

Date : October 02, 2019

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 19I23-PTH04-1-SCC

Customer identification : Blue Tansy - Morocco - B5010689R

Type : Essential oil

Source : *Tanacetum annuum*

Customer : Plant Therapy

ANALYSIS

Method: PC-PA-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 : October 02, 2019

Checked and approved by :

Sylvain Mercier, M. Sc., chimiste 2014-005

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PHYSICOCHEMICAL DATA

Physical aspect: Dark blue liquid

Refractive index: 1.5072 ± 0.0003 (20 °C)

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	%	Classe
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Toluene	tr	Simple phenolic
Unknown	tr	Unknown
Unknown	tr	Unknown
Ethyl 2-methylbutyrate	0.02	Aliphatic ester
Propyl isobutyrate	0.01	Aliphatic ester
Hashishene	0.01	Monoterpene
Tricyclene	0.05	Monoterpene
α -Thujene	0.31	Monoterpene
Ethyl tiglate?	0.01	Aliphatic ester
α -Pinene	1.61	Monoterpene
Camphene	0.89	Monoterpene
α -Fenchene	tr	Monoterpene
Propyl 2-methylbutyrate	0.06	Aliphatic ester
Thuja-2,4(10)-diene	0.01	Monoterpene
Propyl isovalerate	0.01	Aliphatic ester
Sabinene	12.53	Monoterpene
β -Pinene	2.72	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
2-Pentylfuran	0.01	Furan
Myrcene	8.03	Monoterpene
α -Phellandrene	7.02	Monoterpene
Menthatriene isomer I	0.01	Monoterpene
Octanal	0.04	Aliphatic aldehyde
Δ^3 -Carene	0.01	Monoterpene
α -Terpinene	0.96	Monoterpene
Isoamyl isobutyrate	0.01	Aliphatic ester
para-Cymene	5.63	Monoterpene
1,8-Cineole	0.94	Monoterpenic ether
β -Phellandrene	0.27	Monoterpene
Limonene	2.83	Monoterpene
(Z)- β -Ocimene	0.02	Monoterpene
Butyl 2-methylbutyrate	0.03	Aliphatic ester
Butyl isovalerate	0.03	Aliphatic ester
(E)- β -Ocimene	0.04	Monoterpene
γ -Terpinene	1.68	Monoterpene
Prenyl isobutyrate	0.01	Aliphatic ester
cis-Sabinene hydrate	0.03	Monoterpenic alcohol
Octanol	0.06	Aliphatic alcohol
Terpinolene	0.68	Monoterpene
para-Cymenene	0.04	Monoterpene
6,7-Epoxymyrcene	0.05	Monoterpenic ether
trans-Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	0.11	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.14	Aliphatic ester

Amyl isovalerate	0.02	Aliphatic ester
Unknown	0.06	Unknown
<i>cis</i> -para-Menth-2-en-1-ol	0.13	Monoterpenic alcohol
α -Campholenal	0.05	Monoterpenic aldehyde
Limona ketone	0.20	Normonoterpenic ketone
Camphor	7.97	Monoterpenic ketone
<i>trans</i> -Pinocarveol	0.04	Monoterpenic alcohol
α ,4-Dimethyl-3-cyclohexene-1-methanol	0.14	Normonoterpenic alcohol
Sabinaketone	0.04	Normonoterpenic ketone
Pinocavone	0.02	Monoterpenic ketone
Borneol	1.66	Monoterpenic alcohol
Unknown	0.14	Oxygenated monoterpene
Unknown	0.01	Oxygenated monoterpene
Terpinen-4-ol	1.88	Monoterpenic alcohol
Unknown	0.07	Unknown
para-Cymen-8-ol	0.03	Monoterpenic alcohol
α -Terpineol	0.19	Monoterpenic alcohol
Myrtenal	0.04	Monoterpenic aldehyde
Myrtenol	0.02	Monoterpenic alcohol
Unknown	0.06	Unknown
α -Phellandrene epoxide	0.11	Monoterpenic ether
Decanal	0.08	Aliphatic aldehyde
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
Unknown	0.06	Oxygenated monoterpene
(3Z)-Hexenyl 2-methylbutyrate	0.06	Aliphatic ester
Cuminal	0.13	Monoterpenic aldehyde
Hexyl 2-methylbutyrate	0.03	Aliphatic ester
Carvotanacetone	0.14	Monoterpenic ketone
Piperitone	0.06	Monoterpenic ketone
Phellandral	0.07	Monoterpenic aldehyde
α -Terpinen-7-al	0.05	Monoterpenic aldehyde
Anthemol?	0.01	Monoterpenic alcohol
Bornyl acetate	0.03	Monoterpenic ester
Cuminol	0.06	Monoterpenic alcohol
Thymol	0.95	Monoterpenic alcohol
Carvacrol	0.09	Monoterpenic alcohol
6-Hydroxycarvotanacetone	0.03	Monoterpenic alcohol
1,4-para-Menthadien-7-ol	0.06	Monoterpenic alcohol
Bicycloelemene	0.01	Sesquiterpene
α -Terpinyl acetate	0.01	Monoterpenic ester
α -Cubebene	0.03	Sesquiterpene
Modhephene	0.04	Sesquiterpene
α -Copaene	0.07	Sesquiterpene
Methyl para-anisate	0.01	Phenolic ester
(<i>E</i>)- β -Damascenone	0.07	Ionone or analog
7-epi-Sesquithujene?	0.04	Sesquiterpene
β -Elemene	0.29	Sesquiterpene
Benzyl isovalerate	0.03	Phenolic ester
α -Cedrene	0.03	Sesquiterpene
β -Caryophyllene	2.11	Sesquiterpene
β -Copaene	0.11	Sesquiterpene
Octyl 2-methylbutyrate	0.11	Aliphatic ester

<i>trans</i> - α -Bergamotene	0.14	Sesquiterpene
Sesquisabinene A	1.01	Sesquiterpene
α -Humulene	0.25	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.20	Sesquiterpene
4,5-diepi-Aristolochene	0.13	Sesquiterpene
Dehydrosesquicineole	0.06	Sesquiterpenic ether
γ -Muurolene	0.15	Sesquiterpene
Germacrene D	1.90	Sesquiterpene
α -Curcumene	0.43	Sesquiterpene
γ -Curcumene	0.13	Sesquiterpene
β -Selinene	0.33	Sesquiterpene
Phenylethyl isovalerate	0.05	Phenolic ester
Bicyclogermacrene	0.33	Sesquiterpene
Phenylethyl 2-methylbutyrate	0.09	Phenolic ester
δ -Guaiene	0.27	Sesquiterpene
γ -Cadinene	0.24	Sesquiterpene
3,6-Dihydrochamazulene	5.20	Azulene
β -Curcumene	0.01	Sesquiterpene
Dihydrochamazulene isomer I	0.95	Azulene
δ -Cadinene	0.27	Sesquiterpene
β -Sesquiphellandrene	0.88	Sesquiterpene
Dihydrochamazulene isomer II	0.36	Azulene
Dihydrochamazulene isomer III	0.10	Azulene
Phenylethyl angelate?	0.05	Phenolic ester
Isocaryophyllene epoxide B	0.03	Sesquiterpenic ether
α -Elemol	0.08	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.02	Sesquiterpenic alcohol
Spathulenol	0.38	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Caryophyllene oxide	0.32	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
Junenol	0.01	Sesquiterpenic alcohol
5,6-Dihydrochamazulene	0.88	Azulene
Unknown	0.30	Sesquiterpene
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	0.97	Azulene
γ -Eudesmol	0.05	Sesquiterpenic alcohol
Eremoligenol	0.08	Sesquiterpenic alcohol
τ -Cadinol	0.08	Sesquiterpenic alcohol
α -Muurolol	0.05	Sesquiterpenic alcohol
β -Eudesmol	0.74	Sesquiterpenic alcohol
α -Eudesmol	0.03	Sesquiterpenic alcohol
Dihydrochamazulene isomer IV	0.45	Azulene
(3 <i>E</i> ,5 <i>E</i>)-7-Hydroxyfarnesene	0.05	Sesquiterpenic alcohol
Unknown	0.12	Azulene
Chamazulene	10.38	Azulene
α -Phellandrene dimer II	0.08	Diterpene
Dehydrochamazulene	0.03	Azulene
Phytone	0.05	Terpenic ketone
9-(15,16-Dihydro-15-methyleneneryl)- α -terpinene?	0.15	Homoditerpene
9-(15,16-Dihydro-15-methyleneneryl)-para-cymene?	0.07	Homoditerpene

9-(15,16-Dihydro-15-methylenegeranyl)- α -terpinene	0.78	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-paracymene	0.17	Homoditerpene
Unknown	0.15	Unknown
Unknown	0.53	Unknown
Consolidated total	95.34%	

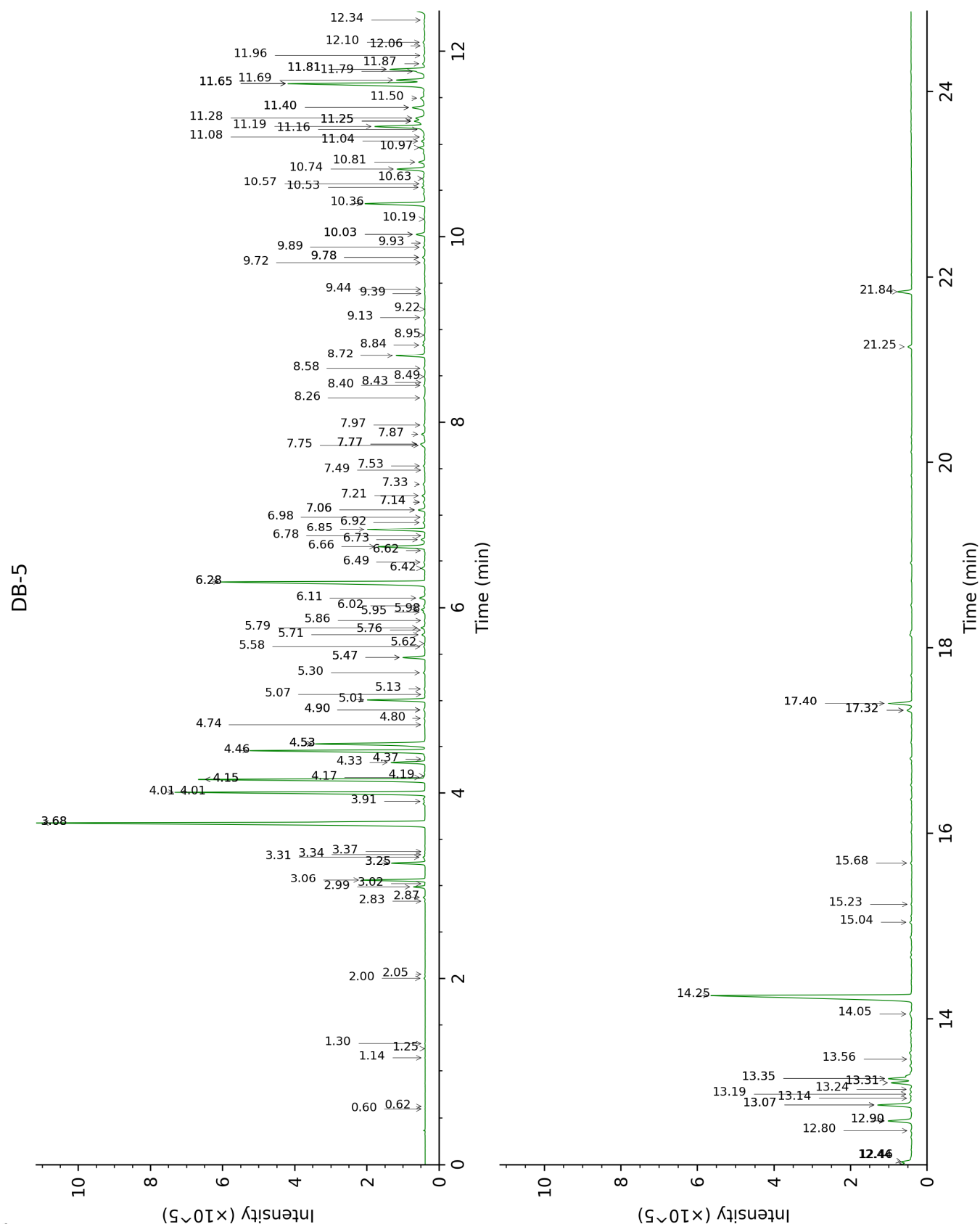
tr: The compound has been detected below 0.005% of total signal.

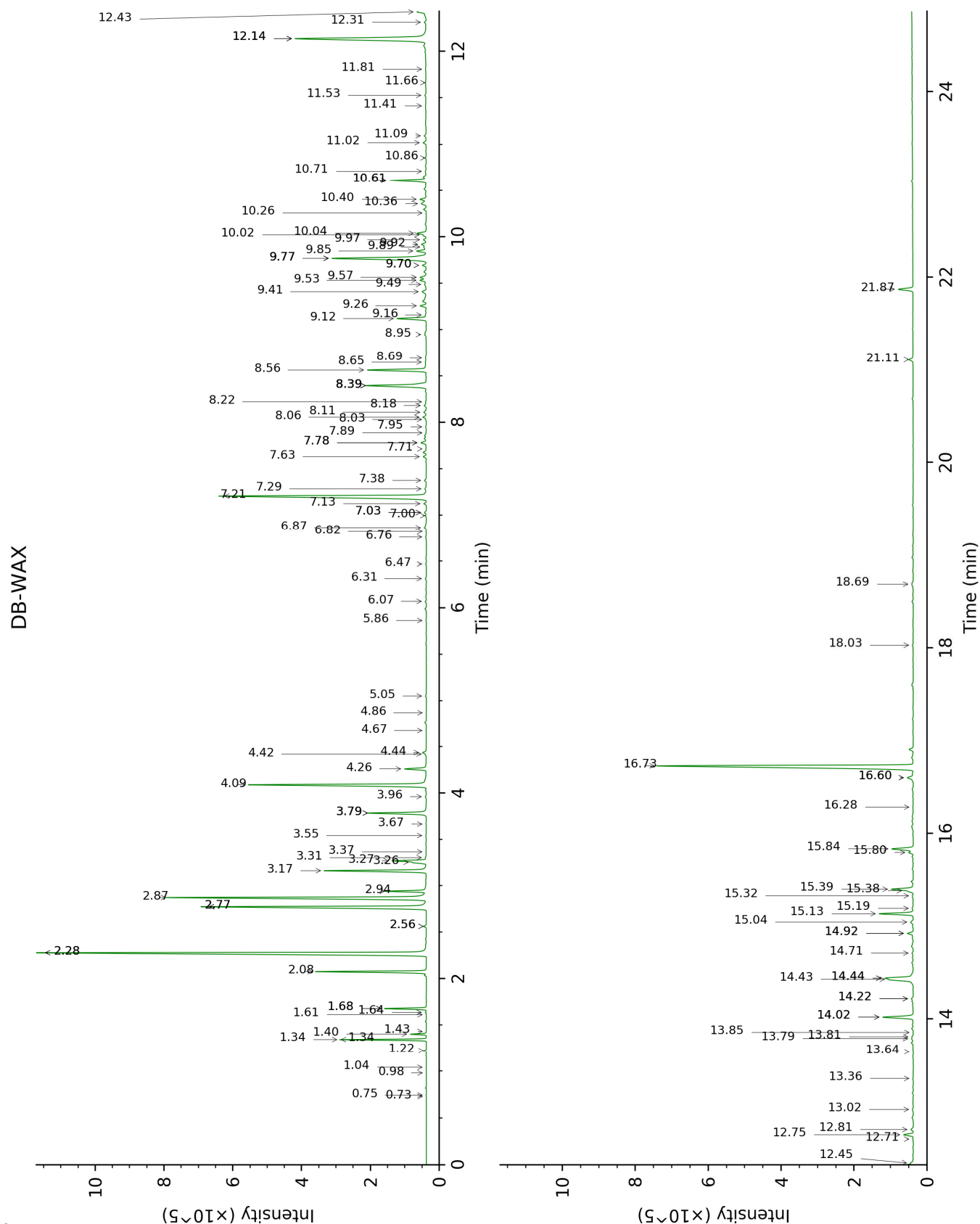
Note: no correction factor was applied

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	0.60	641	tr	0.75	887	tr
2-Methylbutyral	0.62	651	tr	0.73	882	tr
Toluene	1.14	760	tr	1.43	1004	tr
Unknown [m/z 73, 41 (54), 87 (50), 56 (47), 54 (29), 55 (25), 100 (23)... 115? (6)]	1.25	774	tr	0.98	933	tr
Unknown [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.30	782	tr	1.04	943	tr
Ethyl 2-methylbutyrate	2.00	849	0.02	1.64	1024	0.02
Propyl isobutyrate	2.05	853	0.01	1.68*	1028	0.90
Hashishene	2.83	914	0.01	1.34*	992	1.64
Tricyclene	2.87	917	0.05	1.22	972	0.05
α -Thujene	2.99	924	0.31	1.40	1001	0.30
Ethyl tiglate?	3.02	927	0.01	3.55	1187	0.01
α -Pinene	3.06	929	1.61	1.34*	992	[1.64]
Camphene	3.25*	942	0.90	1.68*	1028	[0.90]
α -Fenchene	3.25*	942	[0.90]	1.61	1021	tr
Propyl 2-methylbutyrate	3.31	946	0.06	2.56*	1111	0.07
Thuja-2,4(10)-diene	3.34	948	0.01	2.28*	1086	12.84
Propyl isovalerate	3.37	950	0.01	2.77*	1127	7.02
Sabinene	3.68*	970	15.25	2.28*	1086	[12.84]
β -Pinene	3.68*	970	[15.25]	2.08	1067	2.72
6-Methyl-5-hepten-2-one	3.91	985	0.03	5.05	1297	0.03
2-Pentylfuran	4.01*	992	8.00	3.67	1197	0.01
Myrcene	4.01*	992	[8.00]	2.87	1135	8.03
α -Phellandrene	4.15*	1001	7.06	2.77*	1127	[7.02]
Menthatriene isomer I	4.15*	1001	[7.06]	3.37	1174	0.01
Octanal	4.17	1002	0.04	4.42	1251	0.03
Δ 3-Carene	4.19	1004	0.01	2.56*	1111	[0.07]
α -Terpinene	4.33	1013	0.96	2.94	1140	1.06
Isoamyl isobutyrate	4.37	1015	0.01	3.31	1169	0.02
para-Cymene	4.46	1021	5.63	4.09	1228	5.52
1,8-Cineole	4.53*	1025	4.06	3.27	1166	0.94
β -Phellandrene	4.53*	1025	[4.06]	3.26	1165	0.27
Limonene	4.53*	1025	[4.06]	3.17	1158	2.83
(Z)- β -Ocimene	4.74	1038	0.02	3.79*	1206	1.73
Butyl 2-methylbutyrate	4.80	1043	0.03	3.79*	1206	[1.73]
Butyl isovalerate	4.90*	1048	0.06			
(E)- β -Ocimene	4.90*	1048	[0.06]	3.96	1218	0.04
γ -Terpinene	5.01	1056	1.68	3.79*	1206	[1.73]
Prenyl isobutyrate	5.07	1059	0.01	4.86	1283	0.01
cis-Sabinene hydrate	5.13	1063	0.03	6.82	1426	0.02
Octanol	5.30	1074	0.06	8.18	1527	0.09
Terpinolene	5.47*	1085	0.67	4.26	1240	0.68
para-Cymenene	5.47*	1085	[0.67]	6.31	1389	0.04

6,7-Epoxygeranyl	5.58	1092	0.05	6.07	1371	0.04
<i>trans</i> -Sabinene hydrate	5.62	1094	0.02	7.95	1510	0.03
Linalool	5.71	1100	0.11	8.06	1518	0.12
Nonanal	5.76	1103	0.01	5.86	1356	0.02
2-Methylbutyl 2-methylbutyrate	5.78	1105	0.14	4.44	1252	0.14
Amyl isovalerate	5.86	1110	0.02	4.67	1270	0.02
Unknown [m/z 71, 43 (95), 81 (82), 79 (73), 67 (67), 41 (49), 109 (14)...	5.95	1116	0.06	6.87	1429	0.07
<i>cis</i> -para-Menth-2-en-1-ol	5.98	1118	0.13	8.11	1522	0.10
α -Campholenal	6.02	1120	0.05	7.00	1439	0.03
Limona ketone	6.10	1126	0.20	7.78*†	1497	0.26
Camphor	6.28*	1137	8.18	7.21	1454	7.97
<i>trans</i> -Pinocarveol	6.28*	1137	[8.18]	9.16	1603	0.04
α ,4-Dimethyl-3-cyclohexene-1-methanol	6.42	1147	0.14			
Sabinaketone	6.49	1151	0.04	8.69	1567	0.05
Pinocarpone	6.62	1159	0.02	7.89	1505	0.02
Borneol	6.66	1162	1.66	9.77*	1652	3.80
Unknown [m/z 95, 110 (38), 81 (21), 79 (16)... 152 (7)]	6.73	1167	0.14	7.63	1486	0.10
Unknown [m/z 95, 110 (43), 81 (28), 41 (15)... 152 (8)]	6.78	1170	0.01	7.72	1492	0.02
Terpinen-4-ol	6.85	1174	1.88	8.56	1557	1.87
Unknown [m/z 69, 68 (65), 110 (51), 67 (39), 41 (27), 83 (26)...	6.92	1180	0.07			
para-Cymen-8-ol	6.98	1183	0.03	11.53	1799	0.04
α -Terpineol	7.06*	1189	0.23	9.77*	1652	[3.80]
Myrtenal	7.06*	1189	[0.23]	8.65	1563	0.04
Myrtenol	7.14*	1194	0.08	10.86	1742	0.02
Unknown [m/z 79, 107 (72), 41 (58), 55 (47), 77 (41), 67 (41)...	7.14*	1194	[0.08]			
α -Phellandrene epoxide	7.21	1199	0.11	11.02	1756	0.12
Decanal	7.34	1207	0.08	7.29	1460	0.07
<i>trans</i> -Carveol	7.49	1217	0.02	11.42	1789	0.02
Unknown [m/z 93, 41 (68), 79 (67), 91 (66), 92 (57), 67 (42), 77 (41)... 150 (12)]	7.53	1220	0.06			
(3Z)-Hexenyl 2-methylbutyrate	7.75†	1236	0.22	7.03*	1441	0.07
Cuminal	7.77*†	1237	[0.22]	10.61*	1721	1.21
Hexyl 2-methylbutyrate	7.77*†	1237	[0.22]	6.47	1401	0.03
Carvotanacetone	7.87	1244	0.14	9.49	1630	0.10
Piperitone	7.97	1251	0.06	9.89†	1662	0.29
Phellandral	8.26	1270	0.07	9.97	1668	0.11
α -Terpinen-7-al	8.40	1279	0.05	10.71	1730	0.05

Anthemol?	8.43	1281	0.01			
Bornyl acetate	8.49	1285	0.03	8.22	1530	0.03
Cuminol	8.58	1291	0.06	14.22*†	2044	0.12
Thymol	8.72	1300	0.95	15.13	2133	1.04
Carvacrol	8.84	1308	0.09	15.38	2158	0.15
6-Hydroxycarvotanacetone	8.94	1315	0.03	11.66	1811	0.02
1,4-para-Menthadien-7-ol	9.13	1328	0.06	13.79	2002	0.06
Bicycloelemene	9.22	1335	0.01	7.03*	1441	[0.07]
α-Terpinyl acetate	9.39	1346	0.01	9.70*	1646	0.14
α-Cubebene	9.44	1350	0.03	6.76	1421	0.04
Modhephene	9.72	1370	0.04	7.38	1467	0.06
α-Copaene	9.78*	1374	0.09	7.13	1448	0.07
Methyl para-anisate	9.78*	1374	[0.09]	13.85	2009	0.01
(E)-β-Damascenone	9.89	1381	0.07	11.09	1762	0.07
7-epi-Sesquithujene?	9.93	1384	0.04	7.78*†	1497	[0.26]
β-Elemene	10.03*	1391	0.32	8.40*	1544	2.30
Benzyl isovalerate	10.03*	1391	[0.32]	11.81	1823	0.03
α-Cedrene	10.19	1402	0.03	8.03	1516	0.02
β-Caryophyllene	10.36	1414	2.11	8.40*	1544	[2.30]
β-Copaene	10.53	1427	0.11	8.40*	1544	[2.30]
Octyl 2-methylbutyrate	10.57	1430	0.11	8.95	1587	0.07
trans-α-Bergamotene	10.64	1435	0.14	8.40*	1544	[2.30]
Sesquisabinene A	10.74	1442	1.01	9.12	1600	0.94
α-Humulene	10.81	1448	0.25	9.26	1611	0.20
(E)-β-Farnesene	10.97	1459	0.20	9.53	1633	0.22
4,5-diepi-Aristolochene	11.04	1464	0.13	9.41	1623	0.19
Dehydrosesquicineole	11.08	1468	0.06	10.02†	1673	0.40
γ-Murolene	11.16	1474	0.15	9.57	1636	0.24
Germacrene D	11.19	1476	1.90	9.77*	1652	[3.80]
ar-Curcumene	11.25*†	1480	0.93	10.61*	1721	[1.21]
γ-Curcumene	11.25*†	1480	[0.93]	9.70*	1646	[0.14]
β-Selinene	11.25*†	1480	[0.93]	9.85	1658	0.33
Phenylethyl isovalerate	11.28†	1483	[0.93]	13.02	1932	0.05
Bicyclogermacrene	11.40*	1491	0.60	10.04†	1674	[0.40]
Phenylethyl 2-methylbutyrate	11.40*	1491	[0.60]	12.81	1912	0.09
δ-Guaiene	11.50	1499	0.27	9.92†	1664	[0.29]
γ-Cadinene	11.66*	1510	5.56	10.36	1700	0.24
3,6-Dihydrochamazulene	11.66*	1510	[5.56]	12.14*	1852	6.18
β-Curcumene	11.66*	1510	[5.56]	10.26	1692	0.01
Dihydrochamazulene isomer I	11.69	1513	0.95	12.14*	1852	[6.18]
δ-Cadinene	11.79	1521	0.27	10.40	1704	0.22
β-Sesquiphellandrene	11.81*	1522	1.25	10.61*	1721	[1.21]
Dihydrochamazulene isomer II	11.81*	1522	[1.25]	12.43	1878	0.36
Dihydrochamazulene isomer III	11.87	1527	0.10	12.31	1868	0.06
Phenylethyl angelate?	11.96	1534	0.05	14.22*†	2044	[0.12]
Isocaryophyllene	12.06	1542	0.03	12.14*	1852	[6.18]

epoxide B						
α-Elemol	12.10	1545	0.08	14.02*	2025	1.05
(E)-Nerolidol	12.34	1564	0.02	13.81	2004	0.04
Spathulenol	12.44	1572	0.38	14.42†	2064	1.71
Caryophyllene oxide isomer	12.46*	1574	0.45	12.71	1903	0.03
Caryophyllene oxide	12.46*	1574	[0.45]	12.75	1907	0.32
Humulene epoxide II	12.80	1600	0.04	13.36	1962	0.02
Junenol	12.90*	1608	0.89	13.64	1989	0.01
5,6-Dihydrochamazulene	12.90*	1608	[0.89]	14.44*†	2065	[1.71]
Unknown [m/z 145, 173 (83), 159 (57), 174 (47), 129 (47), 115 (44), 128 (43), 91 (43), 157 (36), 202 (30)]	13.07*	1622	1.27			
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	13.07*	1622	[1.27]	14.02*	2025	[1.05]
γ-Eudesmol	13.14	1628	0.05	14.92*	2112	0.20
Eremoligenol	13.19	1631	0.08	15.04	2124	0.12
τ-Cadinol	13.24	1636	0.08	14.92*	2112	[0.20]
α-Muurolol	13.31*	1641	0.72	15.19	2139	0.05
β-Eudesmol	13.31*	1641	[0.72]	15.39	2160	0.74
α-Eudesmol	13.35*†	1645	0.98	15.32	2152	0.03
Dihydrochamazulene isomer IV	13.35*†	1645	[0.98]	14.44*†	2065	[1.71]
(3E,5E)-7-Hydroxyfarnesene	13.56	1662	0.05	16.28	2250	0.02
Unknown [m/z 143, 142 (92), 157 (79), 158 (61), 141 (59), 128 (57), 159 (43), 115 (41), 202 (41)]	14.05	1703	0.12	18.69	2513	0.11
Chamazulene	14.25	1720	10.38	16.73	2297	10.53
α-Phellandrene dimer II	15.04	1788	0.08	12.45	1880	0.08
Dehydrochamazulene	15.23	1805	0.03	18.03	2439	0.04
Phytone	15.68	1846	0.05	14.71	2091	0.05
9-(15,16-Dihydro-15-methyleneneryl)-α-terpinene?	17.32*	2000	0.22	15.80	2200	0.15
9-(15,16-Dihydro-15-methyleneneryl)-para-cymene?	17.32*	2000	[0.22]	16.60*	2283	0.23
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	17.40*	2008	0.97	15.84	2204	0.78
9-(15,16-Dihydro-15-methylenegeranyl)-para-cymene	17.40*	2008	[0.97]	16.60*	2283	[0.23]
Unknown analog I	21.25	2420	0.15	21.11	2805	0.18
Unknown [m/z 186, 157 (37), 171 (18), 322 (15)]	21.84	2490	0.53	21.87	2903	0.51
Total identified	95.20%			93.78%		

Total reported	96.35%	94.78%
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*: 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