

Date : March 08, 2019

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 19C07-PTH03-1-SCC

Customer identification : Damiana - DD0101810R

Type : Essential oil

Source : *Turnera diffusa*

Customer : Plant Therapy

ANALYSIS

Method: PC-PA-014-17J19 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Benoit Roger, Ph. D.

Analysis date : March 08, 2019

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow viscous liquid

Refractive index: 1.4868 ± 0.0003 (20 °C)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
Dimethylsulfide	tr	tr	Aliphatic sulfide
Isovaleral	0.02	0.02	Aliphatic aldehyde
2-Methylbutyral	0.01	0.01	Aliphatic aldehyde
2-Ethylfuran	0.05	0.05	Furan
Isoamyl alcohol	0.01	0.05	Aliphatic alcohol
Toluene	0.01	0.29*	Simple phenolic
Methyl isovalerate	0.01	3.19*	Aliphatic ester
Hexanal	0.05	0.04	Aliphatic aldehyde
Ethyl 2-methylbutyrate	0.11	0.08	Aliphatic ester
Ethyl isovalerate	0.25*	0.24	Aliphatic ester
Unknown	[0.25]*	0.02	Unknown
(3Z)-Hexenol	0.03	0.02	Aliphatic alcohol
(2E)-Hexenol	0.01	0.01	Aliphatic alcohol
Hexanol	0.07	0.07*	Aliphatic alcohol
Unknown	0.03	0.03	Unknown
Isoamyl acetate	0.01	0.01	Aliphatic ester
Unknown	0.02	0.02	Unknown
Heptanal	tr	0.01	Aliphatic aldehyde
Hashishene	0.01	[3.19]*	Monoterpene
Tricyclene	0.03	0.03	Monoterpene
α -Thujene	0.27	[0.29]*	Monoterpene
α -Pinene	3.12	[3.19]*	Monoterpene
Unknown	0.19	0.18	Monoterpene
Camphene	0.17	0.18	Monoterpene
Thuja-2,4(10)-diene	0.19	0.46*	Monoterpene
Benzaldehyde	0.01	0.02	Simple phenolic
β -Pinene	1.34*	1.09	Monoterpene
Sabinene	[1.34]*	[0.46]*	Monoterpene
cis-Carane	0.01	tr	Monoterpene
6-Methyl-5-hepten-2-one	0.11*	0.09*	Aliphatic ketone
Dehydro-1,8-cineole	[0.11]*	0.04	Monoterpenic ether
Myrcene	0.23*	0.21	Monoterpene
2-Pentylfuran	[0.23]*	0.01	Furan
α -Phellandrene	0.13	0.09	Monoterpene
Δ^3 -Carene	0.22	0.16	Monoterpene
α -Terpinene	0.12	0.12	Monoterpene
Hexyl acetate	0.03	0.02	Aliphatic ester
para-Cymene	0.88	0.86	Monoterpene
Limonene	20.04*	0.22	Monoterpene
1,8-Cineole	[20.04]*	20.59*	Monoterpenic ether
β -Phellandrene	[20.04]*	[20.59]*	Monoterpene
Unknown	[20.04]*	[0.07]*	Monoterpene
(Z)- β -Ocimene	0.04	0.37*	Monoterpene
Unknown	0.03		Unknown
(E)- β -Ocimene	0.02	0.01	Monoterpene
Unknown	0.02*	0.03	Monoterpene
Unknown	[0.02]*	0.25*	Unknown
γ -Terpinene	0.34	[0.37]*	Monoterpene

<i>cis</i> -Sabinene hydrate	0.08	[0.25]*	Monoterpenic alcohol
Unknown	0.02	0.03*	Oxygenated monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	0.01	Monoterpenic alcohol
Unknown	0.02		Unknown
Unknown	0.08*	[0.09]*	Unknown
Unknown	[0.08]*	0.06*	Oxygenated monoterpene
Terpinolene	0.21*	0.09	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	[0.21]*	[0.25]*	Monoterpenic alcohol
para-Cymenene	[0.21]*	0.01	Monoterpene
<i>trans</i> -Sabinene hydrate	0.05	[0.11]	Monoterpenic alcohol
Linalool	0.23*	0.20	Monoterpenic alcohol
α -Thujone	[0.23]*	0.13	Monoterpenic ketone
Nonanal	0.07	0.02	Aliphatic aldehyde
Hotrienol	0.03*	0.04	Monoterpenic alcohol
Isoamyl isovalerate	[0.03]*	[0.03]*	Aliphatic ester
Unknown	0.07*	0.02	Oxygenated monoterpene
β -Thujone	[0.07]*	0.09*	Monoterpenic ketone
Unknown	0.01		Oxygenated monoterpene
<i>cis</i> -para-Menth-2-en-1-ol	0.07	0.05	Monoterpenic alcohol
α -Campholenal	0.25	0.75*	Monoterpenic aldehyde
Nopinone	0.05	0.04	Normonoterpenic ketone
<i>trans</i> -Pinocarveol	0.30	0.36	Monoterpenic alcohol
<i>cis</i> -Verbenol	0.08	0.06	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.28	0.27	Monoterpenic alcohol
meta-Mentha-4,6-dien-8-ol	0.03	0.29*	Monoterpenic alcohol
Sabinaketone	0.03	0.70*	Normonoterpenic ketone
Pinocamphone	0.03	[0.06]*	Monoterpenic ketone
Phellandrenol analog I	0.16*		Monoterpenic alcohol
Pinocarvone	[0.16]*	0.11	Monoterpenic ketone
Borneol	0.10*	2.27*	Monoterpenic alcohol
α -Phellandren-8-ol	[0.10]*	0.06	Monoterpenic alcohol
Terpinen-4-ol	0.22	0.28*	Monoterpenic alcohol
para-Cymen-8-ol	0.05	0.05	Monoterpenic alcohol
α -Terpineol	0.58*	[2.27]*	Monoterpenic alcohol
Myrtenal	[0.58]*	[0.70]*	Monoterpenic aldehyde
Myrtenol	0.18	0.09	Monoterpenic alcohol
Verbenone	0.13	0.09	Monoterpenic ketone
<i>trans</i> -Carveol	0.13	0.13	Monoterpenic alcohol
<i>cis</i> -Carveol	0.02	0.15	Monoterpenic alcohol
Myrtenyl formate?	0.10	0.21*	Monoterpenic ester
Hexyl 2-methylbutyrate?	0.09*	[0.09]*	Aliphatic ester
Carvone	[0.09]*	0.82*	Monoterpenic ketone
Isopentyl hexanoate	0.05		Aliphatic ester
Linalyl acetate	0.05	[0.05]	Monoterpenic ester
Unknown	0.13		Unknown
<i>trans</i> -Linalool oxide acetate (pyr.)	0.03	0.10	Monoterpenic ester
Unknown	0.08	0.11	Unknown
Geranial	0.07	0.83*	Monoterpenic aldehyde
Limonen-10-ol	0.17	0.16	Monoterpenic alcohol
Thymol	0.61	0.69	Monoterpenic alcohol
Carvacrol	0.03	0.08	Monoterpenic alcohol
Myrtenyl acetate	0.04	0.10	Monoterpenic ester

Hexyl tiglate	0.08	0.77*	Aliphatic ester
δ -Elemene	0.09	[0.75]*	Sesquiterpene
α -Terpinyl acetate	0.80*	[2.27]*	Monoterpenic ester
α -Cubebene	[0.80]*	0.43	Sesquiterpene
Cyclosativene I	0.48	[0.75]*	Sesquiterpene
Cyclosativene II	0.23	[0.75]*	Sesquiterpene
α -Ylangene	0.12*	0.12	Sesquiterpene
Unknown	[0.12]*	0.07	Sesquiterpene
α -Copaene	0.71	0.78	Sesquiterpene
<i>cis</i> - β -Elemene	0.26	0.12	Sesquiterpene
β -Bourbonene	[0.26]	0.13	Sesquiterpene
β -Cubebene	0.38	0.36	Sesquiterpene
β -Elemene	0.32	1.75*	Sesquiterpene
Unknown	0.16		Sesquiterpene
(<i>Z</i>)-Jasmone	0.04	0.07	Jasmonate
Unknown	0.09	0.10	Sesquiterpene
α -Gurjunene	0.09	0.09	Sesquiterpene
β -Caryophyllene	1.59	[1.75]*	Sesquiterpene
β -Copaene	0.31	0.27	Sesquiterpene
Aromadendrene	0.04	[0.28]*	Sesquiterpene
6,9-Guaiadiene	0.71*	[0.70]*	Sesquiterpene
α -Guaiene	[0.71]*	[1.75]	Sesquiterpene
Unknown	0.53*	[0.21]*	Sesquiterpene
Unknown	[0.53]*	[0.77]*	Sesquiterpene
α -Humulene	0.35	0.34	Sesquiterpene
Unknown	0.59	0.54	Sesquiterpene
allo-Aromadendrene	0.56	0.59	Sesquiterpene
Geranylacetone	0.11	0.12	Monoterpenic ketone
4,5-diepi-Aristolochene	1.48	1.92	Sesquiterpene
Unknown	2.71*	3.94*	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	[2.71]*	[0.29]*	Sesquiterpene
γ -Murolene	0.77	0.91*	Sesquiterpene
α -Amorphene	0.31	[0.91]*	Sesquiterpene
β -Selinene	0.58	0.90	Sesquiterpene
Unknown	8.73*	5.67	Unknown
δ -Selinene	[8.73]*	[2.27]*	Sesquiterpene
γ -Amorphene	[8.73]	[3.94]*	Sesquiterpene
α -Selinene	1.37*	[0.82]*	Sesquiterpene
4-epi- <i>cis</i> -Dihydroagarofuran	[1.37]*	0.39	Sesquiterpenic ether
epi-Cubebol	[1.37]*	0.54	Sesquiterpenic alcohol
α -Murolene	0.78	[0.83]*	Sesquiterpene
δ -Amorphene	0.33	[0.82]*	Sesquiterpene
γ -Cadinene	1.21*	0.47	Sesquiterpene
Cubebol	[1.21]*	0.52	Sesquiterpenic alcohol
endo-1-Bourbonanol	0.04		Sesquiterpenic alcohol
Zonarene	3.16*	3.05*	Sesquiterpene
δ -Cadinene	[3.16]*	[3.05]*	Sesquiterpene
<i>trans</i> -Calamenene	[3.16]*	0.16	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.35	0.27	Sesquiterpene
Unknown	0.33*	0.18	Sesquiterpene
α -Cadinene	[0.33]*	0.19	Sesquiterpene
α -Calacorene	0.83	1.12*	Sesquiterpene

Isocaryophyllene epoxide B	0.18	[1.12]*	Sesquiterpenic ether
Furopelargone isomer	0.67	2.91*	Sesquiterpenic ketone
Palustrol	0.14	0.16	Sesquiterpenic alcohol
β -Calacorene	0.19	[1.27]	Sesquiterpene
(E)-Nerolidol	2.40	2.25	Sesquiterpenic alcohol
Germacrene D-4-ol	0.41	0.44*	Sesquiterpenic alcohol
Caryophyllene oxide isomer	2.71*	1.27	Sesquiterpenic ether
Spathulenol	[2.71]*	0.59*	Sesquiterpenic alcohol
Caryophyllene oxide	[2.71]*	[2.91]*	Sesquiterpenic ether
Globulol	[2.71]*	0.17	Sesquiterpenic alcohol
Furopelargone A	1.59*	0.45	Sesquiterpenic ketone
Unknown	[1.59]*		Sesquiterpene
Viridiflorol	[1.59]*	0.11	Sesquiterpenic alcohol
Unknown	0.66	0.82	Oxygenated sesquiterpene
Ledol	1.24*	1.32*	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	[1.24]*	[0.59]*	Sesquiterpenic alcohol
Humulene epoxide II	1.56*	[1.32]*	Sesquiterpenic ether
Unknown	[1.56]*		Oxygenated sesquiterpene
Unknown	[1.56]*	1.17	Oxygenated sesquiterpene
Unknown	0.16	0.16	Sesquiterpene
Selin-6-en-4 α -ol?	5.69*	3.73	Sesquiterpenic alcohol
Junenol	[5.69]*	[0.44]*	Sesquiterpenic alcohol
10-epi- γ -Eudesmol	[5.69]*	0.45	Sesquiterpenic alcohol
Unknown	[5.69]	0.42	Oxygenated sesquiterpene
Guaia-6,10(14)-dien-4 β -ol	0.60	0.31	Sesquiterpenic alcohol
Unknown	1.03		Unknown
Isospathulenol	0.24	0.18	Sesquiterpenic alcohol
τ -Muurolol	1.35*	0.94	Sesquiterpenic alcohol
Jinkoh-eremol	[1.35]*	0.22	Sesquiterpenic alcohol
τ -Cadinol	[1.35]*	[0.42]	Sesquiterpenic alcohol
Unknown	1.44*	0.24	Oxygenated sesquiterpene
Valerianol	[1.44]*	1.46*	Sesquiterpenic alcohol
Unknown	[1.44]*	0.39	Oxygenated sesquiterpene
cis-Calamenen-10-ol	0.08*	0.07	Sesquiterpenic alcohol
Intermedeol?	[0.08]*	0.30	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.25	0.30*	Sesquiterpenic alcohol
Unknown	1.44*	1.01	Unknown
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	[1.44]*	[0.30]*	Sesquiterpenic alcohol
Eudesma-4(15),7-dien-1 β -ol	0.38		Sesquiterpenic alcohol
Cyperotundone	0.32	0.23	Sesquiterpenic ketone
Juniper camphor	0.43	0.25	Sesquiterpenic alcohol
Unknown	0.31	0.12	Oxygenated sesquiterpene
Unknown	0.24		Oxygenated sesquiterpene
Oplopanone	0.29	0.20	Sesquiterpenic alcohol
Unknown	0.22		Oxygenated sesquiterpene
Unknown	0.60		Unknown
Unknown	1.04	[1.46]*	Oxygenated sesquiterpene
Unknown	0.34	0.51	Oxygenated sesquiterpene
Dehydrofukinone	0.85	0.90	Sesquiterpenic ketone
Unknown	0.19	0.19	Oxygenated sesquiterpene
Phytol	0.07	0.12	Diterpenic alcohol
Total identified	87.82%	78.20%	

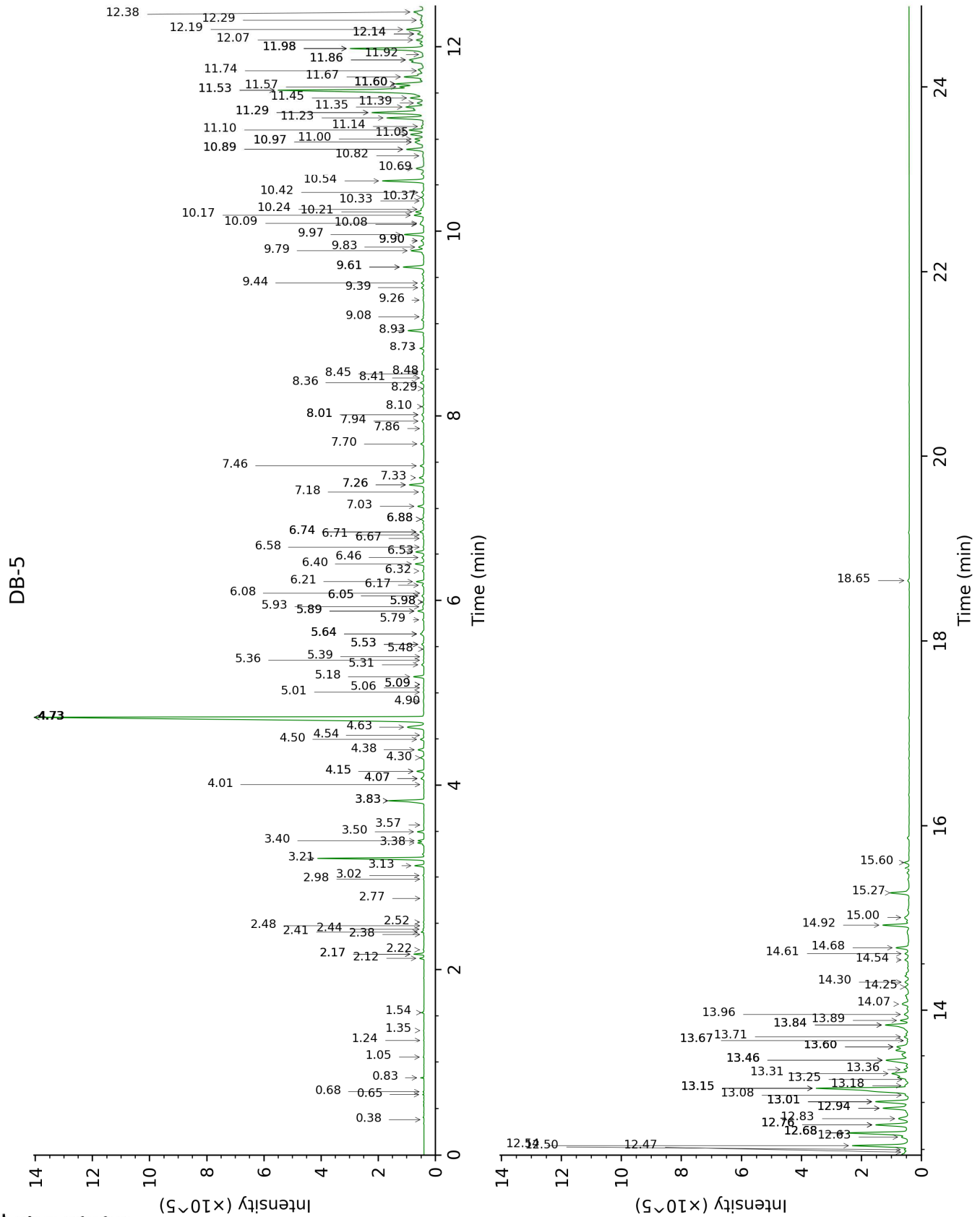
*: Two or more compounds are coeluting on this column

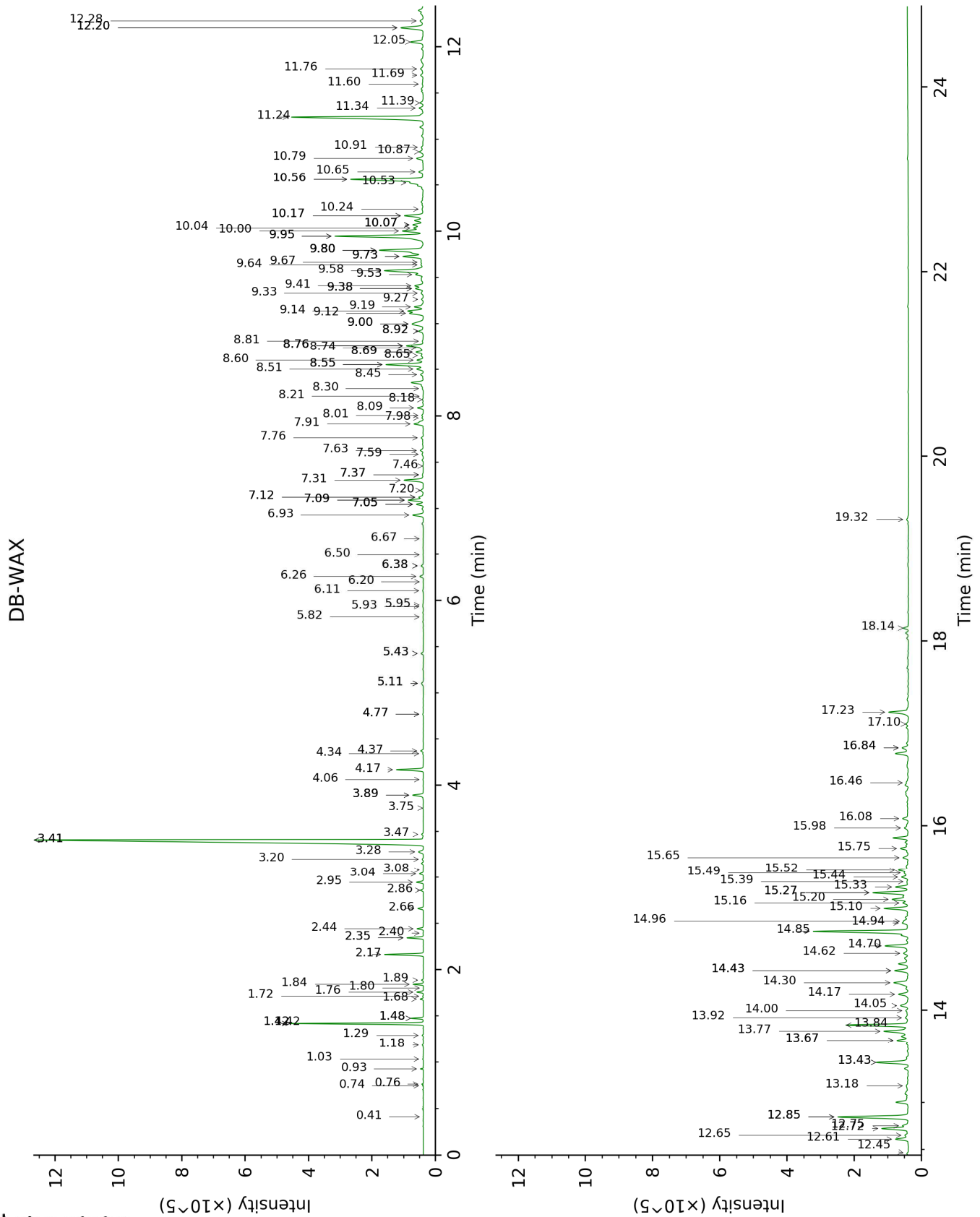
[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Dimethylsulfide	0.38	514	tr	0.41	713	tr
Isovaleral	0.65	640	0.02	0.76	886	0.02
2-Methylbutyral	0.68	649	0.01	0.74	880	0.01
2-Ethylfuran	0.83	693	0.05	0.93	922	0.05
Isoamyl alcohol	1.05	731	0.01	3.47	1175	0.05
Toluene	1.24	756	0.01	1.48*	1002	0.29
Methyl isovalerate	1.35	771	0.01	1.42*	994	3.19
Hexanal	1.54	796	0.05	1.89	1040	0.04
Ethyl 2-methylbutyrate	2.12	847	0.11	1.68	1021	0.08
Ethyl isovalerate	2.17*	851	0.25	1.84	1036	0.24
Unknown [m/z 109, 43 (28), 124 (28), 41 (14), 55 (11), 79 (9), 81 (8)...]	2.17*	851	[0.25]	1.72	1024	0.02
(3Z)-Hexenol	2.22	855	0.03	5.94	1348	0.02
(2E)-Hexenol	2.38	868	0.01	6.20	1368	0.01
Hexanol	2.41	870	0.07	5.43*	1311	0.07
Unknown [m/z 79, 78 (45), 91 (28), 77 (28), 41 (13), 80 (12), 107 (11)... 122 (1)]	2.44	873	0.03	1.18	959	0.03
Isoamyl acetate	2.48	876	0.01	2.40	1088	0.01
Unknown [m/z 81, 79 (20), 80 (12), 82 (9)... 124 (7)]	2.52	879	0.02	1.03	937	0.02
Heptanal	2.77	900	tr	3.08	1144	0.01
Hashishene	2.98	914	0.01	1.42*	994	[3.19]
Tricyclene	3.02	916	0.03	1.29	975	0.03
α -Thujene	3.13	924	0.27	1.48*	1002	[0.29]
α -Pinene	3.21	929	3.12	1.42*	994	[3.19]
Unknown [m/z 91, 92 (47), 65 (11)... 134 (1)]	3.38	940	0.19	2.44	1093	0.18
Camphene	3.40	942	0.17	1.76	1028	0.18
Thuja-2,4(10)-diene	3.50	948	0.19	2.35*	1084	0.46
Benzaldehyde	3.57	952	0.01	7.46	1462	0.02
β -Pinene	3.83*	970	1.34	2.17	1066	1.09
Sabinene	3.83*	970	[1.34]	2.35*	1084	[0.46]
cis-Carane	4.01	981	0.01	1.80	1032	tr
6-Methyl-5-hepten-2-one	4.07*	985	0.11	5.11*	1303	0.09
Dehydro-1,8-cineole	4.07*	985	[0.11]	3.20	1153	0.04
Myrcene	4.15*	990	0.23	2.95	1133	0.21
2-Pentylfuran	4.15*	990	[0.23]	3.75	1198	0.01

α -Phellandrene	4.30	1000	0.13	2.86	1127	0.09
Δ^3 -Carene	4.38	1005	0.22	2.66	1111	0.16
α -Terpinene	4.50	1012	0.12	3.04	1141	0.12
Hexyl acetate	4.54	1015	0.03	4.34	1243	0.02
para-Cymene	4.63	1021	0.88	4.17	1230	0.86
Limonene	4.73*	1027	20.04	3.28	1160	0.22
1,8-Cineole	4.73*	1027	[20.04]	3.41*	1170	20.59
β -Phellandrene	4.73*	1027	[20.04]	3.41*	1170	[20.59]
Unknown [m/z 95, 123 (60), 67 (50), 41 (27)... 138 (20)]	4.73*	1027	[20.04]	5.43*	1311	[0.07]
(Z)- β -Ocimene	4.90	1038	0.04	3.89*	1209	0.37
Unknown [m/z 109, 43 (57), 91 (28), 67 (25), 93 (24), 95 (22), 77 (21), 137 (21), 41 (17), 79 (14)...]	5.01	1045	0.03			
(E)- β -Ocimene	5.06	1048	0.02	4.06	1222	0.01
Unknown [m/z 41, 69 (97), 95 (33), 67 (31), 53 (18)...]	5.10*	1050	0.02	6.11	1361	0.03
Unknown [m/z 109, 45 (67), 41 (40), 67 (39), 81 (33), 79 (27), 95 (24), 91 (23), 82 (21), 55 (21), 93 (20)...]	5.10*	1050	[0.02]	7.05*	1431	0.25
γ -Terpinene	5.18	1055	0.34	3.89*	1209	[0.37]
cis-Sabinene hydrate	5.31	1063	0.08	7.05*	1431	[0.25]
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.36	1066	0.02	4.77*	1276	0.03
cis-Linalool oxide (fur.)	5.39	1068	0.02	6.67	1402	0.01
Unknown [m/z 56, 55 (94), 41 (85), 69 (74), 43 (65), 70 (63)...]	5.48	1074	0.02			
Unknown [m/z 43, 56 (90), 55 (51), 70 (48), 69 (37), 41 (28), 57 (26)...]	5.53*	1077	0.08	5.11*	1303	[0.09]
Unknown [m/z 43, 94 (63), 109 (61), 59 (55), 79 (51)...152 (2)]	5.53*	1077	[0.08]	7.36*	1455	0.06
Terpinolene	5.64*†	1084	0.21	4.37	1245	0.09
trans-Linalool	5.64*†	1084	[0.21]	7.05*	1431	[0.25]

oxide (fur.)						
para-Cymenene	5.64*†	1084	[0.21]	6.50	1389	0.01
<i>trans</i> -Sabinene hydrate	5.79	1093	0.05	8.01†	1504	[0.11]
Linalool	5.89*	1099	0.23	8.09	1511	0.20
α-Thujone	5.89*	1099	[0.23]	6.26	1372	0.13
Nonanal	5.93	1102	0.07	5.95	1350	0.02
Hotrienol	5.98*	1106	0.03	8.81	1568	0.04
Isoamyl isovalerate	5.98*	1106	[0.03]	4.77*	1276	[0.03]
Unknown [m/z 111, 69 (70), 41 (68), 55 (53), 43 (51)... 154 (7)]	6.05*	1110	0.07	5.82	1340	0.02
β-Thujone	6.05*	1110	[0.07]	6.38*	1380	0.09
Unknown [m/z 109, 91 (57), 93 (47), 81 (44), 77 (40)... 154 (1)]	6.08	1112	0.01			
<i>cis</i> -para-Menth-2-en-1-ol	6.17	1117	0.07	8.18†	1518	0.05
α-Campholenal	6.20	1120	0.25	7.09*†	1434	0.75
Nopinone	6.32	1127	0.05	8.30	1527	0.04
<i>trans</i> -Pinocarveol	6.40	1132	0.30	9.18	1597	0.36
<i>cis</i> -Verbenol	6.46	1136	0.08	9.27	1604	0.06
<i>trans</i> -Verbenol	6.52	1140	0.28	9.53	1626	0.27
meta-Mentha-4,6-dien-8-ol	6.58	1143	0.03	9.38*	1613	0.29
Sabinaketone	6.67	1150	0.03	8.76*	1564	0.70
Pinocamphone	6.71	1152	0.03	7.36*	1455	[0.06]
Phellandrenol analog I	6.74*	1154	0.16			
Pinocarvone	6.74*	1154	[0.16]	7.98†	1502	0.11
Borneol	6.88*	1163	0.10	9.80*	1647	2.27
α-Phellandren-8-ol	6.88*	1163	[0.10]	10.24	1684	0.06
Terpinen-4-ol	7.02	1172	0.22	8.69*	1558	0.28
para-Cymen-8-ol	7.18	1182	0.05	11.60	1800	0.05
α-Terpineol	7.26*	1187	0.58	9.80*	1647	[2.27]
Myrtenal	7.26*	1187	[0.58]	8.76*	1564	[0.70]
Myrtenol	7.33	1192	0.18	10.92	1741	0.09
Verbenone	7.46	1200	0.13	9.67	1637	0.09
<i>trans</i> -Carveol	7.70	1216	0.13	11.39	1782	0.13
<i>cis</i> -Carveol	7.86	1228	0.02	11.76	1814	0.15
Myrtenyl formate?	7.94	1233	0.10	8.92*	1576	0.21
Hexyl 2-methylbutyrate?	8.01*	1238	0.09	6.38*	1380	[0.09]
Carvone	8.01*	1238	[0.09]	10.07*†	1670	0.82
Isopentyl hexanoate	8.10	1244	0.05			
Linalyl acetate	8.30	1257	0.05	8.21†	1520	[0.05]
Unknown [m/z 97, 109 (23), 95 (17), 67 (14), 81 (13),	8.36	1261	0.13			

166 (12)...] <i>trans</i> -Linalool oxide acetate (pyr.)	8.41	1264	0.03	9.33	1609	0.10
Unknown [m/z 43, 111 (47), 93 (41), 55 (28), 67 (23), 41 (22)...]	8.45	1267	0.08	8.74	1562	0.11
Geranial	8.48	1269	0.07	10.17*	1678	0.83
Limonen-10-ol	8.73	1286	0.17	13.18	1943	0.16
Thymol	8.93	1300	0.61	15.20	2137	0.69
Carvacrol	9.08	1306	0.03	15.39	2156	0.08
Myrtenyl acetate	9.26	1319	0.04	9.64	1634	0.10
Hexyl tiglate	9.39	1328	0.08	9.00*	1582	0.77
δ-Elemene	9.44	1332	0.09	7.12*†	1437	[0.75]
α-Terpinyl acetate	9.61*	1344	0.80	9.80*	1647	[2.27]
α-Cubebene	9.61*	1344	[0.80]	6.93	1422	0.43
Cyclosativene I	9.79	1357	0.48	7.09*†	1434	[0.75]
Cyclosativene II	9.83	1359	0.23	7.12*†	1437	[0.75]
α-Ylangene	9.90*†	1364	0.12	7.20	1442	0.12
Unknown [m/z 189, 91 (89), 82 (78), 109 (72), 93 (68), 67 (63), 161 (59)... 204 (tr)]	9.90*†	1364	[0.12]	7.59	1472	0.07
α-Copaene	9.97	1369	0.71	7.31	1451	0.78
<i>cis</i> -β-Elemene	10.08†	1377	0.26	8.45	1539	0.12
β-Bourbonene	10.09†	1377	[0.26]	7.63	1475	0.13
β-Cubebene	10.17	1384	0.38	7.91	1497	0.36
β-Elemene	10.21	1386	0.32	8.55*†	1547	1.75
Unknown [m/z 93, 122 (98), 161 (98), 107 (86), 95 (46), 105 (72)... 204 (34)]	10.24	1388	0.16			
(Z)-Jasmone	10.33	1394	0.04	12.45	1876	0.07
Unknown [m/z 117, 118 (95), 159 (82), 131 (81), 91 (71)... 202 (15), 204 (9)]	10.36	1397	0.09	8.65	1555	0.10
α-Gurjunene	10.42	1401	0.09	7.76	1486	0.09
β-Caryophyllene	10.54	1410	1.59	8.55*†	1547	[1.75]
β-Copaene	10.69	1421	0.31	8.51	1544	0.27
Aromadendrene	10.82	1431	0.04	8.69*	1558	[0.28]
6,9-Guaiadiene	10.89*	1436	0.71	8.76*	1564	[0.70]
α-Guaiene	10.89*	1436	[0.71]	8.60†	1551	[1.75]
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.97*	1442	0.53	8.92*	1576	[0.21]
Unknown [m/z 161, 105 (70), 91 (51), 133 (50), 204	10.97*	1442	[0.53]	9.00*	1582	[0.77]

(45), 119 (37)...						
α -Humulene	11.00	1444	0.35	9.41	1616	0.34
Unknown [m/z 105, 161 (78), 93 (70), 133 (67), 91 (66), 204 (63), 119 (41)]	11.05	1448	0.59	9.12	1592	0.54
allo- Aromadendrene	11.10	1452	0.56	9.14	1594	0.59
Geranylacetone	11.14	1454	0.11	11.69	1808	0.12
4,5-diepi- Aristolochene	11.23	1461	1.48	9.58	1629	1.92
Unknown [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	11.29*†	1466	2.71	9.95*	1660	3.94
<i>trans</i> -Cadina- 1(6),4-diene	11.29*†	1466	[2.71]	9.38*	1613	[0.29]
γ -Murolene	11.35	1470	0.77	9.73*	1642	0.91
α -Amorphene	11.39	1473	0.31	9.73*	1642	[0.91]
β -Selinene	11.45	1477	0.58	10.00	1664	0.90
Unknown [m/z 109, 67 (10), 110 (9), 43 (9), 107 (7), 81 (6)...	11.53*†	1484	8.73	11.24	1769	5.67
δ -Selinene	11.53*†	1484	[8.73]	9.80*	1647	[2.27]
γ -Amorphene	11.57†	1486	[8.73]	9.95*	1660	[3.94]
α -Selinene	11.60*†	1489	1.37	10.07*†	1670	[0.82]
4-epi- <i>cis</i> - Dihydroagarofuran	11.60*†	1489	[1.37]	10.04	1667	0.39
epi-Cubebol	11.60*†	1489	[1.37]	12.05	1840	0.54
α -Murolene	11.67	1494	0.78	10.17*	1678	[0.83]
δ -Amorphene	11.74	1499	0.33	10.07*†	1670	[0.82]
γ -Cadinene	11.86*†	1508	1.21	10.52	1708	0.47
Cubebol	11.86*†	1508	[1.21]	12.61	1890	0.52
endo-1- Bourbonanol	11.92	1513	0.04			
Zonarene	11.98*	1518	3.16	10.56*	1711	3.05
δ -Cadinene	11.98*	1518	[3.16]	10.56*	1711	[3.05]
<i>trans</i> -Calamenene	11.98*	1518	[3.16]	11.34	1777	0.16
<i>trans</i> -Cadina-1,4- diene	12.07	1525	0.35	10.80	1731	0.27
Unknown [m/z 189, 204 (92), 161 (65), 133 (51), 105 (51), 91 (51), 119 (45)]	12.14*	1530	0.33	10.65	1718	0.18
α -Cadinene	12.14*	1530	[0.33]	10.87	1737	0.19
α -Calacorene	12.19	1534	0.83	12.20*	1854	1.12
Isocaryophyllene epoxide B	12.29	1542	0.18	12.20*	1854	[1.12]
Furopelargone	12.38	1549	0.67	12.85*	1912	2.91

isomer						
Palustrol	12.47	1556	0.14	12.28	1861	0.16
β -Calacorene	12.50	1558	0.19	12.75†	1903	[1.27]
(E)-Nerolidol	12.54	1562	2.40	13.84	2005	2.25
Germacrene D-4-ol	12.63	1569	0.41	13.67*	1989	0.44
Caryophyllene oxide isomer	12.68*	1572	2.71	12.72†	1900	1.27
Spathulenol	12.68*	1572	[2.71]	14.43*	2062	0.59
Caryophyllene oxide	12.68*	1572	[2.71]	12.85*	1912	[2.91]
Globulol	12.68*	1572	[2.71]	13.92	2012	0.17
Furopelargone A	12.76*	1579	1.59	14.05	2025	0.45
Unknown [m/z 202, 187 (91), 91 (51), 79 (46), 93 (44), 43 (40)...]	12.76*	1579	[1.59]			
Viridiflorol	12.76*	1579	[1.59]	14.00	2020	0.11
Unknown [m/z 111, 126 (82), 109 (60), 162 (54), 81 (54), 55 (53), 121 (52)... 220 (12)]	12.83	1584	0.66	14.30	2049	0.82
Ledol	12.94*	1593	1.24	13.43*	1967	1.32
Eudesm-5-en-11-ol	12.94*	1593	[1.24]	14.43*	2062	[0.59]
Humulene epoxide II	13.01*	1599	1.56	13.43*	1967	[1.32]
Unknown [m/z 149, 43 (95), 93 (84), 177 (66), 109 (62), 67 (60)...220 (11)]	13.01*	1599	[1.56]			
Unknown [m/z 177, 43 (97), 109 (65), 67 (57), 96 (51)... 220 (13)]	13.01*	1599	[1.56]	13.77	1998	1.17
Unknown [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	13.08	1605	0.16	12.65	1894	0.16
Selin-6-en-4 α -ol?	13.16*†	1611	5.69	14.85	2103	3.73
Junenol	13.16*†	1611	[5.69]	13.67*	1989	[0.44]
10-epi- γ -Eudesmol	13.16*†	1611	[5.69]	14.17	2037	0.45
Unknown [m/z 81, 43 (52), 161 (49), 105 (30), 207 (27), 95 (26), 93 (24), 109 (24)...]	13.18†	1613	[5.69]	14.94†	2112	0.42
Guaia-6,10(14)-dien-4 β -ol	13.25	1618	0.60	15.75	2193	0.31
Unknown [m/z 145, 59 (97), 161 (87), 218 (76), 43	13.31	1624	1.03			

(76), 179 (63)...						
Isospathulenol	13.36	1627	0.24	15.49	2166	0.18
τ -Muurolol	13.46*	1635	1.35	15.10	2127	0.94
Jinkoh-eremol	13.46*	1635	[1.35]	15.16	2133	0.22
τ -Cadinol	13.46*	1635	[1.35]	14.96†	2114	[0.42]
Unknown [m/z 161, 59 (67), 95 (45), 93 (40), 105 (40), 149 (39), 81 (39), 43 (38), 204 (37)... 220 (5)]	13.60*†	1647	1.44	14.62	2080	0.24
Valerianol	13.60*†	1647	[1.44]	15.27*	2144	1.46
Unknown [m/z 43, 81 (84), 41 (64), 67 (62), 95 (58), 79 (58)... 204 (48), 220 (2)]	13.60*†	1647	[1.44]	15.52	2169	0.39
<i>cis</i> -Calamenen-10- ol	13.67*	1653	0.08	16.46	2266	0.07
Intermedeol?	13.67*	1653	[0.08]	15.44	2161	0.30
<i>trans</i> -Calamenen- 10-ol	13.71	1657	0.25	16.84*	2306	0.30
Unknown [m/z 175, 176 (14), 218 (13), 105 (11), 91 (11), 119 (10)...	13.84*	1667	1.44	14.70	2087	1.01
(3Z)-Caryophylla- 3,8(13)-dien-5 β -ol	13.84*	1667	[1.44]	16.84*	2306	[0.30]
Eudesma-4(15),7- dien-1 β -ol	13.89	1671	0.38			
Cyperotundone	13.96	1677	0.32	15.65	2183	0.23
Juniper camphor	14.07	1686	0.43	16.08	2226	0.25
Unknown [m/z 91, 105 (66), 133 (48), 159 (46), 117 (39), 119 (34), 189 (34)... 220 (12)]	14.25	1701	0.31	17.10	2333	0.12
Unknown [m/z 123, 136 (49), 43 (38), 107 (37), 119 (36), 109 (33), 91 (33)... 222 (10)]	14.30	1706	0.24			
Oplopanone	14.54	1726	0.29	18.14	2447	0.20
Unknown [m/z 109, 55 (70), 41 (69), 43 (64)... 236 (27)]	14.61	1732	0.22			
Unknown [m/z 135, 150 (35), 218 (17), 203 (15), 91 (13), 136 (12)...	14.68	1738	0.60			
Unknown [m/z	14.92	1759	1.04	15.27*	2144	[1.46]

105, 145 (97), 202 (96), 131 (96), 43 (66), 187 (64)...220 (53)]						
Unknown [m/z 161, 43 (89), 105 (62), 119 (53), 81 (51), 189 (50), 204 (42)]	15.00	1766	0.34	15.33	2150	0.51
Dehydrofukinone	15.27	1789	0.85	17.23	2347	0.90
Unknown [m/z 159, 117 (66), 43 (48), 131 (42), 91 (41), 202 (38)...220 (2)]	15.60	1819	0.19	15.98	2216	0.19
Phytol	18.65	2110	0.07	19.32	2581	0.12
Total identified	87.82%			78.20%		
Total reported	94.17%			89.98%		

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified 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