Date : August 20, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21H17-ORA07
Customer identification : Clary Sage - Hungary - 3 years
Type : Essential oil
Source : *Salvia sclarea*
Customer : Organic Aromas Inc.

Analysis

Method: PC-MAT-014 ISO - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.
Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005
Analysis date : August 19, 2021

Checked and approved by :

Alexis St-Gelais, M. Sc., Chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid
Refractive index: 1.4586 ± 0.0003 (20 °C; method PC-MAT-016)

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
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Pentanone	tr	Aliphatic ketone
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Octane	tr	Alkane
(2*E*)-Hexenal	0.03	Aliphatic aldehyde
(3*Z*)-Hexenol	0.07	Aliphatic alcohol
2-Methyloctane	0.01	Alkane
(2*E*)-Hexenol	0.13	Aliphatic alcohol
Hexanol	0.05	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	0.01	Aliphatic ketone
α-Thujene	tr	Monoterpene
α-Pinene	0.07	Monoterpene
α-Fenchene	tr	Monoterpene
Camphene	0.01	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.02	Monoterpene
β-Pinene	0.08	Monoterpene
Octen-3-ol	0.04	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.44	Monoterpene
trans-Dehydroxylinalool oxide	0.04	Monoterpenic ether
Octan-3-ol	tr	Aliphatic alcohol
Octanal	tr	Aliphatic aldehyde
cis-Dehydroxylinalool oxide	0.03	Monoterpenic ether
α-Terpinene	tr	Monoterpene
para-Cymene	0.04	Monoterpene
Limonene	0.25	Monoterpene
β-Phellandrene	0.02	Monoterpene
(*Z*)-β-Ocimene	0.18	Monoterpene
(*E*)-β-Ocimene	0.30	Monoterpene
γ-Terpinene	0.01	Monoterpene
cis-Linalool oxide (fur.)	0.05	Monoterpenic alcohol
Terpinolene	0.08	Monoterpene
trans-Linalool oxide (fur.)	0.06	Monoterpenic alcohol
Rosefuran	tr	Monoterpenic ether
Linalool	26.20	Monoterpenic alcohol
β-Thujone	0.01	Monoterpenic ketone
Hotrienol	0.02	Monoterpenic alcohol
α-Thujone	0.03	Monoterpenic ketone
Dehydrosabinaketone	0.01	Normonoterpenic ketone

cis-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
allo-Ocimene	0.01	Monoterpene
Camphor	0.02	Monoterpenic ketone
neoiso-Thujol	0.01	Monoterpenic alcohol
(*E*)-Myroxide	0.01	Monoterpenic ether
Nerol oxide	0.02	Aliphatic ether
Borneol	0.04	Monoterpenic alcohol
Terpinen-4-ol	0.03	Monoterpenic alcohol
α-Terpineol	2.40	Monoterpenic alcohol
Hodiendiol	0.06	Monoterpenic alcohol
Linalyl formate	0.23	Monoterpenic ester
Nerol	0.49	Monoterpenic alcohol
Unknown	0.02	Monoterpenic ester
Neral	0.02	Monoterpenic aldehyde
Linalyl acetate	58.40	Monoterpenic ester
Geraniol	1.24	Monoterpenic alcohol
Geranial	0.06	Monoterpenic aldehyde
Unknown	0.02	Unknown
Neryl formate	tr	Monoterpenic ester
Bornyl acetate	0.05	Monoterpenic ester
Unknown	0.03	Unknown
Thymol	0.01	Monoterpenic alcohol
Geranyl formate	0.10	Monoterpenic ester
Carvacrol	tr	Monoterpenic alcohol
δ-Elemene	0.02	Sesquiterpene
Hodiendiol derivative	0.10	Oxygenated monoterpene
α-Cubebene	0.06	Sesquiterpene
Unknown	0.05	Oxygenated monoterpene
Unknown	0.01	Monoterpenic ester
Unknown	0.05	Oxygenated monoterpene
Neryl acetate	0.67	Monoterpenic ester
α-Copaene	0.33	Sesquiterpene
(*Z*)-8-Hydroxylinalool?	0.01	Monoterpenic alcohol
β-Bourbonene	0.09	Sesquiterpene
Geranyl acetate	1.26	Monoterpenic ester
β-Cubebene	tr	Sesquiterpene
β-Elemene	0.07	Sesquiterpene
Isocaryophyllene	0.01	Sesquiterpene
β-Caryophyllene	0.89	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
trans-α-Bergamotene	0.01	Sesquiterpene
α-Humulene	0.05	Sesquiterpene
9-epi-β-Caryophyllene	0.02	Sesquiterpene
Germacrene D	1.32	Sesquiterpene
β-Selinene	0.03	Sesquiterpene
Hodiendiol derivative IV	0.18	Oxygenated monoterpene
Bicyclogermacrene	0.14	Sesquiterpene
Germacrene A	0.03	Sesquiterpene
α-Muurolene	0.02	Sesquiterpene
Hodiendiol derivative II	0.04	Oxygenated monoterpene
Cubebol	0.02	Sesquiterpenic alcohol

γ-Cadinene	0.03	Sesquiterpene
β-Bisabolene	0.02	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	0.05	Sesquiterpene
δ-Cadinene	0.09	Sesquiterpene
α-Calacorene	0.01	Sesquiterpene
α-Elemol	0.01	Sesquiterpenic alcohol
Isocaryophyllene epoxide B	0.01	Sesquiterpenic ether
1,5-Epoxysalvial-4(14)-ene	0.02	Sesquiterpenic ether
Spathulenol	0.16	Sesquiterpenic alcohol
Caryophyllene oxide	0.16	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.02	Aliphatic alcohol
Guaiol	0.02	Sesquiterpenic alcohol
Unknown	0.05	Oxygenated sesquiterpene
Torilenol	0.07	Oxygenated sesquiterpene
Unknown	0.05	Unknown
Hinesol	0.01	Sesquiterpenic alcohol
τ-Cadinol	0.02	Sesquiterpenic alcohol
β-Eudesmol	0.05	Sesquiterpenic alcohol
α-Eudesmol	0.05	Sesquiterpenic alcohol
α-Cadinol	0.01	Sesquiterpenic alcohol
(1βH)-Guai-9-en-11-ol?	tr	Sesquiterpenic alcohol
Eudesma-4(15),7-dien-1β-ol	0.02	Sesquiterpenic alcohol
Cyclocolorenone	0.01	Sesquiterpenic ketone
Unknown	0.04	Unknown
Phytone	0.03	Terpenic ketone
Sclareoloxide	0.06	Terpenic ether
Unknown	0.05	Unknown
Geranyl-α-terpinene	0.01	Diterpene
Geranyl-para-cymene	0.04	Diterpene
Manoyl oxide	0.01	Diterpenic ether
13-epi-Manoyl oxide	tr	Diterpenic ether
Manool	0.02	Diterpenic alcohol
Sclareol	0.28	Diterpenic alcohol
Consolidated total	**98.59%**	

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.

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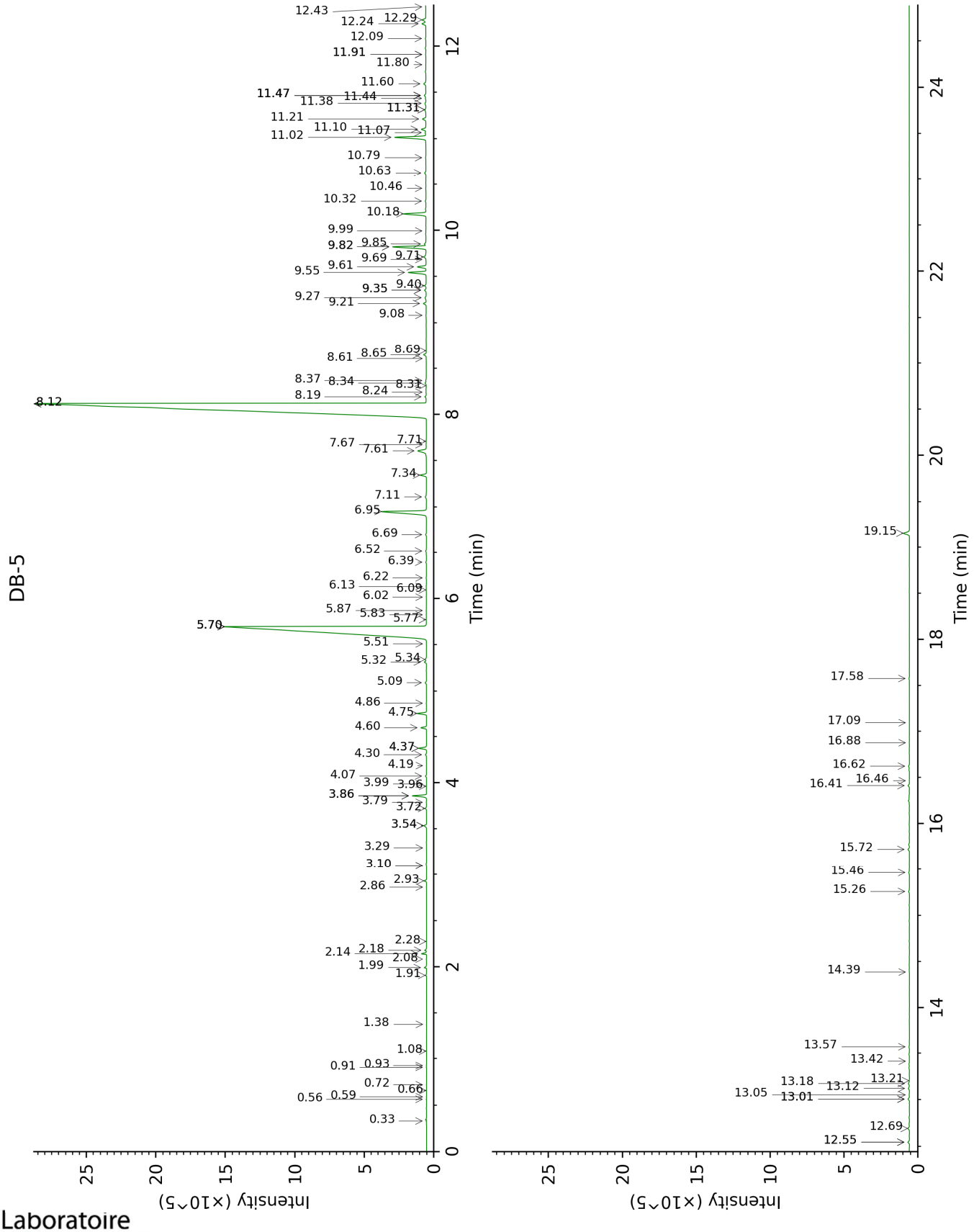
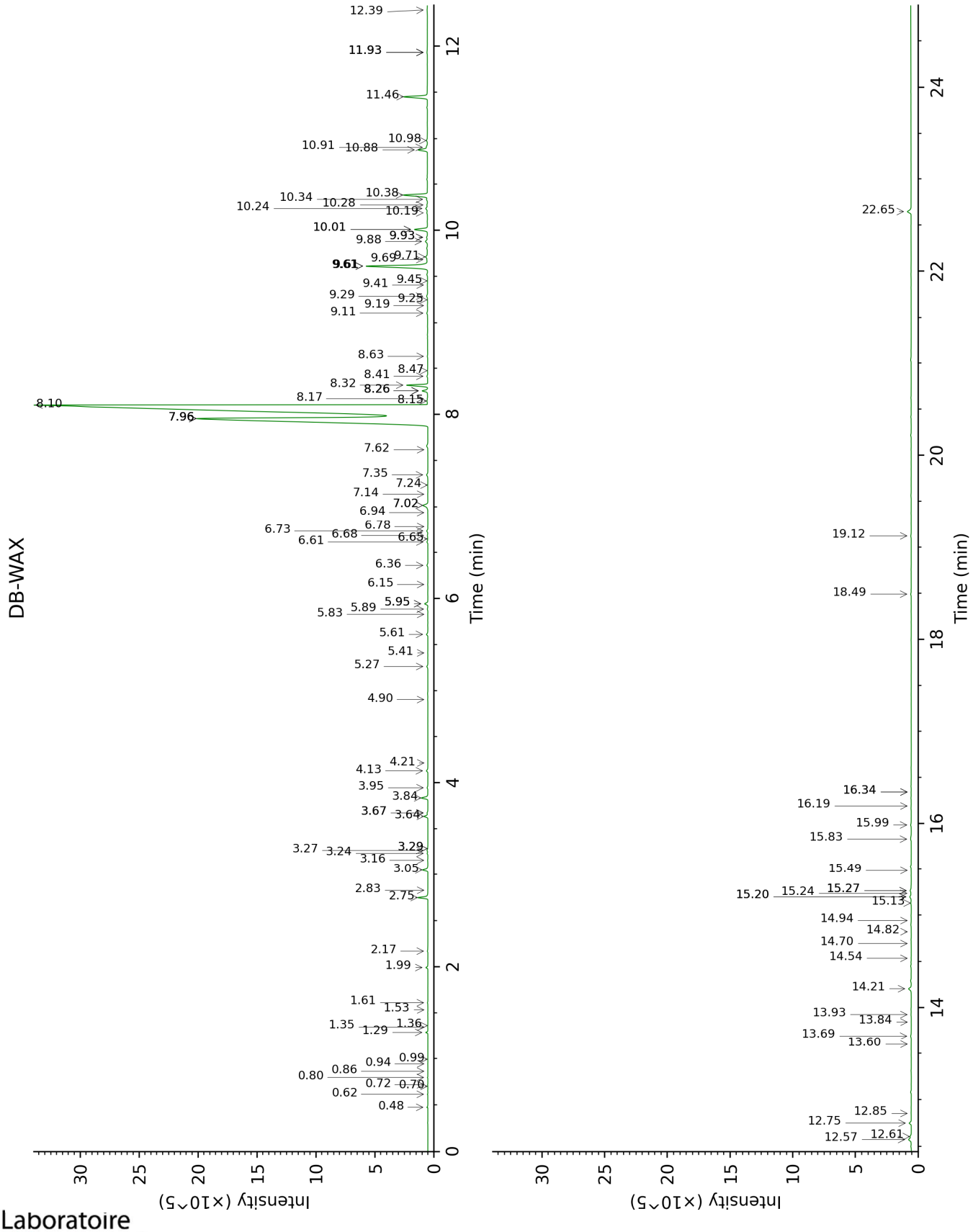

DB-5
Time (min)
Intensity (×10^5)
12.43
12.24
12.29
12.09
11.91
11.80
11.60
11.47
11.38
11.44
11.31
11.21
11.10
11.07
11.02
10.79
10.63
10.46
10.32
10.18
9.99
9.82
9.85
9.69
9.71
9.61
9.55
9.35
9.40
9.27
9.21
9.08
8.61
8.65
8.69
8.37
8.34
8.31
8.19
8.24
8.12
7.67
7.71
7.61
7.34
7.11
6.95
6.69
6.52
6.39
6.22
6.13
6.09
6.02
5.87
5.83
5.77
5.70
5.51
5.32
5.34
5.09
4.86
4.75
4.60
4.37
4.30
4.19
4.07
3.99
3.96
3.86
3.79
3.72
3.54
3.29
3.10
2.93
2.86
2.28
2.14
2.18
2.08
1.99
1.91
1.38
1.08
0.91
0.93
0.72
0.66
0.56
0.59
0.33
19.15
17.58
17.09
16.88
16.62
16.41
16.46
15.72
15.46
15.26
14.39
13.57
13.42
13.18
13.21
13.12
13.05
13.01
12.69
12.55


DB-WAX
Time (min)
Intensity (×10^5)
12.39
11.93
11.46
10.98
10.91
10.88
10.38
10.34
10.28
10.24
10.19
10.01
9.93
9.88
9.71
9.69
9.61
9.45
9.41
9.29
9.25
9.19
9.11
8.63
8.47
8.41
8.32
8.26
8.17
8.15
8.10
7.96
7.62
7.35
7.24
7.14
7.02
6.94
6.78
6.73
6.68
6.65
6.61
6.36
6.15
5.95
5.89
5.83
5.61
5.41
5.27
4.90
4.21
4.13
3.95
3.84
3.67
3.64
3.29
3.27
3.24
3.16
3.05
2.83
2.75
2.17
1.99
1.61
1.53
1.36
1.35
1.29
0.99
0.94
0.86
0.80
0.72
0.70
0.62
0.48
22.65
19.12
18.49
16.34
16.19
15.99
15.83
15.49
15.27
15.24
15.20
15.13
14.94
14.82
14.70
14.54
14.21
13.93
13.84
13.69
13.60
12.85
12.75
12.61
12.57

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.33	499	0.01	0.80	907	0.01
Isovaleral	0.56	642	0.01	0.72	886	tr
2-Methylbutyral	0.59	652	tr	0.70	880	tr
2-Pentanone	0.66	678	tr	0.99	940	tr
2-Ethylfuran	0.72	701	tr	0.86	918	tr
Isoamyl alcohol	0.91	731	0.01	3.29*	1176	0.01
2-Methylbutanol	0.93	734	tr	3.29*	1176	[0.01]
Toluene	1.08	758	tr	1.36	1001	tr
Octane	1.38	803	tr	0.48	783	0.02
(2*E*)-Hexenal	1.91	849	0.03	3.24	1172	0.03
(3*Z*)-Hexenol	1.99	857	0.07	5.61	1346	0.08
2-Methyloctane	2.08	864	0.01	0.62	848	0.01
(2*E*)-Hexenol	2.14	870	0.13	5.94*	1370	0.16
Hexanol	2.18	873	0.05	5.27	1320	0.06
3-Acetyl-3-methylcyclopentene	2.28	881	0.01	0.94	932	tr
α-Thujene	2.86	926	tr	1.35	1000	0.01
α-Pinene	2.93	930	0.07	1.29	991	0.07
α-Fenchene	3.10*†	942	0.02	1.53	1018	tr
Camphene	3.10*†	942	[0.02]	1.61	1026	0.01
Benzaldehyde	3.30	955	0.01	7.14	1458	0.01
Sabinene	3.54*	971	0.10	2.17	1083	0.02
β-Pinene	3.54*	971	[0.10]	1.99	1065	0.08
Octen-3-ol	3.72	984	0.04	6.65	1421	0.01
6-Methyl-5-hepten-2-one	3.79	988	0.01	4.90	1300	0.02
Myrcene	3.86*	993	0.46	2.75	1133	0.44
trans-Dehydroxylinalool oxide	3.86*	993	[0.46]	3.27	1175	0.04
Octan-3-ol	3.96	1000	tr	5.89	1365	0.03
Octanal	3.99	1002	tr	4.21	1248	tr
cis-Dehydroxylinalool oxide	4.07	1007	0.03	3.67*	1207	0.05
α-Terpinene	4.19	1014	tr	2.83	1139	0.01
para-Cymene	4.30	1022	0.04	3.95	1228	0.04
Limonene	4.37*	1026	0.25	3.05	1157	0.25
β-Phellandrene	4.37*	1026	[0.25]	3.16	1166	0.02
(*Z*)-β-Ocimene	4.60	1040	0.18	3.64	1204	0.18
(*E*)-β-Ocimene	4.75	1050	0.30	3.84	1219	0.32
γ-Terpinene	4.86	1057	0.01	3.67*	1207	[0.05]
cis-Linalool oxide (fur.)	5.09	1072	0.05	6.36	1400	0.05
Terpinolene	5.32†	1086	0.12	4.13	1241	0.08
trans-Linalool oxide (fur.)	5.34†	1088	[0.12]	6.73	1428	0.06
Rosefuran	5.51	1098	tr	5.83	1361	0.01
Linalool	5.70*	1110	26.44	7.96*†	1520	84.62

β-Thujone	5.70*	1110	[26.44]	6.15	1385	0.01
Hotrienol	5.70*	1110	[26.44]	8.63	1572	0.02
α-Thujone	5.70*	1110	[26.44]	5.94*	1370	[0.16]
Dehydrosabinaketone	5.77	1115	0.01	8.48	1560	0.01
cis-para-Menth-2-en-1-ol	5.83	1118	0.01	7.96*†	1520	[84.62]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.87	1121	0.01	9.45	1638	0.01
allo-Ocimene	6.02	1131	0.01	5.41	1331	0.01
Camphor	6.10	1136	0.02	7.02*	1449	0.33
neoiso-Thujol	6.13	1138	0.01	9.41	1634	0.01
(*E*)-Myroxide	6.22	1144	0.01	6.94	1443	0.01
Nerol oxide	6.40	1155	0.02	6.68	1424	0.03
Borneol	6.52	1163	0.04	9.61*	1651	3.78
Terpinen-4-ol	6.69	1174	0.03	8.41	1555	0.04
α-Terpineol	6.95	1191	2.40	9.61*	1651	[3.78]
Hodiendiol	7.11	1201	0.06	12.61	1908	0.08
Linalyl formate	7.34	1216	0.23	8.26*	1543	0.27
Nerol	7.61	1234	0.49	10.88	1757	0.48
Unknown [m/z 121, 43 (93), 41 (37), 107 (35), 67 (33), 136 (32)... 154 (1)]	7.67	1239	0.02	7.24	1465	0.01
Neral	7.71	1241	0.02	9.29	1625	0.06
Linalyl acetate	8.12*	1268	59.63	8.10†	1531	[84.62]
Geraniol	8.12*	1268	[59.63]	11.46	1806	1.24
Geranial	8.19	1273	0.06	9.93*	1676	0.05
Unknown [m/z 121, 43 (75), 95 (57), 41 (34), 93 (33), 69 (28)...]	8.24	1277	0.02			
Neryl formate	8.31	1281	tr	9.25	1621	0.01
Bornyl acetate	8.34	1283	0.05	8.15	1535	0.05
Unknown [m/z 43, 121 (74), 93 (42), 95 (38), 107 (29), 41 (29), 136 (28)...]	8.37	1285	0.03			
Thymol	8.61	1301	0.01	14.94	2131	0.01
Geranyl formate	8.65	1304	0.10	9.71	1659	0.12
Carvacrol	8.69	1307	tr	15.20*	2157	0.10
δ-Elemene	9.08	1335	0.02	6.78	1431	tr
Hodiendiol derivative	9.21	1344	0.10	12.75	1922	0.11
α-Cubebene	9.27	1348	0.06	6.61	1419	0.05
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.35*	1354	0.06	10.91	1759	0.05
Unknown [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81 (25)...]	9.35*	1354	[0.06]			

Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.40	1357	0.05	10.98	1765	0.05
Neryl acetate	9.55	1368	0.67	10.01*	1683	0.69
α-Copaene	9.61	1372	0.33	7.02*	1449	[0.33]
(*Z*)-8-Hydroxylinalool?	9.69	1377	0.01	13.60	2001	0.01
β-Bourbonene	9.71	1379	0.09	7.35	1473	0.08
Geranyl acetate	9.82*	1387	1.34	10.38	1714	1.26
β-Cubebene	9.82*	1387	[1.34]	7.62	1494	tr
β-Elemene	9.85	1389	0.07	8.26*	1543	[0.27]
Isocaryophyllene	10.00	1399	0.01	7.96*†	1520	[84.62]
β-Caryophyllene	10.18	1413	0.89	8.32	1548	0.90
β-Copaene	10.32	1423	0.03	8.17	1536	0.02
trans-α-Bergamotene	10.46	1434	0.01	8.26*	1543	[0.27]
α-Humulene	10.63	1446	0.05	9.10	1610	0.05
9-epi-β-Caryophyllene	10.80	1459	0.02	9.19	1616	0.02
Germacrene D	11.02	1475	1.32	9.61*	1651	[3.78]
β-Selinene	11.07	1479	0.03	9.68	1657	0.04
Hodiendiol derivative IV	11.10	1482	0.18			
Bicyclogermacrene	11.21	1490	0.14	9.88	1673	0.13
Germacrene A	11.31*	1497	0.05	10.28	1705	0.03
α-Muurolene	11.31*	1497	[0.05]	9.93*	1676	[0.05]
Hodiendiol derivative II	11.38	1503	0.04			
Cubebol	11.44	1507	0.02	12.40	1889	0.02
γ-Cadinene	11.47*	1509	0.07	10.19	1698	0.03
β-Bisabolene	11.47*	1509	[0.07]	10.01*	1683	[0.69]
(3*E*,6*E*)-α-Farnesene	11.47*	1509	[0.07]	10.34	1710	0.05
δ-Cadinene	11.60	1519	0.09	10.24	1702	0.10
α-Calacorene	11.80	1535	0.01	11.93*	1848	0.03
α-Elemol	11.91*	1544	0.02	13.84	2024	0.01
Isocaryophyllene epoxide B	11.91*	1544	[0.02]	11.93*	1848	[0.03]
1,5-Epoxysalvial-4(14)-ene	12.08	1558	0.02	11.93*	1848	[0.03]
Spathulenol	12.24	1570	0.16	14.21	2059	0.18
Caryophyllene oxide	12.29	1574	0.16	12.57	1906	0.18
Salvial-4(14)-en-1-one	12.43	1585	0.02	12.85	1931	0.02
Guaiol	12.55*	1594	0.07	13.93	2032	0.02
Unknown [m/z 91, 119 (91), 79 (86), 93 (85), 41 (74), 107 (68), 105 (67), 134 (65)... 220 (1)]	12.55*	1594	[0.07]			
Torilenol	12.69	1606	0.07	15.27*	2164	0.09
Unknown [m/z 43, 93 (89), 91 (88), 79 (87), 123 (76), 81 (75)...]	13.01*	1632	0.06	13.69	2009	0.05
Hinesol	13.01*	1632	[0.06]	14.82	2119	0.01

τ-Cadinol	13.05	1636	0.02	14.70	2106	0.01
β-Eudesmol	13.12	1641	0.05	15.20*	2157	[0.10]
α-Eudesmol	13.18	1646	0.05	15.13	2150	0.03
α-Cadinol	13.21	1648	0.01	15.27*	2164	[0.09]
(1βH)-Guai-9-en-11-ol?	13.42	1666	tr	15.49	2186	0.01
Eudesma-4(15),7-dien-1β-ol	13.57	1678	0.02	15.83	2221	0.06
Cyclocolorenone	14.39	1748	0.01	16.34*	2274	0.01
Unknown [m/z 123, 191 (88), 81 (86), 41 (86), 151 (80), 91 (76)...]	15.26	1825	0.04	18.49	2510	0.03
Phytone	15.46	1843	0.03	14.54	2091	0.01
Sclareoloxide	15.72	1867	0.06			
Unknown [m/z 109, 132 (88), 157 (76), 119 (66), 91 (57), 105 (55)...]	16.41	1931	0.05			
Geranyl-α-terpinene	16.46	1936	0.01	15.24	2161	0.02
Geranyl-para-cymene	16.62	1951	0.04	15.99	2237	0.04
Manoyl oxide	16.88	1975	0.01	16.34*	2274	[0.01]
13-epi-Manoyl oxide	17.09	1996	tr	16.19	2258	0.01
Manool	17.58	2044	0.02	19.12	2583	0.03
Sclareol	19.15	2204	0.28	22.65	3025	0.25
Total identified		**98.58%**			**98.12%**	
Total reported		**98.79%**			**98.32%**	

*: 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