

Date : 2024-01-26

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24A19-PTH01

Customer Identification : Lavender Fine - France - LK0107R

Type : Essential Oil

Source : *Lavandula angustifolia*

Customer : Plant Therapy

Checked and approved by:

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. 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.

GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

***ISO**

Results : See analysis summary (next page)

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

Date : 2024-01-23

PHYSICOCHEMICAL DATA

Refractive index : 1.4608 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cindy Caron B. Sc.

Date : 2024-01-23

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	0.01	Aliphatic alcohol
Methacrolein	tr	Aliphatic aldehyde
3-Buten-2-one	0.01	Aliphatic ketone
Ethyl acetate	tr	Aliphatic ester
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isoamyl alcohol	tr	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Prenal	0.01	Aliphatic aldehyde
Butyl acetate	0.02	Aliphatic ester
Methyl hexyl ether	0.06	Aliphatic ether
(3Z)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.05	Aliphatic alcohol
Tricyclene	0.02	Monoterpene
α -Thujene	0.10	Monoterpene
α -Pinene	0.17	Monoterpene
Camphene	0.17	Monoterpene
α -Fenchene	0.01	Monoterpene
5,5-Dimethyl-2(5H)-furanone	0.01	Aliphatic lactone
Butyl isobutyrate	0.01	Aliphatic ester
Sabinene	0.05	Monoterpene
β -Pinene	0.09	Monoterpene
Octen-3-ol	0.35	Aliphatic alcohol
Octan-3-one	1.43	Aliphatic ketone
Dehydro-1,8-cineole	0.02	Monoterpenic ether
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.48	Monoterpene
Butyl butyrate	0.11	Aliphatic ester
Octan-3-ol	0.07	Aliphatic alcohol
α -Phellandrene	0.03	Monoterpene
Pseudolimonene	0.01	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
Δ^3 -Carene	0.33	Monoterpene
(3Z)-Hexenyl acetate	0.02	Aliphatic ester
α -Terpinene	0.02	Monoterpene
Hexyl acetate	0.41	Aliphatic ester
<i>meta</i> -Cymene	0.08	Monoterpene
<i>para</i> -Cymene	0.26	Monoterpene
β -Phellandrene	0.15	Monoterpene
Limonene	0.38	Monoterpene
1,8-Cineole	0.95	Monoterpenic ether

Lavender lactone	0.01	Aliphatic lactone
(Z)- β -Ocimene	3.57	Monoterpene
(E)- β -Ocimene	1.14	Monoterpene
γ -Terpinene	0.07	Monoterpene
<i>cis</i> -Sabinene hydrate	0.06	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.13	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
α -Pinene oxide analog	0.06	Monoterpenic ether
Isoterpinolene	0.02	Monoterpene
Terpinolene	0.06	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.10	Monoterpenic alcohol
Rosefuran	0.03	Monoterpenic ether
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	35.48	Monoterpenic alcohol
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
β -Thujone	0.04	Monoterpenic ketone
Octen-3-yl acetate	1.06	Aliphatic ester
Unknown	0.05	Unknown
Octan-3-yl acetate	0.04	Aliphatic ester
allo-Ocimene	0.07	Monoterpene
(Z)-Myroxide	0.04	Monoterpenic ether
Camphor	0.23	Monoterpenic ketone
neo-allo-Ocimene	0.01	Monoterpene
(E)-Myroxide	0.05	Monoterpenic ether
Hexyl isobutyrate	0.05	Aliphatic ester
Nerol oxide	0.01	Aliphatic ether
Borneol	0.83	Monoterpenic alcohol
Lavandulol	0.84	Monoterpenic alcohol
(3E,5Z)-Undeca-1,3,5-triene	0.05	Alkene
Terpinen-4-ol	2.64	Monoterpenic alcohol
Cryptone	0.18	Normoterpenic ketone
<i>meta</i> -Cymen-8-ol	0.09	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	0.08	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
α -Terpineol	0.67	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.37	Monoterpenic alcohol
Hexyl butyrate	0.03	Aliphatic ester
Verbenone	0.03	Monoterpenic ketone
Unknown	0.03	Unknown
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol
Octyl acetate	0.01	Aliphatic ester
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
Bornyl formate	0.05	Monoterpenic ester
Nerol	0.13	Monoterpenic alcohol

Hexyl 2-methylbutyrate	0.03	Aliphatic ester
Cuminal	0.04	Monoterpenic aldehyde
Neral	0.03	Monoterpenic aldehyde
Carvone	0.05	Monoterpenic ketone
Hexyl isovalerate	0.01	Aliphatic ester
Linalyl acetate	34.48	Monoterpenic ester
Geraniol	0.35	Monoterpenic alcohol
Geranial	0.03	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.02	Monoterpenic alcohol
Bornyl acetate	0.10	Monoterpenic ester
Lavandulyl acetate	3.00	Monoterpenic ester
Thymol	0.05	Monoterpenic alcohol
Unknown	0.01	Oxygenated monoterpene
Hexyl tiglate	0.03	Aliphatic ester
Hodiendiol derivative	0.04	Oxygenated monoterpene
α -Terpinyl acetate	0.01	Monoterpenic ester
Unknown	0.04	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.25	Monoterpenic ester
α -Copaene	0.03	Sesquiterpene
β -Bourbonene	0.02	Sesquiterpene
Geranyl acetate	0.43	Monoterpenic ester
β -Elemene	0.05	Sesquiterpene
7-epi-Sesquithujene	0.03	Sesquiterpene
Hexyl hexanoate	0.03	Aliphatic ester
Sesquithujene	0.04	Sesquiterpene
β -Caryophyllene	2.43	Sesquiterpene
α -Santalene	0.34	Sesquiterpene
Lavandulyl isobutyrate	0.05	Monoterpenic ester
<i>trans</i> - α -Bergamotene	0.10	Sesquiterpene
Sesquisabinene A	0.01	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.03	Sesquiterpene
α -Humulene	0.09	Sesquiterpene
Lavandulyl butyrate?	0.07	Monoterpenic ester
(<i>E</i>)- β -Farnesene	0.91	Sesquiterpene
Dauca-5,8-diene?	0.02	Sesquiterpene
Germacrene D	0.30	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.04	Sesquiterpene
Isodaucene	0.02	Sesquiterpene
β -Bisabolene	0.03	Sesquiterpene
γ -Cadinene	0.10	Sesquiterpene
Lavandulyl isovalerate	0.01	Monoterpenic ester
Unknown	0.05	Oxygenated sesquiterpene
δ -Cadinene	0.03	Sesquiterpene
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether

Caryophyllene oxide	0.46	Sesquiterpenic ether
Caryophyllene oxide isomer	0.07	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
τ -Cadinol	0.10	Sesquiterpenic alcohol
(3Z)-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
α -Bisabolol	0.01	Sesquiterpenic alcohol
Consolidated total	99.04	

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

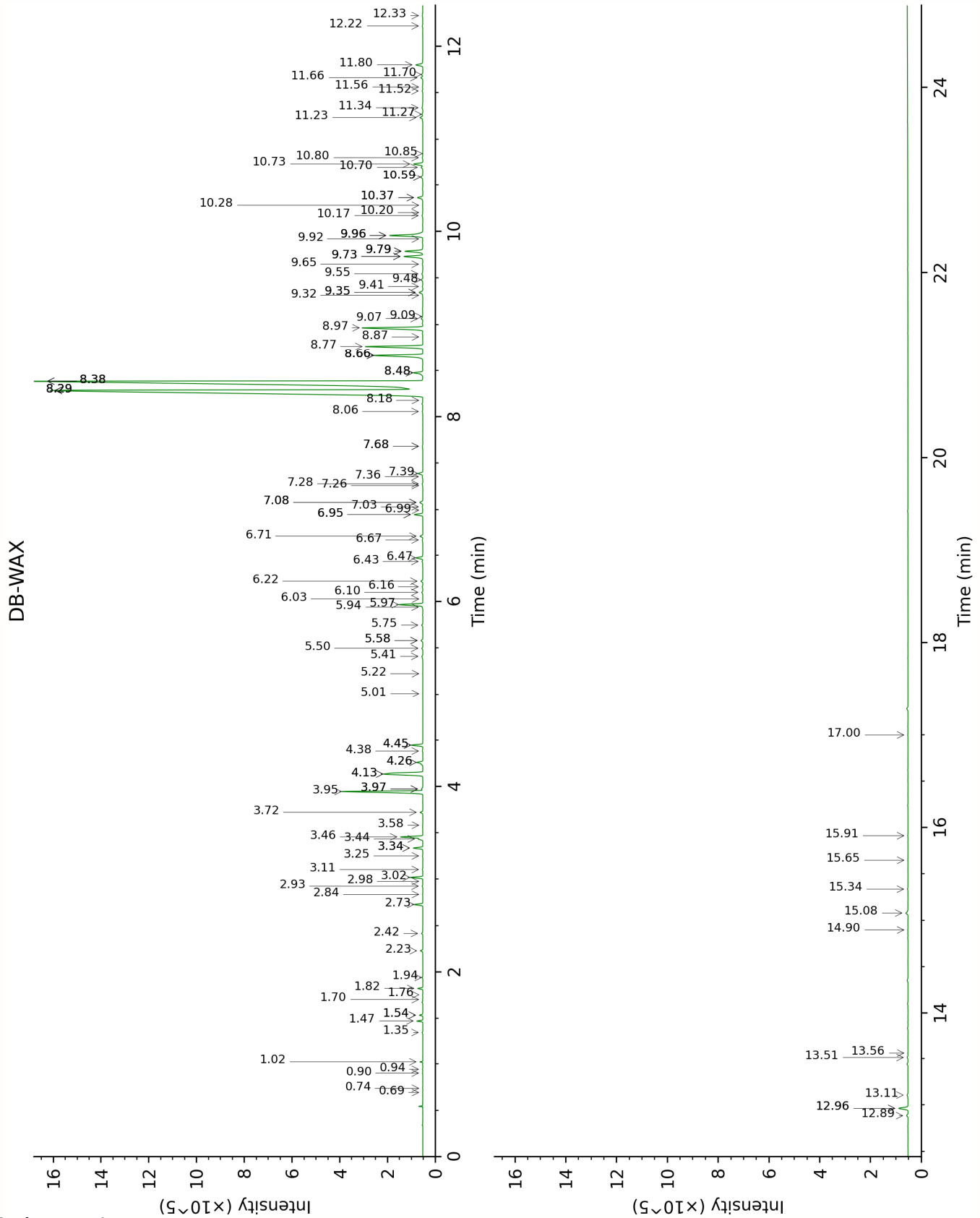
Note: no correction factor was applied

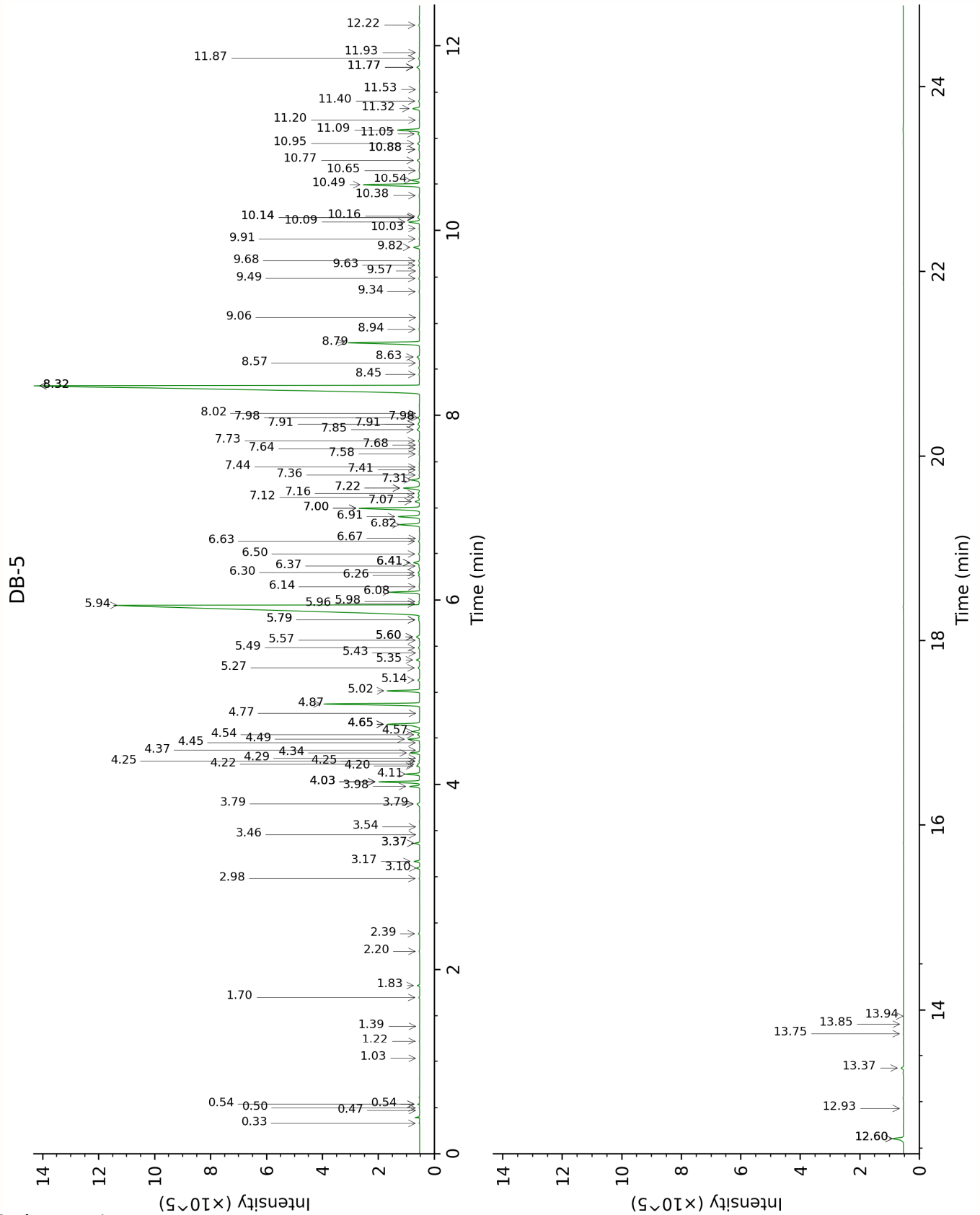
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Ethanol	Column DB-WAX			Column DB-5		
	0.90	904.5	0.01	0.33	500.2	0.01
Methacrolein	0.69	839.3	tr	0.47	550.7	tr
3-Buten-2-one	0.94	910.6	0.01	0.50	573.5	0.01
Ethyl acetate	0.74	854.3	tr	0.54*	606.0	[0.03]
2-Methyl-3-buten-2-ol	1.70	1015.7	0.01	0.54*	606.0	[0.03]
Isoamyl alcohol	3.58	1174.6	0.01	1.03	732.8	tr
Toluene	1.54*	999.8	[0.11]	1.22	758.9	0.01
Prenal	3.34*	1155.9	[0.39]	1.39	781.4	0.01
Butyl acetate	1.94	1038.1	0.02	1.70	816.5	0.02
Methyl hexyl ether	1.02	922.8	0.06	1.83	827.1	0.06
(3Z)-Hexenol	5.94	1345.5	0.02	2.20	857.4	0.03
Hexanol	5.58*	1319.8	[0.09]	2.39	872.9	0.05
Tricyclene	1.35	971.6	0.02	2.98	918.5	0.02
α -Thujene	1.54*	999.8	[0.11]	3.10	926.0	0.10
α -Pinene	1.47	990.4	0.18	3.17	930.7	0.17
Camphene	1.82	1027.0	0.17	3.36*	943.6	[0.18]
α -Fenchene	1.76	1020.5	0.01	3.36*	943.6	[0.18]
5,5-Dimethyl-2(5H)-furanone	8.66*	1546.9	[2.49]	3.46	949.7	0.01
Butyl isobutyrate	2.84	1118.0	0.01	3.54	955.3	0.01
Sabinene	2.42	1082.9	0.05	3.79*	971.5	[0.14]
β -Pinene	2.23	1065.3	0.09	3.79*	971.5	[0.14]
Octen-3-ol	6.95*	1418.0	[0.37]	3.98	984.0	0.35
Octan-3-one	4.14*	1215.3	[2.57]	4.03*	987.3	[1.43]
Dehydro-1,8-cineole	3.25	1149.5	0.02	4.03*	987.3	[1.43]
6-Methyl-5-hepten-2-one	5.22	1292.8	0.01	4.03*	987.3	[1.43]
Myrcene	3.02	1131.9	0.47	4.11	992.8	0.48
Butyl butyrate	3.72	1185.1	0.11	4.20	998.5	0.11
Octan-3-ol	6.22	1365.5	0.08	4.22	999.7	0.07
α -Phellandrene	2.93	1124.7	0.03	4.25*	1001.9	[0.03]
Pseudolimonene	2.98	1128.7	0.01	4.25*	1001.9	[0.03]
<i>cis</i> -Dehydroxylinalool oxide	3.97*	1203.8	[0.07]	4.28	1004.1	0.01
Δ^3 -Carene	2.73	1109.8	0.33	4.34	1007.6	0.33
(3Z)-Hexenyl acetate	5.01	1277.3	0.01	4.37	1009.5	0.02
α -Terpinene	3.11	1138.3	0.02	4.45	1014.5	0.02
Hexyl acetate	4.45*	1237.4	[0.47]	4.49	1016.9	0.41

<i>meta</i> -Cymene	4.26*	1224.2	[0.27]	4.54	1019.9	0.08
<i>para</i> -Cymene	4.26*	1224.2	[0.27]	4.57	1022.1	0.26
β -Phellandrene	3.44	1163.3	0.15	4.65*	1027.0	[1.47]
Limonene	3.34*	1155.9	[0.39]	4.65*	1027.0	[1.47]
1,8-Cineole	3.46	1165.0	0.95	4.65*	1027.0	[1.47]
Lavender lactone	9.41	1604.7	0.03	4.77	1034.4	0.01
(Z)- β -Ocimene	3.95	1201.9	3.59	4.87	1040.7	3.57
(E)- β -Ocimene	4.14*	1215.3	[2.57]	5.02	1050.1	1.14
γ -Terpinene	3.97*	1203.8	[0.07]	5.14	1057.3	0.07
<i>cis</i> -Sabinene hydrate	7.08*	1427.7	[0.16]	5.27	1065.6	0.06
<i>cis</i> -Linalool oxide (fur.)	6.71	1400.2	0.13	5.35	1070.9	0.13
Octanol	8.38*†	1525.3	[34.29]	5.43	1075.6	0.01
α -Pinene oxide analog	5.58*	1319.8	[0.09]	5.48	1079.1	0.06
Isoterpinolene	4.38	1232.9	0.03	5.57	1084.2	0.02
Terpinolene	4.45*	1237.4	[0.47]	5.60*	1086.5	[0.16]
<i>trans</i> -Linalool oxide (fur.)	7.08*	1427.7	[0.16]	5.60*	1086.5	[0.16]
Rosefuran	6.16	1361.2	0.03	5.79*	1097.9	[0.06]
<i>trans</i> -Sabinene hydrate	8.18	1509.4	0.01	5.79*	1097.9	[0.06]
Linalool	8.29*†	1517.7	[35.56]	5.94	1107.9	35.48
(Z)-6-Methyl-3,5-heptadien-2-one	8.38*†	1525.3	[34.29]	5.96	1108.8	0.03
β -Thujone	6.47	1383.5	0.32	5.98	1110.5	0.04
Octen-3-yl acetate	5.97	1347.5	1.04	6.08	1116.9	1.06
Unknown LAAN I [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	9.79*	1635.3	[0.89]	6.14	1120.6	0.05
Octan-3-yl acetate	5.41	1307.6	0.05	6.26	1128.4	0.04
allo-Ocimene	5.75	1331.6	0.05	6.30	1130.4	0.07
(Z)-Myroxide	7.03	1424.2	0.03	6.37	1134.9	0.04
Camphor	7.39	1450.7	0.23	6.40*	1137.3	[0.28]
neo-allo-Ocimene	6.03	1351.8	0.01	6.40*	1137.3	[0.28]
(E)-Myroxide	7.28	1442.4	0.03	6.50	1143.2	0.05
Hexyl isobutyrate	5.50	1313.8	0.05	6.64	1152.0	0.05
Nerol oxide	6.99	1421.4	0.01	6.67	1153.9	0.01
Borneol	9.96*	1648.9	[1.77]	6.82	1163.4	0.83
Lavandulol	9.79*	1635.3	[0.89]	6.91	1169.5	0.84
(3E,5Z)-Undeca-1,3,5-triene	6.10	1356.9	0.05	7.00*	1175.2	[2.69]

Terpinen-4-ol	8.77	1554.7	2.64	7.00*	1175.2	[2.69]
Cryptone	9.35*	1599.6	[0.20]	7.07	1179.8	0.18
<i>meta</i> -Cymen-8-ol	11.66	1790.7	0.09	7.12	1182.8	0.09
<i>para</i> -Cymen-8-ol	11.70	1793.6	0.06	7.16	1185.4	0.08
Myrtenal	8.87	1562.7	0.01	7.22*	1189.1	[0.68]
α -Terpineol	9.96*	1648.9	[1.77]	7.22*	1189.1	[0.68]
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	12.96*	1905.6	[0.48]	7.31	1194.7	0.37
Hexyl butyrate	6.43	1380.7	0.04	7.36	1198.1	0.03
Verbenone	9.79*	1635.3	[0.89]	7.41	1201.6	0.03
Unknown SASC VII [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...] (3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.68*	1472.4	[0.04]	7.44	1203.5	0.03
Octyl acetate	11.52	1778.6	0.04	7.58	1212.9	0.03
<i>trans</i> -Carveol	7.26	1441.1	0.01	7.64	1216.6	0.01
Bornyl formate	11.56	1782.3	0.02	7.68	1219.4	0.02
Nerol	8.29*†	1517.7	[35.56]	7.73	1222.5	0.05
Hexyl 2-methylbutyrate	11.24	1754.5	0.14	7.85	1230.5	0.13
Cuminal	6.67	1397.2	0.03	7.91*	1234.4	[0.09]
Neral	10.80	1717.9	0.04	7.91*	1234.4	[0.09]
Carvone	9.65	1624.0	0.03	7.98*	1239.1	[0.06]
Hexyl isovalerate	10.17	1666.2	0.05	7.98*	1239.1	[0.06]
Linalyl acetate	6.95*	1418.0	[0.37]	8.02	1242.2	0.01
Geraniol	8.38*†	1525.3	[34.29]	8.32*	1262.2	[34.82]
Geranial	11.80	1802.6	0.35	8.32*	1262.2	[34.82]
2,6-Dimethyl-1,7-octadiene-3,6-diol	10.28	1675.1	0.02	8.44	1270.4	0.03
Bornyl acetate	14.90	2087.0	0.02	8.57	1278.6	0.02
Lavandulyl acetate	8.48*	1532.3	[0.46]	8.63	1282.9	0.10
Thymol	8.97	1570.2	2.97	8.80	1293.7	3.00
Unknown CUSE IV [m/z 150, 107 (98), 91 (79), 108 (61)]	15.34	2130.6	0.03	8.94	1303.4	0.05
Hexyl tiglate	12.22	1839.6	0.03	9.06	1312.1	0.01
Hodiendiol derivative	9.09	1579.6	0.02	9.34	1331.8	0.03
α -Terpinyl acetate	13.11	1918.8	0.05	9.49	1341.9	0.04
Unknown SASC II	9.92	1645.9	0.01	9.57	1347.5	0.01
	11.27	1757.4	0.04	9.63	1351.9	0.04

[m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]						
Unknown SASC III [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	11.34	1763.3	0.04	9.68	1355.2	0.04
Neryl acetate	10.36*	1681.8	[0.28]	9.82	1365.5	0.25
α -Copaene	7.36	1448.2	0.04	9.91	1371.8	0.03
β -Bourbonene	7.68*	1472.4	[0.04]	10.02	1379.8	0.02
Geranyl acetate	10.73	1712.2	0.43	10.09	1384.7	0.43
β -Elemene	8.66*	1546.9	[2.49]	10.14*	1388.1	[0.08]
7-epi-Sesquithujene	8.06	1500.2	0.03	10.14*	1388.1	[0.08]
Hexyl hexanoate	9.07	1577.8	0.08	10.16	1389.0	0.03
Sesquithujene	8.29*†	1517.7	[35.56]	10.38	1404.7	0.04
β -Caryophyllene	8.66*	1546.9	[2.49]	10.50	1413.4	2.43
α -Santalene	8.48*	1532.3	[0.46]	10.54	1417.0	0.34
Lavandulyl isobutyrate	9.55	1615.7	0.07	10.65	1425.2	0.05
<i>trans</i> - α -Bergamotene	8.66*	1546.9	[2.49]	10.76	1433.5	0.10
Sesquisabinene A	9.32	1597.1	0.01	10.88*	1442.3	[0.04]
<i>cis</i> - β -Bergamotene?				10.88*	1442.3	[0.04]
α -Humulene	9.48	1610.5	0.08	10.95	1447.0	0.09
Lavandulyl butyrate?	10.70	1709.1	0.09	11.05	1454.7	0.07
(<i>E</i>)- β -Farnesene	9.73*	1630.8	[0.95]	11.09	1457.8	0.91
Dauca-5,8-diene?	9.35*	1599.6	[0.20]	11.20	1465.7	0.02
Germacrene D	9.96*	1648.9	[1.77]	11.32	1475.0	0.30
<i>trans</i> - β -Bergamotene	9.73*	1630.8	[0.95]	11.40	1481.1	0.04
Isodaucene	10.20	1668.8	0.02	11.53	1490.3	0.02
β -Bisabolene	10.36*	1681.8	[0.28]	11.77*	1508.4	[0.14]
γ -Cadinene	10.59*	1699.7	[0.13]	11.77*	1508.4	[0.14]
Lavandulyl isovalerate	10.85	1721.7	0.01	11.77*	1508.4	[0.14]
Unknown CULO LIV [m/z 121, 93 (56), 91 (12), 94 (11), 122 (10)...220]	13.51	1956.1	0.04	11.87	1515.9	0.05

δ -Cadinene	10.59*	1699.7	[0.13]	11.93	1520.8	0.03
Isocaryophyllene epoxide B	12.33	1849.5	0.04	12.22	1544.0	0.04
Caryophyllene oxide	12.96*	1905.6	[0.48]	12.60*	1573.8	[0.53]
Caryophyllene oxide isomer	12.89	1898.4	0.07	12.60*	1573.8	[0.53]
Humulene epoxide II	13.56	1960.5	0.01	12.93	1599.3	0.01
τ -Cadinol	15.08	2104.9	0.13	13.37	1635.1	0.10
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	17.00	2300.9	0.02	13.75	1666.3	0.02
<i>cis</i> -14-nor-Murol-5-en-4-one?	15.91	2188.2	0.02	13.85	1674.9	0.01
α -Bisabolol	15.65	2161.8	0.01	13.94	1682.1	0.01
Total reported		98.53%			99.08%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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