Date : March 18, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22C08-PTH02
Customer identification : Fragonia - Australia - FA01032111R
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 : Seydou Ka, Ph. D.
Analysis date : March 17, 2022

Checked and approved by :

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid
Refractive index: 1.4697 ± 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	0.06	Aliphatic alcohol
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
(*E*)-2-Methyl-1,3-pentadiene	0.01	Alkene
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Unknown	tr	Unknown
(2*E*)-Hexenal	0.01	Aliphatic aldehyde
(3*Z*)-Hexenol	0.08	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Styrene	tr	Simple phenolic
Hashishene	0.01	Monoterpene
α-Thujene	0.26	Monoterpene
α-Pinene	24.98	Monoterpene
α-Fenchene	0.01	Monoterpene
Unknown	tr	Monoterpene
Camphene	0.04	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
Sabinene	0.53	Monoterpene
β-Pinene	1.49	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.88	Monoterpene
trans-Dehydroxylinalool oxide	0.04	Monoterpenic ether
α-Phellandrene	0.14	Monoterpene
Pseudolimonene	0.05	Monoterpene
cis-Dehydroxylinalool oxide	tr	Monoterpenic ether
(3*Z*)-Hexenyl acetate	0.03	Aliphatic ester
α-Terpinene	0.76	Monoterpene
para-Cymene	2.00	Monoterpene
Limonene	2.16	Monoterpene
1,8-Cineole	26.06	Monoterpenic ether
(*Z*)-β-Ocimene	0.02	Monoterpene
(*E*)-β-Ocimene	0.05	Monoterpene
γ-Terpinene	2.08	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
Unknown	0.02	Oxygenated monoterpene
cis-Linalool oxide (fur.)	0.07	Monoterpenic alcohol
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
para-Cymenene	0.05	Monoterpene
Terpinolene	0.41	Monoterpene
trans-Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	9.93	Monoterpenic alcohol
Hotrienol	0.16	Monoterpenic alcohol
endo-Fenchol	0.03	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.05	Monoterpenic alcohol
α-Campholenal	0.05	Monoterpenic aldehyde

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trans-Rose oxide	0.02	Monoterpenic ether
Nopinone	0.03	Normonoterpenic ketone
trans-Pinocarveol	0.20	Monoterpenic alcohol
Camphor	0.01	Monoterpenic ketone
trans-para-Menth-2-en-1-ol	0.03	Monoterpenic alcohol
Isopulegol	0.05	Monoterpenic alcohol
Nerol oxide	0.05	Aliphatic ether
Pinocarvone	0.07	Monoterpenic ketone
Hydrocinnamal	0.01	Phenylpropanoid
Borneol	0.04	Monoterpenic alcohol
δ-Terpineol	0.42	Monoterpenic alcohol
Terpinen-4-ol	2.78	Monoterpenic alcohol
Cryptone	0.02	Normonoterpenic ketone
Myrtenal	0.25	Monoterpenic aldehyde
α-Terpineol	6.47	Monoterpenic alcohol
Myrtenol	4.31	Monoterpenic alcohol
Verbenone	0.02	Monoterpenic ketone
Unknown	0.03	Unknown
trans-Carveol	0.05	Monoterpenic alcohol
Nerol	0.53	Monoterpenic alcohol
Citronellol	0.55	Monoterpenic alcohol
Cuminal	0.01	Monoterpenic aldehyde
Carvone	0.01	Monoterpenic ketone
Neral	0.02	Monoterpenic aldehyde
cis-Myrtanol	0.31	Monoterpenic alcohol
Geraniol	1.61	Monoterpenic alcohol
Geranial	0.10	Monoterpenic aldehyde
trans-Pinocarvyl acetate	0.02	Monoterpenic ester
Myrtenyl acetate	1.11	Monoterpenic ester
Methyl geranate	0.18	Monoterpenic ester
Bicycloelemene	0.04	Sesquiterpene
α-Cubebene	0.01	Sesquiterpene
Citronellyl acetate	0.04	Monoterpenic ester
Neryl acetate	0.08	Monoterpenic ester
α-Copaene	0.05	Sesquiterpene
7-Cubebene	0.02	Sesquiterpene
β-Bourbonene	0.02	Sesquiterpene
Methyl (*E*)-cinnamate	0.04	Phenylpropanoid ester
Geranyl acetate	0.16	Monoterpenic ester
β-Elemene	0.03	Sesquiterpene
(*Z*)-Jasmone	0.01	Jasmonate
α-Gurjunene	0.06	Sesquiterpene
β-Caryophyllene	0.68	Sesquiterpene
γ-Maaliene	0.02	Sesquiterpene
Aromadendrene	0.22	Sesquiterpene
Selina-5,11-diene	0.03	Sesquiterpene
α-Humulene	1.19	Sesquiterpene
allo-Aromadendrene	0.01	Sesquiterpene
trans-Cadina-1(6),4-diene	0.05	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
β-Selinene	0.05	Sesquiterpene
Viridiflorene	0.36	Sesquiterpene

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α-Selinene	0.03	Sesquiterpene
Bicyclogermacrene	1.01	Sesquiterpene
α-Muurolene	0.04	Sesquiterpene
δ-Amorphene	0.05	Sesquiterpene
γ-Cadinene	0.02	Sesquiterpene
trans-Calamenene	0.10	Sesquiterpene
Zonarene	0.07	Sesquiterpene
δ-Cadinene	0.05	Sesquiterpene
trans-Cadina-1,4-diene	0.07	Sesquiterpene
α-Calacorene	0.02	Sesquiterpene
Germacrene B	0.03	Sesquiterpene
Epiglobulol	0.01	Sesquiterpenic alcohol
Palustrol	0.06	Sesquiterpenic alcohol
Spathulenol	0.09	Sesquiterpenic alcohol
Caryophyllene oxide	0.06	Sesquiterpenic ether
Globulol	0.21	Sesquiterpenic alcohol
Viridiflorol	0.07	Sesquiterpenic alcohol
Cubeban-11-ol	0.02	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.06	Sesquiterpenic alcohol
Humulene epoxide II	0.08	Sesquiterpenic ether
Rosifoliol	0.06	Sesquiterpenic alcohol
1-epi-Cubenol	0.02	Sesquiterpenic alcohol
γ-Eudesmol	0.04	Sesquiterpenic alcohol
Isospathulenol	0.05	Sesquiterpenic alcohol
β-Eudesmol	0.05	Sesquiterpenic alcohol
α-Eudesmol	0.04	Sesquiterpenic alcohol
Heptadecane	0.01	Alkane
Consolidated total	**98.60%**	

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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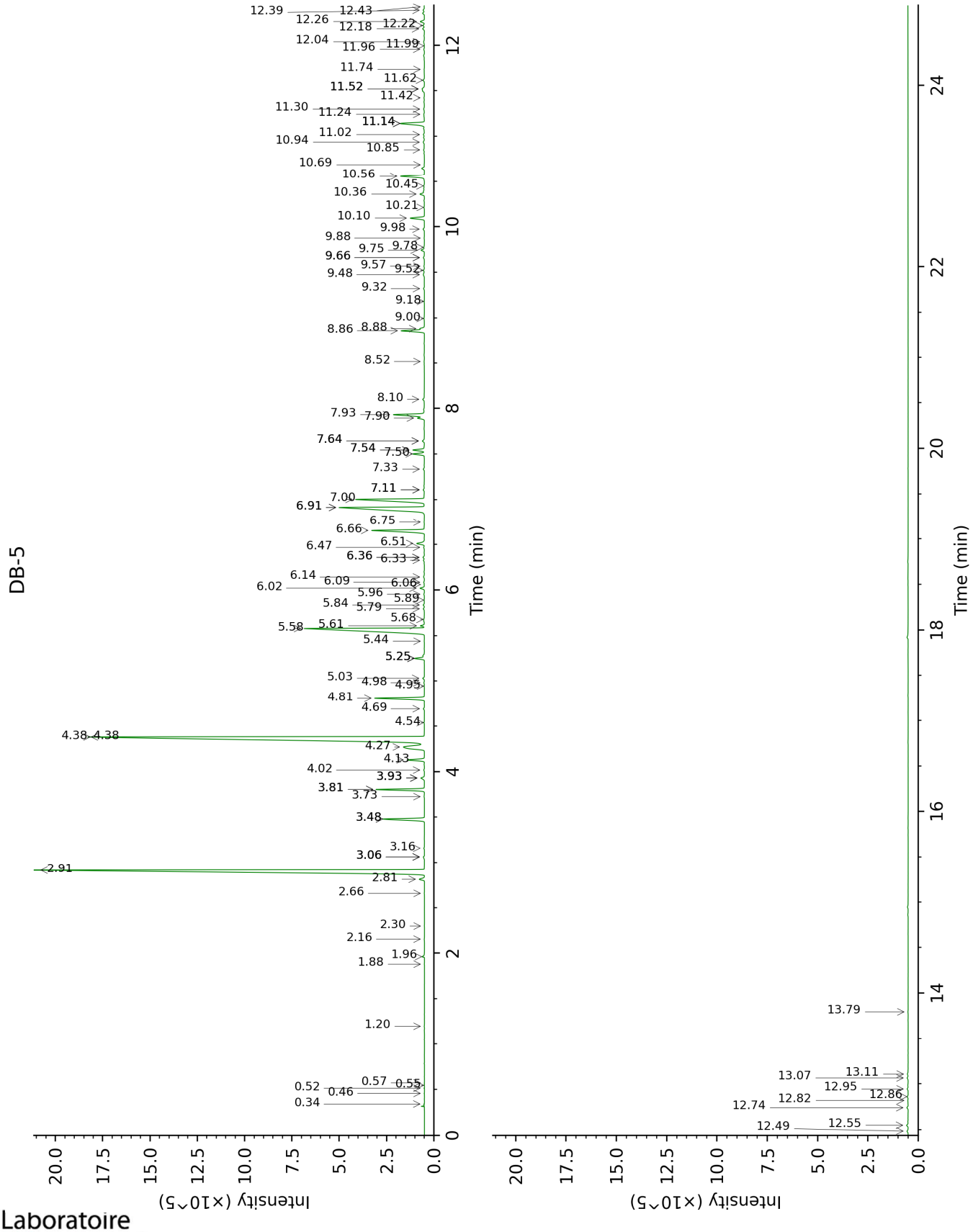
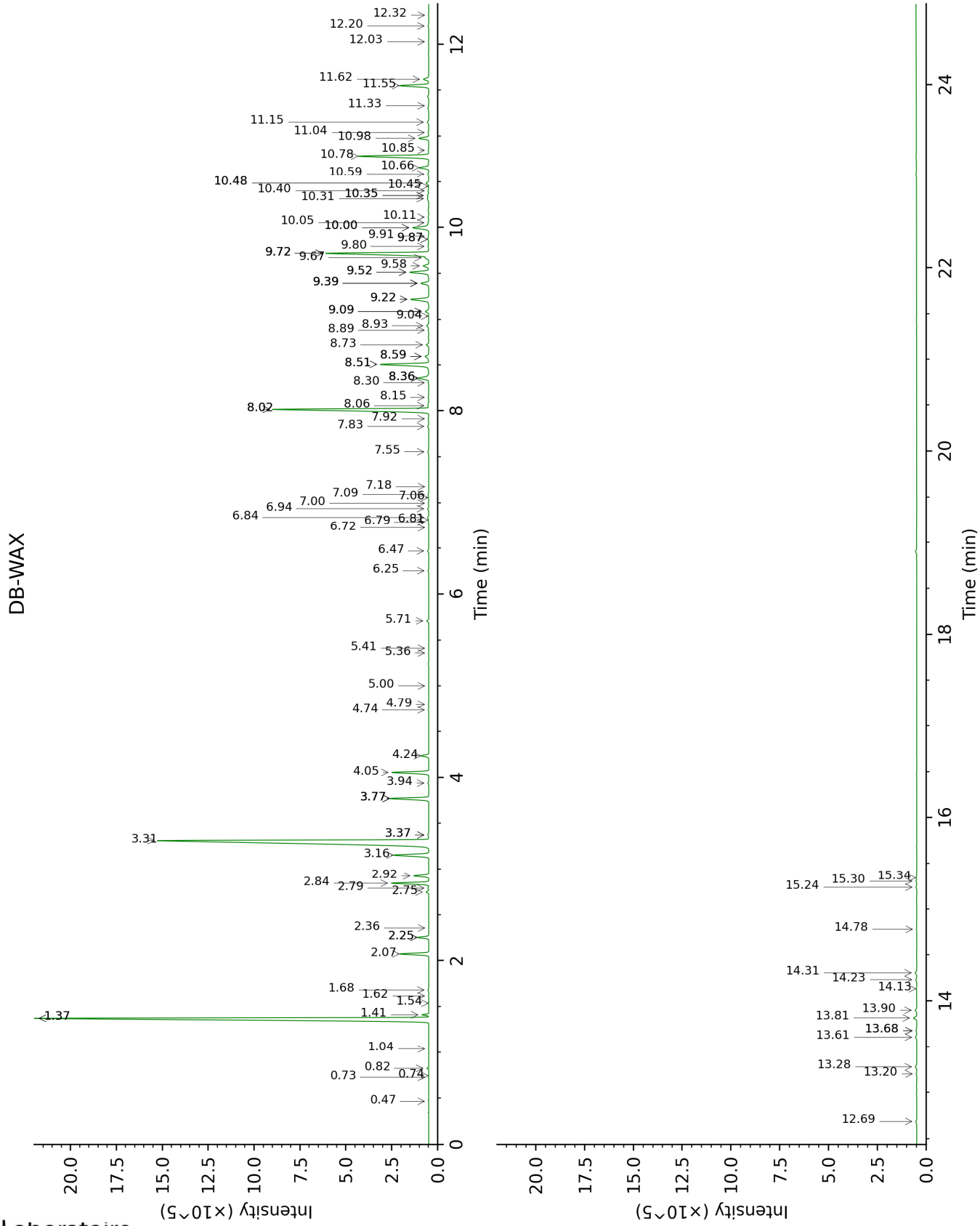

DB-5
Intensity (×10^5)
Time (min)
12.39
12.43
12.26
12.18
12.22
12.04
11.96
11.99
11.74
11.62
11.52
11.42
11.30
11.24
11.14
11.02
10.94
10.85
10.69
10.56
10.45
10.36
10.21
10.10
9.98
9.88
9.75
9.78
9.66
9.57
9.52
9.48
9.32
9.18
9.00
8.86
8.88
8.52
8.10
7.93
7.90
7.64
7.54
7.50
7.33
7.11
7.00
6.91
6.75
6.66
6.51
6.47
6.36
6.33
6.14
6.09
6.06
6.02
5.96
5.89
5.84
5.79
5.68
5.58
5.61
5.44
5.25
5.03
4.98
4.95
4.81
4.69
4.54
4.38
4.38
4.27
4.13
4.02
3.93
3.81
3.73
3.48
3.16
3.06
2.91
2.81
2.66
2.30
2.16
1.96
1.88
1.20
0.57
0.55
0.52
0.46
0.34
13.79
13.07
13.11
12.95
12.86
12.82
12.74
12.49
12.55


DB-WAX
Intensity (×10^5)
Time (min)
12.32
12.20
12.03
11.62
11.55
11.33
11.15
11.04
10.98
10.85
10.78
10.66
10.59
10.48
10.45
10.40
10.35
10.31
10.11
10.05
10.00
9.91
9.87
9.80
9.72
9.67
9.58
9.52
9.39
9.22
9.09
9.04
8.93
8.89
8.73
8.59
8.51
8.36
8.30
8.15
8.06
8.02
7.92
7.83
7.55
7.18
7.09
7.06
7.00
6.94
6.84
6.81
6.79
6.72
6.47
6.25
5.71
5.41
5.36
5.00
4.79
4.74
4.24
4.05
3.94
3.77
3.37
3.31
3.16
2.92
2.84
2.79
2.75
2.36
2.25
2.07
1.68
1.62
1.54
1.41
1.37
1.04
0.82
0.74
0.73
0.47
15.34
15.30
15.24
14.78
14.31
14.23
14.13
13.90
13.81
13.68
13.61
13.28
13.20
12.69

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.34	499	0.06	0.82	908	0.04
2-Methyl-3-buten-2-ol	0.46	605	tr	1.54	1014	tr
(*E*)-2-Methyl-1,3-pentadiene	0.52	628	0.01	0.47	767	0.01
Isovaleral	0.55	640	tr	0.74	886	tr
2-Methylbutyral	0.57	650	tr	0.73	880	tr
Unknown [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.20	780	tr	1.04	942	0.01
(2*E*)-Hexenal	1.88	850	0.01	3.37*	1176	0.05
(3*Z*)-Hexenol	1.96	857	0.08	5.71	1347	0.11
Hexanol	2.16	874	0.01	5.36	1322	0.02
Styrene	2.30	886	tr	3.77*	1207	2.14
Hashishene	2.66	915	0.01	1.37*	996	24.77
α-Thujene	2.81	925	0.26	1.41	1001	0.26
α-Pinene	2.91	932	24.98	1.37*	996	[24.77]
α-Fenchene	3.06*	942	0.06	1.62	1021	0.01
Unknown [m/z 91, 92 (47), 65 (11)... 134 (1)]	3.06*	942	[0.06]	2.36	1094	tr
Camphene	3.06*	942	[0.06]	1.68	1028	0.04
Thuja-2,4(10)-diene	3.16	949	0.02	2.25*	1084	0.56
Sabinene	3.48*	970	2.04	2.25*	1084	[0.56]
β-Pinene	3.48*	970	[2.04]	2.07	1066	1.49
6-Methyl-5-hepten-2-one	3.73	987	0.02	5.00	1298	0.01
Myrcene	3.81*	992	1.92	2.84	1134	1.88
trans-Dehydroxylinalool oxide	3.81*	992	[1.92]	3.37*	1176	[0.05]
α-Phellandrene	3.93*	1001	0.19	2.75	1126	0.14
Pseudolimonene	3.93*	1001	[0.19]	2.79	1130	0.05
cis-Dehydroxylinalool oxide	3.93*	1001	[0.19]	3.77*	1207	[2.14]
(3*Z*)-Hexenyl acetate	4.02	1007	0.03	4.79	1283	0.02
α-Terpinene	4.13	1014	0.76	2.92	1140	0.77
para-Cymene	4.27	1023	2.00	4.06	1228	2.00
Limonene	4.38*	1030	28.28	3.16	1158	2.16
1,8-Cineole	4.38*	1030	[28.28]	3.31	1171	26.06
(*Z*)-β-Ocimene	4.54	1040	0.02	3.77*	1207	[2.14]
(*E*)-β-Ocimene	4.69	1049	0.05	3.94	1219	0.05
γ-Terpinene	4.81	1057	2.08	3.77*	1207	[2.14]
cis-Sabinene hydrate	4.95	1065	0.01	6.84	1429	0.06

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Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	4.98	1068	0.02	4.74	1278	0.03
cis-Linalool oxide (fur.)	5.03	1071	0.07	6.47	1402	0.07
trans-Linalool oxide (fur.)	5.25*†	1085	0.51	6.81	1427	0.02
para-Cymenene	5.25*†	1085	[0.51]	6.26	1386	0.05
Terpinolene	5.25*†	1085	[0.51]	4.24	1241	0.41
trans-Sabinene hydrate	5.44	1097	0.01	7.92	1509	0.05
Linalool	5.58	1106	9.93	8.02*	1517	9.97
Hotrienol	5.61	1107	0.16	8.73	1572	0.14
endo-Fenchol	5.68	1112	0.03	8.30	1540	0.03
cis-para-Menth-2-en-1-ol	5.80	1119	0.05	8.06	1520	0.09
α-Campholenal	5.84	1122	0.05	6.94	1436	0.06
trans-Rose oxide	5.89	1126	0.02	5.41	1326	0.01
Nopinone	5.96	1130	0.03	8.15	1527	0.04
trans-Pinocarveol	6.02	1134	0.20	9.09*	1600	0.22
Camphor	6.06	1136	0.01	7.18	1454	0.01
trans-para-Menth-2-en-1-ol	6.09	1138	0.03	8.89	1585	0.05
Isopulegol	6.14	1142	0.05	8.02*	1517	[9.97]
Nerol oxide	6.33	1154	0.05	6.79	1425	0.02
Pinocarvone	6.36*	1156	0.07	7.83	1503	0.07
Hydrocinnamal	6.36*	1156	[0.07]	10.45	1711	0.01
Borneol	6.47	1163	0.04	9.72*	1652	6.59
δ-Terpineol	6.51	1165	0.42	9.40*	1625	0.48
Terpinen-4-ol	6.66	1175	2.78	8.51*	1555	3.04
Cryptone	6.75	1181	0.02	9.09*	1600	[0.22]
Myrtenal	6.91*	1191	6.65	8.59*	1562	0.28
α-Terpineol	6.91*	1191	[6.65]	9.72*	1652	[6.59]
Myrtenol	7.00	1197	4.31	10.78	1740	4.34
Verbenone	7.11*	1204	0.06	9.52*	1635	1.22
Unknown [m/z 95, 93 (32), 121 (24), 79 (22), 91 (21), 105 (16)... 154 (2)]	7.11*	1204	[0.06]	10.85	1745	0.03
trans-Carveol	7.34	1219	0.05	11.33	1786	0.02
Nerol	7.50	1230	0.53	10.98	1756	0.56
Citronellol	7.54*	1233	0.54	10.66	1729	0.55
Cuminal	7.54*	1233	[0.54]	10.48*	1714	0.16
Carvone	7.64*	1240	0.11	9.87*	1664	0.07
Neral	7.64*	1240	[0.11]	9.40*	1625	[0.48]
cis-Myrtanol	7.90	1256	0.31	11.62	1812	0.34
Geraniol	7.93	1259	1.61	11.55	1805	1.69
Geranial	8.10	1270	0.10	10.05	1679	0.05
trans-Pinocarvyl acetate	8.52	1298	0.02	9.04	1596	0.01

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Myrtenyl acetate	8.86	1322	1.11	9.52*	1635	[1.22]
Methyl geranate	8.88	1324	0.18	9.67	1648	0.16
Bicycloelemene	9.00	1332	0.04	7.00	1441	0.03
α-Cubebene	9.18	1345	0.01	6.72	1421	0.01
Citronellyl acetate	9.32	1355	0.04	9.40*	1625	[0.48]
Neryl acetate	9.48	1366	0.08	10.11	1684	0.03
α-Copaene	9.52	1369	0.05	7.09	1448	0.04
7-Cubebene	9.57	1372	0.02	7.06	1445	0.02
β-Bourbonene	9.66*	1379	0.06			
Methyl (*E*)-cinnamate	9.66*	1379	[0.06]	13.68*	1999	0.06
Geranyl acetate	9.75	1385	0.16	10.48*	1714	[0.16]
β-Elemene	9.78	1387	0.03	8.36*	1544	0.74
(*Z*)-Jasmone	9.88	1394	0.01	12.32	1874	0.01
α-Gurjunene	9.98	1401	0.06	7.56	1482	0.07
β-Caryophyllene	10.10	1410	0.68	8.36*	1544	[0.74]
γ-Maaliene	10.21	1419	0.02	8.36*	1544	[0.74]
Aromadendrene	10.36	1430	0.22	8.51*	1555	[3.04]
Selina-5,11-diene	10.45	1436	0.03	8.59*	1562	[0.28]
α-Humulene	10.56	1444	1.19	9.22*	1611	1.21
allo-Aromadendrene	10.69	1454	0.01	8.93	1588	0.14
trans-Cadina-1(6),4-diene	10.85	1466	0.05	9.22*	1611	[1.21]
Germacrene D	10.94	1473	0.08	9.72*	1652	[6.59]
β-Selinene	11.02	1479	0.05	9.80	1658	0.06
Viridiflorene	11.14*	1488	1.39	9.58	1641	0.36
α-Selinene	11.14*	1488	[1.39]	9.91	1667	0.03
Bicyclogermacrene	11.14*	1488	[1.39]	10.00*	1674	1.14
α-Muurolene	11.24	1496	0.04	10.00*	1674	[1.14]
δ-Amorphene	11.30	1500	0.05	9.87*	1664	[0.07]
γ-Cadinene	11.42	1509	0.02	10.35*	1703	0.09
trans-Calamenene	11.52*	1517	0.14	11.15	1771	0.10
Zonarene	11.52*	1517	[0.14]	10.35*	1703	[0.09]
δ-Cadinene	11.52*	1517	[0.14]	10.40	1707	0.05
trans-Cadina-1,4-diene	11.62	1525	0.07	10.59	1723	0.06
α-Calacorene	11.74	1534	0.02	12.03	1848	0.02
Germacrene B	11.96	1551	0.03	11.04	1762	0.05
Epiglobulol	11.99	1554	0.01	13.20	1955	0.03
Palustrol	12.04	1558	0.06	12.20	1863	0.04
Spathulenol	12.18	1569	0.09	14.31	2060	0.09
Caryophyllene oxide	12.22	1572	0.06	12.69	1907	0.06
Globulol	12.26	1575	0.21	13.82	2012	0.20
Viridiflorol	12.39	1585	0.07	13.90	2021	0.09
Cubeban-11-ol	12.43	1588	0.02	13.60	1992	0.09
Eudesm-5-en-11-ol analog	12.49	1593	0.06	14.13	2043	0.03
Humulene epoxide II	12.55	1598	0.08	13.28	1962	0.09
Rosifoliol	12.74	1614	0.06	14.23	2053	0.06

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1-epi-Cubenol	12.82	1620	0.02	13.68*	1999	[0.06]
γ-Eudesmol	12.86	1624	0.04	14.78	2106	0.02
Isospathulenol	12.95	1630	0.05	15.34	2163	0.04
β-Eudesmol	13.07	1640	0.05	15.30	2159	0.04
α-Eudesmol	13.11	1644	0.04	15.24	2153	0.05
Heptadecane	13.80	1701	0.01	10.32	1700	0.12
Total identified		**98.58%**			**99.00%**	
Total reported		**98.61%**			**99.08%**	

*: 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

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