

Date : September 04, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20H26-PTH08


Customer identification : Helichrysum Italicum ORG - H9010899R

Type : Essential oil

Source : *Helichrysum italicum*

Customer : Plant Therapy

ANALYSIS

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

Analyst : Sylvain Mercier, M. Sc., Chimiste

Analysis date : August 31, 2020

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4766 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No 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-pentanone	tr	Aliphatic ketone
Octane	tr	Alkane
2-Methyl-2-heptene	0.01	Alkene
4-Methyl-3-hexanone	0.02	Aliphatic ketone
Nonane	0.01	Alkane
Bornylene	0.01	Monoterpene
Tricyclene	tr	Monoterpene
α -Thujene	tr	Monoterpene
α -Pinene	6.26	Monoterpene
α -Fenchene	0.09	Monoterpene
Camphene	0.05	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
β -Pinene	0.15	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.02	Monoterpene
<i>trans</i> -Dehydroxylinalool oxide	tr	Monoterpenic ether
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
Pseudolimonene	tr	Monoterpene
2-Carene	tr	Monoterpene
α -Phellandrene	0.01	Monoterpene
Isobutyl 2-methylbutyrate	0.02	Aliphatic ester
(3Z)-Hexenyl acetate	tr	Aliphatic ester
α -Terpinene	0.08	Monoterpene
para-Methylanisole	tr	Simple phenolic
para-Cymene	0.12	Monoterpene
Limonene	1.26	Monoterpene
β -Phellandrene	0.01	Monoterpene
1,8-Cineole	0.19	Monoterpenic ether
(Z)- β -Ocimene	0.01	Monoterpene
(E)- β -Ocimene	0.02	Monoterpene
Isobutyl angelate	0.16	Aliphatic ester
γ -Terpinene	0.25	Monoterpene
Octanol	tr	Aliphatic alcohol
Terpinolene	0.11	Monoterpene
2-Nonanone	0.03	Aliphatic ketone
2,4-Dimethylheptane-3,5-dione	0.04	β -Diketone
Linalool	0.51	Monoterpenic alcohol
Nonanal	0.05	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.06	Aliphatic ester
endo-Fenchol	0.06	Monoterpenic alcohol
α -Campholenal	0.01	Monoterpenic aldehyde
<i>trans</i> -Pinocarveol	0.06	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.03	Monoterpenic alcohol
para-Vinylnisole	0.02	Simple phenolic

Nerol oxide	0.03	Aliphatic ether
Isoamyl angelate	0.64*	Aliphatic ester
2-Methylbutyl angelate	[0.64]*	Aliphatic ester
Borneol	0.07	Monoterpenic alcohol
Unknown	0.02	Aliphatic ester
Terpinen-4-ol	0.21	Monoterpenic alcohol
4,6-Dimethyloctane-3,5-dione epimer I	0.14	β -Diketone
4,6-Dimethyloctane-3,5-dione epimer II	0.18	β -Diketone
α -Terpineol	0.25	Monoterpenic alcohol
Myrtenol	0.01	Monoterpenic alcohol
2-Methylbutyl tiglate	0.02	Aliphatic ester
Verbenone	0.02	Monoterpenic ketone
Unknown	0.03	Unknown
Decanal	0.04	Aliphatic aldehyde
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.30	β -Diketone
Nerol	0.19	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.03	Aliphatic ester
Isoamyl hexanoate	0.03	Aliphatic ester
3-Methylpentyl angelate	0.02	Aliphatic ester
Unknown	0.05	Aliphatic ester
Unknown	0.04	Aliphatic ester
(3Z)-Hexenyl angelate	0.03	Aliphatic ester
Hexyl angelate	0.30	Aliphatic ester
2-Undecanone	0.04	Aliphatic ketone
2-Acetyl-para-cresol?	0.03	Simple phenolic
Myrtenyl acetate	0.02	Monoterpenic ester
Hexyl tiglate	0.05	Aliphatic ester
Bicycloelemene	0.01	Sesquiterpene
α -Terpinyl acetate	0.25	Monoterpenic ester
Cyclosativene I	0.12	Sesquiterpene
Cyclosativene II	0.28	Sesquiterpene
α -Ylangene	0.01	Sesquiterpene
Neryl acetate	30.75	Monoterpenic ester
Italicene isomer	0.83	Sesquiterpene
α -Copaene	1.44	Sesquiterpene
Geranyl acetate	0.42	Monoterpenic ester
Hexyl hexanoate	0.01	Aliphatic ester
α -Funebrene	0.16	Sesquiterpene
Isoitalicene	0.16	Sesquiterpene
Italicene	3.07	Sesquiterpene
Isocaryophyllene	0.07	Sesquiterpene
α -Gurjunene	0.02	Sesquiterpene
Tetradecane	0.03	Alkane
α -Cedrene	0.04	Sesquiterpene
β -Caryophyllene	4.22	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.91	Sesquiterpene
β -Copaene	0.06	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.90	Sesquiterpene
Italidione I (4,6,9-Trimethyldec-8-ene-3,5-dione)	2.42	β -Diketone
6,9-Guaiadiene	0.02	Sesquiterpene

Unknown	0.12	Sesquiterpene
α -Humulene	0.31	Sesquiterpene
Cadina-4,11-diene	0.01	Sesquiterpene
Neryl propionate	tr	Monoterpenic ester
allo-Aromadendrene	0.12	Sesquiterpene
(<i>E</i>)- β -Farnesene	1.21	Sesquiterpene
α -Acoradiene	0.36	Sesquiterpene
4,5-diepi-Aristolochene	0.11	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.12	Sesquiterpene
Unknown	1.65*	Sesquiterpene
Selina-4,11-diene	[1.65]*	Sesquiterpene
γ -Curcumene	10.47	Sesquiterpene
β -Selinene	5.37	Sesquiterpene
Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione)	2.39	β -Diketone
ar-Curcumene	2.66	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.90	Sesquiterpene
Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione)	1.19	β -Diketone
α -Selinene	3.69	Sesquiterpene
Eudesma-2,4(15),11-triene	0.20	Sesquiterpene
Italidione II analog	0.33	β -Diketone
δ -Amorphene	0.33	Sesquiterpene
10-epi-Italicene ether	0.06	Sesquiterpenic ether
γ -Cadinene	0.23	Sesquiterpene
β -Bisabolene	1.18*	Sesquiterpene
β -Curcumene	[1.18]*	Sesquiterpene
7-epi- α -Selinene	0.30	Sesquiterpene
Sesquicineole	0.39	Sesquiterpenic ether
δ -Cadinene	0.53	Sesquiterpene
<i>trans</i> -Calamenene	0.04	Sesquiterpene
Italicene ether	0.12	Sesquiterpenic ether
(<i>E</i>)- γ -Bisabolene	0.10	Sesquiterpene
α -Cadinene	0.06	Sesquiterpene
Selina-3,7(11)-diene	0.13	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.14	Sesquiterpene
Caryophyllenyl alcohol	0.02	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.16	Sesquiterpenic alcohol
Italidione III isomer I	0.59	β -Diketone
Italidione III isomer II	0.58*	β -Diketone
Caryophyllene oxide	[0.58]*	Sesquiterpenic ether
Italidione III isomer III	0.25	β -Diketone
Guaiol	0.15	Sesquiterpenic alcohol
Copaborneol	0.25	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.28	Sesquiterpenic alcohol
Unknown	0.14	Oxygenated sesquiterpene
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.17	Unknown
Neryl angelate?	0.09	Monoterpenic ester
Caryophylladienol I	0.04	Sesquiterpenic alcohol
γ -Eudesmol	0.03	Sesquiterpenic alcohol
1-epi-Cubenol	0.02	Sesquiterpenic alcohol

Eudesmol analog?	0.16	Sesquiterpenic alcohol
τ-Muurolol	0.02	Sesquiterpenic alcohol
τ-Cadinol	0.02	Sesquiterpenic alcohol
Cubenol	0.02	Sesquiterpenic alcohol
β-Eudesmol	0.10	Sesquiterpenic alcohol
α-Eudesmol	0.06	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.18	Sesquiterpenic alcohol
Bulnesol	0.04	Sesquiterpenic alcohol
β-Bisabolol	0.16	Sesquiterpenic alcohol
epi-α-Bisabolol	0.05	Sesquiterpenic alcohol
α-Bisabolol	0.03	Sesquiterpenic alcohol
Neryl 4-methylvalerate?	0.05	Monoterpenic ester
Unknown	0.05	Unknown
Geranyl 4-methylvalerate?	0.03	Monoterpenic ester
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.11	Unknown
Consolidated total	98.20%	

*: 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

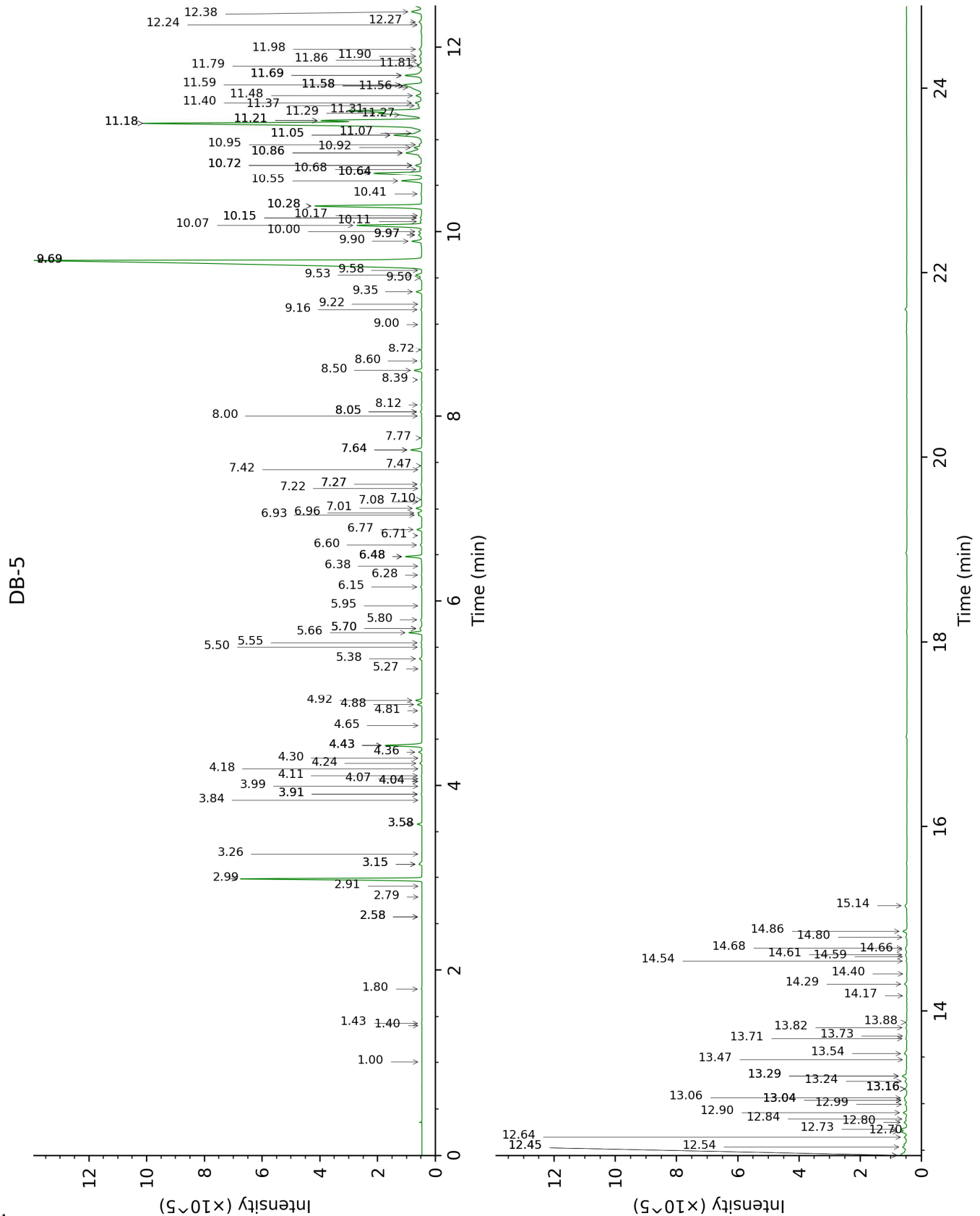
tr: The compound has been detected below 0.005% of total signal.

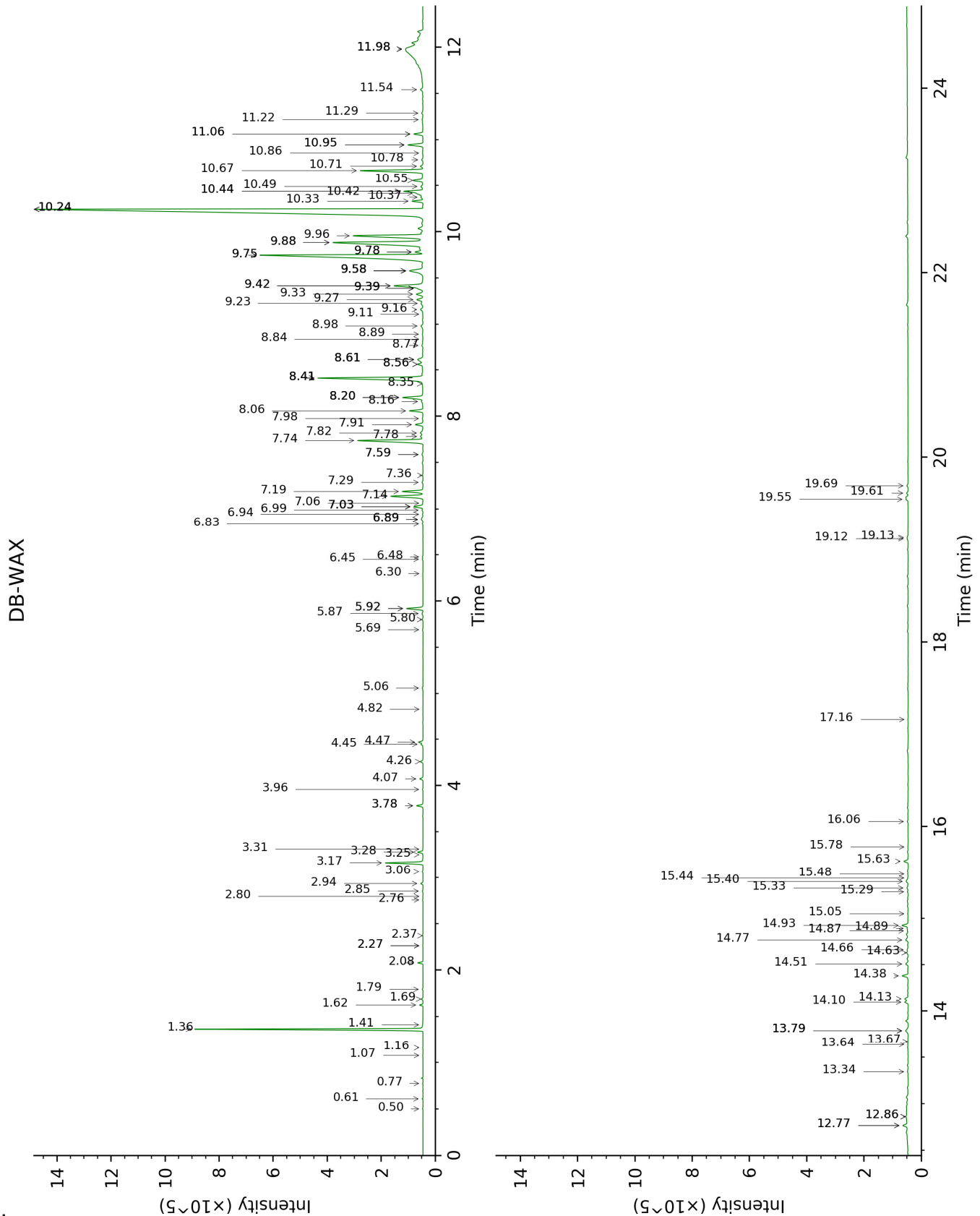
Note: no correction factor was applied

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.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2-Methyl-3-pentanone	1.00	742	tr	1.16	959	tr
Octane	1.40	802	tr	0.50	784	tr
2-Methyl-2-heptene	1.43	804	0.01	0.61	831	0.01
4-Methyl-3-hexanone	1.80	836	0.02	1.79	1037	0.02
Nonane	2.58*	902	0.01	0.77	892	0.01
Bornylene	2.58*	902	[0.01]	1.08	945	0.01
Tricyclene	2.79	917	tr			
α-Thujene	2.91	924	tr	1.41	999	0.01
α-Pinene	2.99	930	6.26	1.36	993	6.13
α-Fenchene	3.15*†	941	0.15	1.62	1020	0.09
Camphene	3.15*†	941	[0.15]	1.69	1027	0.05
Thuja-2,4(10)-diene	3.26	948	0.01	2.26*	1084	0.01
β-Pinene	3.58*	970	0.16	2.08	1066	0.15
Sabinene	3.58*	970	[0.16]	2.26*	1084	[0.01]
6-Methyl-5-hepten-2-one	3.84	987	0.01	5.06	1294	0.04
Myrcene	3.91*	991	0.03	2.85	1133	0.02
<i>trans</i> -Dehydroxylinalool oxide	3.91*	991	[0.03]	3.31	1169	tr
6-Methyl-5-hepten-2-ol	3.99	997	0.01	6.94	1432	0.02
Pseudolimonene	4.04*†	1000	0.01	2.80	1128	tr
2-Carene	4.04*†	1000	[0.01]	2.37	1095	tr
α-Phellandrene	4.07†	1002	[0.01]	2.76	1125	0.01
Isobutyl 2-methylbutyrate	4.11	1004	0.02	3.06	1149	0.02
(3Z)-Hexenyl acetate	4.18	1009	tr	4.82	1280	0.01
α-Terpinene	4.24	1013	0.08	2.94	1139	0.07
para-Methylanisole	4.30	1016	tr	6.30	1384	0.01
para-Cymene	4.36	1020	0.12	4.07	1226	0.13
Limonene	4.43*	1025	1.49	3.17	1157	1.26
β-Phellandrene	4.43*	1025	[1.49]	3.25	1164	0.01
1,8-Cineole	4.43*	1025	[1.49]	3.28	1166	0.19
(Z)-β-Ocimene	4.65	1038	0.01	3.78*	1205	0.25
(E)-β-Ocimene	4.81	1048	0.02	3.96	1217	0.02
Isobutyl angelate	4.88†	1052	0.40	4.47†	1254	[0.24]
γ-Terpinene	4.92†	1055	[0.40]	3.78*	1205	[0.25]
Octanol	5.27	1077	tr	8.20*	1527	0.95
Terpinolene	5.38	1084	0.11	4.26	1239	0.10
2-Nonanone	5.50	1092	0.03	5.80	1348	0.03
2,4-	5.55	1095	0.04	7.59*	1480	0.05

Dimethylheptane-3,5-dione						
Linalool	5.66	1102	0.51	8.06	1516	0.52
Nonanal	5.70*	1104	0.11	5.86	1353	0.05
2-Methylbutyl 2-methylbutyrate	5.70*	1104	[0.11]	4.45†	1253	0.24
endo-Fenchol	5.80	1110	0.06	8.41*	1544	5.18
α-Campholenal	5.95	1120	0.01	7.03*	1438	0.40
trans-Pinocarveol	6.15	1133	0.06	9.16	1602	0.14
trans-Verbenol	6.28	1141	0.03	9.58*	1636	0.97
para-Vinylanisole	6.38	1147	0.02	9.39*†	1620	1.75
Nerol oxide	6.48*	1154	0.67	6.83	1424	0.03
Isoamyl angelate	6.48*	1154	[0.67]	5.92*	1357	0.64
2-Methylbutyl angelate	6.48*	1154	[0.67]	5.92*	1357	[0.64]
Borneol	6.60	1162	0.07	9.78*	1652	0.34
Unknown [m/z 83, 100 (34), 55 (33), 43 (21), 84 (21)...]	6.71	1168	0.02	5.69	1340	0.02
Terpinen-4-ol	6.77	1172	0.21	8.56*	1555	0.23
4,6-Dimethyloctane-3,5-dione epimer I	6.94	1183	0.14	8.61*	1559	0.38
4,6-Dimethyloctane-3,5-dione epimer II	6.96	1184	0.18	8.61*	1559	[0.38]
α-Terpineol	7.01	1188	0.25	9.78*	1652	[0.34]
Myrtenol	7.08	1192	0.01	10.86	1741	0.02
2-Methylbutyl tiglate	7.10	1194	0.02	6.89*	1428	0.11
Verbenone	7.22	1201	0.02	9.58*	1636	[0.97]
Unknown [m/z 95, 93 (32), 121 (24), 79 (22), 91 (21), 105 (16)... 154 (2)]	7.27*	1204	0.07	10.94*	1749	0.63
Decanal	7.27*	1204	[0.07]	7.29	1458	0.04
Unknown [m/z 81, 57 (91), 168 (73), 67 (52), 140 (45), 41 (36), 113 (27)...]	7.42	1215	0.01			
Unknown [m/z 81, 109 (85), 168 (72), 57 (69), 67 (58), 41 (49), 140 (45)...]	7.47	1217	0.02			
Unknown [m/z 113, 57 (55), 85 (16), 170 (16)]	7.64*	1229	0.49			
Nerol	7.64*	1229	[0.49]	11.06*	1759	0.39
Hexyl 2-methylbutyrate	7.77	1237	0.03	6.48	1397	0.02
Isoamyl	8.00	1253	0.03	6.89*	1428	[0.11]

hexanoate						
3-Methylpentyl angelate	8.05*	1256	0.07	7.36	1463	0.02
Unknown [m/z 83, 55 (29), 57 (24), 100 (21), 104 (13)...]	8.05*	1256	[0.07]	6.89*	1428	[0.11]
Unknown [m/z 83, 55 (30), 57 (23), 100 (20), 98 (14)...]	8.12	1261	0.04	6.99	1435	0.04
(3Z)-Hexenyl angelate	8.40	1279	0.03	8.20*	1527	[0.95]
Hexyl angelate	8.50	1286	0.30	7.91	1504	0.32
2-Undecanone	8.60	1293	0.04	8.61*	1559	[0.38]
2-Acetyl-para-cresol?	8.72	1300	0.03			
Myrtenyl acetate	9.00	1320	0.02	9.58*	1636	[0.97]
Hexyl tiglate	9.16	1331	0.05	8.90	1581	0.05
Bicycloelemene	9.22	1335	0.01	7.06	1441	0.02
α -Terpinyl acetate	9.35	1345	0.25	9.75*	1649	10.72
Cyclosativene I	9.50	1355	0.12	7.03*	1438	[0.40]
Cyclosativene II	9.53	1357	0.28	7.03*	1438	[0.40]
α -Ylangene	9.58	1361	0.01	7.03*	1438	[0.40]
Neryl acetate	9.69*	1368	33.03	10.24*	1690	30.98
Italicene isomer	9.69*	1368	[33.03]	7.19	1450	0.83
α -Copaene	9.69*	1368	[33.03]	7.14	1446	1.44
Geranyl acetate	9.90	1383	0.42	10.56	1716	0.43
Hexyl hexanoate	9.97*	1388	0.19	8.84	1577	0.01
α -Funebrene	9.97*	1388	[0.19]	7.82	1497	0.16
Isoitalicene	10.00	1390	0.16	7.78	1494	0.14
Italicene	10.07	1395	3.07	7.74	1491	3.04
Isocaryophyllene	10.11	1398	0.07	8.16	1524	0.10
α -Gurjunene	10.15*†	1401	0.11	7.59*	1480	[0.05]
Tetradecane	10.15*†	1401	[0.11]	6.45	1395	0.03
α -Cedrene	10.17†	1403	[0.11]	7.98	1510	0.04
β -Caryophyllene	10.28*	1410	5.13	8.41*	1544	[5.18]
<i>cis</i> - α -Bergamotene	10.28*	1410	[5.13]	8.20*	1527	[0.95]
β -Copaene	10.41	1420	0.06	8.35	1539	0.03
<i>trans</i> - α -Bergamotene	10.55	1430	0.90	8.41*	1544	[5.18]
Italidione I (4,6,9-Trimethyldec-8-ene-3,5-dione)	10.64*	1437	2.44	11.98*†	1838	7.36
6,9-Guaiadiene	10.64*	1437	[2.44]	8.56*	1555	[0.23]
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.68	1440	0.12	8.77	1571	0.06
α -Humulene	10.72*	1444	0.32	9.27	1610	0.31
Cadina-4,11-diene	10.72*	1444	[0.32]	9.11	1598	0.01
Neryl propionate	10.72*	1444	[0.32]	10.94*	1749	[0.63]

allo-Aromadendrene	10.86*†	1453	1.33	8.98	1588	0.12
(E)-β-Farnesene	10.86*†	1453	[1.33]	9.42*†	1623	[1.75]
α-Acoradiene	10.92	1458	0.36	9.33	1615	0.34
4,5-diepi-Aristolochene	10.95	1460	0.11	9.39*†	1620	[1.75]
trans-Cadina-1(6),4-diene	11.05*†	1468	1.77	9.23	1607	0.12
Unknown [m/z 119, 91 (85), 93 (77), 105 (76), 79 (61), 134 (60), 94 (49), 204 (46)]	11.05*†	1468	[1.77]	9.39*†	1620	[1.75]
Selina-4,11-diene	11.07†	1469	[1.77]	9.42*†	1623	[1.75]
γ-Curcumene	11.18*†	1477	20.89	9.75*	1649	[10.72]
β-Selinene	11.18*†	1477	[20.89]	9.88*	1660	5.70
Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione)	11.21*†	1480	[20.89]	11.98*†	1838	[7.36]
ar-Curcumene	11.21*†	1480	[20.89]	10.67	1725	2.66
trans-β-Bergamotene	11.27†	1484	5.79	9.58*	1636	[0.97]
Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione)	11.29†	1485	[5.79]	11.98*†	1838	[7.36]
α-Selinene	11.31†	1487	[5.79]	9.96	1666	3.69
Eudesma-2,4(15),11-triene	11.37	1492	0.20	11.06*	1759	[0.39]
Italidione II analog	11.40	1494	0.33	12.77*†	1908	1.41
δ-Amorphene	11.48	1500	0.33	9.88*	1660	[5.70]
10-epi-Italicene ether	11.56†	1506	1.77	11.29	1778	0.06
γ-Cadinene	11.58*†	1508	[1.77]	10.42	1704	0.23
β-Bisabolene	11.58*†	1508	[1.77]	10.24*	1690	[30.98]
β-Curcumene	11.58*†	1508	[1.77]	10.24*	1690	[30.98]
7-epi-α-Selinene	11.59†	1509	[1.77]	10.44*	1706	0.83
Sesquicineole	11.69*	1516	0.96	10.33	1697	0.39
δ-Cadinene	11.69*	1516	[0.96]	10.44*	1706	[0.83]
trans-Calamenene	11.69*	1516	[0.96]	11.22	1772	0.04
Italicene ether	11.79†	1524	0.29	11.54	1800	0.12
(E)-γ-Bisabolene	11.81†	1526	[0.29]	10.37	1700	0.10
α-Cadinene	11.86	1530	0.06	10.78	1735	0.05
Selina-3,7(11)-diene	11.90	1533	0.13	10.49	1710	0.11
(E)-α-Bisabolene	11.98	1539	0.14	10.72	1729	0.11
Caryophyllenyl alcohol	12.24	1560	0.02	13.64	1989	0.02
(E)-Nerolidol	12.27	1562	0.16	13.79*	2003	0.17
Italidione III	12.38	1571	0.59	12.86*†	1917	[1.41]

isomer I						
Italidione III	12.45*†	1576	0.58	12.86*†	1917	[1.41]
isomer II						
Caryophyllene oxide	12.45*†	1576	[0.58]	12.77*†	1908	[1.41]
Italidione III						
isomer III	12.54	1583	0.25			
Guaiol	12.64	1591	0.15	14.13	2036	0.16
Copaborneol	12.70	1595	0.25	14.93	2113	0.25
Eudesm-5-en-11-ol	12.73	1598	0.28	14.38	2060	0.26
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.80	1604	0.14	14.51	2072	0.11
Unknown [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	12.84	1607	0.08	14.63	2084	0.07
Unknown [m/z 182, 109 (58), 69 (50), 41 (42), 43 (40), 139 (31)... 235 (17), 250 (1)...]	12.90	1612	0.17	14.10	2033	0.15
Neryl angelate?	12.99	1620	0.09			
Caryophylladienol I	13.04*	1623	0.09	16.06	2227	0.04
γ-Eudesmol	13.04*	1623	[0.09]	14.89	2110	0.03
1-epi-Cubenol	13.04*	1623	[0.09]	13.79*	2003	[0.17]
Eudesmol analog?	13.06	1625	0.16			
τ-Muurolol	13.16*	1633	0.09	15.05	2126	0.02
τ-Cadinol	13.16*	1633	[0.09]	14.87	2107	0.02
Cubenol	13.16*	1633	[0.09]	13.67	1992	0.02
β-Eudesmol	13.24	1640	0.10	15.40	2160	0.13
α-Eudesmol	13.30*	1645	0.27	15.33	2153	0.06
Selin-11-en-4α-ol	13.30*	1645	[0.27]	15.63	2183	0.18
Bulnesol	13.47	1659	0.04	15.29	2149	0.03
β-Bisabolol	13.54	1665	0.16	14.77	2097	0.13
epi-α-Bisabolol	13.70	1678	0.05	15.48	2168	0.02
α-Bisabolol	13.73	1681	0.03	15.44	2164	0.01
Neryl 4-methylvalerate?	13.82	1688	0.05	13.34	1962	0.04
Unknown [m/z 196, 69 (62), 109 (58), 41 (54), 139 (41)... 249 (21)...]	13.88	1693	0.05	14.66	2087	0.04
Geranyl 4-methylvalerate?	14.17	1718	0.03	13.79*	2003	[0.17]
Unknown [m/z 43, 69 (32), 198 (29),	14.29	1729	0.12			

41 (27), 93 (26)... 202 (20)...]						
Unknown [m/z 82, 125 (40), 41 (35), 69 (31), 67 (27)... 236? (t)]	14.40	1738	0.02	15.78	2198	0.02
Unknown [m/z 109, 127 (46), 138 (45), 81 (27), 123 (25)... 220? (2)]	14.54	1750	0.04	19.12	2561	0.04
Unknown [m/z 136, 121 (74), 135 (55), 218 (36), 148 (33), 40 (42)... 236? (1)]	14.59†	1754	0.10			
Unknown [m/z 109, 138 (71), 82 (42), 123 (41), 127 (38)...]	14.61†	1756	[0.10]	19.13	2562	0.03
Unknown [m/z 96, 41 (29), 178 (28), 43 (27)... 236 (2)]	14.66	1761	0.04	17.16	2343	0.02
Unknown [m/z 109, 127 (46), 138 (45), 82 (34), 81 (31)... 236? (t)]	14.68	1762	0.07	19.62	2619	0.06
Unknown [m/z 109, 138 (75), 123 (45), 127 (42), 81 (30)...]	14.80	1772	0.07	19.69	2628	0.06
Unknown [m/z 98, 82 (77), 83 (42), 137 (37), 41 (28)... 238 (1)]	14.86	1778	0.18	19.55	2611	0.18
Unknown [m/z 43, 82 (69), 41 (66), 93 (62), 96 (55), 55 (49), 67 (45), 154 (44)...]	15.14	1802	0.11			
Total identified		97.04%			95.49%	
Total reported		98.45%			96.39%	

*: 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