymen-8-ol	7.20	1183	0.06	11.43	1798	0.06
para-Cymen-8-ol	7.24	1185	0.08	11.47	1801	0.05
Butyl hexanoate	7.27	1188	0.02	6.17	1381	0.05
α -Terpineol	7.31	1190	1.12	9.71*	1654	[1.83]
Hodiendiol	7.39	1195	0.06	12.66*	1909	0.47
Hexyl butyrate	7.40	1196	0.43	6.21*	1384	[0.42]
Verbenone	7.51	1203	0.03	9.55*	1640	[1.28]
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.55	1206	0.03	11.07*	1767	0.04
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.66	1213	0.05	11.29	1785	0.04
<i>trans</i> -Carveol	7.76	1220	0.03	11.32	1789	0.03

Bornyl formate	7.83*	1224	0.05	7.92	1512	0.01
exo-2-Hydroxcineole	7.83*	1224	[0.05]	11.56*	1810	0.48
Nerol	7.93	1231	0.21	10.99*	1760	0.24
Hexyl 2-methylbutyrate	8.00	1235	0.12	6.40	1398	0.05
Neral	8.07*	1240	0.10	9.40	1628	0.03
Carvone	8.07*	1240	[0.10]	9.91	1670	0.04
Hexyl isovalerate	8.12	1244	0.02	6.64	1416	0.01
Linalyl acetate	8.41*	1263	26.07	8.11*†	1527	[56.13]
Geraniol	8.41*	1263	[26.07]	11.56*	1810	[0.48]
Geranial	8.54	1271	0.05	10.02	1678	0.01
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.66	1280	0.02	14.59*	2088	0.02
Bornyl acetate	8.74	1285	0.14	8.19*	1533	0.72
Cuminol	8.84	1292	0.04	14.12	2043	0.04
Lavandulyl acetate	8.90	1295	3.20	8.70	1573	3.20
Unknown [m/z 150, 107 (98), 91 (79), 108 (61)]	9.20	1314	0.02	11.95	1844	0.01
Hexyl tiglate	9.44	1331	0.05	8.82	1582	0.04
Hodiendiol derivative	9.58	1341	0.03	12.85	1926	0.03
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.73	1351	0.05	10.99*	1760	[0.24]
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.78	1355	0.04	11.07*	1767	[0.04]
Neryl acetate	9.92	1365	0.33	10.10	1685	0.34
α-Copaene	10.02	1372	0.03	7.07	1448	0.03
Daucene	10.08	1376	0.01	7.12*	1452	[0.20]
β-Bourbonene	10.14	1380	0.08	7.40	1472	0.08
1,5-diepi-β-Bourbonene	10.15	1381	0.01	7.33	1467	0.01
Geranyl acetate	10.20	1384	0.55	10.47*	1716	0.65
7-epi-Sesquithujene	10.25*	1388	0.15	7.79	1501	0.11
β-Elemene	10.25*	1388	[0.15]	8.32†	1542	4.13
Hexyl hexanoate	10.27	1390	0.11	8.79	1579	0.15
α-Funebrene	10.30	1392	0.01	7.76	1500	0.02
Isocaryophyllene	10.44	1402	0.02	8.11*†	1527	[56.13]
β-Caryophyllene	10.61	1414	4.01	8.38*†	1547	[4.13]
α-Santalene	10.66	1418	0.53	8.19*	1533	[0.72]
Lavandulyl isobutyrate	10.73	1423	0.04	9.27	1618	0.13
Coumarin	10.74	1424	0.03	17.04	2339	0.06
trans-α-Bergamotene	10.88	1434	0.17	8.38*†	1547	[4.13]
Sesquisabinene A	10.98	1442	0.03	9.05	1600	0.02

<i>cis</i> - β -Bergamotene?	10.99	1443	0.05			
α -Humulene	11.06	1448	0.14	9.19*	1611	[0.13]
Lavandulyl butyrate?	11.16	1455	0.14	10.47*	1716	[0.65]
(<i>E</i>)- β -Farnesene	11.21	1459	4.26	9.48	1634	4.39
<i>trans</i> -Cadina-1(6),4-diene	11.35	1470	0.01	9.19*	1611	[0.13]
Germacrene D	11.44	1476	0.52	9.69	1652	0.41
Isodaucene	11.65	1491	0.02	9.97	1674	0.04
β -Bisabolene	11.86	1508	0.04	10.06	1682	0.06
γ -Cadinene	11.88*	1510	0.17	10.30	1701	0.16
Lavandulyl isovalerate	11.88*	1510	[0.17]	10.56	1724	0.04
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.97	1516	0.05	13.24	1961	0.05
δ -Cadinene	12.02	1520	0.01	10.36	1706	0.01
β -Sesquiphellandrene	12.04	1522	0.02	10.53	1721	0.03
Isocaryophyllene epoxide B	12.34	1545	0.05	12.03	1851	0.06
(<i>E</i>)-Nerolidol	12.58	1564	0.03	13.69	2002	0.02
Dendrolasin	12.70	1573	0.05	12.45	1888	0.04
Caryophyllene oxide	12.72*	1575	0.51	12.66*	1909	[0.47]
Caryophyllene oxide isomer	12.72*	1575	[0.51]	12.58	1902	0.06
Humulene epoxide II	13.05	1601	0.02	13.21	1958	0.01
τ -Cadinol	13.48	1636	0.09	14.79	2108	0.10
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	13.85	1667	0.02	16.72	2304	0.02
Phytone	15.92	1845	0.01	14.59*	2088	[0.02]
9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	17.68	2009	0.01	15.70	2198	0.05
Total identified	98.15%			98.37%		
Total reported	98.41%			98.44%		

*: 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