Date : March 17, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21B23-FEP18
Customer identification : Neroli - Tunisia - 985116-19
Type : Essential oil
Source : *Citrus aurantium* subsp. *amara*
Customer : Fern & Petal

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
Analysis date : March 17, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid
Refractive index: 1.4694 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No clear 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	0.06	Aliphatic alcohol
Methacrolein	0.01	Aliphatic aldehyde
3-Buten-2-one	0.03	Aliphatic ketone
2-Methyl-3-buten-2-ol	0.04	Aliphatic alcohol
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Octane	0.01	Alkane
(3*Z*)-Hexenol	0.02	Aliphatic alcohol
(2*E*)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.04	Aliphatic alcohol
α-Thujene	0.02	Monoterpene
α-Pinene	0.24	Monoterpene
Camphene	0.02	Monoterpene
Benzaldehyde	0.04	Simple phenolic
Sabinene	0.41	Monoterpene
β-Pinene	3.02	Monoterpene
6-Methyl-5-hepten-2-one	0.04	Aliphatic ketone
Myrcene	1.15	Monoterpene
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
(3*Z*)-Hexenyl acetate	0.02	Aliphatic ester
para-Cymene	0.12	Monoterpene
Limonene	5.93	Monoterpene
β-Phellandrene	0.05	Monoterpene
Benzyl alcohol	0.01	Simple phenolic
(*Z*)-β-Ocimene	0.27	Monoterpene
(*E*)-β-Ocimene	1.16	Monoterpene
Unknown	0.01	Monoterpene
γ-Terpinene	0.01	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.61	Monoterpenic alcohol
α-Pinene oxide analog	0.05	Monoterpenic ether
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.07	Monoterpene
trans-Linalool oxide (fur.)	0.45	Monoterpenic alcohol
trans-Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	49.13	Monoterpenic alcohol
Phenylethyl alcohol	0.07	Simple phenolic
(*E*)-4,8-Dimethylnona-1,3,7-triene	0.02	Terpene derivative
cis-para-Menth-2-en-1-ol	0.05	Monoterpenic alcohol
cis-Limonene oxide	0.02	Monoterpenic ether
Benzeneacetonitrile	0.37	Simple phenolic
trans-Pinocarveol	0.02	Monoterpenic alcohol
(*Z*)-Myroxide	0.05	Monoterpenic ether
trans-para-Menth-2-en-1-ol	0.02	Monoterpenic alcohol
neo-allo-Ocimene	0.02	Monoterpene

(*E*)-Myroxide	0.05	Monoterpenic ether
Citronellal	0.01	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.32	Monoterpenic alcohol
para-Cymen-8-ol	0.04	Monoterpenic alcohol
α-Terpineol	8.01	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Myrtenol	0.02	Monoterpenic alcohol
Hodiendiol	0.11	Monoterpenic alcohol
Safranal	0.01	Monoterpenic aldehyde
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol
Linalyl formate	0.03	Monoterpenic ester
1-para-Menthen-9-al	0.02	Monoterpenic aldehyde
Nerol	1.55	Monoterpenic alcohol
Citronellol	0.04	Monoterpenic alcohol
6,7-Dihydro-7-hydroxylinalool	0.02	Monoterpenic alcohol
Neral	0.13	Monoterpenic aldehyde
Phenylethyl acetate	0.06	Phenolic ester
Geraniol	4.07	Monoterpenic alcohol
Linalyl acetate	6.27	Monoterpenic ester
Geranial	0.19	Monoterpenic aldehyde
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.09	Monoterpenic alcohol
Bornyl acetate	0.15	Monoterpenic ester
1-Nitro-2-phenylethane	0.04	Simple phenolic
Indole	0.08	Indole
4-Vinylguaiacol	0.02	Simple phenolic
Methyl anthranilate	0.22	Phenolic ester
Linalyl propionate	0.06	Monoterpenic ester
Hodiendiol derivative	0.08	Oxygenated monoterpene
α-Terpinyl acetate	0.15	Monoterpenic ester
Neryl acetate	1.67	Monoterpenic ester
Geranyl acetate	3.31	Monoterpenic ester
β-Elemene	0.03	Sesquiterpene
(*Z*)-Jasmone	0.06	Jasmonate
Dimethyl anthranilate	0.04	Phenolic ester
Ethyl anthranilate	0.01	Phenolic ester
β-Caryophyllene	0.46	Sesquiterpene
(*Z*)-β-Farnesene?	0.02	Sesquiterpene
α-Humulene	0.07	Sesquiterpene
Geranylacetone	0.04	Monoterpenic ketone
(*E*)-β-Farnesene	0.07	Sesquiterpene
Cabreuva oxide D?	0.03	Sesquiterpenic ether
Germacrene D	0.07	Sesquiterpene
Valencene	0.03	Sesquiterpene
Bicyclogermacrene	0.05	Sesquiterpene
γ-Cadinene	0.01	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	0.03	Sesquiterpene
trans-Calamenene	0.01	Sesquiterpene
δ-Cadinene	0.04	Sesquiterpene
α-Cadinene	0.01	Sesquiterpene
(*Z*)-Nerolidol	0.01	Sesquiterpenic alcohol

Methyl N-formylanthranilate	0.03	Phenolic ester
(*E*)-Nerolidol	2.35	Sesquiterpenic alcohol
Spathulenol	0.11	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Caryophyllene oxide isomer	0.05	Sesquiterpenic ether
Viridiflorol	0.01	Sesquiterpenic alcohol
Humulene epoxide II	0.02	Sesquiterpenic ether
τ-Cadinol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Sesquiterpenic alcohol
α-Cadinol	0.02	Sesquiterpenic alcohol
α-Bisabolol	0.05	Sesquiterpenic alcohol
2,3-Dihydrofarnesol	0.02	Sesquiterpenic alcohol
β-Sinensal	0.01	Sesquiterpenic aldehyde
(2*E*,6*Z*)-Farnesol	0.04	Sesquiterpenic alcohol
Heptadecane	0.03	Alkane
(2*E*,6*Z*)-Farnesal	0.04	Sesquiterpenic aldehyde
(2*E*,6*E*)-Farnesol	1.67	Sesquiterpenic alcohol
(2*E*,6*E*)-Farnesal	0.08	Sesquiterpenic aldehyde
(2*E*,6*E*)-Farnesyl acetate	0.07	Sesquiterpenic ester
Nonadecane	0.01	Alkane
Unknown	0.02	Unknown
Phytol	0.03	Diterpenic alcohol
Tricosane	0.04	Alkane
Pentacosane	0.03	Alkane
Consolidated total	**96.48%**	

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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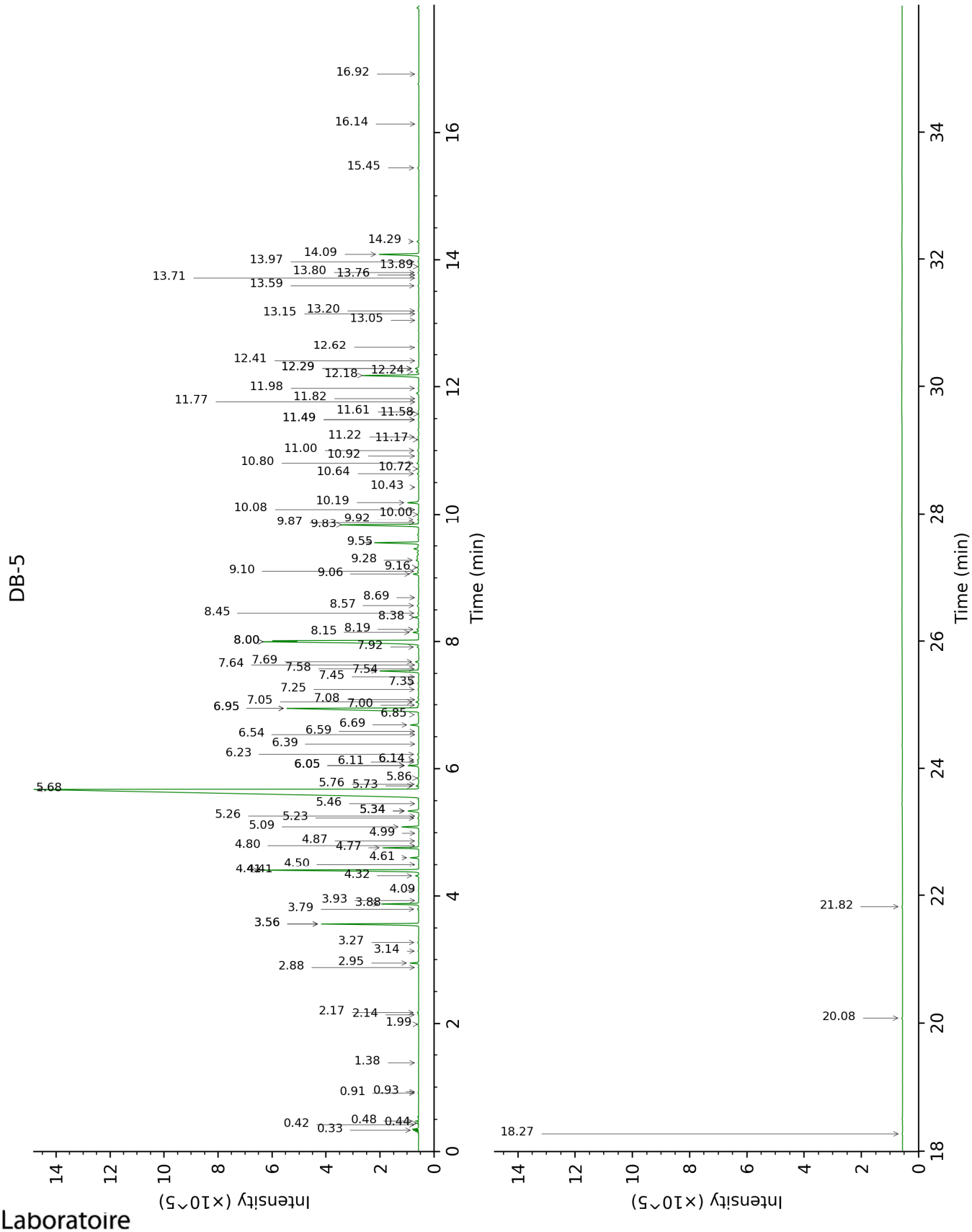
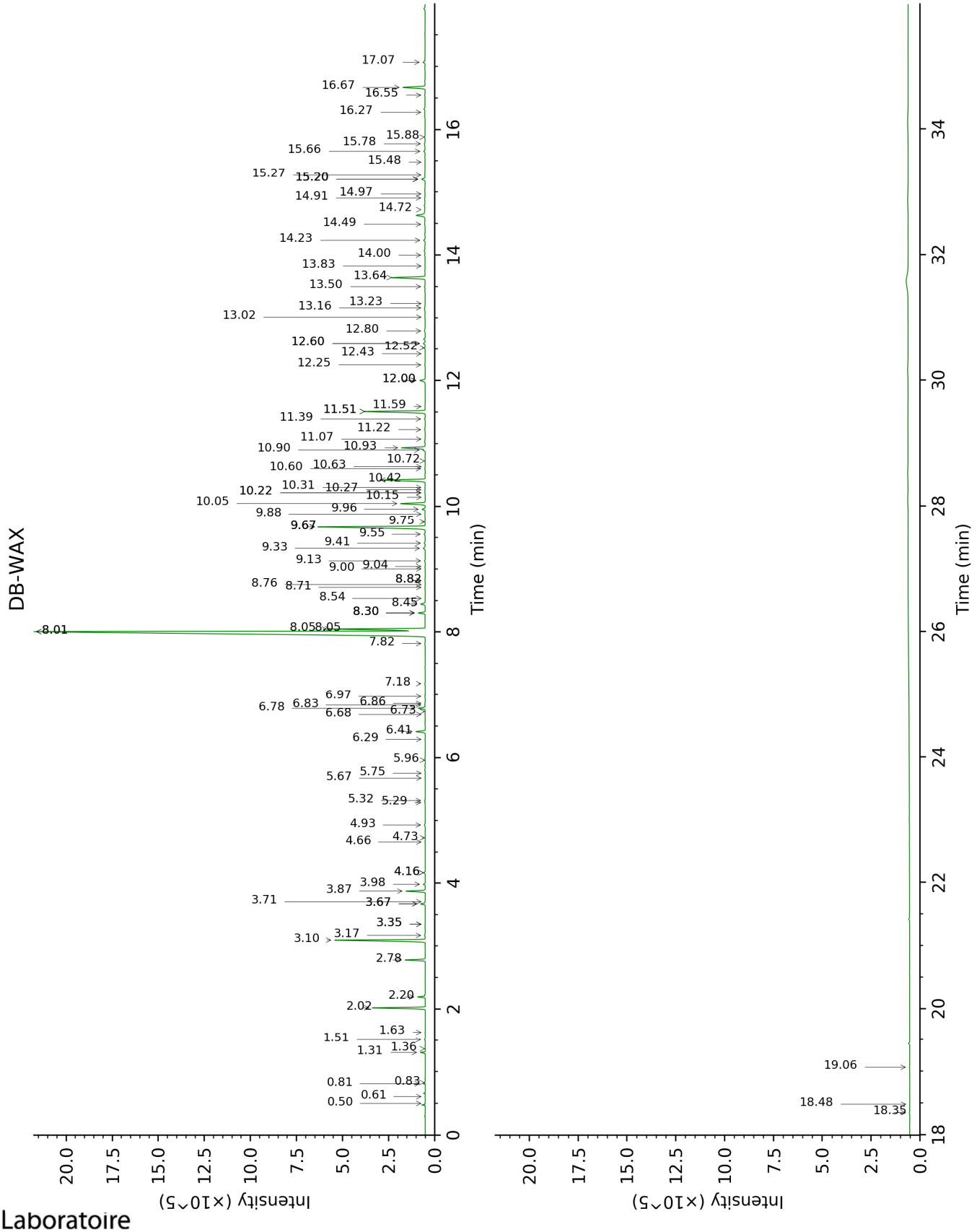

DB-5
Intensity (×10^5)
Time (min)
16.92
16.14
15.45
14.29
14.09
13.97
13.89
13.80
13.76
13.71
13.59
13.20
13.15
13.05
12.62
12.41
12.29
12.18
12.24
11.98
11.82
11.77
11.61
11.58
11.49
11.22
11.17
11.00
10.92
10.80
10.72
10.64
10.43
10.19
10.08
10.00
9.92
9.87
9.83
9.55
9.28
9.16
9.10
9.06
8.69
8.57
8.45
8.38
8.19
8.15
8.00
7.92
7.69
7.64
7.58
7.54
7.45
7.35
7.25
7.08
7.05
7.00
6.95
6.85
6.69
6.59
6.54
6.39
6.23
6.14
6.11
6.05
5.86
5.76
5.73
5.68
5.46
5.34
5.26
5.23
5.09
4.99
4.87
4.80
4.77
4.61
4.50
4.41
4.32
4.09
3.93
3.88
3.79
3.56
3.27
3.14
2.95
2.88
2.17
2.14
1.99
1.38
0.93
0.91
0.48
0.44
0.42
0.33
21.82
20.08
18.27


DB-WAX
Time (min)
Intensity (×10^5)
17.07
16.67
16.55
16.27
15.88
15.78
15.66
15.48
15.27
15.20
14.97
14.91
14.72
14.49
14.23
14.00
13.83
13.64
13.50
13.23
13.16
13.02
12.80
12.60
12.52
12.43
12.25
12.00
11.59
11.51
11.39
11.22
11.07
10.93
10.90
10.72
10.63
10.60
10.42
10.31
10.27
10.22
10.15
10.05
9.96
9.88
9.75
9.67
9.55
9.41
9.33
9.13
9.04
9.00
8.82
8.76
8.71
8.54
8.45
8.30
8.05
8.01
7.82
7.18
6.97
6.86
6.83
6.78
6.73
6.68
6.41
6.29
5.96
5.75
5.67
5.32
5.29
4.93
4.73
4.66
4.16
3.98
3.87
3.71
3.67
3.35
3.17
3.10
2.78
2.20
2.02
1.63
1.51
1.36
1.31
0.83
0.81
0.61
0.50
19.06
18.48
18.35

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.33	499	0.06	0.81	908	0.06
Methacrolein	0.42	552	0.01	0.61	843	0.01
3-Buten-2-one	0.44	573	0.03	0.83	911	0.02
2-Methyl-3-buten-2-ol	0.48	605	0.04	1.51	1016	0.04
Isoamyl alcohol	0.91	731	0.01	3.35*	1179	0.02
2-Methylbutanol	0.93	734	tr	3.35*	1179	[0.02]
Octane	1.38	802	0.01	0.50	802	0.01
(3*Z*)-Hexenol	1.99	856	0.02	5.67	1349	0.02
(2*E*)-Hexenol	2.14	868	0.01	5.96	1370	0.01
Hexanol	2.18	872	0.04	5.32	1324	0.04
α-Thujene	2.88	926	0.02	1.36	1001	0.01
α-Pinene	2.95	931	0.24	1.31	992	0.24
Camphene	3.14	944	0.02	1.63	1028	0.02
Benzaldehyde	3.27	953	0.04	7.18	1461	0.04
Sabinene	3.56*	972	3.49	2.20	1085	0.41
β-Pinene	3.56*	972	[3.49]	2.02	1067	3.02
6-Methyl-5-hepten-2-one	3.79	988	0.04	4.93	1296	0.08
Myrcene	3.88	994	1.15	2.78	1134	1.10
6-Methyl-5-hepten-2-ol	3.93	997	0.01	6.83	1434	0.04
(3*Z*)-Hexenyl acetate	4.09	1008	0.02	4.73	1281	0.01
para-Cymene	4.32	1022	0.12	3.98	1227	0.12
Limonene	4.41*	1028	6.09	3.10	1159	5.93
β-Phellandrene	4.41*	1028	[6.09]	3.17	1165	0.05
Benzyl alcohol	4.50	1034	0.01	11.59	1818	0.04
(*Z*)-β-Ocimene	4.61	1041	0.27	3.67*	1204	0.28
(*E*)-β-Ocimene	4.77	1051	1.16	3.87	1219	1.14
Unknown [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	4.80	1053	0.01	3.70	1207	0.01
γ-Terpinene	4.87	1057	0.01	3.67*	1204	[0.28]
cis-Sabinene hydrate	4.99	1065	0.01	6.73	1427	0.01
cis-Linalool oxide (fur.)	5.09	1071	0.61	6.41	1403	0.62
α-Pinene oxide analog	5.23	1080	0.05	5.29	1321	0.03
Isoterpinolene	5.26	1082	0.01	4.16*	1240	0.08
Terpinolene	5.34*	1087	0.51	4.16*	1240	[0.08]
trans-Linalool oxide (fur.)	5.34*	1087	[0.51]	6.78	1431	0.45
trans-Sabinene hydrate	5.46	1094	0.01	7.82	1509	0.05
Linalool	5.68	1108	49.13	8.01*†	1523	55.59

Phenylethyl alcohol	5.73	1112	0.07	12.00*	1855	0.44
(*E*)-4,8-Dimethylnona-1,3,7-triene	5.76	1114	0.02	4.66	1276	0.02
cis-para-Menth-2-en-1-ol	5.86	1120	0.05	8.01*†	1523	[55.59]
cis-Limonene oxide	6.05*	1132	0.42	6.29	1394	0.02
Benzeneacetonitrile	6.05*	1132	[0.42]	12.00*	1855	[0.44]
trans-Pinocarveol	6.05*	1132	[0.42]	9.00	1601	0.02
(*Z*)-Myroxide	6.11	1136	0.05	6.68	1423	0.03
trans-para-Menth-2-en-1-ol	6.14*	1138	0.05	8.82*	1587	0.04
neo-allo-Ocimene	6.14*	1138	[0.05]	5.75	1355	0.02
(*E*)-Myroxide	6.23	1144	0.05	6.97	1445	0.04
Citronellal	6.39	1154	0.01	6.86	1437	0.03
Borneol	6.54	1164	0.01	9.67*	1656	8.09
cis-Linalool oxide (pyr.)	6.59	1167	0.01	10.15	1695	0.01
Terpinen-4-ol	6.69	1173	0.32	8.45	1558	0.31
para-Cymen-8-ol	6.85	1184	0.04	11.39	1800	0.05
α-Terpineol	6.95*	1190	8.17	9.67*	1656	[8.09]
Myrtenal	6.95*	1190	[8.17]	8.54	1564	0.01
Myrtenol	7.00	1193	0.02	10.72	1744	0.02
Hodiendiol	7.05	1196	0.11	12.60*	1908	0.13
Safranal	7.08	1199	0.01	8.76	1582	0.01
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.25	1210	0.03	11.22	1786	0.04
Linalyl formate	7.35	1217	0.03	8.30*	1546	0.46
1-para-Menthen-9-al	7.45	1223	0.02	8.82*	1587	[0.04]
Nerol	7.54	1230	1.55	10.93	1762	1.56
Citronellol	7.58	1232	0.04	10.60	1733	0.04
6,7-Dihydro-7-hydroxylinalool	7.64	1236	0.02	13.02	1947	0.03
Neral	7.69	1239	0.13	9.33	1628	0.17
Phenylethyl acetate	7.92	1255	0.06	10.90	1758	0.13
Geraniol	8.00*	1260	11.31	11.51*	1811	4.11
Linalyl acetate	8.00*	1260	[11.31]	8.05*†	1527	[55.59]
Geranial	8.15	1270	0.19	9.96	1679	0.21
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.19	1273	0.09	14.49	2088	0.08
Bornyl acetate	8.38	1286	0.15	8.05*†	1527	[55.59]
1-Nitro-2-phenylethane	8.45	1290	0.04	14.00	2040	0.06
Indole	8.57	1298	0.08	17.07	2354	0.16
4-Vinylguaiacol	8.69	1307	0.02	14.91	2129	0.02
Methyl anthranilate	9.06	1333	0.22	15.20*	2159	0.27
Linalyl propionate	9.10	1336	0.06	8.71	1578	0.02
Hodiendiol derivative	9.16	1340	0.08	12.80	1927	0.05
α-Terpinyl acetate	9.28	1348	0.15	9.55	1646	0.08

Neryl acetate	9.55	1368	1.67	10.05	1687	1.65
Geranyl acetate	9.83	1387	3.31	10.42	1718	3.17
β-Elemene	9.87	1390	0.03	8.30*	1546	[0.46]
(*Z*)-Jasmone	9.92	1394	0.06	12.25	1877	0.05
Dimethyl anthranilate	10.00	1400	0.04	13.50	1992	0.05
Ethyl anthranilate	10.08	1405	0.01	15.48	2187	0.02
β-Caryophyllene	10.19	1413	0.46	8.30*	1546	[0.46]
(*Z*)-β-Farnesene?	10.43	1431	0.02	9.04	1604	0.02
α-Humulene	10.64	1447	0.07	9.13	1612	0.06
Geranylacetone	10.72	1453	0.04	11.51*	1811	[4.11]
(*E*)-β-Farnesene	10.80	1459	0.07	9.41	1634	0.08
Cabreuva oxide D?	10.92	1468	0.03			
Germacrene D	11.00	1474	0.07	9.67*	1656	[8.09]
Valencene	11.17	1487	0.03	9.75	1662	0.04
Bicyclogermacrene	11.22	1490	0.05	9.88	1673	0.03
γ-Cadinene	11.49*	1510	0.04	10.22*	1701	0.04
(3*E*,6*E*)-α-Farnesene	11.49*	1510	[0.04]	10.31	1708	0.03
trans-Calamenene	11.58	1518	0.01	11.07	1773	0.02
δ-Cadinene	11.61	1520	0.04	10.27	1705	0.03
α-Cadinene	11.76	1532	0.01	10.64	1736	0.01
(*Z*)-Nerolidol	11.82	1536	0.01	13.23	1967	0.01
Methyl N-formylanthranilate	11.98	1549	0.03	18.48	2512	0.01
(*E*)-Nerolidol	12.18	1565	2.35	13.64	2006	2.36
Spathulenol	12.24	1570	0.11	14.24	2063	0.11
Caryophyllene oxide	12.29*	1574	0.17	12.60*	1908	[0.13]
Caryophyllene oxide isomer	12.29*	1574	[0.17]	12.52	1901	0.05
Viridiflorol	12.41	1583	0.01	13.83	2024	0.03
Humulene epoxide II	12.62	1600	0.02	13.16	1961	0.04
τ-Cadinol	13.05	1635	0.02	14.72	2111	0.02
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109)40)... 204 (35), 222 (2)]	13.15	1644	0.01	14.97	2136	0.02
α-Cadinol	13.20	1648	0.02	15.27	2166	0.03
α-Bisabolol	13.59	1680	0.05	15.20*	2159	[0.27]
2,3-Dihydrofarnesol	13.71	1690	0.02	15.88	2228	0.04
β-Sinensal	13.76	1694	0.01	15.20*	2159	[0.27]
(2*E*,6*Z*)-Farnesol	13.80	1697	0.04	16.28	2270	0.05
Heptadecane	13.89	1705	0.03	10.22*	1701	[0.04]
(2*E*,6*Z*)-Farnesal	13.97	1712	0.04	15.20*	2159	[0.27]
(2*E*,6*E*)-Farnesol	14.09	1722	1.67	16.67	2311	1.63
(2*E*,6*E*)-Farnesal	14.29	1739	0.08	15.66	2205	0.10
(2*E*,6*E*)-Farnesyl acetate	15.45	1842	0.07	15.78	2217	0.06
Nonadecane	16.14	1905	0.01	12.43	1893	0.02

Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	16.92	1979	0.02			
Phytol	18.27	2113	0.03	19.06	2579	0.04
Tricosane	20.08	2305	0.04	16.55	2298	0.04
Pentacosane	21.82	2505	0.03	18.35	2496	0.04
Total identified		**97.86%**			**96.38%**	
Total reported		**97.90%**			**96.40%**	

*: 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