

Date : March 20, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23C13-PTH01

Customer identification : Blue Tansy - Morocco - B50111R

Type : Essential oil

Source : *Tanacetum annuum*

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 : Amélie Simard, Analyste

Analysis date : March 17, 2023

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Dark blue liquid

Refractive index: 1.5167 ± 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
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Toluene	tr	Simple phenolic
Unknown	tr	Unknown
Hexanal	tr	Aliphatic aldehyde
Ethyl 2-methylbutyrate	0.01	Aliphatic ester
Hexanol	0.01	Aliphatic alcohol
Nonane	0.01	Alkane
Hashishene	0.01	Monoterpene
Tricyclene	0.04	Monoterpene
α -Thujene	0.25	Monoterpene
Ethyl tiglate?	0.01	Aliphatic ester
α -Pinene	1.86	Monoterpene
Camphene	0.68	Monoterpene
α -Fenchene	0.01	Monoterpene
Propyl 2-methylbutyrate	0.02	Aliphatic ester
Thuja-2,4(10)-diene	0.03	Monoterpene
Sabinene	14.71	Monoterpene
β -Pinene	4.96	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
2-Pentylfuran	0.02	Furan
Myrcene	3.18	Monoterpene
α -Phellandrene	4.51	Monoterpene
Menthatriene isomer I	0.01	Monoterpene
Pseudolimonene	0.01	Monoterpene
Octanal	0.01	Aliphatic aldehyde
Δ^3 -Carene	0.02	Monoterpene
α -Terpinene	0.77	Monoterpene
Isoamyl isobutyrate	0.01	Aliphatic ester
para-Cymene	4.59	Monoterpene
Limonene	2.12	Monoterpene
β -Phellandrene	0.38	Monoterpene
1,8-Cineole	0.23	Monoterpenic ether
Unknown	0.01	Unknown
(Z)- β -Ocimene	0.02	Monoterpene
Butyl 2-methylbutyrate	0.02	Aliphatic ester
Butyl isovalerate	0.02	Aliphatic ester
(E)- β -Ocimene	0.02	Monoterpene
γ -Terpinene	1.36	Monoterpene
Prenyl isobutyrate	0.01	Aliphatic ester
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.05	Aliphatic alcohol
Terpinolene	0.50	Monoterpene
para-Cymenene	0.04	Monoterpene

<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
6,7-Epoxymyrcene	0.17	Monoterpenic ether
<i>trans</i> -Sabinene hydrate	0.05	Monoterpenic alcohol
Linalool	0.10	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.04	Aliphatic ester
Isoamyl isovalerate	0.01	Aliphatic ester
Unknown	0.17	Unknown
<i>cis</i> -para-Menth-2-en-1-ol	0.08	Monoterpenic alcohol
α -Campholenal	0.06	Monoterpenic aldehyde
Limona ketone	0.24	Normonoterpenic ketone
<i>trans</i> -Pinocarveol	0.02	Monoterpenic alcohol
Camphor	10.12	Monoterpenic ketone
α ,4-Dimethyl-3-cyclohexene-1-methanol	0.05	Normonoterpenic alcohol
Sabinaketone	0.06	Normonoterpenic ketone
Citronellal	0.01	Monoterpenic aldehyde
Pinocarvone	0.02	Monoterpenic ketone
Unknown	0.07	Oxygenated monoterpene
Borneol	1.72	Monoterpenic alcohol
Unknown	0.13	Oxygenated monoterpene
Terpinen-4-ol	1.44	Monoterpenic alcohol
Unknown	0.11	Unknown
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α -Terpineol	0.18	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Myrtenol	0.04	Monoterpenic alcohol
Unknown	0.08	Unknown
<i>cis</i> - α -Phellandrene epoxide (iPr vs Me)	0.14	Monoterpenic ether
Decanal	0.06	Aliphatic aldehyde
<i>trans</i> -Piperitol	0.07	Monoterpenic alcohol
<i>trans</i> -Carveol	0.08	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
(3Z)-Hexenyl 2-methylbutyrate	0.01	Aliphatic ester
Cuminal	0.15	Monoterpenic aldehyde
Hexyl 2-methylbutyrate	0.03	Aliphatic ester
Pulegone	0.09	Monoterpenic ketone
Neral	0.04	Monoterpenic aldehyde
(2E)-Hexenyl isovalerate	0.02	Aliphatic ester
Carvotanacetone	0.10	Monoterpenic ketone
Piperitone	0.04	Monoterpenic ketone
Phellandral	0.07	Monoterpenic aldehyde
Geranial	0.02	Monoterpenic aldehyde
α -Terpinen-7-al	0.06	Monoterpenic aldehyde
Anthemol?	0.02	Monoterpenic alcohol
Bornyl acetate	0.01	Monoterpenic ester
Cuminol	0.06	Monoterpenic alcohol
Perilla alcohol	0.03	Monoterpenic alcohol
Thymol	0.98	Monoterpenic alcohol
4-Methylhexyl 2-methylbutyrate	0.06	Aliphatic ester
Carvacrol	0.02	Monoterpenic alcohol
para-Menth-5-en-1,2-diol isomer III	0.04	Monoterpenic alcohol
6-Hydroxycarvotanacetone	0.03	Monoterpenic alcohol

1,4-para-Menthadien-7-ol	0.07	Monoterpenic alcohol
Bicycloelemene	0.02	Sesquiterpene
α -Cubebene	0.03	Sesquiterpene
Modhephene	0.02	Sesquiterpene
α -Copaene	0.07	Sesquiterpene
Methyl para-anisate	0.03	Phenolic ester
(<i>E</i>)- β -Damascenone	0.05	Apocarotenoid
7-epi-Sesquithujene?	0.04	Sesquiterpene
β -Elemene	0.29	Sesquiterpene
Benzyl isovalerate	0.03	Phenolic ester
α -Cedrene	0.03	Sesquiterpene
β -Caryophyllene	1.75	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
Octyl 2-methylbutyrate	0.16	Aliphatic ester
<i>trans</i> - α -Bergamotene	0.11	Sesquiterpene
Sesquisabinene A	1.22	Sesquiterpene
α -Humulene	0.21	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.10	Sesquiterpene
4,5-diepi-Aristolochene	0.09	Sesquiterpene
Dehydrosesquicineole	0.06	Sesquiterpenic ether
γ -Muurolene	0.13	Sesquiterpene
Germacrene D	1.35	Sesquiterpene
γ -Curcumene	0.14	Sesquiterpene
β -Selinene	0.45	Sesquiterpene
<i>ar</i> -Curcumene	0.19	Sesquiterpene
Eremophilene	0.01	Sesquiterpene
Phenylethyl isovalerate	0.03	Phenolic ester
Phenylethyl 2-methylbutyrate	0.03	Phenolic ester
Bicyclogermacrene	0.21	Sesquiterpene
α -Muurolene	0.07	Sesquiterpene
δ -Guaiene	0.10	Sesquiterpene
3,6-Dihydrochamazulene	7.20	Azulene
β -Curcumene	0.01	Sesquiterpene
γ -Cadinene	0.01	Sesquiterpene
Dihydrochamazulene isomer I	1.45	Azulene
δ -Cadinene	0.20	Sesquiterpene
Dihydrochamazulene isomer II	0.15	Azulene
β -Sesquiphellandrene	0.39	Sesquiterpene
Dihydrochamazulene isomer III	0.10	Azulene
Phenylethyl angelate?	0.03	Phenolic ester
Isocaryophyllene epoxide B	0.04	Sesquiterpenic ether
α -Elemol	0.06	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.03	Sesquiterpenic alcohol
Spathulenol	0.11	Sesquiterpenic alcohol
Caryophyllene oxide	0.30	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
10-epi-Junenol	0.04	Sesquiterpenic alcohol
Humulene epoxide II	0.06	Sesquiterpenic ether
Junenol	0.03	Sesquiterpenic alcohol
5,6-Dihydrochamazulene	0.74	Azulene
Unknown	0.05	Sesquiterpene
γ -Eudesmol	0.16	Sesquiterpenic alcohol

7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	1.88	Azulene
Eremoligenol	0.08	Sesquiterpenic alcohol
τ -Cadinol	0.04	Sesquiterpenic alcohol
β -Eudesmol	0.70	Sesquiterpenic alcohol
α -Eudesmol	0.03	Sesquiterpenic alcohol
Dihydrochamazulene isomer IV	1.57	Azulene
(3E,5E)-7-Hydroxyfarnesene	0.13	Sesquiterpenic alcohol
Unknown	0.30	Azulene
Chamazulene	10.92	Azulene
α -Phellandrene dimer II	0.05	Diterpene
Dehydrochamazulene	0.02	Azulene
Phytone	0.07	Terpenic ketone
9-(15,16-Dihydro-15-methyleneneryl)- α -terpinene?	0.24	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-paracycymene	0.23	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	0.86	Homoditerpene
Unknown	0.27	Unknown
Unknown	0.94	Unknown
Unknown	0.10	Unknown
Unknown	0.07	Unknown
Consolidated total	94.67%	

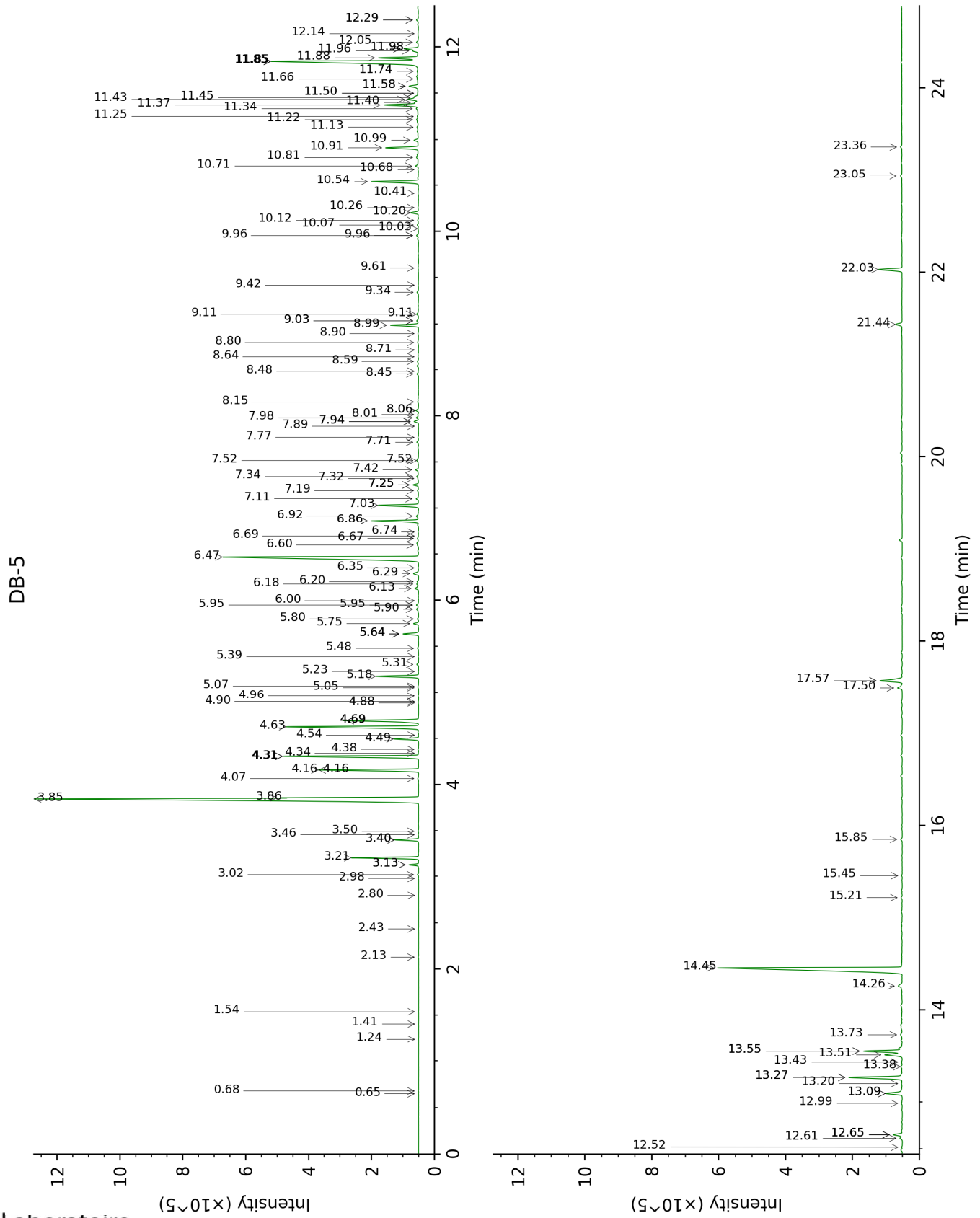
tr: The compound has been detected below 0.005% of total signal.

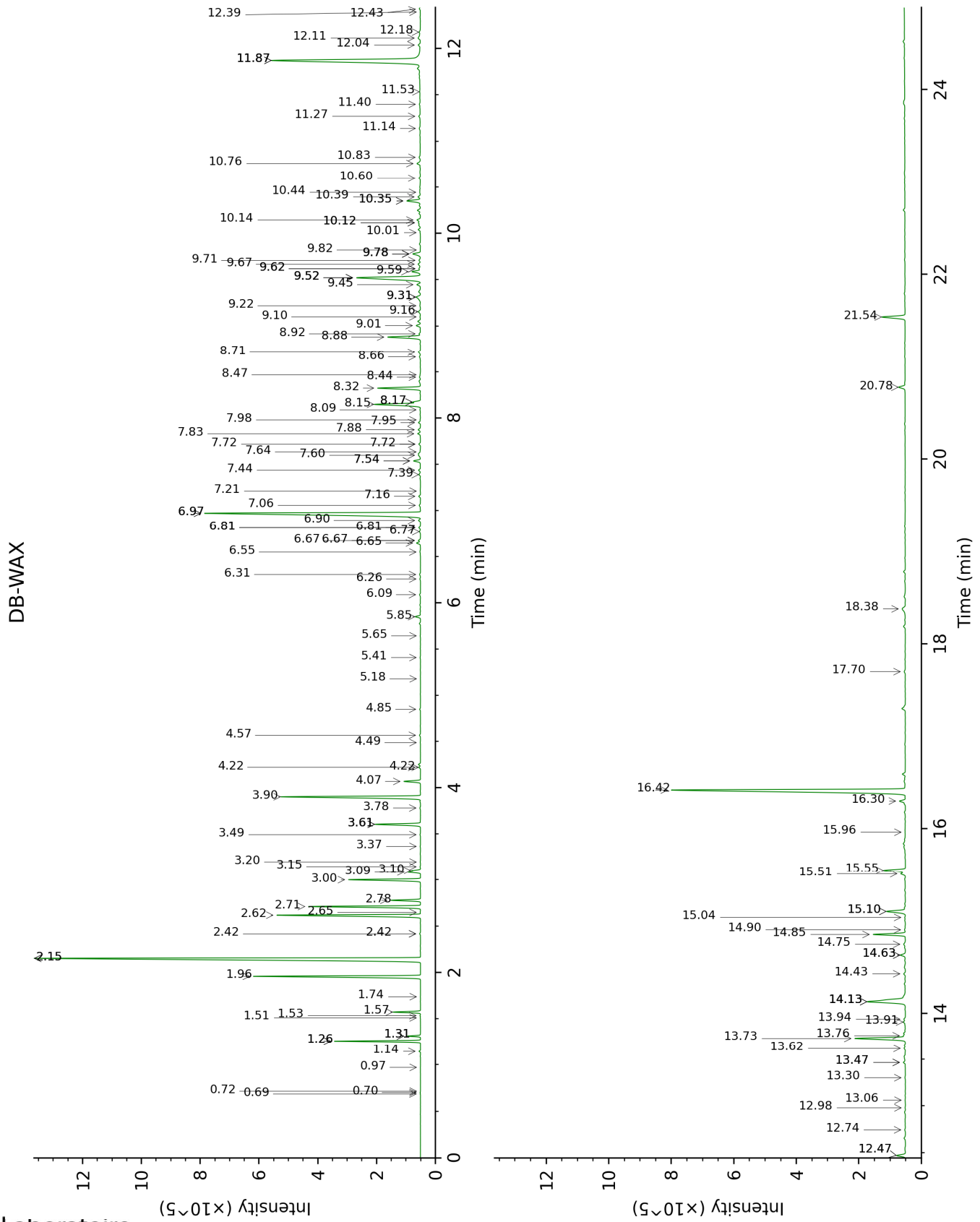
Note: no correction factor was applied

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	%
Isovaleral	0.65	641	tr	0.70	888	0.01
2-Methylbutyral	0.68	651	tr	0.69	882	tr
Toluene	1.24	759	tr	1.31*	1000	0.27
Unknown [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.41	781	tr	0.97	941	tr
Hexanal	1.54	799	tr	1.74	1044	tr
Ethyl 2-methylbutyrate	2.13	850	0.01	1.54	1022	0.01
Hexanol	2.43	874	0.01	5.18	1321	0.01
Nonane	2.80	904	0.01	0.72	894	tr
Hashishene	2.98	916	0.01	1.26*	991	1.91
Tricyclene	3.02	919	0.04	1.14	971	0.03
α -Thujene	3.13*	926	0.27	1.31*	1000	[0.27]
Ethyl tiglate?	3.13*	926	[0.27]	3.37	1189	0.01
α -Pinene	3.21	931	1.86	1.26*	991	[1.91]
Camphene	3.40*	944	0.69	1.57	1026	0.68
α -Fenchene	3.40*	944	[0.69]	1.51	1020	0.01
Propyl 2-methylbutyrate	3.46	948	0.02	2.42*	1111	0.03
Thuja-2,4(10)-diene	3.50	950	0.03	2.15*	1087	15.14
Sabinene	3.85†	973	19.68	2.15*	1087	[15.14]
β -Pinene	3.86†	974	[19.68]	1.96	1066	4.96
6-Methyl-5-hepten-2-one	4.07	987	0.03	4.85	1304	0.03
2-Pentylfuran	4.16*	993	3.12	3.49	1200	0.02
Myrcene	4.16*	993	[3.12]	2.71	1135	3.18
α -Phellandrene	4.31*	1003	4.48	2.62	1127	4.51
Menthatriene isomer I	4.31*	1003	[4.48]	3.20	1175	0.01
Pseudolimonene	4.31*	1003	[4.48]	2.65	1130	0.01
Octanal	4.34	1005	0.01	4.22*	1255	0.05
Δ 3-Carene	4.38	1008	0.02	2.42*	1111	[0.03]
α -Terpinene	4.49	1015	0.77	2.78	1140	0.77
Isoamyl isobutyrate	4.54	1018	0.01	3.15	1171	0.02
para-Cymene	4.63	1023	4.59	3.90	1231	4.67
Limonene	4.69*	1027	2.67	3.00	1159	2.12
β -Phellandrene	4.69*	1027	[2.67]	3.09	1166	0.38
1,8-Cineole	4.69*	1027	[2.67]	3.10	1167	0.23
Unknown [m/z 43, 55 (65), 41 (34), 67 (32), 107 (30), 122 (26)... 125 (10)]	4.88	1039	0.01	5.41	1338	0.02
(Z)- β -Ocimene	4.90	1040	0.02	3.61*	1208	1.41
Butyl 2-methylbutyrate	4.96	1044	0.02	3.61*	1208	[1.41]
Butyl isovalerate	5.06	1050	0.02			
(E)- β -Ocimene	5.07	1051	0.02	3.78	1222	0.03
γ -Terpinene	5.18	1058	1.36	3.61*	1208	[1.41]
Prenyl isobutyrate	5.23	1061	0.01	4.57	1282	0.04
cis-Sabinene hydrate	5.31	1066	0.06	6.67*	1430	0.07
cis-Linalool oxide (fur.)	5.39	1071	0.02	6.31	1403	0.04
Octanol	5.48	1077	0.05	7.95	1527	0.07

Terpinolene	5.64*	1086	0.53	4.07	1244	0.50
para-Cymenene	5.64*	1086	[0.53]	6.09	1387	0.04
<i>trans</i> -Linalool oxide (fur.)	5.64*	1086	[0.53]	6.67*	1430	[0.07]
6,7-Epoxymyrcene	5.75	1093	0.17	5.85	1370	0.17
<i>trans</i> -Sabinene hydrate	5.80	1096	0.05	7.72*	1509	0.06
Linalool	5.90	1103	0.10	7.83	1518	0.11
Nonanal	5.95*	1106	0.10	5.65	1355	0.01
2-Methylbutyl 2-methylbutyrate	5.95*	1106	[0.10]	4.22*	1255	[0.05]
Isoamyl isovalerate	6.00	1109	0.01	4.49	1276	0.01
Unknown [m/z 71, 43 (95), 81 (82), 79 (73), 67 (67), 41 (49), 109 (14)...]	6.13	1117	0.17	6.65	1428	0.14
<i>cis</i> -para-Menth-2-en-1-ol	6.18	1120	0.08	7.88	1521	0.10
α -Campholenal	6.20	1122	0.06	6.77	1438	0.04
Limona ketone	6.29	1128	0.24	7.54*	1495	0.25
<i>trans</i> -Pinocarveol	6.35	1131	0.02	8.92	1603	0.05
Camphor	6.47	1139	10.12	6.97*	1453	10.14
α ,4-Dimethyl-3-cyclohexene-1-methanol	6.60	1147	0.05			
Sabinaketone	6.67	1152	0.06	8.44	1566	0.04
Citronellal	6.69	1153	0.01	6.81*	1441	0.06
Pinocarvone	6.74	1156	0.02	7.64	1503	0.02
Unknown [m/z 95, 110 (38), 81 (21), 79 (16)... 152 (7)]	6.86*	1164	1.78	7.39	1484	0.07
Borneol	6.86*	1164	[1.78]	9.52*	1652	3.35
Unknown [m/z 95, 110 (43), 81 (28), 41 (15)... 152 (8)]	6.92	1167	0.13	7.44	1488	0.07
Terpinen-4-ol	7.03	1175	1.44	8.32	1556	1.44
Unknown [m/z 69, 68 (65), 110 (51), 67 (39), 41 (27), 83 (26)...]	7.10	1179	0.11	7.60	1500	0.08
para-Cymen-8-ol	7.19	1185	0.05	11.27	1800	0.05
α -Terpineol	7.25*	1189	0.20	9.52*	1652	[3.35]
Myrtenal	7.25*	1189	[0.20]	8.47	1568	0.02
Myrtenol	7.32	1193	0.04	10.60	1742	0.05
Unknown [m/z 79, 107 (72), 41 (58), 55 (47), 77 (41), 67 (41)...]	7.34	1195	0.08			
<i>cis</i> - α -Phellandrene epoxide (iPr vs Me)	7.42	1199	0.14	10.76	1756	0.13
Decanal	7.52*	1206	0.13	7.06	1459	0.06
<i>trans</i> -Piperitol	7.52*	1206	[0.13]	10.12*	1701	0.08
<i>trans</i> -Carveol	7.71	1219	0.08	11.14	1788	0.04
Unknown [m/z 93, 41 (68), 79 (67), 91 (66), 92 (57), 67 (42), 77 (41)... 150 (12)]	7.77	1222	0.03			
(3 <i>Z</i>)-Hexenyl 2-methylbutyrate	7.89	1230	0.01	6.81*	1441	[0.06]

Cuminal	7.94*	1234	0.17	10.35*	1721	0.54
Hexyl 2-methylbutyrate	7.94*	1234	[0.17]	6.26	1399	0.03
Pulegone	7.98	1236	0.09	8.72	1587	0.10
Neral	8.01	1239	0.04	9.22	1628	0.03
(2E)-Hexenyl isovalerate	8.06*	1242	0.11	6.97*	1453	[10.14]
Carvotanacetone	8.06*	1242	[0.11]	9.16	1622	0.10
Piperitone	8.15	1248	0.04	9.62*	1660	0.06
Phellandral	8.45	1268	0.07	9.71	1668	0.07
Geranial	8.48	1270	0.02	9.82	1677	0.01
α -Terpinen-7-al	8.59	1277	0.06	10.44	1729	0.03
Anthemol?	8.64	1280	0.02			
Bornyl acetate	8.71	1285	0.01	7.98	1530	0.02
Cuminol	8.80	1291	0.06	13.91	2042	0.08
Perilla alcohol	8.90	1298	0.03	12.98	1954	0.02
Thymol	8.99	1304	0.98	14.85	2135	1.03
4-Methylhexyl 2-methylbutyrate	9.03*	1307	0.08	7.16	1467	0.06
Carvacrol	9.03*	1307	[0.08]	15.10*	2160	0.79
para-Menth-5-en-1,2-diol isomer III	9.11*	1312	0.10	14.90	2140	0.04
6-Hydroxycarvotanacetone	9.11*	1312	[0.10]	11.40	1811	0.03
1,4-para-Menthadien-7-ol	9.34	1329	0.07	13.47*	2000	0.08
Bicycloelemene	9.42	1334	0.02	6.81*	1441	[0.06]
α -Cubebene	9.60	1347	0.03	6.55	1421	0.03
Modhephene	9.96*	1372	0.08	7.21	1471	0.02
α -Copaene	9.96*	1372	[0.08]	6.90	1447	0.07
Methyl para-anisate	10.03	1377	0.03	13.62	2014	0.06
(E)- β -Damascenone	10.07	1380	0.05	10.83	1762	0.05
7-epi-Sesquithujene?	10.12	1384	0.04	7.54*	1495	[0.25]
β -Elemene	10.20	1389	0.29	8.17*†	1545	[2.02]
Benzyl isovalerate	10.26	1393	0.03	11.53	1823	0.03
α -Cedrene	10.41	1404	0.03	7.72*	1509	[0.06]
β -Caryophyllene	10.54	1413	1.75	8.15†	1543	2.02
β -Copaene	10.68	1424	0.02	8.09	1538	0.03
Octyl 2-methylbutyrate	10.71	1426	0.16	8.66	1583	0.05
trans- α -Bergamotene	10.81	1434	0.11	8.17*†	1545	[2.02]
Sesquisabinene A	10.91	1441	1.22	8.88	1600	1.23
α -Humulene	10.99	1447	0.21	9.01	1610	0.16
(E)- β -Farnesene	11.13	1458	0.10	9.31*	1635	0.26
4,5-diepi-Aristolochene	11.22	1464	0.09	9.10	1618	0.02
Dehydrosesquiceneole	11.25	1466	0.06	9.78*	1673	0.33
γ -Muurolene	11.34	1473	0.13	9.31*	1635	[0.26]
Germacrene D	11.37	1476	1.35	9.52*	1652	[3.35]
γ -Curcumene	11.40	1478	0.14	9.45	1646	0.14
β -Selinene	11.43	1480	0.45	9.59	1658	0.33
ar-Curcumene	11.45	1481	0.19	10.39	1725	0.09
Eremophilene	11.50*	1485	0.04	9.62*	1660	[0.06]
Phenylethyl isovalerate	11.50*	1485	[0.04]	12.74	1932	0.03
Phenylethyl 2-methylbutyrate	11.58*	1491	0.47	12.47*	1907	0.32

Bicyclogermacrene	11.58*	1491	[0.47]	9.78*	1673	[0.33]
α-Muurolene	11.66	1497	0.07	9.78*	1673	[0.33]
δ-Guaiene	11.74	1503	0.10	9.67	1664	0.11
3,6-Dihydrochamazulene	11.84*	1511	7.44	11.87*	1853	8.68
β-Curcumene	11.84*	1511	[7.44]	10.01	1692	0.01
γ-Cadinene	11.84*	1511	[7.44]	10.12*	1701	[0.08]
Dihydrochamazulene isomer I	11.88	1514	1.45	11.87*	1853	[8.68]
δ-Cadinene	11.96	1520	0.20	10.14	1704	0.13
Dihydrochamazulene isomer II	11.98*	1522	0.54	12.11	1875	0.15
β-Sesquiphellandrene	11.98*	1522	[0.54]	10.35*	1721	[0.54]
Dihydrochamazulene isomer III	12.05	1527	0.10	12.04	1868	0.09
Phenylethyl angelate?	12.14	1534	0.03	13.94	2045	0.07
Isocaryophyllene epoxide B	12.29*	1546	0.09	11.87*	1853	[8.68]
α-Elemol	12.29*	1546	[0.09]	13.76	2028	0.06
(E)-Nerolidol	12.52	1564	0.03	13.47*	2000	[0.08]
Spathulenol	12.61	1571	0.11	14.13*	2063	2.20
Caryophyllene oxide	12.65*	1574	0.35	12.47*	1907	[0.32]
Caryophyllene oxide isomer	12.65*	1574	[0.35]	12.40	1900	0.01
10-epi-Junenol	12.65*	1574	[0.35]	12.43	1903	0.04
Humulene epoxide II	12.99	1601	0.06	13.06	1962	0.03
Junenol	13.09*	1609	0.77	13.30	1984	0.03
5,6-Dihydrochamazulene	13.09*	1609	[0.77]	14.13*	2063	[2.20]
Unknown [m/z 145, 173 (83), 159 (57), 174 (47), 129 (47), 115 (44), 128 (43), 91 (43), 157 (36), 202 (30)]	13.20	1618	0.05			
γ-Eudesmol	13.27*	1623	2.10	14.63*	2112	0.20
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	13.27*	1623	[2.10]	13.73	2025	1.88
Eremoligenol	13.38	1633	0.08	14.75	2124	0.09
τ-Cadinol	13.43	1637	0.04	14.63*	2112	[0.20]
β-Eudesmol	13.51	1643	0.70	15.10*	2160	[0.79]
α-Eudesmol	13.55*†	1647	1.60	15.04	2153	0.03
Dihydrochamazulene isomer IV	13.55*†	1647	[1.60]	14.13*	2063	[2.20]
(3E,5E)-7-Hydroxyfarnesene	13.73	1662	0.13	15.96	2248	0.01
Unknown [m/z 143, 142 (92), 157 (79), 158 (61), 141 (59), 128 (57), 159 (43), 115 (41), 202 (41)]	14.26	1705	0.30	18.38	2513	0.25
Chamazulene	14.45	1722	10.92	16.42	2296	11.22
α-Phellandrene dimer II	15.21	1788	0.05	12.18	1880	0.05
Dehydrochamazulene	15.45	1809	0.02	17.70	2436	0.06
Phytone	15.85	1845	0.07	14.43	2092	0.07

9-(15,16-Dihydro-15-methyleneneryl)- α -terpinene?	17.50	1998	0.24	15.51	2201	0.17
9-(15,16-Dihydro-15-methylenegeranyl)-paracycymene	17.57*	2006	1.04	16.30	2284	0.23
9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	17.57*	2006	[1.04]	15.55	2205	0.86
Unknown analog I	21.44	2414	0.27	20.78	2802	0.29
Unknown [m/z 186, 157 (37), 171 (18), 322 (15)]	22.03	2483	0.94	21.54	2900	0.95
Unknown analog II	23.05	2605	0.10			
Unknown analog III	23.36	2644	0.07			
Total identified		92.74%			92.46%	
Total reported		94.98%			94.34%	

*: 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