

Date : 2024-08-29

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24H16-NSO01

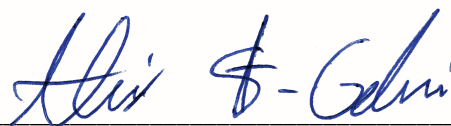
Customer Identification : Helichrysum - Lot: 36377-M1

Type : Essential Oil

Source : *Helichrysum italicum*

Customer : Natural Sourcing LLC

Checked and approved by:



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

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

✖ISO

Results : See analysis summary (next page)

Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005

Date : 2024-08-28

PHYSICOCHEMICAL DATA

Refractive index : 1.4785 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cassandra Baker

Date : 2024-08-19

CONCLUSION

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

ANALYSIS SUMMARY - CONSOLIDATED CONTENTS

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

Identification	%	Class
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
3-Pentanone	0.01	Aliphatic ketone
2-Ethylfuran	0.01	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
2-Methyl-3-pentanone	0.04	Aliphatic ketone
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Hexanal	tr	Aliphatic aldehyde
Octane	0.02	Alkane
2-Methyl-2-heptene	0.08	Alkene
4-Methyl-3-hexanone	0.10	Aliphatic ketone
Hexanol	0.01	Aliphatic alcohol
Isoamyl acetate	tr	Aliphatic ester
Bornylene	0.02	Monoterpene
Nonane	0.02	Alkane
Tricyclene	0.06	Monoterpene
α -Thujene	0.01	Monoterpene
α -Pinene	19.68	Monoterpene
α -Fenchene	0.31	Monoterpene
Camphene	1.10	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
β -Pinene	1.00	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	0.04	Monoterpene
2-Pentylfuran	0.02	Furan
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
2-Carene	0.02	Monoterpene
Unknown	0.03	Monoterpene
α -Phellandrene	0.01	Monoterpene
Isobutyl 2-methylbutyrate	0.03	Aliphatic ester
Isobutyl isovalerate	0.01	Aliphatic ester
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
α -Terpinene	0.08	Monoterpene
<i>para</i> -Methylanisole	0.01	Simple phenolic
<i>para</i> -Cymene	0.26	Monoterpene
1,8-Cineole	1.51	Monoterpenic ether
Limonene	3.98	Monoterpene

(Z)- β -Ocimene	0.02	Monoterpene
(E)- β -Ocimene	0.03	Monoterpene
Isobutyl angelate	0.20	Aliphatic ester
γ -Terpinene	0.28	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.54	Monoterpene
<i>para</i> -Cymenene	0.02	Monoterpene
2-Nonanone	0.05	Aliphatic ketone
2,4-Dimethylheptane-3,5-dione	0.03	β -Diketone
Linalool	1.87	Monoterpenic alcohol
Nonanal	0.04	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.07	Aliphatic ester
endo-Fenchol	0.07	Monoterpenic alcohol
α -Campholenal	0.01	Monoterpenic aldehyde
<i>trans</i> -Pinocarveol	0.05	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.04	Monoterpenic alcohol
<i>para</i> -Vinylanisole	0.05	Simple phenolic
Nerol oxide	0.03	Aliphatic ether
Isoamyl angelate	0.62	Aliphatic ester
2-Methylbutyl angelate	0.03	Aliphatic ester
Borneol	0.08	Monoterpenic alcohol
Unknown	0.01	Aliphatic ester
Nonanol	0.12	Aliphatic alcohol
Terpinen-4-ol	0.18	Monoterpenic alcohol
4,6-Dimethyloctane-3,5-dione epimer I	0.13	β -Diketone
4,6-Dimethyloctane-3,5-dione epimer II	0.15	β -Diketone
α -Terpineol	0.27	Monoterpenic alcohol
Myrtenol	0.03	Monoterpenic alcohol
2-Methylbutyl tiglate	0.03	Aliphatic ester
Unknown	0.02	Unknown
Decanal	0.03	Aliphatic aldehyde
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Nerol	0.34	Monoterpenic alcohol
Unknown	0.09	β -Diketone
Hexyl 2-methylbutyrate?	0.04	Aliphatic ester
3-Methylpentyl angelate	0.03	Aliphatic ester
Geraniol	2.13	Monoterpenic alcohol
Unknown	0.06	Aliphatic ester
Neryl methyl ether	0.09	Monoterpenic ether
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.01	Monoterpenic alcohol
Neryl formate	0.08	Monoterpenic ester
(3Z)-Hexenyl angelate	tr	Aliphatic ester
Hexyl angelate	0.25	Aliphatic ester

2-Undecanone	0.05	Aliphatic ketone
2-Acetyl- <i>para</i> -cresol?	0.08	Simple phenolic
Myrtenyl acetate	0.01	Monoterpenic ester
Unknown	0.01	Unknown
Hexyl tiglate	0.01	Aliphatic ester
α -Terpinyl acetate	0.02	Monoterpenic ester
Cyclosativene I	0.02	Sesquiterpene
Cyclosativene II	0.02	Sesquiterpene
Longicyclene	0.24	Sesquiterpene
Neryl acetate	9.42	Monoterpenic ester
α -Ylangene	0.05	Sesquiterpene
α -Copaene	1.34	Sesquiterpene
Italicene isomer	0.75	Sesquiterpene
Geranyl acetate	2.04	Monoterpenic ester
Hexyl hexanoate	0.05	Aliphatic ester
α -Funebrene	0.14	Sesquiterpene
Isoitalicene	0.14	Sesquiterpene
Italicene	2.79	Sesquiterpene
Isocaryophyllene	0.08	Sesquiterpene
Tetradecane	0.06	Alkane
α -Gurjunene	0.04	Sesquiterpene
α -Cedrene	0.03	Sesquiterpene
β -Caryophyllene	9.42	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.87	Sesquiterpene
β -Ylangene	0.03	Sesquiterpene
β -Copaene	0.07	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.79	Sesquiterpene
6,9-Guaiadiene	0.19	Sesquiterpene
Italidione I (4,6,9-Trimethyldec-8-ene-3,5-dione)	0.81	β -Diketone
Unknown	0.04	Sesquiterpene
Cadina-4,11-diene	0.07	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.23	Sesquiterpene
α -Humulene	0.30	Sesquiterpene
Neryl propionate	0.84	Monoterpenic ester
allo-Aromadendrene	0.09	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.44	Sesquiterpene
β -Acoradiene	0.35	Sesquiterpene
4,5-diepi-Aristolochene	[0.12]	Sesquiterpene
Unknown	[0.12]	Sesquiterpene
Selina-4,11-diene	1.26	Sesquiterpene
γ -Curcumene	7.57	Sesquiterpene
α -Curcumene	2.48	Sesquiterpene
Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione)	2.35	β -Diketone

Unknown	0.02	Sesquiterpene
β-Selinene	3.67	Sesquiterpene
<i>trans</i> -β-Bergamotene	0.24	Sesquiterpene
Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione)	0.88	β-Diketone
α-Selinene	2.39	Sesquiterpene
Valencene	0.68	Sesquiterpene
α-Muurolene	0.24	Sesquiterpene
Italidione II analog	0.41	β-Diketone
δ-Amorphene	0.33	Sesquiterpene
10-epi-Italicene ether	0.16	Sesquiterpenic ether
γ-Cadinene	[0.68]	Sesquiterpene
β-Curcumene	[0.68]	Sesquiterpene
β-Bisabolene	0.10	Sesquiterpene
7-epi-α-Selinene	0.03	Sesquiterpene
δ-Cadinene	[0.78]	Sesquiterpene
Sesquicineole	[0.78]	Sesquiterpenic ether
<i>trans</i> -Calamenene	0.05	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.14	Sesquiterpene
Italicene ether	0.09	Sesquiterpenic ether
(<i>E</i>)-γ-Bisabolene	0.06	Sesquiterpene
α-Cadinene	0.11	Sesquiterpene
Selina-3,7(11)-diene	0.03	Sesquiterpene
Phenylethyl angelate?	0.05	Phenolic ester
(<i>E</i>)-α-Bisabolene	0.10	Sesquiterpene
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether
Caryophyllenyl alcohol	0.03	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.12	Sesquiterpenic alcohol
Italidione III isomer I	0.56	β-Diketone
Caryophyllene oxide	[0.40]	Sesquiterpenic ether
Caryophyllene oxide isomer	[0.40]	Sesquiterpenic ether
Italidione III isomer II	0.44	β-Diketone
Italidione III isomer III	0.09	β-Diketone
Guaiol	0.13	Sesquiterpenic alcohol
Copaborneol	0.28	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.31	Sesquiterpenic alcohol
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.05	Unknown
Neryl angelate?	0.08	Monoterpenic ester
1-epi-Cubenol	0.02	Sesquiterpenic alcohol
γ-Eudesmol	0.25	Sesquiterpenic alcohol
Caryophylladienol I	0.04	Sesquiterpenic alcohol
Hinesol	0.01	Sesquiterpenic alcohol
τ-Cadinol	0.06	Sesquiterpenic alcohol

τ-Muurolol	0.04	Sesquiterpenic alcohol
β-Eudesmol	0.13	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.19	Sesquiterpenic alcohol
α-Eudesmol	0.09	Sesquiterpenic alcohol
Isoguaiol D	0.05	Sesquiterpenic alcohol
Unknown	0.02	Unknown
Bulnesol	0.03	Sesquiterpenic alcohol
β-Bisabolol	0.13	Sesquiterpenic alcohol
α-Bisabolol	0.05	Sesquiterpenic alcohol
epi-α-Bisabolol	0.04	Sesquiterpenic alcohol
Neryl 4-methylvalerate?	0.02	Monoterpenic ester
Unknown	0.03	Unknown
Geranyl 4-methylvalerate?	0.02	Monoterpenic ester
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Geranyl hexanoate	0.02	Monoterpenic ester
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
<i>trans</i> -Bisabola-1(6),10-diene-2,3-diol	0.33	Sesquiterpenic alcohol
Unknown	0.07	Unknown
Phytone	0.05	Terpenic ketone
Unknown	0.13	Unknown
Consolidated total	98.77	

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

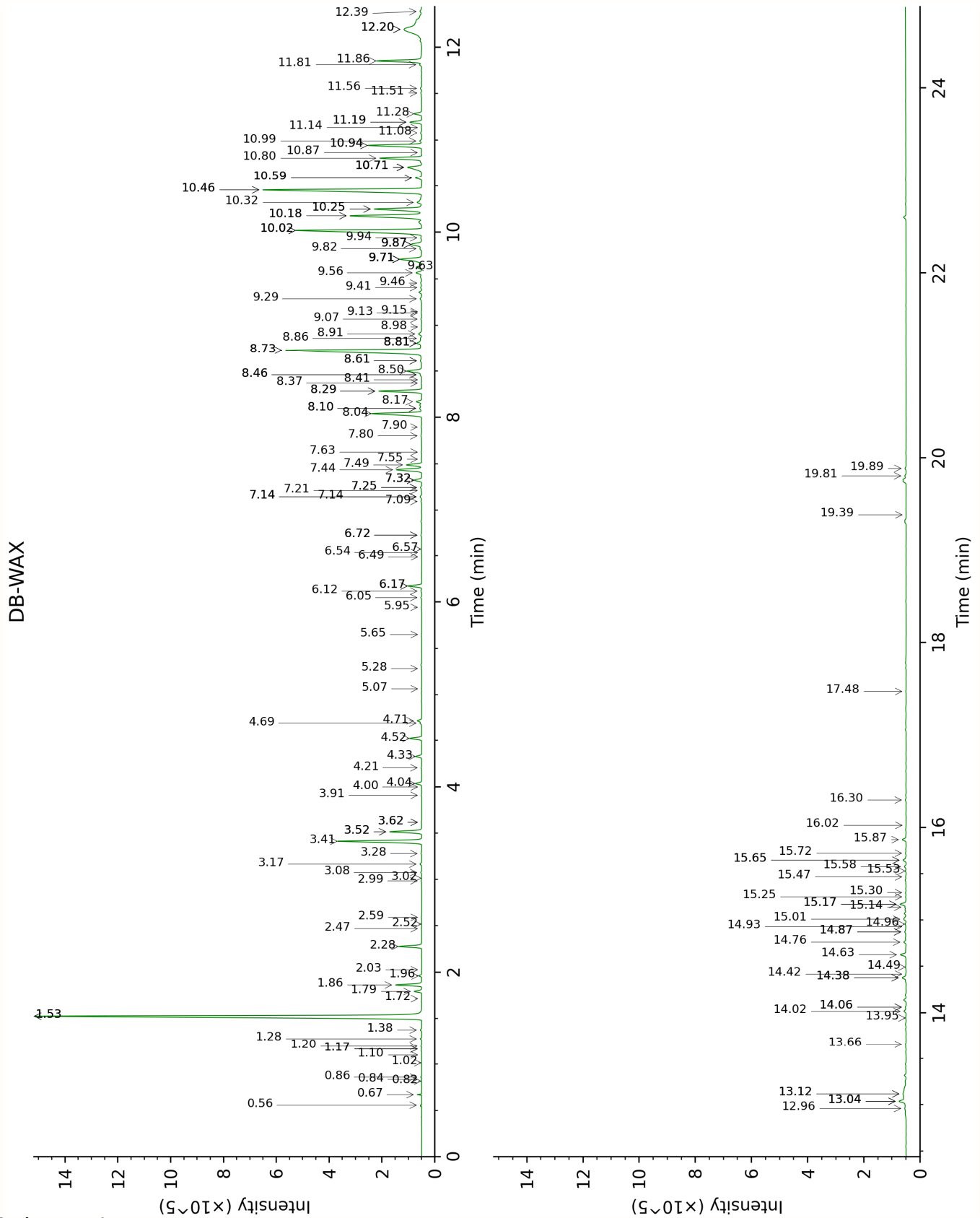
Note: no correction factor was applied

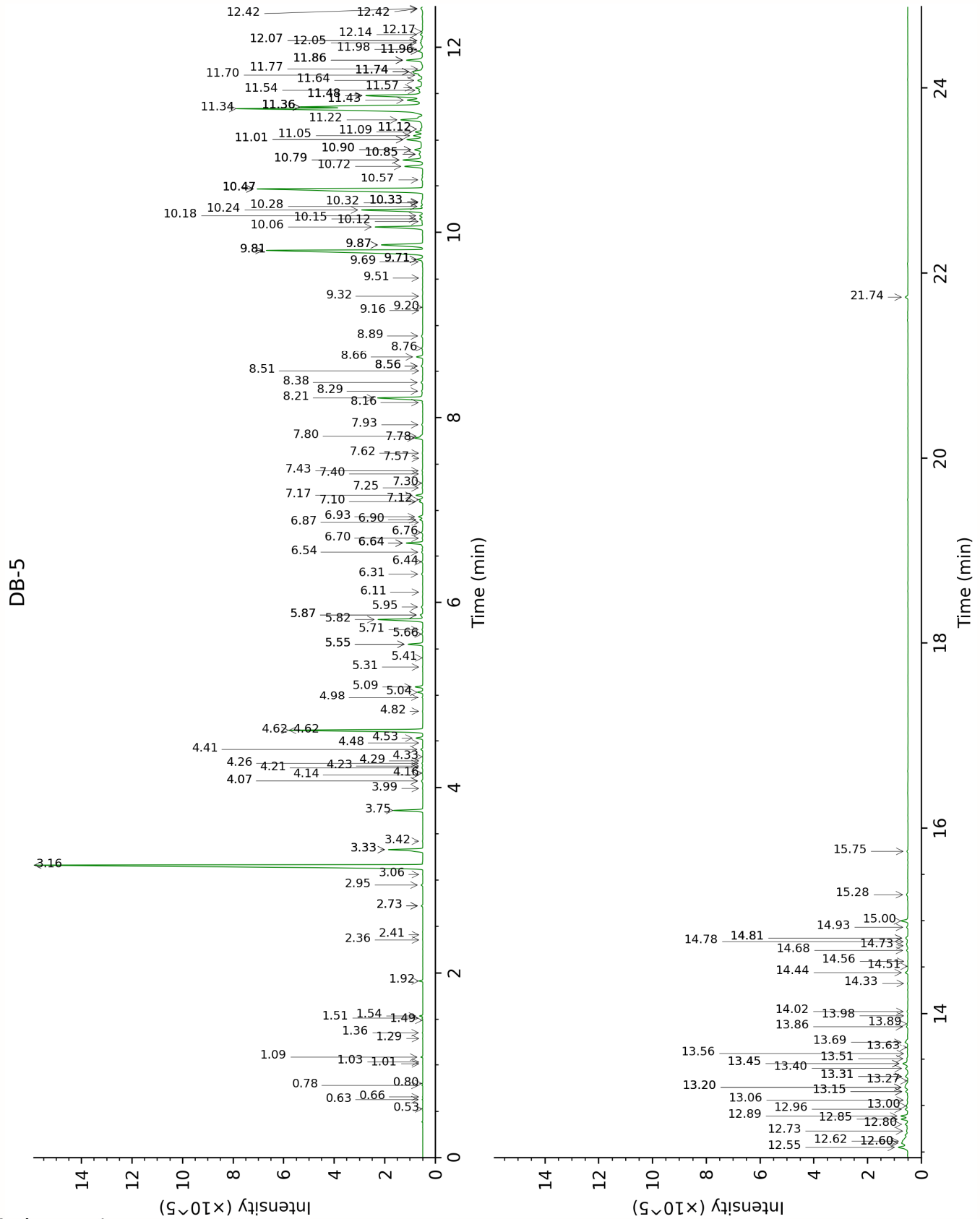
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

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FULL ANALYSIS DATA

2-Methyl-3-buten-2-ol	Column DB-WAX			Column DB-5		
	1.72	1013.4	tr	0.53	605.6	tr
Isovaleral	0.84	884.5	0.01	0.63	640.2	0.01
2-Methylbutyral	0.82	878.3	0.01	0.66	650.6	tr
3-Pentanone	1.17*	940.9	[0.01]	0.78	693.5	0.01
2-Ethylfuran	1.02	917.7	0.01	0.80	700.4	0.01
Isoamyl alcohol	3.62*	1174.8	[0.02]	1.01	732.4	tr
2-Methylbutanol	3.62*	1174.8	[0.02]	1.03	735.1	tr
2-Methyl-3-pentanone	1.28	958.2	0.04	1.09	742.5	0.04
Unknown HEIT III [m/z 73, 41 (54), 87 (50), 56 (47), 54 (29), 55 (25), 100 (23)... 115? (6)]	1.10	930.8	tr	1.30	771.7	0.01
Unknown HEIT II [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.17*	940.9	[0.01]	1.36	780.3	0.01
Hexanal	2.03	1043.1	0.01	1.49	799.2	tr
Octane	0.56	784.2	0.02	1.52	802.5	0.02
2-Methyl-2-heptene	0.67	828.6	0.08	1.54	805.0	0.08
4-Methyl-3-hexanone	1.96	1036.9	0.11	1.92	836.1	0.10
Hexanol	5.65	1321.4	0.01	2.36	872.8	0.01
Isoamyl acetate	2.52	1090.0	0.01	2.41	877.3	tr
Bornylene	1.20	945.4	0.02	2.72*	903.2	[0.05]
Nonane	0.86	893.0	0.02	2.72*	903.2	[0.05]
Tricyclene	1.38	972.8	0.06	2.95	918.0	0.06
α-Thujene	1.53*	995.4	[19.71]	3.06	925.6	0.01
α-Pinene	1.53*	995.4	[19.71]	3.16	932.2	19.68
α-Fenchene	1.79	1020.8	0.31	3.33*	943.2	[1.41]
Camphene	1.86	1027.5	1.10	3.33*	943.2	[1.41]
Thuja-2,4(10)-diene	2.47	1085.3	0.02	3.42	949.2	0.02
β-Pinene	2.28	1067.0	1.00	3.75	971.1	1.00
6-Methyl-5-hepten-2-one	5.28	1295.2	0.02	3.99	986.7	0.02
Myrcene	3.08	1133.5	0.04	4.07*	992.1	[0.06]
2-Pentylfuran	3.91	1196.9	0.02	4.07*	992.1	[0.06]
6-Methyl-5-hepten-2-ol	7.14*	1428.9	[0.10]	4.14	996.3	0.01
2-Carene	2.59	1096.6	0.02	4.16	997.7	0.02

Unknown HEIT I [m/z = 123, 43 (16), 152 (14), 124 (9), 137 (6)]	2.99	1126.6	0.03	4.21	1001.4	0.03
α -Phellandrene	3.02	1128.8	0.01	4.23	1002.7	0.01
Isobutyl 2- methylbutyrate	3.28	1149.1	0.04	4.26	1004.5	0.03
Isobutyl isovalerate	3.52*	1167.0	[1.53]	4.29	1006.2	0.01
(3Z)-Hexenyl acetate	5.07	1279.5	0.01	4.33	1008.9	0.01
α -Terpinene	3.17	1140.4	0.08	4.41	1013.9	0.08
<i>para</i> - Methylanisole	6.54	1384.3	0.01	4.48	1018.3	0.01
<i>para</i> -Cymene	4.33	1226.8	0.26	4.53	1021.6	0.26
1,8-Cineole	3.52*	1167.0	[1.53]	4.62*	1026.8	[5.50]
Limonene	3.41	1159.2	3.98	4.62*	1026.8	[5.50]
(Z)- β -Ocimene	4.00	1203.3	0.01	4.82	1039.6	0.02
(E)- β -Ocimene	4.21	1218.1	0.03	4.98	1049.2	0.03
Isobutyl angelate	4.71	1254.3	0.20	5.04	1052.9	0.20
γ -Terpinene	4.04	1206.0	0.28	5.09	1056.5	0.28
<i>cis</i> -Linalool oxide (fur.)	6.72*	1397.9	[0.05]	5.31	1069.9	0.01
Octanol	8.41	1523.2	0.02	5.41	1076.1	0.01
Terpinolene	4.52	1240.8	0.54	5.55*	1085.3	[0.55]
<i>para</i> -Cymenene	6.57	1387.0	0.02	5.55*	1085.3	[0.55]
2-Nonanone	6.05	1349.8	0.04	5.66	1092.1	0.05
2,4- Dimethylheptane- 3,5-dione	7.80	1477.3	0.08	5.71	1095.1	0.03
Linalool	8.28*	1513.8	[1.90]	5.82	1102.0	1.87
Nonanal	6.12	1354.7	0.04	5.87*	1105.1	[0.13]
2-Methylbutyl 2- methylbutyrate	4.69	1252.6	0.07	5.87*	1105.1	[0.13]
endo-Fenchol	8.61*	1538.9	[0.11]	5.95	1110.6	0.07
α -Campholenal	7.24*	1436.3	[0.07]	6.11	1120.7	0.01
<i>trans</i> -Pinocarveol	9.41	1600.4	0.06	6.31	1133.2	0.05
<i>trans</i> -Verbenol	9.82	1634.1	0.10	6.44	1141.7	0.04
<i>para</i> -Vinylanisole	9.63	1618.0	0.29	6.54	1148.2	0.05
Nerol oxide	7.09	1425.2	0.03	6.64*	1154.5	[0.66]
Isoamyl angelate	6.18*	1358.7	[0.63]	6.64*	1154.5	[0.66]
2-Methylbutyl angelate	6.18*	1358.7	[0.63]	6.70	1157.8	0.03
Borneol	10.02*	1649.8	[7.92]	6.76	1161.8	0.08
Unknown HEIT IV	5.94	1342.3	0.02	6.87	1169.2	0.01

[m/z 83, 100 (34), 55 (33), 43 (21), 84 (21)...]						
Nonanol	9.71*	1624.9	[1.41]	6.90	1171.0	0.12
Terpinen-4-ol	8.81*	1554.0	[0.36]	6.93	1173.1	0.18
4,6-Dimethyloctane-3,5-dione epimer I	8.81*	1554.0	[0.36]	7.10	1183.4	0.13
4,6-Dimethyloctane-3,5-dione epimer II	8.81*	1554.0	[0.36]	7.12	1184.8	0.15
α-Terpineol	10.02*	1649.8	[7.92]	7.17	1187.8	0.27
Myrtenol	11.14	1741.8	0.02	7.25	1192.9	0.03
2-Methylbutyl tiglate	7.14*	1428.9	[0.10]	7.30	1196.2	0.03
Unknown PIMA 7 [m/z 95, 93 (32), 121 (24), 79 (22), 91 (21), 105 (16)... 154 (2)]	11.19*	1746.7	[0.55]	7.40	1202.5	0.02
Decanal	7.55	1458.8	0.02	7.43	1204.8	0.03
Unknown HEIT XXII [m/z 81, 57 (91), 168 (73), 67 (52), 140 (45), 41 (36), 113 (27)...]				7.56	1213.8	0.01
Unknown HEIT XXI [m/z 81, 109 (85), 168 (72), 57 (69), 67 (58), 41 (49), 140 (45)...]				7.62	1217.5	0.02
Nerol	11.28	1754.3	0.38	7.78	1228.3	0.34
Unknown HEIT V [m/z 113, 57 (55), 85 (16), 170 (16)]				7.80	1229.6	0.09
Hexyl 2-methylbutyrate?	6.49	1381.1	tr	7.93	1237.9	0.04
3-Methylpentyl angelate	7.63	1464.4	0.03	8.16	1253.8	0.03
Geraniol	11.86	1802.9	2.17	8.22	1257.2	2.13
Unknown HEIT VII [m/z 83, 55 (30), 57 (23), 100 (20), 98 (14)...]	7.24*	1436.3	[0.07]	8.29	1262.1	0.06

Neryl methyl ether	7.32*	1442.1	[0.38]	8.38	1268.3	0.09
2,6-Dimethyl-1,7-octadiene-3,6-diol	14.93	2085.4	0.01	8.51	1276.7	0.01
Neryl formate	9.71*	1624.9	[1.41]	8.56*	1280.1	[0.08]
(3Z)-Hexenyl angelate	8.46*	1527.3	[0.08]	8.56*	1280.1	[0.08]
Hexyl angelate	8.17*†	1505.0	[0.26]	8.66	1286.7	0.25
2-Undecanone	8.86	1558.0	0.06	8.76	1293.4	0.05
2-Acetyl- <i>para</i> -cresol?				8.89	1302.3	0.08
Myrtenyl acetate	9.87*	1637.8	[0.70]	9.16	1321.4	0.01
Unknown HEIT XXXIV [m/z 141, 43 (58), 81 (49), 67 (27), 41 (19)...]				9.20	1324.0	0.01
Hexyl tiglate	9.15	1580.2	0.02	9.32	1332.3	0.01
α -Terpinyl acetate	9.94	1643.5	0.06	9.51	1346.0	0.02
Cyclosativene I	7.14*	1428.9	[0.10]	9.69	1358.3	0.02
Cyclosativene II	7.21	1433.9	0.02	9.71*	1360.1	[0.26]
Longicyclene	7.32*	1442.1	[0.38]	9.71*	1360.1	[0.26]
Neryl acetate	10.46*	1684.9	[9.52]	9.81*	1366.9	[9.47]
α -Ylangene	7.32*	1442.1	[0.38]	9.81*	1366.9	[9.47]
α -Copaene	7.44	1450.4	1.34	9.87*	1371.1	[2.11]
Italicene isomer	7.49	1454.3	0.75	9.87*	1371.1	[2.11]
Geranyl acetate	10.80	1713.9	2.03	10.06	1384.6	2.04
Hexyl hexanoate	9.13	1579.1	0.03	10.12	1388.7	0.05
α -Funebrene	8.10*†	1499.5	[0.13]	10.15	1390.7	0.14
Isoitalicene	8.10*†	1499.5	[0.13]	10.18	1393.1	0.14
Italicene	8.04	1495.1	2.75	10.24	1397.5	2.79
Isocaryophyllene	8.46*	1527.3	[0.08]	10.28	1400.2	0.08
Tetradecane	6.72*	1397.9	[0.05]	10.32	1402.9	0.06
α -Gurjunene	7.90	1484.3	0.04	10.33*	1403.7	[0.06]
α -Cedrene	8.28*	1513.8	[1.90]	10.33*	1403.7	[0.06]
β -Caryophyllene	8.73*	1548.0	[10.21]	10.47*	1414.0	[10.09]
<i>cis</i> - α -Bergamotene	8.50	1530.4	0.87	10.47*	1414.0	[10.09]
β -Ylangene	8.37	1520.4	0.03	10.47*	1414.0	[10.09]
β -Copaene	8.61*	1538.9	[0.11]	10.57	1421.2	0.07
<i>trans</i> - α -Bergamotene	8.73*	1548.0	[10.21]	10.72	1432.6	0.79
6,9-Guaiadiene	8.91	1561.7	0.19	10.79*	1437.7	[1.00]
Italidione I (4,6,9-Trimethyldec-8-ene-3,5-dione)	12.20*	1832.8	[4.04]	10.79*	1437.7	[1.00]

Unknown BOCA IV [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	9.07	1574.0	0.04	10.85*	1442.3	[0.32]
Cadina-4,11-diene	9.46	1604.3	0.07	10.85*	1442.3	[0.32]
<i>cis</i> - β -Bergamotene?				10.90*	1445.9	[0.53]
α -Humulene	9.56	1613.2	0.30	10.90*	1445.9	[0.53]
Neryl propionate	11.19*	1746.7	[0.55]	11.01*	1454.1	[0.94]
allo-Aromadendrene	9.29	1590.8	0.09	11.01*	1454.1	[0.94]
(<i>E</i>)- β -Farnesene	9.87*	1637.8	[0.70]	11.05	1457.2	0.44
β -Acoradiene	9.71*	1624.9	[1.41]	11.09	1460.1	0.35
4,5-diepi-Aristolochene	9.71*	1624.9	[1.41]	11.12*	1462.5	[0.12]
Unknown CEDE VI [m/z 119, 91 (85), 93 (77), 105 (76), 79 (61), 134 (60), 94 (49), 204 (46)]	9.71*	1624.9	[1.41]	11.12*	1462.5	[0.12]
Selina-4,11-diene	9.71*	1624.9	[1.41]	11.22	1469.8	1.26
γ -Curcumene	10.02*	1649.8	[7.92]	11.34*†	1478.8	[9.82]
α -Curcumene	10.94*	1725.6	[2.63]	11.36*†	1480.2	[5.92]
Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione)	12.20*	1832.8	[4.04]	11.36*†	1480.2	[5.92]
Unknown CILI III [m/z 41, 69 (90), 79 (78), 93 (72), 91 (70)...204]	8.98	1567.5	0.02	11.36*†	1480.2	[5.92]
β -Selinene	10.18*	1662.5	[4.35]	11.36*†	1480.2	[5.92]
<i>trans</i> - β -Bergamotene	9.87*	1637.8	[0.70]	11.36*†	1480.2	[5.92]
Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione)	12.20*	1832.8	[4.04]	11.43	1485.6	0.88
α -Selinene	10.25*	1668.3	[2.72]	11.48*	1489.3	[3.07]
Valencene	10.18*	1662.5	[4.35]	11.48*	1489.3	[3.07]
α -Muurolene	10.32	1674.0	0.24	11.54*†	1493.5	[0.23]
Italidione II analog	13.04*†	1907.7	[0.56]	11.57*†	1495.5	[0.42]
δ -Amorphene	10.25*	1668.3	[2.72]	11.64	1501.4	0.33

10-epi-Italicene ether	11.56	1777.4	0.07	11.70	1505.9	0.16
γ-Cadinene	10.71*	1705.7	[1.05]	11.74*	1508.8	[0.77]
β-Curcumene	10.59*	1695.6	[0.32]	11.74*	1508.8	[0.77]
β-Bisabolene	10.46*	1684.9	[9.52]	11.74*	1508.8	[0.77]
7-epi-α-Selinene	10.71*	1705.7	[1.05]	11.77	1510.9	0.03
δ-Cadinene	10.71*	1705.7	[1.05]	11.86*	1518.5	[0.83]
Sesquicineole	10.59*	1695.6	[0.32]	11.86*	1518.5	[0.83]
trans-Calamenene	11.51	1773.1	0.05	11.86*	1518.5	[0.83]
trans-Cadina-1,4-diene	10.94*	1725.6	[2.63]	11.96*	1526.2	[0.23]
Italicene ether	11.81	1799.3	0.09	11.96*	1526.2	[0.23]
(E)-γ-Bisabolene	10.71*	1705.7	[1.05]	11.98	1527.7	0.06
α-Cadinene	11.08	1736.9	0.06	12.05	1533.2	0.11
Selina-3,7(11)-diene	10.87	1719.1	0.03	12.07*	1535.0	[0.11]
Phenylethyl angelate?	14.49	2043.7	0.05	12.07*	1535.0	[0.11]
(E)-α-Bisabolene	10.99	1729.6	0.09	12.14	1540.1	0.10
Isocaryophyllene epoxide B	12.39	1850.0	0.12	12.17	1542.7	0.04
Caryophyllenyl alcohol	13.94	1991.2	0.03	12.42*	1562.2	[0.11]
(E)-Nerolidol	14.02	1998.0	0.12	12.42*	1562.2	[0.11]
Italidione III isomer I	13.12*†	1915.1	[0.62]	12.55	1572.3	0.56
Caryophyllene oxide	13.04*†	1907.7	[0.56]	12.60*	1575.9	[0.40]
Caryophyllene oxide isomer	12.96*†	1900.6	[0.13]	12.60*	1575.9	[0.40]
Italidione III isomer II	13.12*†	1915.1	[0.62]	12.62	1577.5	0.44
Italidione III isomer III	13.04*†	1907.7	[0.56]	12.73	1586.1	0.09
Guaiol	14.38*	2032.6	[0.21]	12.80	1591.8	0.13
Copaborneol	15.17*	2109.4	[0.33]	12.85	1596.1	0.28
Eudesm-5-en-11-ol	14.63	2056.5	0.31	12.89	1598.8	0.31
Unknown MIAL II [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	14.76	2069.5	0.12	12.96	1604.7	0.12
Unknown MECA V [m/z 179, 161 (66)]	14.87*	2080.0	[0.11]	13.00	1607.7	0.10

119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]						
Unknown HEIT VIII [m/z 182, 109 (58), 69 (50), 41 (42), 43 (40), 139 (31)... 235 (17), 250 (1)...]	14.38*	2032.6	[0.21]	13.06	1612.8	0.05
Neryl angelate?				13.15*	1620.4	[0.10]
1-epi-Cubenol	14.06*	2002.3	[0.04]	13.15*	1620.4	[0.10]
γ-Eudesmol	15.17*	2109.4	[0.33]	13.20*	1624.1	[0.29]
Caryophylladienol I	16.30	2222.7	0.04	13.20*	1624.1	[0.29]
Hinesol	15.25	2117.4	0.03	13.27	1630.0	0.01
τ-Cadinol	15.14	2106.3	0.06	13.32*	1633.8	[0.13]
τ-Muurolol	15.30	2122.0	0.04	13.32*	1633.8	[0.13]
β-Eudesmol	15.65*	2156.7	[0.18]	13.40	1641.0	0.13
Selin-11-en-4α-ol	15.87	2178.7	0.19	13.45*	1645.3	[0.30]
α-Eudesmol	15.58	2149.7	0.09	13.45*	1645.3	[0.30]
Isoguaiol D	15.47	2138.8	0.04	13.51	1649.7	0.05
Unknown HEIT XXXV [m/z 151, 180 (68), 179 (17), 152 (10), 95 (9)...]				13.56	1654.2	0.02
Bulnesol	15.53	2145.1	0.04	13.63	1659.7	0.03
β-Bisabolol	15.01	2093.5	0.17	13.69	1664.9	0.13
α-Bisabolol	15.65*	2156.7	[0.18]	13.86*†	1678.7	[0.05]
epi-α-Bisabolol	15.72	2164.2	0.04	13.89*†	1681.3	[0.04]
Neryl 4- methylvalerate?	13.66	1964.6	0.04	13.98	1688.4	0.02
Unknown HEIT IX [m/z 196, 69 (62), 109 (58), 41 (54), 139 (41)... 249 (21)...]	14.87*	2080.0	[0.11]	14.02	1692.2	0.03
Geranyl 4- methylvalerate?	14.06*	2002.3	[0.04]	14.33	1718.0	0.02
Unknown HEIT X [m/z 43, 69 (32), 198 (29), 41 (27), 93 (26)... 202 (20)...]				14.44	1728.1	0.12
Unknown HEIT XI [m/z 82, 125 (40),	16.02	2194.5	0.01	14.51	1734.0	0.01

41 (35), 69 (31), 67 (27)... 236? (t)]						
Geranyl hexanoate	14.42	2036.4	0.02	14.56	1738.7	0.02
Unknown HEIT XII [m/z 109, 127 (46), 138 (45), 81 (27), 123 (25)... 220? (2)]				14.68	1748.8	0.06
Unknown HEIT XIII [m/z 136, 121 (74), 135 (55), 218 (36), 148 (33), 40 (42)... 236? (1)]				14.73	1753.2	0.03
Unknown HEIT XIV [m/z 109, 138 (71), 82 (42), 123 (41), 127 (38)...]	19.39	2561.2	0.01	14.78	1757.0	0.03
Unknown HEIT XVI [m/z 109, 127 (46), 138 (45), 82 (34), 81 (31)... 236? (t)]	19.81	2610.6	0.07	14.82*	1760.3	[0.13]
Unknown HEIT XV [m/z 96, 41 (29), 178 (28), 43 (27)... 236 (2)]	17.48	2346.9	0.03	14.82*	1760.3	[0.13]
Unknown HEIT XVII [m/z 109, 138 (75), 123 (45), 127 (42), 81 (30)...]	19.89	2620.1	0.06	14.93	1770.4	0.06
<i>trans</i> -Bisabola-1(6),10-diene-2,3-diol				15.00	1776.4	0.33
Unknown HEIT XIX [m/z 43, 82 (69), 41 (66), 93 (62), 96 (55), 55 (49), 67 (45), 154 (44)...]				15.28	1800.8	0.07
Phytone	14.96	2088.2	0.05	15.75	1843.2	0.05
Unknown HEIT XXIX [m/z 81, 69 (80), 137 (48), 95 (35), 41 (35), 98				21.74	2459.8	0.13

(33)...					
Total reported	96.17%			98.25%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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