Date : January 14, 2021

Certificate of Analysis – GC Profiling

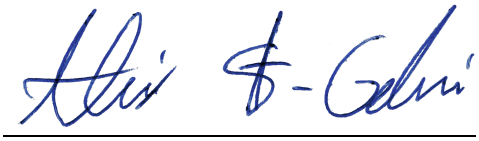
Sample identification

Internal code : 20L21-PSC02
Customer identification : Petitgrain Mandarin - CIRE-2020-01
Type : Essential oil
Source : *Citrus reticulata* cv. Mandarine
Customer : Pacha Soap Co.

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 : Alexis St-Gelais, M. Sc., chimiste
Analysis date : January 13, 2021

Checked and approved by :



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

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Méthode certifiée ISO 17025:2017 Certified method

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Physicochemical data

Physical aspect: Faintly yellow liquid
Refractive index: 1.4780 ± 0.0003 (20 °C; method PC-MAT-016)
Optical rotation: +31.8° (21 °C, methanol, *c* = 1.3)

ISO 8898 - Oil of mandarin petitgrain

Compound	Min. %	Max. %	Observed %	Complies?
Methyl anthranilate		0.20	0	Yes
Dimethyl anthranilate	40	55	1	No
para-Cymene	4	6	2	No
γ-Terpinene	22	27	10	No
Limonene	8	11	16	No
β-Pinene	2	3	2	Yes
α-Pinene	2	3	3	Yes
Optical rotation	+2.0°	+13.0°	+31.8°	No
Refractive index	1.4980	1.5470	1.4780	No

Conclusion

The observed proportions of the constituents are not in line with expectations for this essential oil. The dimethyl anthranilate content is too low, whereas the oil features too much linalool, among others.[1]

Reference

(1) Dugo, G.; Cotroneo, A.; Bonaccorsi, I. Composition of Petitgrain Oils. In *Citrus oils: Composition, advanced analytical techniques, contaminants, and biological activity*; Dugo, G., Mondello, L., Eds.; CRC Press: Boca Raton, FL, 2011; pp 253–331.

Analysis summary – Consolidated contents

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
1-Methylpyrrole	0.01	Pyrrole
(3*Z*)-Hexenol	0.02	Aliphatic alcohol
Heptanal	0.01	Aliphatic aldehyde
Tricyclene	tr	Monoterpene
α-Thujene	1.09	Monoterpene
α-Pinene	2.85	Monoterpene
Camphene	0.04	Monoterpene
α-Fenchene	0.01	Monoterpene
Sabinene	9.68	Monoterpene
β-Pinene	2.48	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.82	Monoterpene
α-Phellandrene	0.14	Monoterpene
Pseudolimonene	0.02	Monoterpene
Octanal	0.04	Aliphatic aldehyde
Δ3-Carene	0.03	Monoterpene
α-Terpinene	1.26	Monoterpene
para-Cymene	1.98	Monoterpene
Limonene	15.99	Monoterpene
β-Phellandrene	0.47*	Monoterpene
1,8-Cineole	[0.47]*	Monoterpenic ether
(*Z*)-β-Ocimene	0.55	Monoterpene
(*E*)-β-Ocimene	9.46	Monoterpene
γ-Terpinene	10.10	Monoterpene
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene	1.22	Monoterpene
trans-Linalool oxide (fur.)	0.07	Monoterpenic alcohol
para-Cymenene	0.39	Monoterpene
trans-Sabinene hydrate	0.03	Monoterpenic alcohol
Linalool	20.32	Monoterpenic alcohol
para-Mentha-1,3,8-triene	0.02	Monoterpene
Nonanal	0.01	Aliphatic aldehyde
endo-Fenchol	0.02	Monoterpenic alcohol
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.04	Monoterpene
cis-para-Menth-2-en-1-ol	0.10	Monoterpenic alcohol
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
allo-Ocimene	0.01	Monoterpene
cis-Limonene oxide	0.02	Monoterpenic ether
trans-Limonene oxide	0.01	Monoterpenic ether
Cosmene isomer I	0.13	Monoterpene
trans-para-Menth-2-en-1-ol	0.06	Monoterpenic alcohol

Camphor	0.02	Monoterpenic ketone
Epoxyterpinolene	0.01	Monoterpenic ether
Unknown	0.01	Unknown
Umbellulone	0.03	Monoterpenic ketone
Terpinen-4-ol	2.67	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α-Terpineol	0.69	Monoterpenic alcohol
Methyl salicylate	0.02	Phenolic ester
cis-Piperitol	0.03	Monoterpenic alcohol
Decanal	0.01	Aliphatic aldehyde
trans-Piperitol	0.02	Monoterpenic alcohol
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.03	Monoterpenic alcohol
Citronellol	0.08	Monoterpenic alcohol
Thymol methyl ether	1.42	Monoterpenic ether
Neral	0.02	Monoterpenic aldehyde
8,9-Dehydrothymol methyl ether	0.04	Monoterpenic ether
Geraniol	0.17	Monoterpenic alcohol
Perillaldehyde	0.02	Monoterpenic aldehyde
Geranial	0.02	Monoterpenic aldehyde
Thymol	3.98	Monoterpenic alcohol
4-Vinylguaiacol	0.22	Simple phenolic
δ-Elemene	0.23	Sesquiterpene
α-Ylangene	0.01	Sesquiterpene
Neryl acetate	0.01	Monoterpenic ester
α-Copaene	0.06	Sesquiterpene
Geranyl acetate	0.02	Monoterpenic ester
β-Elemene	0.20	Sesquiterpene
Dimethyl anthranilate	0.89	Phenolic ester
β-Caryophyllene	3.33	Sesquiterpene
γ-Elemene	0.05	Sesquiterpene
Aromadendrene	0.03	Sesquiterpene
α-Humulene	0.35	Sesquiterpene
Germacrene D	0.21	Sesquiterpene
Bicyclogermacrene	0.54	Sesquiterpene
γ-Cadinene	0.08	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	1.00	Sesquiterpene
δ-Cadinene	0.14	Sesquiterpene
Germacrene B	0.42	Sesquiterpene
α-Elemol	0.02	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.07	Sesquiterpenic alcohol
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.04	Sesquiterpenic ether
Globulol	0.07	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.01	Sesquiterpenic alcohol
τ-Muurolol	tr	Sesquiterpenic alcohol
τ-Cadinol	0.04	Sesquiterpenic alcohol
α-Cadinol	0.02	Sesquiterpenic alcohol
α-Sinensal	0.73	Sesquiterpenic aldehyde
Phytol	0.09	Diterpenic alcohol
Consolidated total	**98.87%**	

*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

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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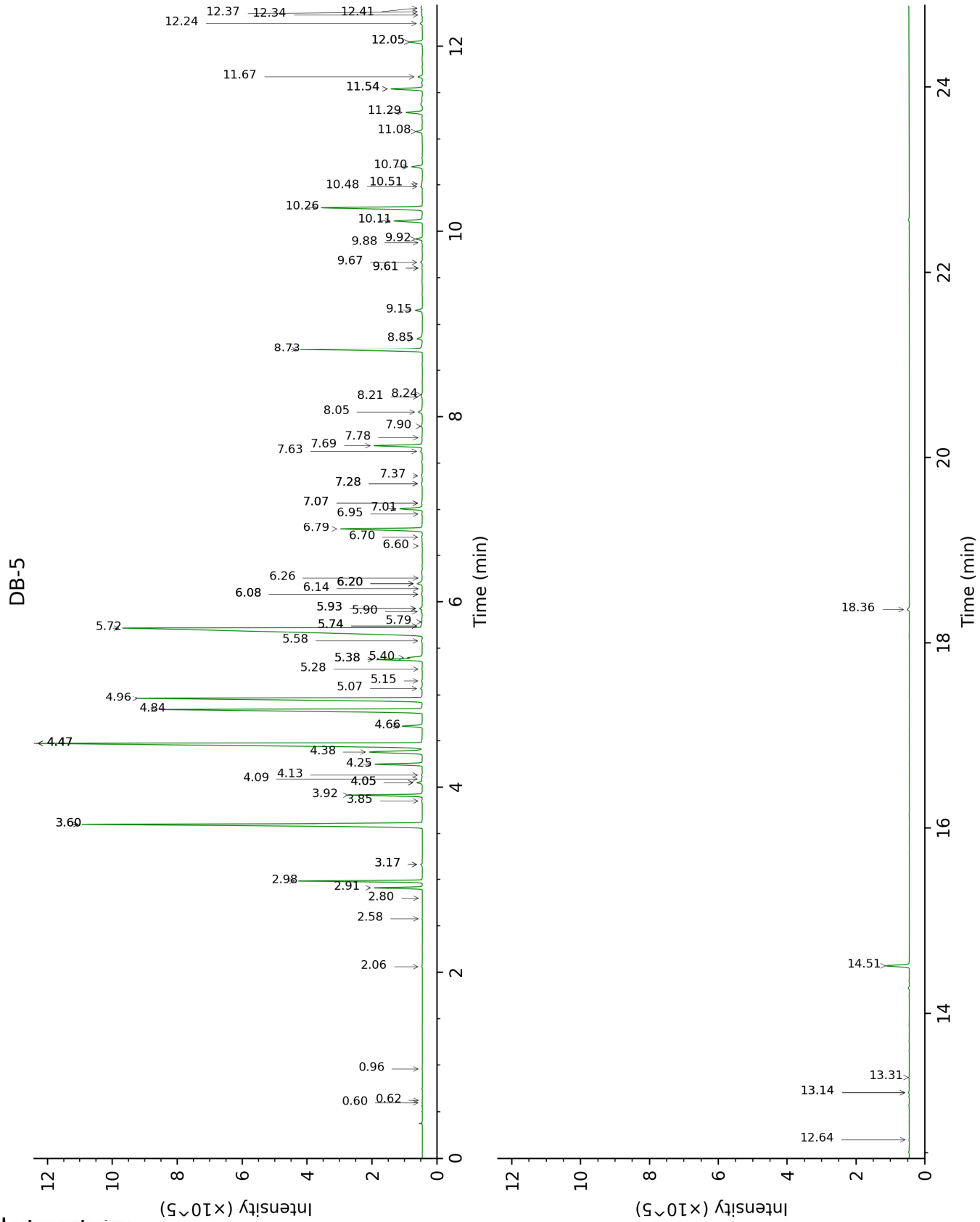
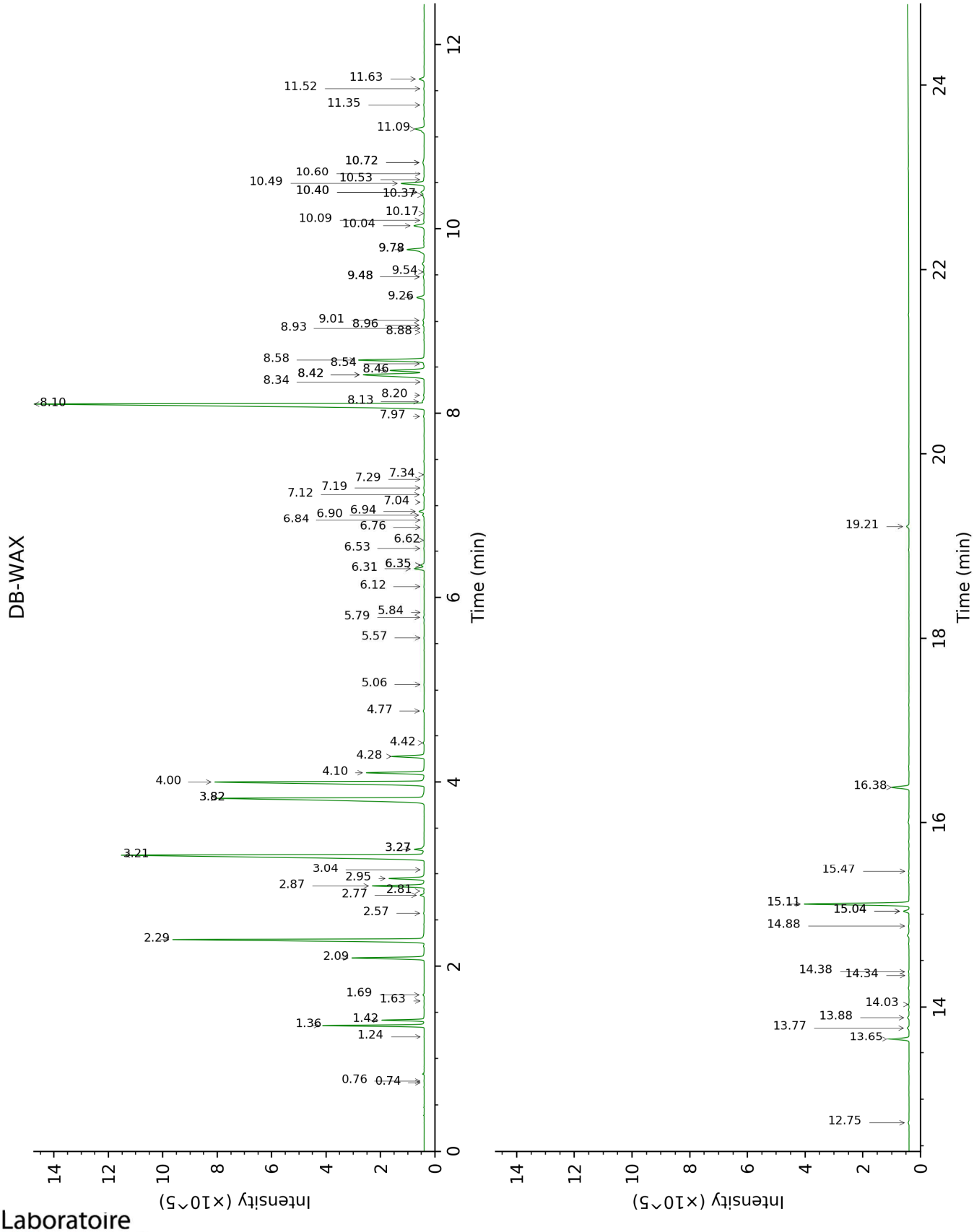

DB-5
Intensity (×10^5)
Time (min)
12.37
12.34
12.41
12.24
12.05
11.67
11.54
11.29
11.08
10.70
10.48
10.51
10.26
10.11
9.88
9.92
9.67
9.61
9.15
8.85
8.73
8.21
8.24
8.05
7.90
7.78
7.69
7.63
7.37
7.28
7.07
7.01
6.95
6.79
6.70
6.60
6.26
6.20
6.14
6.08
5.93
5.90
5.79
5.74
5.72
5.58
5.38
5.40
5.28
5.15
5.07
4.96
4.84
4.66
4.47
4.38
4.25
4.13
4.09
4.05
3.92
3.85
3.60
3.17
2.98
2.91
2.80
2.58
2.06
0.96
0.62
0.60
18.36
14.51
13.31
13.14
12.64


DB-WAX
Time (min)
Intensity (×10^5)
11.63
11.52
11.35
11.09
10.72
10.60
10.49
10.53
10.40
10.37
10.17
10.09
10.04
9.78
9.54
9.48
9.26
9.01
8.93
8.96
8.88
8.58
8.54
8.46
8.42
8.34
8.20
8.13
8.10
7.97
7.34
7.29
7.19
7.12
7.04
6.94
6.90
6.84
6.76
6.62
6.53
6.35
6.31
6.12
5.84
5.79
5.57
5.06
4.77
4.42
4.28
4.10
4.00
3.82
3.27
3.21
3.04
2.95
2.87
2.81
2.77
2.57
2.29
2.09
1.69
1.63
1.42
1.36
1.24
0.76
0.74
19.21
16.38
15.47
15.11
15.04
14.88
14.38
14.34
14.03
13.88
13.77
13.65
12.75

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isovaleral	0.60	640	tr	0.76	887	tr
2-Methylbutyral	0.62	651	tr	0.74	880	tr
1-Methylpyrrole	0.96	740	0.01			
(3*Z*)-Hexenol	2.06	861	0.02	5.79	1348	0.03
Heptanal	2.58	904	0.01	3.04	1147	0.01
Tricyclene	2.80	918	tr	1.24	971	tr
α-Thujene	2.91	926	1.09	1.42	999	1.10
α-Pinene	2.98	931	2.85	1.36	991	2.81
Camphene	3.17*	943	0.05	1.69	1026	0.04
α-Fenchene	3.17*	943	[0.05]	1.63	1019	0.01
Sabinene	3.60*	971	12.28	2.29	1085	9.68
β-Pinene	3.60*	971	[12.28]	2.09	1066	2.48
6-Methyl-5-hepten-2-one	3.85	988	0.02	5.06	1296	0.01
Myrcene	3.92	992	1.82	2.87	1133	1.81
α-Phellandrene	4.05*	1001	0.15	2.77	1125	0.14
Pseudolimonene	4.05*	1001	[0.15]	2.81	1129	0.02
Octanal	4.09	1004	0.04	4.42	1252	0.03
Δ3-Carene	4.13	1006	0.03	2.57	1110	0.02
α-Terpinene	4.25	1014	1.26	2.95	1140	1.27
para-Cymene	4.38	1022	1.98	4.10	1228	1.98
Limonene	4.47*	1028	16.47	3.21	1160	15.99
β-Phellandrene	4.47*	1028	[16.47]	3.27*	1165	0.39
1,8-Cineole	4.47*	1028	[16.47]	3.27*	1165	[0.39]
(*Z*)-β-Ocimene	4.66	1039	0.55	3.82*	1208	10.59
(*E*)-β-Ocimene	4.84	1050	9.46	4.00	1221	9.47
γ-Terpinene	4.96	1058	10.10	3.82*	1208	[10.59]
cis-Sabinene hydrate	5.07	1065	0.06	6.84	1425	0.01
cis-Linalool oxide (fur.)	5.15	1070	0.02	6.53	1402	0.02
Octanol	5.28	1078	0.02	8.20	1527	0.03
Terpinolene	5.38*†	1085	1.60	4.28	1242	1.22
trans-Linalool oxide (fur.)	5.38*†	1085	[1.60]	6.90	1429	0.07
para-Cymenene	5.40†	1086	[1.60]	6.31	1386	0.39
trans-Sabinene hydrate	5.58	1097	0.03	7.97	1509	0.03
Linalool	5.72	1106	20.32	8.10	1519	20.20
para-Mentha-1,3,8-triene	5.74*	1108	0.06	6.12	1372	0.02
Nonanal	5.74*	1108	[0.06]	5.84	1352	0.01
endo-Fenchol	5.78	1110	0.02	8.34	1538	0.01
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	5.90	1117	0.04	4.77	1278	0.04
cis-para-Menth-2-en-1-ol	5.93*	1120	0.09	8.13	1521	0.10

trans-para-Mentha-2,8-dien-1-ol	5.93*	1120	[0.09]	8.92	1583	0.01
allo-Ocimene	6.08*	1129	0.03	5.57	1332	0.01
cis-Limonene oxide	6.08*	1129	[0.03]	6.35*	1389	0.14
trans-Limonene oxide	6.14	1133	0.01	6.62	1408	0.01
Cosmene isomer I	6.20*	1137	0.21	6.35*	1389	[0.14]
trans-para-Menth-2-en-1-ol	6.20*	1137	[0.21]	8.96	1586	0.06
Camphor	6.20*	1137	[0.21]	7.19	1451	0.02
Epoxyterpinolene	6.26	1141	0.01	6.76	1419	0.01
Unknown [m/z 43, 109 (68), 67 (62), 81 (36), 41 (31), 137 (29), 79 (26)...]	6.60	1163	0.01	7.29	1458	0.01
Umbellulone	6.70	1169	0.03	8.88	1580	0.03
Terpinen-4-ol	6.79	1175	2.67	8.58	1556	2.65
para-Cymen-8-ol	6.95	1186	0.02	11.52	1797	0.02
α-Terpineol	7.01	1189	0.69	9.78*	1651	0.87
Methyl salicylate	7.07*	1193	0.03	10.53	1713	0.02
cis-Piperitol	7.07*	1193	[0.03]	9.54	1632	0.03
Decanal	7.28*	1207	0.04	7.34	1462	0.01
trans-Piperitol	7.28*	1207	[0.04]	10.40*	1702	0.16
(3*E*,5*E*)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.37	1213	0.03	11.35	1782	0.02
Citronellol	7.63	1230	0.08	10.72*	1730	0.12
Thymol methyl ether	7.69	1235	1.42	8.46	1547	1.38
Neral	7.78	1240	0.02	9.48*	1628	0.06
8,9-Dehydrothymol methyl ether	7.90	1249	0.04	9.48*	1628	[0.06]
Geraniol	8.05	1259	0.17	11.63	1807	0.23
Perillaldehyde	8.21	1270	0.02	10.72*	1730	[0.12]
Geranial	8.24	1272	0.02	10.09	1677	0.04
Thymol	8.73	1301	3.98	15.11	2131	3.99
4-Vinylguaiacol	8.85	1309	0.22	15.04*	2124	0.23
δ-Elemene	9.15	1331	0.23	6.94	1432	0.22
α-Ylangene	9.61*	1364	0.03	7.04	1440	0.01
Neryl acetate	9.61*	1364	[0.03]	10.17	1683	0.01
α-Copaene	9.67	1368	0.06	7.12	1446	0.05
Geranyl acetate	9.88	1383	0.02	10.60	1719	0.01
β-Elemene	9.92	1386	0.20	8.42*	1544	3.46
Dimethyl anthranilate	10.11	1400	0.89	13.65	1989	0.91
β-Caryophyllene	10.26	1411	3.33	8.42*	1544	[3.46]
γ-Elemene	10.48	1428	0.05	9.01	1590	0.08
Aromadendrene	10.51	1430	0.03	8.54	1553	0.03
α-Humulene	10.70	1444	0.35	9.26	1610	0.33

Germacrene D	11.08	1473	0.21	9.78*	1651	[0.87]
Bicyclogermacrene	11.29	1488	0.54	10.04	1672	0.49
γ-Cadinene	11.54*	1508	0.96	10.36	1699	0.08
(3*E*,6*E*)-α-Farnesene	11.54*	1508	[0.96]	10.49	1710	1.00
δ-Cadinene	11.67	1518	0.14	10.40*	1702	[0.16]
Germacrene B	12.05*	1548	0.42	11.09	1760	0.42
α-Elemol	12.05*	1548	[0.42]	14.03	2026	0.02
(*E*)-Nerolidol	12.24	1563	0.07	13.77	2001	0.08
Spathulenol	12.34	1571	0.03	14.38	2059	0.03
Caryophyllene oxide	12.37	1573	0.04	12.75	1906	0.05
Globulol	12.41	1577	0.07	13.88	2012	0.07
Eudesm-5-en-11-ol	12.64	1594	0.01	14.34	2056	0.01
τ-Muurolol	13.14*	1636	0.03	15.04*	2124	[0.23]
τ-Cadinol	13.14*	1636	[0.03]	14.88	2108	0.04
α-Cadinol	13.31	1649	0.02	15.47	2167	0.02
α-Sinensal	14.51	1751	0.73	16.38	2260	0.75
Phytol	18.36	2109	0.09	19.21	2573	0.11
Total identified		**98.75%**			**98.42%**	
Total reported		**98.76%**			**98.44%**	

*: 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