Date : September 23, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21I13-PTH05
Customer identification : Fragonia - FA01022011R
Type : Essential oil
Source : *Agonis fragrans*
Customer : Plant Therapy

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 2013-174
Analysis date : September 23, 2021

Checked and approved by :

Alexis St-Gelais, M. Sc., 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid
Refractive index: 1.4700 ± 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	0.10	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Unknown	0.01	Unknown
(3*Z*)-Hexenol	0.04	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Hashishene	0.01	Monoterpene
α-Thujene	0.26	Monoterpene
α-Pinene	26.32	Monoterpene
Camphene	0.05	Monoterpene
α-Fenchene	0.02	Monoterpene
Thuja-2,4(10)-diene	0.03	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.18	Monoterpene
β-Pinene	1.59	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.55	Monoterpene
Pseudolimonene	0.05	Monoterpene
α-Phellandrene	0.09	Monoterpene
α-Terpinene	0.41	Monoterpene
para-Cymene	2.82	Monoterpene
Limonene	2.20	Monoterpene
1,8-Cineole	26.75	Monoterpenic ether
(*Z*)-β-Ocimene	0.02	Monoterpene
(*E*)-β-Ocimene	0.03	Monoterpene
γ-Terpinene	1.35	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
cis-Linalool oxide (fur.)	0.09	Monoterpenic alcohol
Terpinolene	0.30	Monoterpene
para-Cymenene	0.06	Monoterpene
trans-Linalool oxide (fur.)	0.07	Monoterpenic alcohol
trans-Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	10.20	Monoterpenic alcohol
Hotrienol	0.11	Monoterpenic alcohol
endo-Fenchol	0.05	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.04	Monoterpenic alcohol
α-Campholenal	0.03	Monoterpenic aldehyde
trans-Rose oxide	0.02	Monoterpenic ether
Nopinone	0.03	Normonoterpenic ketone
trans-Pinocarveol	0.13	Monoterpenic alcohol
trans-para-Menth-2-en-1-ol	0.04	Monoterpenic alcohol
Camphene hydrate	0.06	Monoterpenic alcohol
Isopulegol	0.02	Monoterpenic alcohol
Nerol oxide	0.02	Aliphatic ether
Pinocarvone	0.03	Monoterpenic ketone

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Hydrocinnamal	0.02	Phenylpropanoid
Borneol	0.04	Monoterpenic alcohol
δ-Terpineol	0.36	Monoterpenic alcohol
Terpinen-4-ol	2.80	Monoterpenic alcohol
Cryptone	0.02	Normonoterpenic ketone
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α-Terpineol	5.70	Monoterpenic alcohol
Myrtenal	0.21	Monoterpenic aldehyde
Myrtenol	4.27	Monoterpenic alcohol
Unknown	0.03	Unknown
Verbenone	0.02	Monoterpenic ketone
trans-Carveol	0.05	Monoterpenic alcohol
Nerol	0.52	Monoterpenic alcohol
Citronellol	0.50	Monoterpenic alcohol
Carvone	0.08	Monoterpenic ketone
cis-Myrtanol	0.28	Monoterpenic alcohol
Geraniol	1.52	Monoterpenic alcohol
Geranial	0.07	Monoterpenic aldehyde
Cuminol	0.01	Monoterpenic alcohol
trans-Pinocarvyl acetate	0.03	Monoterpenic ester
Thymol	0.02	Monoterpenic alcohol
Carvacrol	0.01	Monoterpenic alcohol
Myrtenyl acetate	0.23	Monoterpenic ester
Methyl geranate	0.18	Monoterpenic ester
Bicycloelemene	0.03	Sesquiterpene
α-Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.02	Monoterpenic ester
Neryl acetate	0.04	Monoterpenic ester
α-Copaene	0.05	Sesquiterpene
7-Cubebene	0.03	Sesquiterpene
Methyl (*E*)-cinnamate	0.03	Phenylpropanoid ester
β-Bourbonene	0.04	Sesquiterpene
Geranyl acetate	0.04	Monoterpenic ester
β-Elemene	0.05	Sesquiterpene
(*Z*)-Jasmone	0.02	Jasmonate
α-Gurjunene	0.09	Sesquiterpene
β-Caryophyllene	0.78	Sesquiterpene
γ-Maaliene	0.04	Sesquiterpene
Aromadendrene	0.30	Sesquiterpene
α-Humulene	1.28	Sesquiterpene
allo-Aromadendrene	0.18	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
β-Selinene	0.06	Sesquiterpene
allo-Aromadendr-9-ene	0.07	Sesquiterpene
α-Selinene	0.08	Sesquiterpene
Bicyclogermacrene	0.64	Sesquiterpene
Viridiflorene	0.46	Sesquiterpene
α-Muurolene	0.04	Sesquiterpene
Unknown	0.04	Sesquiterpene
γ-Cadinene	0.03	Sesquiterpene
trans-Calamenene	0.15	Sesquiterpene
Zonarene	0.03	Sesquiterpene

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δ-Cadinene	0.10	Sesquiterpene
trans-Cadina-1,4-diene	0.06	Sesquiterpene
α-Calacorene	0.02	Sesquiterpene
Germacrene B	0.04	Sesquiterpene
Epiglobulol	0.04	Sesquiterpenic alcohol
Palustrol	0.09	Sesquiterpenic alcohol
Spathulenol	0.18	Sesquiterpenic alcohol
Caryophyllene oxide	0.09	Sesquiterpenic ether
Globulol	0.24	Sesquiterpenic alcohol
Viridiflorol	0.12	Sesquiterpenic alcohol
Cubeban-11-ol	0.09	Sesquiterpenic alcohol
Humulene epoxide I	0.03	Sesquiterpenic ether
Eudesm-5-en-11-ol analog	0.08	Sesquiterpenic alcohol
Humulene epoxide II	0.12	Sesquiterpenic ether
Rosifoliol	0.09	Sesquiterpenic alcohol
1-epi-Cubenol	0.02	Sesquiterpenic alcohol
γ-Eudesmol	0.05	Sesquiterpenic alcohol
Isospathulenol	0.17	Sesquiterpenic alcohol
β-Eudesmol	0.06	Sesquiterpenic alcohol
α-Eudesmol	0.05	Sesquiterpenic alcohol
Heptadecane	0.01	Alkane
Consolidated total	**98.78%**	

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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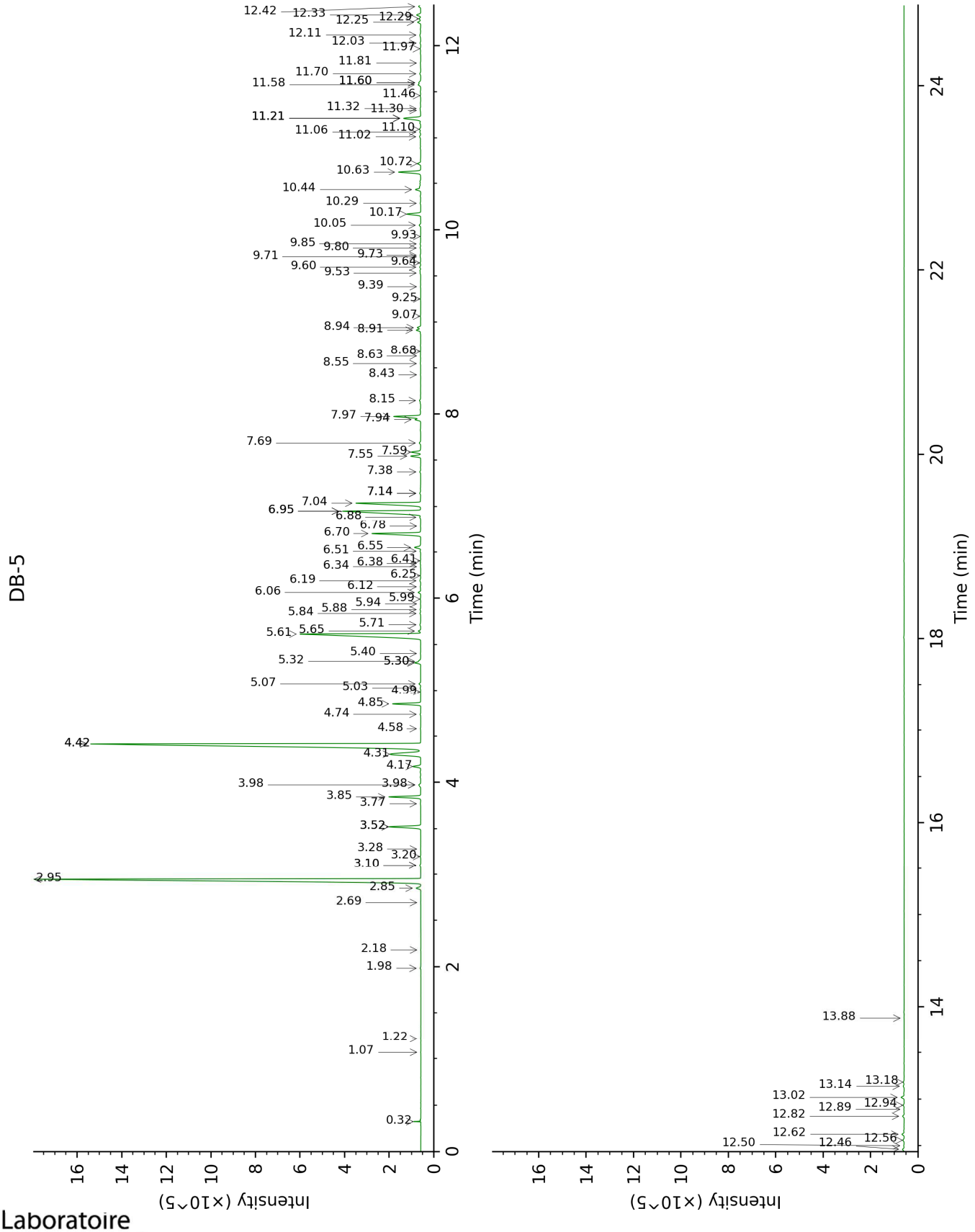
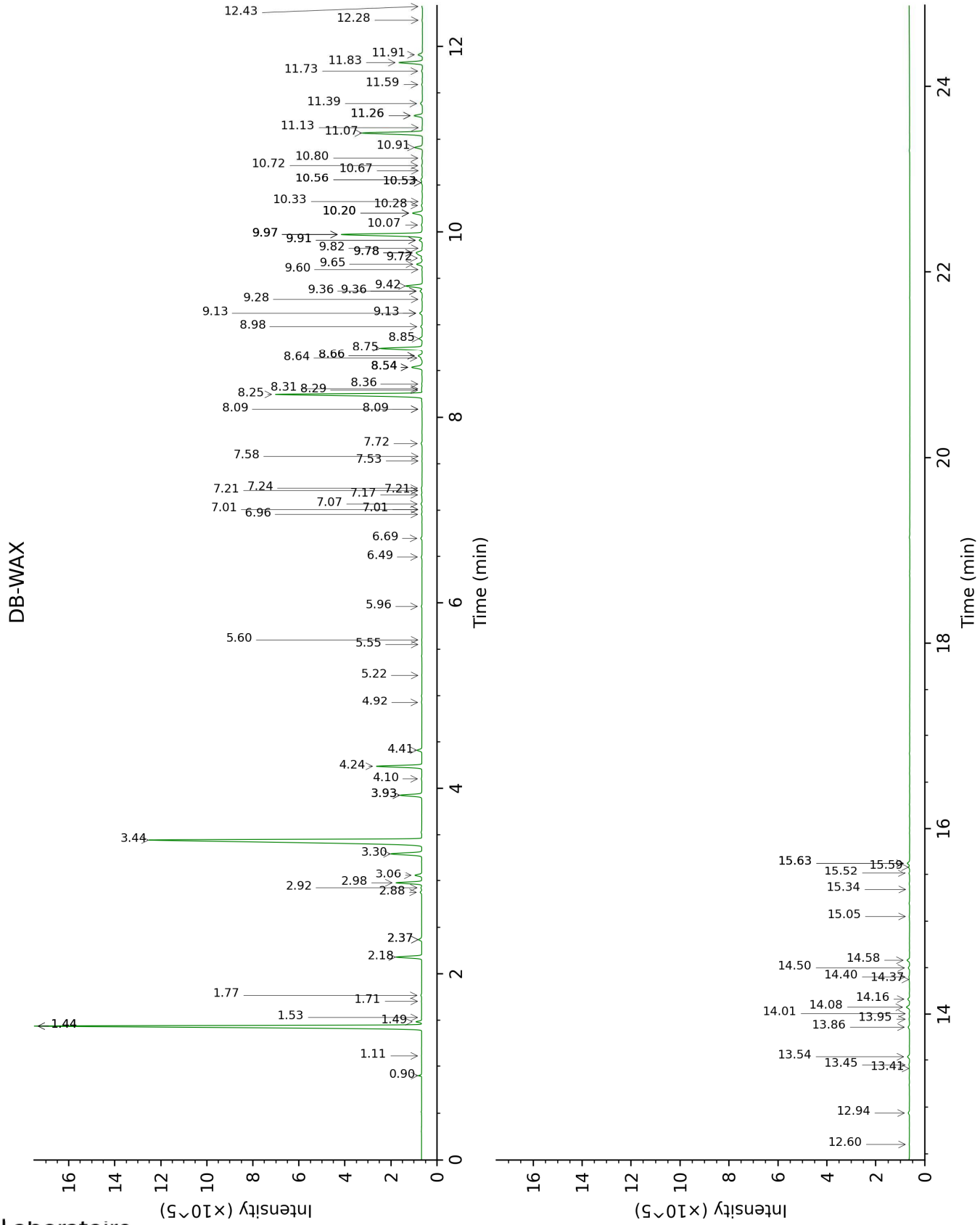

DB-5
Intensity (×10^5)
Time (min)
12.42
12.33
12.25
12.29
12.11
12.03
11.97
11.81
11.70
11.58
11.60
11.46
11.32
11.30
11.21
11.06
11.10
11.02
10.72
10.63
10.44
10.29
10.17
10.05
9.93
9.85
9.80
9.71
9.73
9.64
9.60
9.53
9.39
9.25
9.07
8.94
8.91
8.63
8.68
8.55
8.43
8.15
7.97
7.94
7.69
7.55
7.59
7.38
7.14
7.04
6.95
6.88
6.78
6.70
6.51
6.55
6.34
6.38
6.41
6.25
6.19
6.12
6.06
5.94
5.99
5.84
5.88
5.71
5.61
5.65
5.40
5.32
5.30
5.07
5.03
4.99
4.85
4.74
4.58
4.42
4.31
4.17
3.98
3.98
3.85
3.77
3.52
3.28
3.20
3.10
2.95
2.85
2.69
2.18
1.98
1.22
1.07
0.32
13.88
13.14
13.18
13.02
12.89
12.94
12.82
12.62
12.50
12.46
12.56


DB-WAX
Intensity (×10^5)
Time (min)
12.43
12.28
11.91
11.83
11.73
11.59
11.39
11.26
11.13
11.07
10.91
10.80
10.72
10.67
10.56
10.53
10.33
10.28
10.20
10.07
9.97
9.91
9.82
9.78
9.72
9.65
9.60
9.42
9.36
9.36
9.28
9.13
9.13
8.98
8.85
8.75
8.66
8.64
8.54
8.36
8.31
8.29
8.25
8.09
8.09
7.72
7.58
7.53
7.24
7.21
7.21
7.17
7.07
7.01
7.01
6.96
6.69
6.49
5.96
5.60
5.55
5.22
4.92
4.41
4.24
4.10
3.93
3.44
3.30
3.06
2.98
2.92
2.88
2.37
2.18
1.77
1.71
1.53
1.49
1.44
1.11
0.90
15.63
15.59
15.52
15.34
15.05
14.58
14.50
14.40
14.37
14.16
14.08
14.01
13.95
13.86
13.54
13.45
13.41
12.94
12.60

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.32	499	0.10	0.90	907	0.11
Toluene	1.07	758	0.01	1.53	1001	0.01
Unknown [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.22	781	0.01	1.11	941	0.01
(3*Z*)-Hexenol	1.98	857	0.04	5.96	1351	0.05
Hexanol	2.18	874	0.01	5.55	1321	0.01
Hashishene	2.69	915	0.01	1.44*	992	26.51
α-Thujene	2.85	926	0.26	1.49	997	0.27
α-Pinene	2.95	932	26.32	1.44*	992	[26.51]
Camphene	3.10*	943	0.06	1.77	1025	0.05
α-Fenchene	3.10*	943	[0.06]	1.70	1018	0.02
Thuja-2,4(10)-diene	3.20	949	0.03	2.37*	1084	0.21
Benzaldehyde	3.28	955	0.01	7.53	1465	0.01
Sabinene	3.52*	971	1.77	2.37*	1084	[0.21]
β-Pinene	3.52*	971	[1.77]	2.18	1065	1.59
6-Methyl-5-hepten-2-one	3.77	988	0.02	5.22	1298	0.01
Myrcene	3.84	993	1.55	2.98	1133	1.52
Pseudolimonene	3.98*	1002	0.14	2.92	1129	0.05
α-Phellandrene	3.98*	1002	[0.14]	2.88	1125	0.09
α-Terpinene	4.17	1014	0.41	3.06	1140	0.41
para-Cymene	4.31	1023	2.82	4.24	1230	2.83
Limonene	4.42*	1030	28.74	3.30	1158	2.20
1,8-Cineole	4.42*	1030	[28.74]	3.44	1170	26.75
(*Z*)-β-Ocimene	4.58	1040	0.02	3.93*	1207	1.38
(*E*)-β-Ocimene	4.74	1050	0.03	4.10	1220	0.03
γ-Terpinene	4.85	1057	1.35	3.93*	1207	[1.38]
cis-Sabinene hydrate	4.99	1066	0.01	7.01*	1427	0.02
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.03	1068	0.03	4.92	1281	0.03
cis-Linalool oxide (fur.)	5.07	1071	0.09	6.69	1403	0.09
Terpinolene	5.30*†	1085	0.41	4.41	1243	0.30
para-Cymenene	5.30*†	1085	[0.41]	6.49	1389	0.06
trans-Linalool oxide (fur.)	5.32†	1086	[0.41]	7.07	1431	0.07
trans-Sabinene hydrate	5.40	1092	0.02	8.09*	1507	0.03
Linalool	5.61	1105	10.20	8.25	1519	10.09
Hotrienol	5.65	1107	0.11	8.98	1576	0.10
endo-Fenchol	5.71	1112	0.05	8.54*	1541	0.83

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cis-para-Menth-2-en-1-ol	5.84	1119	0.04	8.29	1523	0.04
α-Campholenal	5.88	1122	0.03	7.17	1438	0.05
trans-Rose oxide	5.94	1126	0.02	5.60	1325	0.02
Nopinone	5.99	1129	0.03	8.36	1528	0.03
trans-Pinocarveol	6.06	1134	0.13	9.36*	1606	0.16
trans-para-Menth-2-en-1-ol	6.12	1138	0.04	9.13*	1587	0.20
Camphene hydrate	6.19	1142	0.06	8.64†	1549	0.38
Isopulegol	6.24	1145	0.02	8.31	1524	0.03
Nerol oxide	6.34	1152	0.02	7.01*	1427	[0.02]
Pinocarvone	6.38	1154	0.03	8.09*	1507	[0.03]
Hydrocinnamal	6.41	1156	0.02	10.67	1711	0.02
Borneol	6.51	1162	0.04	9.97*	1654	5.79
δ-Terpineol	6.55	1165	0.36	9.65	1629	0.42
Terpinen-4-ol	6.70	1175	2.80	8.75	1558	2.84
Cryptone	6.78	1180	0.02	9.36*	1606	[0.16]
para-Cymen-8-ol	6.88	1186	0.05	11.74	1801	0.06
α-Terpineol	6.95*	1191	5.99	9.97*	1654	[5.79]
Myrtenal	6.95*	1191	[5.99]	8.85	1566	0.21
Myrtenol	7.04	1196	4.27	11.07	1745	4.19
Unknown [m/z 95, 93 (32), 121 (24), 79 (22), 91 (21), 105 (16)... 154 (2)]	7.14*	1203	0.06	11.13	1750	0.03
Verbenone	7.14*	1203	[0.06]	9.82	1642	0.02
trans-Carveol	7.38	1218	0.05	11.59	1788	0.05
Nerol	7.55	1230	0.52	11.26*	1760	0.57
Citronellol	7.59	1233	0.50	10.92	1732	0.52
Carvone	7.69	1239	0.08	10.20*	1673	0.76
cis-Myrtanol	7.94	1256	0.28	11.91	1817	0.32
Geraniol	7.97	1258	1.52	11.83	1809	1.54
Geranial	8.15	1270	0.07	10.28	1679	0.07
Cuminol	8.43	1288	0.01	14.37	2040	0.03
trans-Pinocarvyl acetate	8.55	1296	0.03	9.28	1598	0.03
Thymol	8.63	1302	0.02	15.34	2134	0.01
Carvacrol	8.68	1306	0.01	15.63*	2162	0.17
Myrtenyl acetate	8.92	1322	0.23	9.78*	1639	0.69
Methyl geranate	8.94	1324	0.18	9.91*	1649	0.22
Bicycloelemene	9.07	1333	0.03	7.21*	1442	0.03
α-Cubebene	9.25	1346	0.02	6.96	1423	0.04
Citronellyl acetate	9.39	1355	0.02	9.60	1624	0.03
Neryl acetate	9.53	1366	0.04	10.33	1683	0.04
α-Copaene	9.60	1370	0.05	7.24	1444	0.05
7-Cubebene	9.64	1374	0.03	7.21*	1442	[0.03]
Methyl (*E*)-cinnamate	9.71	1378	0.03	14.01	2005	0.02
β-Bourbonene	9.73	1379	0.04	7.58	1469	0.02
Geranyl acetate	9.80	1385	0.04	10.72	1716	0.07
β-Elemene	9.85	1388	0.05	8.54*	1541	[0.83]

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(*Z*)-Jasmone	9.93	1394	0.02	12.60	1877	0.02
α-Gurjunene	10.05	1402	0.09	7.72	1479	0.08
β-Caryophyllene	10.17	1411	0.78	8.54*	1541	[0.83]
γ-Maaliene	10.29	1420	0.04	8.66*†	1551	[0.38]
Aromadendrene	10.44	1431	0.30	8.66*†	1551	[0.38]
α-Humulene	10.63	1446	1.28	9.42	1610	1.20
allo-Aromadendrene	10.72	1452	0.18	9.13*	1587	[0.20]
Germacrene D	11.02	1474	0.08	9.91*	1649	[0.22]
β-Selinene	11.06	1478	0.06	9.97*	1654	[5.79]
allo-Aromadendr-9-ene	11.10	1480	0.07	9.72	1634	0.07
α-Selinene	11.21*	1489	1.19	10.07	1662	0.08
Bicyclogermacrene	11.21*	1489	[1.19]	10.20*	1673	[0.76]
Viridiflorene	11.21*	1489	[1.19]	9.78*	1639	[0.69]
α-Muurolene	11.30	1495	0.04	10.20*	1673	[0.76]
Unknown [m/z 105, 91 (85), 93 (75), 119 (74), 107 (68), 145 (62), 202 (59)]	11.32	1497	0.04			
γ-Cadinene	11.46	1507	0.03	10.53*	1700	0.06
trans-Calamenene	11.58	1516	0.15	11.39	1771	0.15
Zonarene	11.60*	1518	0.13	10.53*	1700	[0.06]
δ-Cadinene	11.60*	1518	[0.13]	10.56*	1702	0.11
trans-Cadina-1,4-diene	11.70	1526	0.06	10.80	1722	0.06
α-Calacorene	11.81	1535	0.02	12.28	1849	0.05
Germacrene B	11.97	1547	0.04	11.26*	1760	[0.57]
Epiglobulol	12.03	1552	0.04	13.45	1954	0.04
Palustrol	12.11	1558	0.09	12.43	1862	0.06
Spathulenol	12.25	1569	0.18	14.58	2060	0.18
Caryophyllene oxide	12.29	1572	0.09	12.94	1907	0.09
Globulol	12.33	1576	0.24	14.08	2012	0.22
Viridiflorol	12.42	1583	0.12	14.16	2020	0.12
Cubeban-11-ol	12.46	1586	0.09	13.86	1992	0.10
Humulene epoxide I	12.50	1589	0.03	13.41	1950	0.02
Eudesm-5-en-11-ol analog	12.56	1593	0.08	14.40	2043	0.06
Humulene epoxide II	12.62	1598	0.12	13.54	1962	0.14
Rosifoliol	12.82	1614	0.09	14.50	2052	0.09
1-epi-Cubenol	12.89	1620	0.02	13.95	2000	0.05
γ-Eudesmol	12.94	1624	0.05	15.05	2105	0.04
Isospathulenol	13.02	1631	0.17	15.63*	2162	[0.17]
β-Eudesmol	13.14	1641	0.06	15.59	2158	0.06
α-Eudesmol	13.18	1644	0.05	15.52	2151	0.05
Heptadecane	13.88	1702	0.01	10.56*	1702	[0.11]
Total identified		**98.56%**			**98.68%**	

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Total reported	**98.64%**	**98.74%**

*: 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

Note: no correction factor was applied
R.T.: Retention time (minutes)
R.I.: Retention index

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