

Date : July 07, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21F22-PTH06


Customer identification : Lavender ORGANIC - Greece - L50114207R

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 : Sarah-Eve Tremblay, M. Sc. A., Chimiste

Analysis date : July 06, 2021

Checked and approved by :



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

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid

Refractive index: 1.4624 ± 0.0003 (20 °C; method PC-MAT-016)

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
Methacrolein	tr	Aliphatic aldehyde
3-Buten-2-one	0.01	Aliphatic ketone
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	tr	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Prenal	0.01	Aliphatic aldehyde
Hexanal	tr	Aliphatic aldehyde
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.11	Aliphatic ether
(2E)-Hexenal	tr	Aliphatic aldehyde
(3Z)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.08	Aliphatic alcohol
Unknown	tr	Unknown
Hashishene	tr	Monoterpene
Tricyclene	0.02	Monoterpene
α -Thujene	0.14	Monoterpene
α -Pinene	0.28	Monoterpene
Camphene	0.16	Monoterpene
α -Fenchene	0.01	Monoterpene
Thuja-2,4(10)-diene	tr	Monoterpene
Butyl isobutyrate	0.01	Aliphatic ester
endo-Isocamphane	tr	Monoterpene
β -Pinene	0.04	Monoterpene
Sabinene	0.04	Monoterpene
Octen-3-ol	0.23	Aliphatic alcohol
Octan-3-one	0.95	Aliphatic ketone
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.66	Monoterpene
Butyl butyrate	0.11	Aliphatic ester
Octan-3-ol	0.19	Aliphatic alcohol
α -Phellandrene	0.04	Monoterpene
Δ^3 -Carene	0.13	Monoterpene
(3Z)-Hexenyl acetate	tr	Aliphatic ester
α -Terpinene	0.05	Monoterpene
Hexyl acetate	0.56	Aliphatic ester
ortho-Cymene	0.04	Monoterpene
para-Cymene	0.22	Monoterpene
Limonene	0.32	Monoterpene
β -Phellandrene	0.14	Monoterpene
1,8-Cineole	0.81	Monoterpenic ether
Lavender lactone	0.01	Aliphatic lactone

(Z)-β-Ocimene	5.83	Monoterpene
(E)-β-Ocimene	3.02	Monoterpene
γ-Terpinene	0.19	Monoterpene
cis-Sabinene hydrate	0.07	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.13	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.)	0.06	Monoterpenic alcohol
Rosefuran	0.05	Monoterpenic ether
Linalool	31.78	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
β-Thujone	0.04	Monoterpenic ketone
Octen-3-yl acetate	0.04	Aliphatic ester
Unknown	0.84	Unknown
α-Campholenal	0.04	Monoterpenic aldehyde
Octan-3-yl acetate	0.10	Aliphatic ester
allo-Ocimene	0.06	Monoterpene
(Z)-Myroxide	0.03	Monoterpenic ether
Camphor	0.29	Monoterpenic ketone
(E)-Myroxide	0.02	Monoterpenic ether
Hexyl isobutyrate	tr	Aliphatic ester
Nerol oxide	tr	Aliphatic ether
Borneol	0.55	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Lavandulol	0.85	Monoterpenic alcohol
Terpinen-4-ol	5.44	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	tr	Alkene
meta-Cymen-8-ol	0.06	Monoterpenic alcohol
Cryptone	0.14	Normonoterpenic ketone
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α-Terpineol	1.14	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Hodiendiol	0.02	Monoterpenic alcohol
Hexyl butyrate	0.39	Aliphatic ester
Verbenone	0.02	Monoterpenic ketone
Unknown	0.03	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol
7-Methyl-2-octyl acetate	tr	Aliphatic ester
trans-Carveol	0.02	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
Nerol	0.18	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.06	Aliphatic ester
Carvone	0.03	Monoterpenic ketone
Neral	0.03	Monoterpenic aldehyde
Hexyl isovalerate	0.01	Aliphatic ester
Geraniol	0.45	Monoterpenic alcohol
Linalyl acetate	27.61	Monoterpenic ester
Geranial	0.01	Monoterpenic aldehyde
Bornyl acetate	0.08	Monoterpenic ester
Cuminol	0.01	Monoterpenic alcohol

Lavandulyl acetate	3.42	Monoterpenic ester
Hexyl tiglate	0.04	Aliphatic ester
Hodiendiol derivative	0.03	Oxygenated monoterpene
Unknown	0.03	Oxygenated monoterpene
Unknown	0.02	Oxygenated monoterpene
Neryl acetate	0.30	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
7-Cubebene	0.01	Sesquiterpene
β -Bourbonene	0.03	Sesquiterpene
Geranyl acetate	0.55	Monoterpenic ester
Hexyl hexanoate	0.08	Aliphatic ester
7-epi-Sesquithujene	0.08	Sesquiterpene
β -Elemene	tr	Sesquiterpene
Isocaryophyllene	0.02	Sesquiterpene
Sesquithujene	0.03	Sesquiterpene
β -Caryophyllene	3.25	Sesquiterpene
α -Santalene	0.41	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.14	Sesquiterpene
Sesquisabinene A	0.01	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.07	Sesquiterpene
α -Humulene	0.10	Sesquiterpene
Lavandulyl butyrate?	0.11	Monoterpenic ester
(<i>E</i>)- β -Farnesene	2.76	Sesquiterpene
Germacrene D	0.27	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.07	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	tr	Sesquiterpene
γ -Cadinene	0.10	Sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
δ -Cadinene	0.02	Sesquiterpene
β -Sesquiphellandrene	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.05	Sesquiterpenic ether
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
Caryophyllene oxide	0.22	Sesquiterpenic ether
τ -Cadinol	0.04	Sesquiterpenic alcohol
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
<i>cis</i> -14-nor-Muurool-5-en-4-one?	0.01	Norsesquiterpenic ketone
Herniarin	0.02	Coumarin
Consolidated total	97.98%	

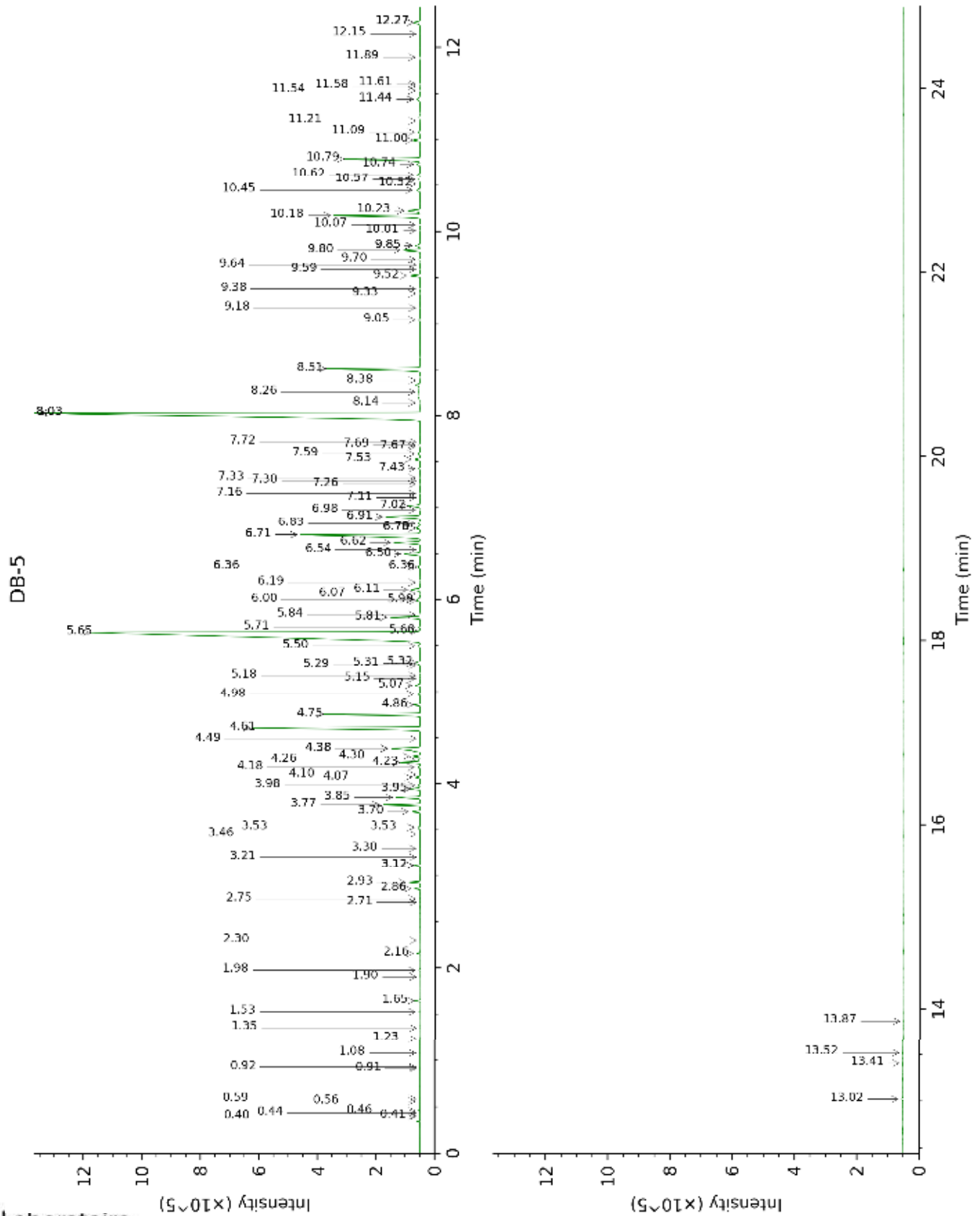
tr: The compound has been detected below 0.005% of total signal.

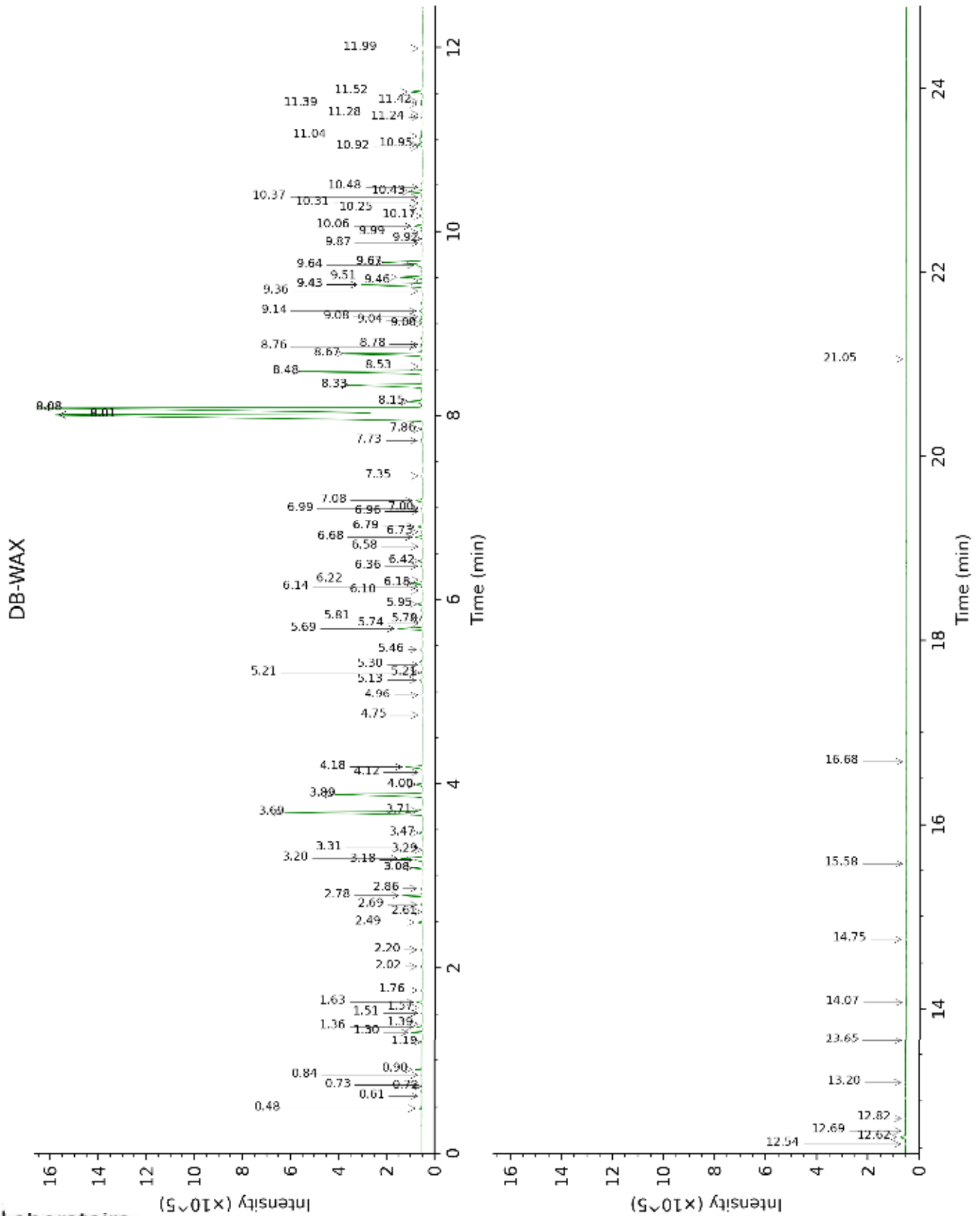
Note: no correction factor was applied

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	540	tr	0.48	783	0.04
Methacrolein	0.41	551	tr	0.62	842	tr
3-Buten-2-one	0.44	577	0.01	0.84	911	0.01
2-Methyl-3-buten-2-ol	0.46	597	tr	1.51*	1014	0.02
Isovaleral	0.56	642	tr	0.73	887	0.01
2-Methylbutylal	0.59	653	tr	0.72	882	tr
Isoamyl alcohol	0.91	732	tr	3.31*	1176	0.01
2-Methylbutanol	0.92	735	tr	3.31*	1176	[0.01]
Toluene	1.08	758	0.01	1.39	1002	0.01
Prenal	1.23	781	0.01	3.08*	1158	0.33
Hexanal	1.35	799	tr	1.76*	1039	0.03
Butyl acetate	1.53	816	0.02	1.76*	1039	[0.03]
Methyl hexyl ether	1.65	827	0.11	0.90	921	0.11
(2E)-Hexenal	1.90	849	tr	3.29	1174	tr
(3Z)-Hexenol	1.98	855	0.03	5.69*	1350	0.90
Hexanol	2.16	871	0.08	5.21*	1316	0.08
Unknown [m/z 59, 85 (88), 41 (57), 43 (43)...]	2.30	883	tr	5.78	1357	tr
Hashishene	2.71	916	tr	1.30*	991	0.28
Tricyclene	2.75	918	0.02	1.19	971	0.02
α -Thujene	2.86	926	0.14	1.36	998	0.13
α -Pinene	2.93	930	0.28	1.30*	991	[0.28]
Camphene	3.12*	943	0.16	1.63	1026	0.16
α -Fenchene	3.12*	943	[0.16]	1.57	1020	0.01
Thuja-2,4(10)-diene	3.21	949	tr	2.20*	1084	0.05
Butyl isobutyrate	3.30	956	0.01	2.61	1120	0.01
endo-Isocamphane	3.46	966	tr	1.51*	1014	[0.02]
β -Pinene	3.53*	971	0.09	2.02	1065	0.04
Sabinene	3.53*	971	[0.09]	2.20*	1084	[0.05]
Octen-3-ol	3.70	983	0.23	6.68*	1422	0.23
Octan-3-one	3.78*	988	1.02	3.89*	1221	3.97
6-Methyl-5-hepten-2-one	3.78*	988	[1.02]	4.96	1297	0.01
Myrcene	3.85	993	0.66	2.78	1134	0.65
Butyl butyrate	3.95*	999	0.28	3.47	1189	0.11
Octan-3-ol	3.95*	999	[0.28]	5.95	1369	0.19
α -Phellandrene	3.98	1002	0.04	2.69	1126	0.04
Δ 3-Carene	4.07	1008	0.13	2.49	1110	0.13
(3Z)-Hexenyl acetate	4.10	1010	tr	4.74	1286	tr
α -Terpinene	4.18	1014	0.05	2.86	1140	0.06
Hexyl acetate	4.23	1018	0.56	4.18*	1243	0.65
ortho-Cymene	4.26	1020	0.04	4.00*	1229	0.25
para-Cymene	4.30	1022	0.22	4.00*	1229	[0.25]
Limonene	4.38*†	1027	1.28	3.08*	1158	[0.33]
β -Phellandrene	4.38*†	1027	[1.28]	3.18	1166	0.14

1,8-Cineole	4.38*†	1027	[1.28]	3.20	1167	0.81
Lavender lactone	4.49	1034	0.01	9.08	1606	0.04
(Z)-β-Ocimene	4.61	1042	5.83	3.69	1207	5.83
(E)-β-Ocimene	4.75	1051	3.02	3.89*	1221	[3.97]
γ-Terpinene	4.86	1058	0.19	3.71	1208	0.10
cis-Sabinene hydrate	4.98	1065	0.07	6.79*	1431	0.17
cis-Linalool oxide (fur.)	5.07	1071	0.13	6.42	1403	0.13
Octanol	5.15	1076	0.02	8.08*†	1528	[59.49]
α-Pinene oxide analog	5.18	1078	0.02	5.30	1322	0.02
Isoterpinolene	5.29	1085	0.01	4.12	1239	0.01
Terpinolene	5.31†	1086	0.20	4.18*	1243	[0.65]
trans-Linalool oxide (fur.)	5.32†	1087	[0.20]	6.79*	1431	[0.17]
Rosefuran	5.50	1099	0.05	5.81	1359	0.05
Linalool	5.65	1108	31.78	8.01*†	1522	59.49
(Z)-6-Methyl-3,5-heptadien-2-one	5.66	1109	0.03	8.08*†	1528	[59.49]
β-Thujone	5.71	1112	0.04	6.14	1383	0.04
Octen-3-yl acetate	5.81*	1119	0.89	5.69*	1350	[0.90]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.81*	1119	[0.89]	9.51	1640	0.84
α-Campholenal	5.84	1121	0.04	6.79*	1431	[0.17]
Octan-3-yl acetate	5.99	1131	0.10	5.13	1310	0.12
allo-Ocimene	6.00	1131	0.06	5.46	1334	0.07
(Z)-Myroxide	6.07	1135	0.03	6.73	1426	0.04
Camphor	6.11	1138	0.29	7.08	1452	0.27
(E)-Myroxide	6.19	1143	0.02	6.96	1443	0.02
Hexyl isobutyrate	6.36*	1154	0.09	5.21*	1316	[0.08]
Nerol oxide	6.36*	1154	[0.09]	6.68*	1422	[0.23]
Borneol	6.50	1163	0.55	9.67*	1653	1.75
cis-Linalool oxide (pyr.)	6.54	1166	0.01	10.17	1694	0.02
Lavandulol	6.62	1171	0.85	9.43*	1634	2.82
Terpinen-4-ol	6.71*	1177	5.51	8.48	1559	5.44
(3E,5Z)-Undeca-1,3,5-triene	6.71*	1177	[5.51]	5.74	1354	tr
meta-Cymen-8-ol	6.78*	1182	0.16	11.39	1797	0.06
Cryptone	6.78*	1182	[0.16]	9.04	1602	0.14
para-Cymen-8-ol	6.83	1185	0.05	11.42	1800	0.05
α-Terpineol	6.91*	1190	1.15	9.67*	1653	[1.75]
Myrtenal	6.91*	1190	[1.15]	8.53	1563	0.01
Hodiendiol	6.98	1195	0.02	12.69	1912	0.02
Hexyl butyrate	7.02	1198	0.39	6.18	1385	0.36
Verbenone	7.11	1204	0.02	9.46	1637	0.01
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.16	1206	0.03	6.10	1380	0.01

(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.26	1213	0.03	11.24	1785	0.04
7-Methyl-2-octyl acetate	7.30	1216	tr	6.22	1388	0.01
<i>trans</i> -Carveol	7.33	1218	0.02	11.28	1788	0.02
Bornyl formate	7.43	1225	0.05	7.86	1510	0.06
Nerol	7.53	1232	0.18	10.95	1760	0.23
Hexyl 2-methylbutyrate	7.59	1236	0.06	6.36	1399	0.04
Carvone	7.67	1241	0.03	9.87	1670	0.03
Neral	7.69	1243	0.03	9.36	1628	0.02
Hexyl isovalerate	7.72	1245	0.01	6.58	1415	tr
Geraniol	8.03*	1266	28.33	11.52	1809	0.45
Linalyl acetate	8.03*	1266	[28.33]	8.08*†	1528	[59.49]
Geranial	8.14	1274	0.01	9.99	1679	0.01
Bornyl acetate	8.26	1282	0.08	8.16*	1534	0.60
Cuminol	8.38	1290	0.01	14.07	2042	0.02
Lavandulyl acetate	8.51	1299	3.42	8.67	1574	3.44
Hexyl tiglate	9.05	1333	0.04	8.78	1582	0.04
Hodiendiol derivative	9.18	1342	0.03	12.82	1925	0.03
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.33	1353	0.03	10.92	1758	0.01
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.38	1357	0.02	11.04	1768	0.08
Neryl acetate	9.52	1367	0.30	10.06*	1685	0.31
α -Copaene	9.59	1372	0.01	7.00	1446	0.02
7-Cubebene	9.64	1375	0.01	6.99	1446	0.03
β -Bourbonene	9.70	1379	0.03	7.35	1472	0.04
Geranyl acetate	9.80	1386	0.55	10.43	1716	0.54
Hexyl hexanoate	9.85*	1390	0.15	8.76	1580	0.08
7-epi-Sesquithujene	9.85*	1390	[0.15]	7.73	1501	0.08
β -Elemene	9.85*	1390	[0.15]	8.33*	1547	3.30
Isocaryophyllene	10.01	1401	0.02	8.01*†	1522	[59.49]
Sesquithujene	10.07	1406	0.03	8.01*†	1522	[59.49]
β -Caryophyllene	10.18	1414	3.25	8.33*	1547	[3.30]
α -Santalene	10.23	1417	0.41	8.16*	1534	[0.60]
<i>trans</i> - α -Bergamotene	10.45	1434	0.14	8.33*	1547	[3.30]
Sesquisabinene A	10.52	1439	0.01	9.00	1599	0.02
<i>cis</i> - β -Bergamotene?	10.57	1443	0.07			
α -Humulene	10.62	1447	0.10	9.14	1611	0.10
Lavandulyl butyrate?	10.74	1456	0.11	10.37	1711	0.02
(<i>E</i>)- β -Farnesene	10.79	1460	2.76	9.43*	1634	[2.82]
Germacrene D	11.00	1475	0.27	9.64	1651	0.22

<i>trans</i> -β-Bergamotene	11.08	1482	0.07	9.43*	1634	[2.82]
Isodaucene	11.21	1491	0.02	9.92	1674	0.01
β-Bisabolene	11.44*	1508	0.15	10.06*	1685	[0.31]
γ-Cadinene	11.44*	1508	[0.15]	10.25	1700	0.10
Unknown [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	11.54	1516	0.03	13.20	1960	0.03
δ-Cadinene	11.58	1520	0.02	10.31	1706	0.01
β-Sesquiphellandrene	11.61	1522	0.02	10.48	1720	0.02
Isocaryophyllene epoxide B	11.89	1544	0.05	11.99	1850	0.02
(<i>E</i>)-Nerolidol	12.15	1564	0.02	13.65	2002	0.01
Caryophyllene oxide isomer	12.27*	1574	0.28	12.54	1899	0.04
Caryophyllene oxide	12.27*	1574	[0.28]	12.62	1906	0.22
τ-Cadinol	13.02	1635	0.04	14.75	2108	0.06
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5β-ol	13.41	1667	0.02	16.68	2305	0.01
<i>cis</i> -14-nor-Muurool-5-en-4-one?	13.52	1676	0.01	15.58	2190	0.01
Herniarin	13.87	1705	0.02	21.05	2809	tr
Total identified		98.38%			96.86%	
Total reported		98.49%			97.84%	

*: 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