Date : 2023-11-10

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 23K03-PTH07
Customer Identification : Organic Clary Sage - Spain - CC4106R
Type : Essential Oil
Source : *Salvia sclarea*
Customer : Plant Therapy

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

Méthode certifiée ISO 17025:2017 Certified method

Laboratoire PhytoChemia

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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 : 2023-11-08

Physicochemical data

Refractive index : 1.4601 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2023-11-06

Conclusion

No adulterant, contaminant or diluent has been detected using this method.

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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
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	tr	Simple phenolic
(2*E*)-Hexenal	0.04	Aliphatic aldehyde
(3*Z*)-Hexenol	0.10	Aliphatic alcohol
(2*E*)-Hexenol	0.13	Aliphatic alcohol
Hexanol	0.09	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	tr	Aliphatic ketone
α-Thujene	0.01	Monoterpene
α-Pinene	0.24	Monoterpene
Unknown	tr	Unknown
Camphene	0.03	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.07	Monoterpene
β-Pinene	0.17	Monoterpene
Octen-3-ol	0.05	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
trans-Dehydroxylinalool oxide	0.05	Monoterpenic ether
Myrcene	0.69	Monoterpene
cis-Dehydroxylinalool oxide	0.04	Monoterpenic ether
α-Terpinene	0.01	Monoterpene
para-Cymene	0.04	Monoterpene
β-Phellandrene	0.01	Monoterpene
1,8-Cineole	0.02	Monoterpenic ether
Limonene	0.40	Monoterpene
(*Z*)-β-Ocimene	0.30	Monoterpene
(*E*)-β-Ocimene	0.52	Monoterpene
γ-Terpinene	0.03	Monoterpene
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
trans-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.14	Monoterpene
Linalool	21.23	Monoterpenic alcohol
Hotrienol	0.03	Monoterpenic alcohol

Dehydrosabinaketone	0.01	Normonoterpenic ketone
Unknown	0.01	Unknown
allo-Ocimene	0.01	Monoterpene
trans-Pinocarveol	0.01	Monoterpenic alcohol
Camphor	0.04	Monoterpenic ketone
(*E*)-Myroxide	0.01	Monoterpenic ether
Nerol oxide	0.03	Aliphatic ether
Borneol	0.05	Monoterpenic alcohol
Terpinen-4-ol	0.05	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α-Terpineol	3.01	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.04	Monoterpenic alcohol
Unknown	0.02	Unknown
Linalyl formate	0.22	Monoterpenic ester
Nerol	0.52	Monoterpenic alcohol
Unknown	0.01	Unknown
Neral	0.03	Monoterpenic aldehyde
Geraniol	1.45	Monoterpenic alcohol
Linalyl acetate	58.19	Monoterpenic ester
Geranial	0.06	Monoterpenic aldehyde
Unknown	0.02	Unknown
Neryl formate	0.04	Monoterpenic ester
Bornyl acetate	0.04	Monoterpenic ester
Thymol	0.01	Monoterpenic alcohol
Geranyl formate	0.10	Monoterpenic ester
δ-Elemene	0.01	Sesquiterpene
Hodiendiol derivative	0.09	Oxygenated monoterpene
α-Terpinyl acetate	0.06	Monoterpenic ester
α-Cubebene	0.02	Sesquiterpene
Unknown	0.04	Monoterpenic ester
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.75	Monoterpenic ester
α-Copaene	0.43	Sesquiterpene
(*Z*)-8-Hydroxylinalool?	0.01	Monoterpenic alcohol
β-Bourbonene	0.09	Sesquiterpene
Geranyl acetate	1.40	Monoterpenic ester
β-Cubebene	0.11	Sesquiterpene
β-Elemene	0.10	Sesquiterpene
γ-4-Dimethylbenzenebutyral	0.02	Simple phenolic
β-Caryophyllene	1.18	Sesquiterpene
β-Copaene	0.04	Sesquiterpene
trans-α-Bergamotene	0.02	Sesquiterpene
α-Humulene	0.06	Sesquiterpene
9-epi-β-Caryophyllene	0.04	Sesquiterpene

(*E*)-β-Farnesene	0.01	Sesquiterpene
γ-Muurolene	0.01	Sesquiterpene
Germacrene D	2.58	Sesquiterpene
α-Amorphene	0.03	Sesquiterpene
β-Selinene	0.03	Sesquiterpene
Hodiendiol derivative IV	0.20	Oxygenated monoterpene
α-Selinene	0.02	Sesquiterpene
Bicyclogermacrene	0.30	Sesquiterpene
α-Muurolene	0.06	Sesquiterpene
Germacrene A	0.06	Sesquiterpene
(*Z*)-α-Bisabolene	0.03	Sesquiterpene
β-Bisabolene	tr	Sesquiterpene
Cubebol	0.02	Sesquiterpenic alcohol
γ-Cadinene	0.01	Sesquiterpene
δ-Cadinene	0.13	Sesquiterpene
Octyl tiglate?	0.02	Aliphatic ester
α-Elemol	0.02	Sesquiterpenic alcohol
1,5-Epoxysalvial-4(14)-ene	0.02	Sesquiterpenic ether
Spathulenol	0.17	Sesquiterpenic alcohol
Caryophyllene oxide	0.12	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.02	Aliphatic alcohol
Guaiol	0.02	Sesquiterpenic alcohol
Unknown	0.07	Oxygenated sesquiterpene
Torilenol	0.06	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Hinesol	0.04	Sesquiterpenic alcohol
Unknown	0.06	Unknown
τ-Cadinol	0.02	Sesquiterpenic alcohol
β-Eudesmol	0.06	Sesquiterpenic alcohol
α-Eudesmol	0.07	Sesquiterpenic alcohol
Unknown	0.03	Unknown
(1βH)-Guai-9-en-11-ol?	0.01	Sesquiterpenic alcohol
Eudesma-4(15),7-dien-1β-ol	0.03	Sesquiterpenic alcohol
Cyclocolorenone	0.01	Sesquiterpenic ketone
Unknown	0.03	Unknown
Phytone	0.03	Terpenic ketone
Unknown	0.07	Unknown
Unknown	0.06	Unknown
Geranyl-*para*-cymene	0.04	Diterpene
Manoyl oxide	0.01	Diterpenic ether
13-epi-Manoyl oxide	0.01	Diterpenic ether
Manool	0.03	Diterpenic alcohol
Sclareol	1.38	Diterpenic alcohol
Consolidated total	**99.12**	

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.

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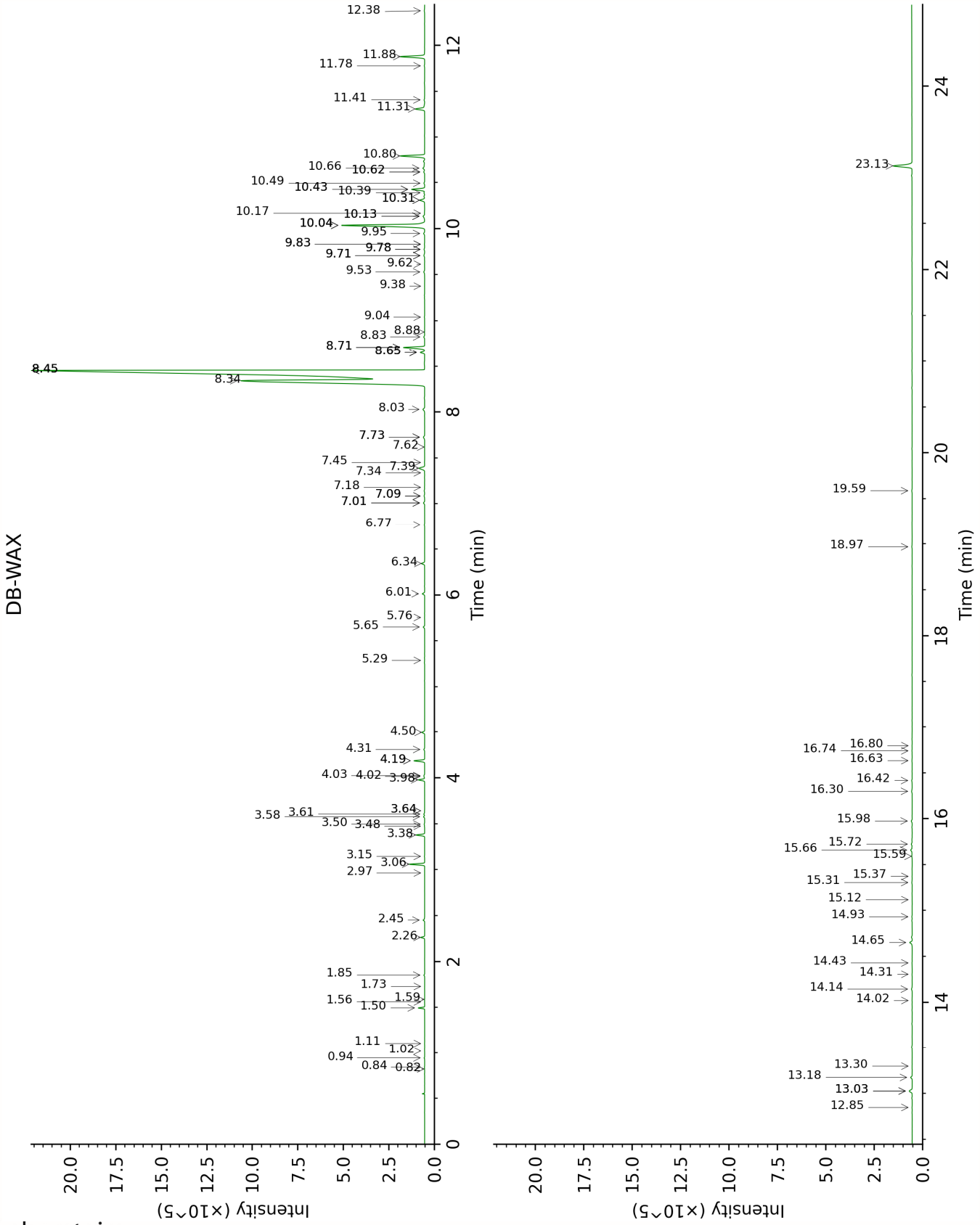
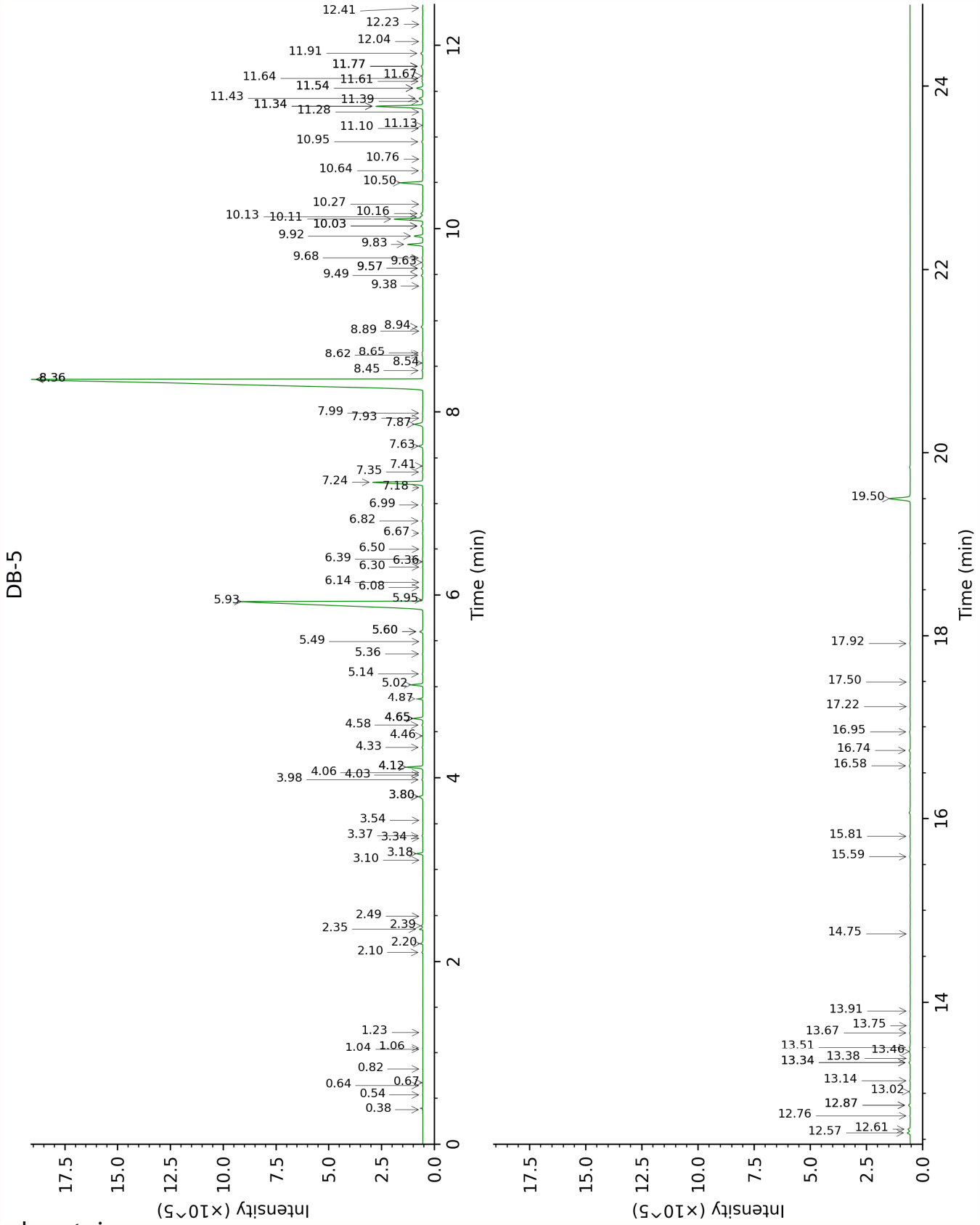

DB-WAX
Time (min)
Intensity (×10^5)
12.38
11.88
11.78
11.41
11.31
10.80
10.66
10.62
10.49
10.43
10.39
10.31
10.17
10.13
10.04
9.95
9.83
9.78
9.71
9.62
9.53
9.38
9.04
8.88
8.83
8.71
8.65
8.45
8.34
8.03
7.73
7.62
7.45
7.39
7.34
7.18
7.09
7.01
6.77
6.34
6.01
5.76
5.65
5.29
4.50
4.31
4.19
4.03
4.02
3.98
3.64
3.61
3.58
3.50
3.48
3.38
3.15
3.06
2.97
2.45
2.26
1.85
1.73
1.59
1.56
1.50
1.11
1.02
0.94
0.84
0.82
23.13
19.59
18.97
16.80
16.74
16.63
16.42
16.30
15.98
15.72
15.66
15.59
15.37
15.31
15.12
14.93
14.65
14.43
14.31
14.14
14.02
13.30
13.18
13.03
12.85


DB-5
Time (min)
Intensity (×10^5)
12.41
12.23
12.04
11.91
11.77
11.64
11.61
11.67
11.54
11.43
11.34
11.39
11.28
11.10
11.13
10.95
10.76
10.64
10.50
10.27
10.13
10.11
10.16
10.03
9.92
9.83
9.68
9.57
9.63
9.49
9.38
8.89
8.94
8.62
8.65
8.54
8.45
8.36
7.99
7.93
7.87
7.63
7.35
7.41
7.24
7.18
6.99
6.82
6.67
6.50
6.39
6.36
6.30
6.14
6.08
5.95
5.93
5.60
5.49
5.36
5.14
5.02
4.87
4.65
4.58
4.46
4.33
4.12
4.06
4.03
3.98
3.80
3.54
3.37
3.34
3.18
3.10
2.49
2.39
2.35
2.20
2.10
1.23
1.04
1.06
0.82
0.67
0.64
0.54
0.38
19.50
17.92
17.50
17.22
16.95
16.74
16.58
15.81
15.59
14.75
13.91
13.75
13.67
13.51
13.46
13.34
13.38
13.14
13.02
12.87
12.76
12.57
12.61

FULL ANALYSIS DATA

	Column DB-WAX			Column DB-5		
Ethanol	0.94	909.1	0.01	0.38	501.8	0.01
2-Methyl-3-buten-2-ol	1.73	1016.6	tr	0.54	607.8	0.01
Isovaleral	0.84	887.5	0.01	0.64	642.2	0.01
2-Methylbutyral	0.82	880.8	tr	0.67	652.5	tr
2-Ethylfuran	1.02	920.7	tr	0.82	702.5	tr
Isoamyl alcohol	3.64*	1177.2	[0.01]	1.04	734.1	0.01
2-Methylbutanol	3.64*	1177.2	[0.01]	1.06	737.0	0.01
Toluene	1.59	1003.3	tr	1.23	760.2	tr
(2*E*)-Hexenal	3.61	1174.4	0.05	2.10	849.9	0.04
(3*Z*)-Hexenol	6.01	1349.2	0.13	2.20	857.8	0.10
(2*E*)-Hexenol	6.34	1372.6	0.17	2.35	870.6	0.13
Hexanol	5.65	1323.6	0.08	2.39	873.6	0.09
3-Acetyl-3-methylcyclopentene	1.11	933.7	tr	2.49	882.1	tr
α-Thujene	1.56	1000.7	tr	3.10	926.8	0.01
α-Pinene	1.50	992.4	0.24	3.18	931.5	0.24
Unknown ERPU I [m/z 137, 82 (95), 67 (94), 43 (73), 55 (49), 93 (35)...]	2.97	1126.0	tr	3.34*†	942.4	[0.01]
Camphene	1.85	1028.2	0.03	3.37*†	944.3	[0.04]
Benzaldehyde	7.62	1465.2	0.01	3.54	955.3	0.01
Sabinene	2.45	1084.7	0.07	3.80*	972.3	[0.24]
β-Pinene	2.26	1066.9	0.17	3.80*	972.3	[0.24]
Octen-3-ol	7.01*	1420.6	[0.07]	3.98	984.3	0.05
Octan-3-one	4.19*	1216.9	[0.52]	4.03	987.7	0.01
6-Methyl-5-hepten-2-one	5.29	1294.6	0.01	4.06	989.4	0.01
trans-Dehydroxylinalool oxide	3.58	1172.2	0.05	4.12*	993.4	[0.73]
Myrcene	3.06	1133.2	0.69	4.12*	993.4	[0.73]
cis-Dehydroxylinalool oxide	4.03	1205.4	0.04	4.33	1007.4	0.04
α-Terpinene	3.15	1139.6	0.01	4.46	1015.2	0.01
para-Cymene	4.31	1225.6	0.04	4.58	1022.5	0.04
β-Phellandrene	3.48	1164.4	0.01	4.65*	1027.0	[0.43]
1,8-Cineole	3.50	1166.1	0.02	4.65*	1027.0	[0.43]
Limonene	3.38	1157.3	0.40	4.65*	1027.0	[0.43]
(*Z*)-β-Ocimene	3.98	1202.2	0.30	4.87	1040.6	0.30
(*E*)-β-Ocimene	4.19*	1216.9	[0.52]	5.02	1050.4	0.52
γ-Terpinene	4.02	1204.8	0.02	5.14	1057.8	0.03
cis-Linalool oxide (fur.)	6.77	1402.9	0.03	5.36	1071.3	0.02
Octanol	8.45*†	1527.8	[56.91]	5.49	1079.7	0.01
trans-Linalool oxide (fur.)	7.09*	1426.1	[0.04]	5.60*	1086.5	[0.16]

Terpinolene	4.50	1238.8	0.14	5.60*	1086.5	[0.16]
Linalool	8.34*†	1519.2	[22.29]	5.93	1106.9	21.23
Hotrienol	9.04	1572.7	0.01	5.95	1108.1	0.03
Dehydrosabinaketone	8.88	1560.3	0.01	6.08	1116.7	0.01
Unknown LAAN I [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	9.83*	1635.1	[0.02]	6.14	1120.2	0.01
allo-Ocimene	5.76	1330.9	0.01	6.30	1130.8	0.01
trans-Pinocarveol	9.38	1598.6	0.01	6.36	1134.5	0.01
Camphor	7.45	1452.9	0.01	6.39	1136.3	0.04
(*E*)-Myroxide	7.34	1444.7	0.01	6.50	1143.2	0.01
Nerol oxide	7.09*	1426.1	[0.04]	6.67	1154.3	0.03
Borneol	10.04*	1651.5	[5.78]	6.82	1163.3	0.05
Terpinen-4-ol	8.83	1556.2	0.05	6.99	1174.4	0.05
para-Cymen-8-ol	11.78	1796.1	0.02	7.18	1186.4	0.02
α-Terpineol	10.04*	1651.5	[5.78]	7.24	1190.1	3.01
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	13.03*	1906.3	[0.23]	7.35	1197.2	0.04
Unknown SASC VI [m/z 43, 71 (80), 67 (55), 59 (51), 68 (44), 41 (43)...]				7.41	1201.4	0.02
Linalyl formate	8.65*	1542.9	[0.23]	7.63	1215.7	0.22
Nerol	11.31	1756.5	0.60	7.87	1231.6	0.52
Unknown SASC IV [m/z 43, 93 (49), 41 (22), 80 (22), 69 (17), 121 (14)...]	7.73*	1473.1	[0.09]	7.93	1235.9	0.01
Neral	9.71*	1625.2	[0.06]	7.99	1239.7	0.03
Geraniol	11.88	1804.9	1.45	8.36*	1264.2	[59.63]
Linalyl acetate	8.45*†	1527.8	[56.91]	8.36*	1264.2	[59.63]
Geranial	10.39	1679.9	0.04	8.45	1270.6	0.06
Unknown MISC V [m/z 121, 43 (75), 95 (57), 41 (34), 93 (33), 69 (28)...]				8.54	1276.1	0.02
Neryl formate	9.71*	1625.2	[0.06]	8.62	1281.8	0.04
Bornyl acetate	8.45*†	1527.8	[56.91]	8.65	1283.4	0.04
Thymol	15.37	2128.7	0.01	8.89	1299.7	0.01
Geranyl formate	10.14*	1659.4	[0.12]	8.94	1302.8	0.10
δ-Elemene	7.18	1433.0	0.01	9.38	1333.8	0.01
Hodiendiol derivative	13.18	1919.9	0.10	9.49	1341.9	0.09
α-Terpinyl acetate	9.95	1644.4	0.06	9.57*	1347.4	[0.08]
α-Cubebene	7.01*	1420.6	[0.07]	9.57*	1347.4	[0.08]
Unknown MISC VII [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81				9.63	1351.8	0.04

(25)...]						
Unknown SASC III [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	11.41	1764.8	0.04	9.68	1355.3	0.04
Neryl acetate	10.43*	1682.8	[0.75]	9.83	1365.6	0.75
α-Copaene	7.39	1448.4	0.42	9.92	1372.0	0.43
(*Z*)-8-Hydroxylinalool?	14.02	1997.8	0.01	10.03*	1379.6	[0.10]
β-Bourbonene	7.73*	1473.1	[0.09]	10.03*	1379.6	[0.10]
Geranyl acetate	10.80	1713.6	1.40	10.10	1385.0	1.40
β-Cubebene	8.03	1495.3	0.12	10.13	1386.6	0.11
β-Elemene	8.71*	1547.5	[1.21]	10.16	1389.2	0.10
γ-4-Dimethylbenzenebutyral				10.27	1396.3	0.02
β-Caryophyllene	8.71*	1547.5	[1.21]	10.50	1413.1	1.18
β-Copaene	8.65*	1542.9	[0.23]	10.64	1423.4	0.04
trans-α-Bergamotene	8.65*	1542.9	[0.23]	10.76	1432.7	0.02
α-Humulene	9.53	1610.9	0.07	10.95	1446.8	0.06
9-epi-β-Caryophyllene	9.62	1617.7	0.01	11.10	1457.6	0.04
(*E*)-β-Farnesene	9.78*	1630.6	[0.04]	11.13	1460.1	0.01
γ-Muurolene	9.83*	1635.1	[0.02]	11.28	1470.9	0.01
Germacrene D	10.04*	1651.5	[5.78]	11.34*	1475.6	[2.61]
α-Amorphene	9.78*	1630.6	[0.04]	11.34*	1475.6	[2.61]
β-Selinene	10.14*	1659.4	[0.12]	11.39	1479.5	0.03
Hodiendiol derivative IV				11.42	1481.9	0.20
α-Selinene	10.17	1662.0	0.02	11.54*	1490.2	[0.33]
Bicyclogermacrene	10.31*	1673.4	[0.31]	11.54*	1490.2	[0.33]
α-Muurolene	10.31*	1673.4	[0.31]	11.61	1495.7	0.06
Germacrene A	10.62*	1698.9	[0.06]	11.64	1498.0	0.06
(*Z*)-α-Bisabolene	10.49	1688.2	0.04	11.67	1500.1	0.03
β-Bisabolene	10.43*	1682.8	[0.75]	11.77*	1508.1	[0.11]
Cubebol	12.85	1889.9	0.02	11.77*	1508.1	[0.11]
γ-Cadinene	10.62*	1698.9	[0.06]	11.77*	1508.1	[0.11]
δ-Cadinene	10.66	1702.4	0.16	11.92	1519.1	0.13
Octyl tiglate?				12.04	1529.2	0.02
α-Elemol	14.31	2025.2	0.01	12.23	1543.8	0.02
1,5-Epoxysalvial-4(14)-ene	12.38	1848.8	0.04	12.41	1557.9	0.02
Spathulenol	14.65	2058.2	0.17	12.57	1570.4	0.17
Caryophyllene oxide	13.03*	1906.3	[0.23]	12.61	1573.5	0.12
Salvial-4(14)-en-1-one	13.30	1931.2	0.01	12.76	1585.0	0.02
Guaiol	14.43	2036.9	0.02	12.87*	1594.0	[0.09]
Unknown MISC CLIX [m/z 91, 119 (91), 79 (86), 93 (85), 41 (74), 107 (68),				12.87*	1594.0	[0.09]

105 (67), 134 (65)... 220 (1)]						
Torilenol	15.72	2163.8	0.06	13.02	1605.7	0.06
Unknown CASA XLIV [m/z 135, 93 (66), 79 (58), 107 (54), 41 (42), 81 (41), 67 (41)... 220 (2)]				13.14	1615.5	0.02
Hinesol	15.31	2122.1	0.04	13.34*	1631.8	[0.07]
Unknown SCTE X [m/z 43, 93 (89), 91 (88), 79 (87), 123 (76), 81 (75)...]	14.14	2009.7	0.06	13.34*	1631.8	[0.07]
τ-Cadinol	15.12	2103.4	0.01	13.38	1635.7	0.02
β-Eudesmol	15.66	2157.3	0.12	13.46	1641.9	0.06
α-Eudesmol	15.59	2150.6	0.05	13.51	1645.9	0.07
Unknown SASC VIII [m/z 81, 41 (46), 79 (46), 93 (39), 91 (33), 107 (33)... 206 (8)]				13.67	1659.2	0.03
(1βH)-Guai-9-en-11-ol?	15.98	2189.0	0.06	13.75	1665.6	0.01
Eudesma-4(15),7-dien-1β-ol	16.30	2222.5	0.05	13.91	1678.7	0.03
Cyclocolorenone	16.80	2274.0	0.02	14.75	1750.2	0.01
Unknown THAR V [m/z 123, 191 (88), 81 (86), 41 (86), 151 (80), 91 (76)...]	18.97	2513.3	0.03	15.59	1824.0	0.03
Phytone	14.93	2085.1	0.02	15.81	1844.2	0.03
Unknown SASC XI [m/z 69, 81 (84), 109 (80), 43 (64), 95 (59)...]				16.58	1914.4	0.07
Unknown UNKN CXC [m/z 109, 132 (88), 157 (76), 119 (66), 91 (57), 105 (55)...]				16.74	1930.3	0.06
Geranyl-*para*-cymene	16.42	2234.7	0.04	16.95	1949.6	0.04
Manoyl oxide	16.74	2268.2	0.02	17.22	1975.7	0.01
13-epi-Manoyl oxide	16.63	2257.1	0.03	17.50	2001.8	0.01
Manool	19.59	2585.0	0.03	17.92	2043.3	0.03
Sclareol	23.13	3035.6	1.39	19.50	2205.0	1.38
Total reported		98.54%			99.18%	

*: 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

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