Date : 2024-08-29

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 24H16-PTH05
Customer Identification : Clary Sage - Ukraine - CF0119R
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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 : 2024-08-26

Physicochemical data

Refractive index : 1.4593 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Kassandra Baker
Date : 2024-08-19

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
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Pentanone	tr	Aliphatic ketone
2-Ethylfuran	0.01	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
Octane	0.01	Alkane
(2*E*)-Hexenal	0.02	Aliphatic aldehyde
(3*Z*)-Hexenol	0.11	Aliphatic alcohol
(2*E*)-Hexenol	0.04	Aliphatic alcohol
Hexanol	0.06	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	tr	Aliphatic ketone
α-Pinene	0.02	Monoterpene
Unknown	0.01	Unknown
Camphene	0.01	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.02	Monoterpene
β-Pinene	0.03	Monoterpene
Octen-3-ol	0.04	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.99	Monoterpene
trans-Dehydroxylinalool oxide	0.15	Monoterpenic ether
Octan-3-ol	0.01	Aliphatic alcohol
cis-Dehydroxylinalool oxide	0.12	Monoterpenic ether
para-Cymene	0.02	Monoterpene
Limonene	0.74	Monoterpene
β-Phellandrene	0.01	Monoterpene
(*Z*)-β-Ocimene	0.37	Monoterpene
(*E*)-β-Ocimene	0.72	Monoterpene
γ-Terpinene	0.02	Monoterpene
cis-Linalool oxide (fur.)	0.09	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
trans-Linalool oxide (fur.)	0.06	Monoterpenic alcohol
Terpinolene	0.20	Monoterpene
Linalool	18.46	Monoterpenic alcohol
Hotrienol	0.10	Monoterpenic alcohol
Unknown	tr	Unknown
allo-Ocimene	0.02	Monoterpene
Camphor	0.02	Monoterpenic ketone

(*E*)-Myroxide	0.01	Monoterpenic ether
Nerol oxide	0.11	Aliphatic ether
Borneol	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.04	Monoterpenic alcohol
α-Terpineol	2.35	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.01	Monoterpenic alcohol
Linalyl formate	0.15	Monoterpenic ester
Nerol	0.49	Monoterpenic alcohol
Thymol methyl ether	0.05	Monoterpenic ether
Neral	0.02	Monoterpenic aldehyde
Linalyl acetate	59.45	Monoterpenic ester
Geraniol	1.42	Monoterpenic alcohol
Geranial	0.03	Monoterpenic aldehyde
Neryl formate	0.04	Monoterpenic ester
Thymol	0.01	Monoterpenic alcohol
Geranyl formate	0.07	Monoterpenic ester
δ-Elemene	0.01	Sesquiterpene
Hodiendiol derivative	0.06	Oxygenated monoterpene
α-Terpinyl acetate	0.05	Monoterpenic ester
α-Cubebene	0.05	Sesquiterpene
Unknown	0.02	Monoterpenic ester
Unknown	0.03	Oxygenated monoterpene
Neryl acetate	0.94	Monoterpenic ester
α-Copaene	0.57	Sesquiterpene
β-Bourbonene	0.24	Sesquiterpene
1,5-diepi-β-Bourbonene	0.02	Sesquiterpene
Geranyl acetate	1.82	Monoterpenic ester
β-Cubebene	0.08	Sesquiterpene
β-Elemene	0.10	Sesquiterpene
γ-4-Dimethylbenzenebutyral	0.04	Simple phenolic
Isocaryophyllene	0.01	Sesquiterpene
β-Caryophyllene	1.91	Sesquiterpene
β-Copaene	0.06	Sesquiterpene
trans-α-Bergamotene	0.05	Sesquiterpene
α-Humulene	0.11	Sesquiterpene
(*E*)-β-Farnesene	0.03	Sesquiterpene
γ-Muurolene	0.03	Sesquiterpene
Germacrene D	1.88	Sesquiterpene
Hodiendiol derivative IV	0.08	Oxygenated monoterpene
β-Selinene	0.03	Sesquiterpene
α-Selinene	0.02	Sesquiterpene
Bicyclogermacrene	0.36	Sesquiterpene
α-Muurolene	0.05	Sesquiterpene
(*Z*)-α-Bisabolene	0.05	Sesquiterpene

Cubebol	0.02	Sesquiterpenic alcohol
γ-Cadinene	0.12	Sesquiterpene
β-Bisabolene	0.03	Sesquiterpene
(*Z*)-γ-Bisabolene	0.02	Sesquiterpene
δ-Cadinene	0.15	Sesquiterpene
trans-Calamenene	0.01	Sesquiterpene
α-Elemol	0.02	Sesquiterpenic alcohol
1,5-Epoxysalvial-4(14)-ene	0.07	Sesquiterpenic ether
Spathulenol	0.20	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Caryophyllene oxide	0.50	Sesquiterpenic ether
Guaiol	0.02	Sesquiterpenic alcohol
Unknown	0.05	Oxygenated sesquiterpene
Torilenol	0.05	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
allo-Aromadendrene epoxide?	0.14	Sesquiterpenic ether
τ-Cadinol	0.04	Sesquiterpenic alcohol
β-Eudesmol	0.10	Sesquiterpenic alcohol
α-Eudesmol	0.06	Sesquiterpenic alcohol
α-Cadinol	0.02	Sesquiterpenic alcohol
Bulnesol	0.02	Sesquiterpenic alcohol
Unknown	0.01	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
Benzyl benzoate	0.04	Phenolic ester
Phytone	0.03	Terpenic ketone
Sclareoloxide	0.29	Terpenic ether
Unknown	0.05	Unknown
Unknown	0.06	Unknown
Geranyl-*para*-cymene	0.06	Diterpene
Manoyl oxide	0.03	Diterpenic ether
13-epi-Manoyl oxide	0.01	Diterpenic ether
Manool	0.05	Diterpenic alcohol
Sclareol	0.63	Diterpenic alcohol
Consolidated total	**98.57**	

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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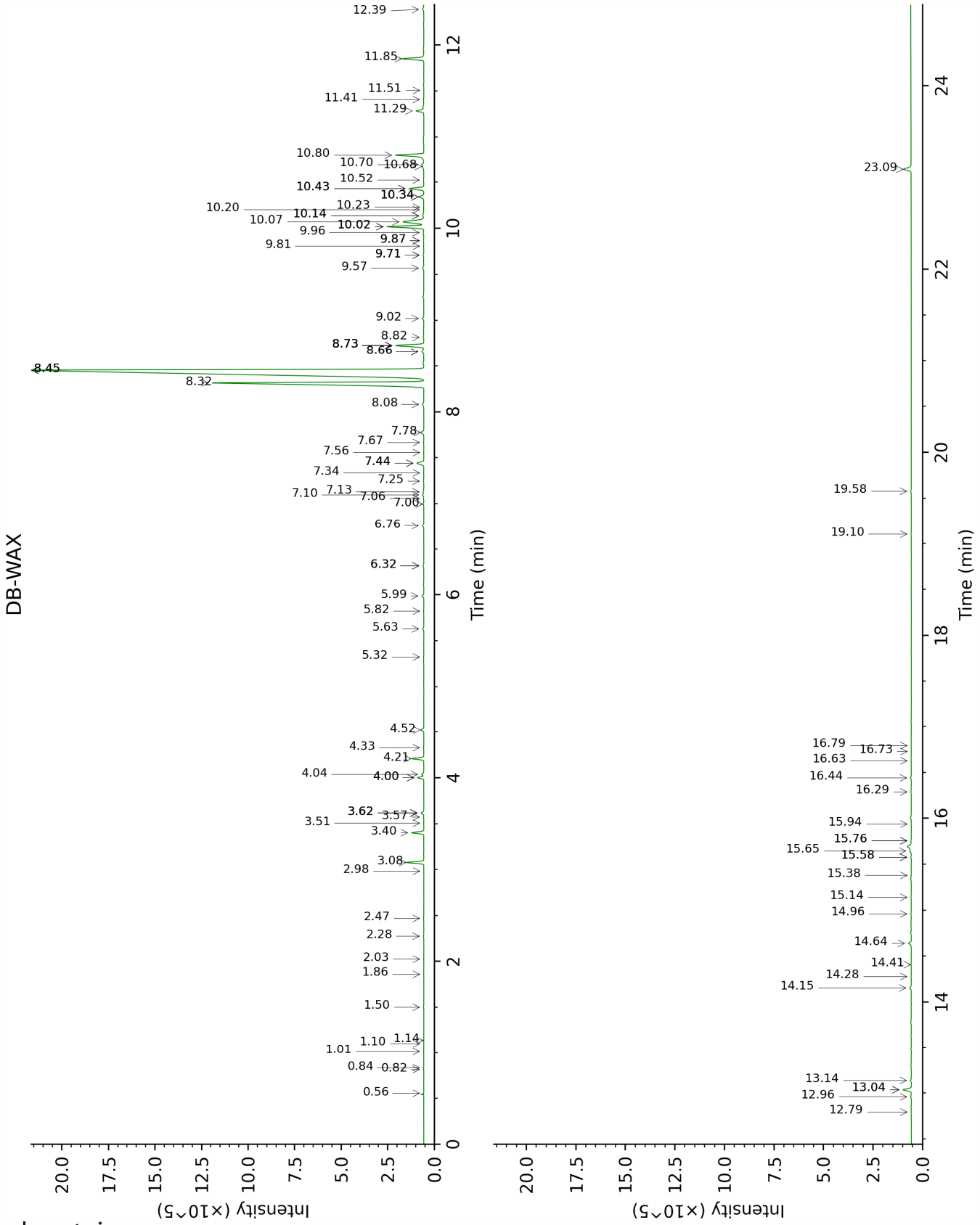
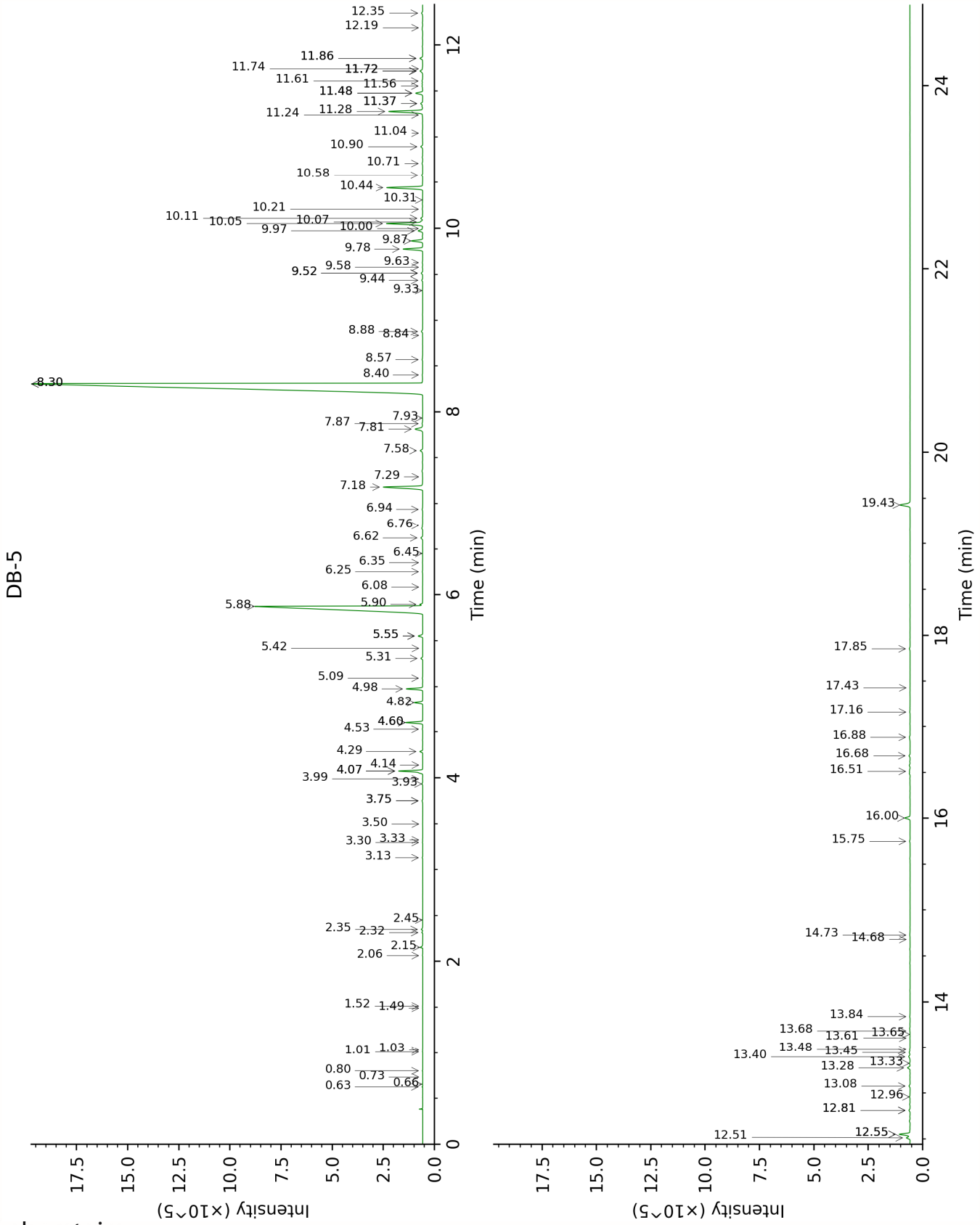

DB-WAX
Time (min)
Intensity (×10^5)
12.39
11.85
11.51
11.41
11.29
10.80
10.70
10.68
10.52
10.43
10.34
10.20
10.23
10.07
10.14
10.02
9.96
9.87
9.81
9.71
9.57
9.02
8.82
8.73
8.66
8.45
8.32
8.08
7.78
7.67
7.56
7.44
7.34
7.25
7.10
7.13
7.06
7.00
6.76
6.32
5.99
5.82
5.63
5.32
4.52
4.33
4.21
4.04
4.00
3.62
3.57
3.51
3.40
3.08
2.98
2.47
2.28
2.03
1.86
1.50
1.14
1.10
1.01
0.84
0.82
0.56
23.09
19.58
19.10
16.79
16.73
16.63
16.44
16.29
15.94
15.76
15.65
15.58
15.38
15.14
14.96
14.64
14.41
14.28
14.15
13.14
13.04
12.96
12.79


DB-5
Time (min)
Intensity (×10^5)
12.35
12.19
11.86
11.74
11.72
11.61
11.56
11.48
11.37
11.24
11.28
11.04
10.90
10.71
10.58
10.44
10.31
10.21
10.11
10.05
10.07
9.97
10.00
9.87
9.78
9.63
9.52
9.58
9.44
9.33
8.88
8.84
8.57
8.40
8.30
7.93
7.87
7.81
7.58
7.29
7.18
6.94
6.76
6.62
6.45
6.35
6.25
6.08
5.88
5.90
5.55
5.42
5.31
5.09
4.98
4.82
4.60
4.53
4.29
4.14
4.07
3.99
3.93
3.75
3.50
3.30
3.33
3.13
2.45
2.35
2.32
2.15
2.06
1.52
1.49
1.01
1.03
0.80
0.73
0.66
0.63
19.43
17.85
17.43
17.16
16.88
16.68
16.51
16.00
15.75
14.73
14.68
13.84
13.68
13.61
13.65
13.48
13.40
13.45
13.28
13.33
13.08
12.96
12.81
12.51
12.55

FULL ANALYSIS DATA

Isovaleral	**Column DB-WAX**			**Column DB-5**		
	0.84	884.5	0.01	0.63	640.2	0.01
2-Methylbutyral	0.82	877.8	0.01	0.66	650.3	0.01
2-Pentanone	1.14	936.8	tr	0.74	677.3	tr
2-Ethylfuran	1.02	917.5	0.01	0.80	701.0	0.01
Isoamyl alcohol	3.62*	1174.8	[0.17]	1.01	731.9	0.01
2-Methylbutanol	3.62*	1174.8	[0.17]	1.03	734.8	tr
Hexanal	2.03	1043.1	0.01	1.49	799.4	0.01
Octane	0.56	783.5	tr	1.52	802.6	0.01
(2*E*)-Hexenal	3.57	1171.4	0.02	2.06	848.6	0.02
(3*Z*)-Hexenol	5.99	1345.3	0.12	2.16	856.0	0.11
(2*E*)-Hexenol	6.32*	1368.8	[0.06]	2.32	869.3	0.04
Hexanol	5.63	1319.8	0.07	2.35	872.1	0.06
3-Acetyl-3-methylcyclopentene	1.10	931.2	tr	2.45	880.6	tr
α-Pinene	1.50	992.2	0.02	3.13	930.0	0.02
Unknown ERPU I [m/z 137, 82 (95), 67 (94), 43 (73), 55 (49), 93 (35)...]	2.98	1126.5	tr	3.30	941.0	0.01
Camphene	1.86	1027.3	0.01	3.32	942.8	0.01
Benzaldehyde	7.56	1459.3	0.01	3.50	954.2	0.01
Sabinene	2.47	1085.3	0.02	3.75*	970.9	[0.04]
β-Pinene	2.28	1066.9	0.03	3.75*	970.9	[0.04]
Octen-3-ol	7.06	1422.6	0.03	3.93	983.0	0.04
6-Methyl-5-hepten-2-one	5.32	1298.0	0.02	3.99	986.7	0.01
Myrcene	3.08	1133.7	0.99	4.07*	992.3	[1.14]
trans-Dehydroxylinalool oxide	3.62*	1174.8	[0.17]	4.07*	992.3	[1.14]
Octan-3-ol	6.32*	1368.8	[0.06]	4.14	996.6	0.01
cis-Dehydroxylinalool oxide	4.04*†	1206.1	[0.15]	4.29	1006.1	0.12
para-Cymene	4.33	1226.9	0.02	4.53	1021.3	0.02
Limonene	3.40	1158.4	0.74	4.60*	1025.9	[0.74]
β-Phellandrene	3.51	1166.3	0.01	4.60*	1025.9	[0.74]
(*Z*)-β-Ocimene	4.00*†	1203.5	[0.36]	4.82	1039.5	0.37
(*E*)-β-Ocimene	4.21	1218.4	0.73	4.98	1049.3	0.72
γ-Terpinene	4.00*†	1203.5	[0.36]	5.09	1056.6	0.02
cis-Linalool oxide (fur.)	6.76	1400.3	0.10	5.31	1070.0	0.09
Octanol	8.45*	1526.8	[59.33]	5.42	1076.9	0.01
trans-Linalool oxide (fur.)	7.13	1427.8	0.06	5.55*	1085.3	[0.22]
Terpinolene	4.52	1240.6	0.20	5.55*	1085.3	[0.22]
Linalool	8.32	1516.1	18.42	5.88	1105.5	18.46
Hotrienol	9.02	1570.6	0.08	5.90	1106.9	0.10

Unknown LAAN I [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	9.87*	1637.5	[0.05]	6.08	1118.9	tr
allo-Ocimene	5.82	1333.6	0.02	6.25	1129.6	0.02
Camphor	7.44*	1450.8	[0.58]	6.35	1135.9	0.02
(*E*)-Myroxide	7.34	1443.0	0.02	6.45	1142.3	0.01
Nerol oxide	7.10	1425.4	0.09	6.62	1153.1	0.11
Borneol	10.02*	1649.7	[2.35]	6.76	1161.8	0.02
Terpinen-4-ol	8.82	1554.8	0.03	6.94	1173.3	0.04
α-Terpineol	10.02*	1649.7	[2.35]	7.18	1188.8	2.35
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	13.04*	1907.7	[0.58]	7.29	1195.9	0.01
Linalyl formate	8.66*	1542.4	[0.17]	7.58	1214.7	0.15
Nerol	11.29	1754.3	0.51	7.81	1230.4	0.49
Thymol methyl ether	8.73*	1548.1	[1.93]	7.87	1234.3	0.05
Neral	9.71*	1624.8	[0.05]	7.93	1238.4	0.02
Linalyl acetate	8.45*	1526.8	[59.33]	8.30*	1263.1	[60.86]
Geraniol	11.85	1802.8	1.42	8.30*	1263.1	[60.86]
Geranial	10.34*	1675.7	[0.39]	8.40	1269.7	0.03
Neryl formate	9.71*	1624.8	[0.05]	8.57	1280.8	0.04
Thymol	15.38	2130.1	0.01	8.84	1299.0	0.01
Geranyl formate	10.14*	1659.1	[0.11]	8.88	1301.8	0.07
δ-Elemene	7.25	1436.4	0.04	9.33	1333.0	0.01
Hodiendiol derivative	13.14	1917.0	0.06	9.44	1340.8	0.06
α-Terpinyl acetate	9.96	1644.5	0.05	9.52*	1346.3	[0.08]
α-Cubebene	7.00	1417.9	0.05	9.52*	1346.3	[0.08]
Unknown MISC VII [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81 (25)...]				9.58	1350.8	0.02
Unknown SASC III [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	11.41	1764.7	0.02	9.63	1354.3	0.03
Neryl acetate	10.43*	1682.9	[0.98]	9.78	1364.7	0.94
α-Copaene	7.44*	1450.8	[0.58]	9.87	1370.9	0.57
β-Bourbonene	7.78	1475.4	0.22	9.97	1378.6	0.24
1,5-diepi-β-Bourbonene	7.67	1467.3	0.02	10.00	1380.3	0.02
Geranyl acetate	10.80	1713.8	1.95	10.05	1384.2	1.82
β-Cubebene	8.08	1498.1	0.11	10.07	1385.3	0.08
β-Elemene	8.73*	1548.1	[1.93]	10.11	1388.1	0.10
γ-4-Dimethylbenzenebutyral				10.21	1395.1	0.04
Isocaryophyllene	8.45*	1526.8	[59.33]	10.31	1402.2	0.01

β-Caryophyllene	8.73*	1548.1	[1.93]	10.44	1412.1	1.91
β-Copaene	8.66*	1542.4	[0.17]	10.58	1422.4	0.06
trans-α-Bergamotene	8.73*	1548.1	[1.93]	10.71	1432.1	0.05
α-Humulene	9.57	1613.5	0.10	10.90	1445.7	0.11
(*E*)-β-Farnesene	9.81	1632.7	0.02	11.04	1456.7	0.03
γ-Muurolene	9.87*	1637.5	[0.05]	11.24	1471.4	0.03
Germacrene D	10.07	1654.0	1.95	11.28	1474.2	1.88
Hodiendiol derivative IV				11.37*	1480.6	[0.11]
β-Selinene	10.14*	1659.1	[0.11]	11.37*	1480.6	[0.11]
α-Selinene	10.23	1666.7	0.02	11.48*	1489.0	[0.38]
Bicyclogermacrene	10.34*	1675.7	[0.39]	11.48*	1489.0	[0.38]
α-Muurolene	10.34*	1675.7	[0.39]	11.56	1494.8	0.05
(*Z*)-α-Bisabolene	10.52	1690.3	0.05	11.61	1498.8	0.05
Cubebol	12.79	1885.5	0.02	11.72*	1507.2	[0.17]
γ-Cadinene	10.68	1703.4	0.12	11.72*	1507.2	[0.17]
β-Bisabolene	10.43*	1682.9	[0.98]	11.72*	1507.2	[0.17]
(*Z*)-γ-Bisabolene	10.20	1664.5	0.02	11.74	1509.1	0.02
δ-Cadinene	10.70	1705.0	0.15	11.86*	1518.1	[0.16]
trans-Calamenene	11.51	1773.1	0.01	11.86*	1518.1	[0.16]
α-Elemol	14.28	2023.1	0.02	12.19	1544.1	0.02
1,5-Epoxysalvial-4(14)-ene	12.39	1850.3	0.11	12.35	1556.6	0.07
Spathulenol	14.64	2057.6	0.21	12.51	1569.4	0.20
Caryophyllene oxide isomer	12.96	1900.6	0.06	12.55*	1572.4	[0.56]
Caryophyllene oxide	13.04*	1907.7	[0.58]	12.55*	1572.4	[0.56]
Guaiol	14.41	2035.4	0.02	12.81*	1592.8	[0.07]
Unknown MISC CLIX [m/z 91, 119 (91), 79 (86), 93 (85), 41 (74), 107 (68), 105 (67), 134 (65)... 220 (1)]				12.81*	1592.8	[0.07]
Torilenol	15.76*	2167.6	[0.03]	12.96	1604.5	0.05
Unknown CASA XLIV [m/z 135, 93 (66), 79 (58), 107 (54), 41 (42), 81 (41), 67 (41)... 220 (2)]				13.08	1614.3	0.06
allo-Aromadendrene epoxide?	14.15	2011.2	0.13	13.28	1630.6	0.14
τ-Cadinol	15.14	2106.4	0.02	13.33	1634.7	0.04
β-Eudesmol	15.65	2156.5	0.13	13.40	1640.6	0.10
α-Eudesmol	15.58*	2149.7	[0.03]	13.45	1644.6	0.06
α-Cadinol	15.76*	2167.6	[0.03]	13.48	1647.3	0.02
Bulnesol	15.58*	2149.7	[0.03]	13.61	1657.9	0.02
Unknown SASC VIII [m/z				13.65	1661.3	0.01

81, 41 (46), 79 (46), 93 (39), 91 (33), 107 (33)... 206 (8)]						
(1βH)-Guai-9-en-11-ol?	15.94	2185.7	0.02	13.68	1664.3	0.01
Eudesma-4(15),7-dien-1β-ol	16.29	2221.9	0.05	13.84	1677.2	0.03
Cyclocolorenone	16.79	2274.1	0.02	14.68	1748.8	0.01
Benzyl benzoate	19.10	2528.5	0.02	14.73	1752.9	0.04
Phytone	14.96	2088.4	0.04	15.75	1843.2	0.03
Sclareoloxide				16.00	1866.2	0.29
Unknown SASC XI [m/z 69, 81 (84), 109 (80), 43 (64), 95 (59)...]				16.51	1912.8	0.05
Unknown UNKN CXC [m/z 109, 132 (88), 157 (76), 119 (66), 91 (57), 105 (55)...]				16.68	1928.9	0.06
Geranyl-*para*-cymene	16.44	2237.7	0.06	16.88	1948.0	0.06
Manoyl oxide	16.73	2267.4	0.01	17.16	1974.0	0.03
13-epi-Manoyl oxide	16.63	2257.0	0.02	17.43	1999.7	0.01
Manool	19.58	2583.2	0.05	17.85	2041.9	0.05
Sclareol	23.09	3025.9	0.63	19.43	2202.2	0.63
Total reported		97.75%			98.50%	

*: 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