

Date : April 08, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21C23-PTH02

Customer identification : Magnolia Flower - China - MQ0102206R

Type : Essential oil

Source : *Michelia x alba*

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 : Seydou Ka, M. Sc.

Analysis date : April 08, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Dark orange liquid

Refractive index: 1.4662 ± 0.0003 (20 °C; method PC-MAT-016)

ISO 17382:2007 - OIL OF MAGNOLIA FLOWER, CHINA TYPE

Compound	Min. %	Max. %	Observed %	Complies?
Methyl 2-methylbutyrate	0.7	6.3	5.7	Yes
1,8-Cineole	0.3	0.8	0.3	Yes
(E)-β-Ocimene	1.1	3.4	2.2	Yes
(Z)-β-Ocimene	0.9	2.4	1.7	Yes
α-Copaene	0.1	0.8	0.4	Yes
Linalool	50.0	72.0	61.2	Yes
β-Elemene	2.1	10.0	2.9	Yes
β-Caryophyllene	1.2	7.0	3.5	Yes
δ-Cadinene	0.3	2.5	1.0	Yes
Nerol	0.001	0.300	0.116	Yes
Methyleugenol	1.2	4.4	2.1	Yes
(E)-Nerolidol	0.2	0.6	0.4	Yes
Methyl (E)-isoeugenol	0.3	1.8	0.5	Yes
Refractive index	1.4650	1.4900	1.4662	Yes

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
Ethanol	tr	Aliphatic alcohol
Isobutyral	tr	Aliphatic aldehyde
Methyl propionate	0.06	Aliphatic ester
1,3-Cyclohexadiene	tr	Alkene
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	0.05	Aliphatic aldehyde
Methyl isobutyrate	0.01	Aliphatic ester
2-Methylbutanenitrile	0.01	Aliphatic nitrile
Methyl butyrate	0.07	Aliphatic ester
Isoamyl alcohol	0.02	Aliphatic alcohol
2-Methylbutanol	0.06	Aliphatic alcohol
Methyl 2-methylbutyrate	5.67	Aliphatic ester
Ethyl 2-methylbutyrate	tr	Aliphatic ester
Methyl tiglate	0.10	Aliphatic ester
Isovaleric acid	0.40*	Aliphatic acid
Hexanol	0.01	Aliphatic alcohol
2-Methylbutyric acid	[0.40]*	Aliphatic acid
2-Heptanone	0.01	Aliphatic ketone
Heptanal	0.01	Aliphatic aldehyde
Methyl hexanoate	0.03	Aliphatic ester
α -Thujene	tr	Monoterpene
α -Pinene	0.14	Monoterpene
Camphene	0.05	Monoterpene
Sabinene	tr	Monoterpene
β -Pinene	0.40	Monoterpene
6-Methyl-5-hepten-2-one	tr	Aliphatic ketone
Myrcene	0.08	Monoterpene
(3Z)-Hexenyl acetate	tr	Aliphatic ester
α -Terpinene	0.03	Monoterpene
Caproic acid	0.04	Aliphatic acid
para-Cymene	0.03	Monoterpene
Limonene	0.02	Monoterpene
1,8-Cineole	0.34	Monoterpenic ether
(Z)- β -Ocimene	1.68	Monoterpene
(E)- β -Ocimene	2.22	Monoterpene
γ -Terpinene	0.04	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.12	Monoterpenic alcohol
trans-Linalool oxide (fur.)	0.16	Monoterpenic alcohol
Terpinolene	0.04	Monoterpene
Methyl benzoate	0.03	Phenolic ester
trans-Sabinene hydrate	0.01	Monoterpenic alcohol
Rosefuran	0.01	Monoterpenic ether
Hotrienol	0.09	Monoterpenic alcohol
Linalool	61.17	Monoterpenic alcohol

endo-Fenchol	0.08	Monoterpenic alcohol
Phenylethyl alcohol	0.26	Simple phenolic
Methyl octanoate	0.02	Aliphatic ester
allo-Ocimene	0.04	Monoterpene
(Z)-Myroxide	0.01	Monoterpenic ether
Camphor	0.03	Monoterpenic ketone
Camphene hydrate	0.01	Monoterpenic alcohol
Nerol oxide	0.01	Aliphatic ether
Borneol	0.05	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.08	Monoterpenic alcohol
trans-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
α-Terpineol	0.52	Monoterpenic alcohol
Methylchavicol	0.08	Phenylpropanoid
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	tr	Monoterpenic alcohol
Nerol	0.12	Monoterpenic alcohol
Phenylethyl acetate	0.06	Phenolic ester
Geraniol	0.33	Monoterpenic alcohol
Undec-(5Z)-en-2-one	0.03	Aliphatic ketone
Safrole	0.07	Phenylpropanoid
Indole	0.06	Indole
1-Nitro-2-phenylethane	0.03	Simple phenolic
Methyl anthranilate	0.02	Phenolic ester
α-Cubebene	0.13	Sesquiterpene
Hodiendiol derivative III	0.02	Oxygenated monoterpene
α-Copaene	0.37	Sesquiterpene
cis-β-Elemene	0.10	Sesquiterpene
β-Elemene	2.85	Sesquiterpene
Methyleugenol	2.10	Phenylpropanoid
β-Caryophyllene	3.52	Sesquiterpene
cis-α-Bergamotene	0.07	Sesquiterpene
α-Santalene	0.08	Sesquiterpene
β-Copaene	0.04	Sesquiterpene
α-Guaiene	0.20*	Sesquiterpene
trans-α-Bergamotene	[0.20]*	Sesquiterpene
Phenylethyl butyrate	0.05	Phenolic ester
α-Humulene	1.27	Sesquiterpene
allo-Aromadendrene	0.02	Sesquiterpene
(E)-β-Farnesene	0.05	Sesquiterpene
trans-Cadina-1(6),4-diene	0.06	Sesquiterpene
Selina-4,11-diene	0.36	Sesquiterpene
γ-Murolene	0.09	Sesquiterpene
Germacrene D	0.68*	Sesquiterpene
α-Amorphene	[0.68]*	Sesquiterpene
Unknown	0.03	Sesquiterpene
β-Selinene	1.39	Sesquiterpene
Phenylethyl isovalerate	0.20	Phenolic ester
Valencene	0.05	Sesquiterpene
α-Selinene	1.20	Sesquiterpene
epi-Cubebol	0.03	Sesquiterpenic alcohol
α-Murolene	0.12	Sesquiterpene
Methyl (E)-isoeugenol	0.49	Phenylpropanoid

Germacrene A	0.29	Sesquiterpene
δ-Guaiene	0.05	Sesquiterpene
β-Bisabolene	0.30	Sesquiterpene
γ-Cadinene	0.07	Sesquiterpene
Cubebol	0.04	Sesquiterpenic alcohol
(3E,6E)-α-Farnesene	0.14	Sesquiterpene
Unknown	0.02	Sesquiterpene
<i>trans</i> -Calamenene	0.04	Sesquiterpene
δ-Cadinene	0.97	Sesquiterpene
Zonarene	0.01	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.18	Sesquiterpene
α-Cadinene	0.03	Sesquiterpene
α-Calacorene	0.05	Sesquiterpene
Isocaryophyllene epoxide B	0.07	Sesquiterpenic ether
α-Elemol	0.04	Sesquiterpenic alcohol
Elemicin	0.03	Phenylpropanoid
(E)-Nerolidol	0.37	Sesquiterpenic alcohol
Caryophyllene oxide	0.40	Sesquiterpenic ether
Viridiflorol	0.02	Sesquiterpenic alcohol
Humulene epoxide II	0.10	Sesquiterpenic ether
Unknown	0.12	Oxygenated sesquiterpene
Junenol	0.04	Sesquiterpenic alcohol
1-epi-Cubenol	0.12	Sesquiterpenic alcohol
τ-Muurolol	0.30	Sesquiterpenic alcohol
τ-Cadinol	0.33	Sesquiterpenic alcohol
Phenylethyl hexanoate	0.32	Phenolic ester
Selin-11-en-4α-ol	0.46	Sesquiterpenic alcohol
α-Cadinol	0.07	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	0.16	Sesquiterpenic alcohol
Germacra-4(15),5,10(14)-trien-1β-ol?	0.01	Sesquiterpenic alcohol
Unknown	0.05	Lignan
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.17	Aliphatic ester
Unknown	0.21	Aliphatic ester
Nonadecane	0.02	Alkane
Methyl palmitate	0.04	Aliphatic ester
Eicosane	0.01	Alkane
Methyl linoleate	0.43	Aliphatic ester
Methyl α-linolenate	0.25	Aliphatic ester
Heneicosane	0.03	Alkane
Docosane	0.01	Alkane
Tricosane	0.03	Alkane
Consolidated total	97.24%	

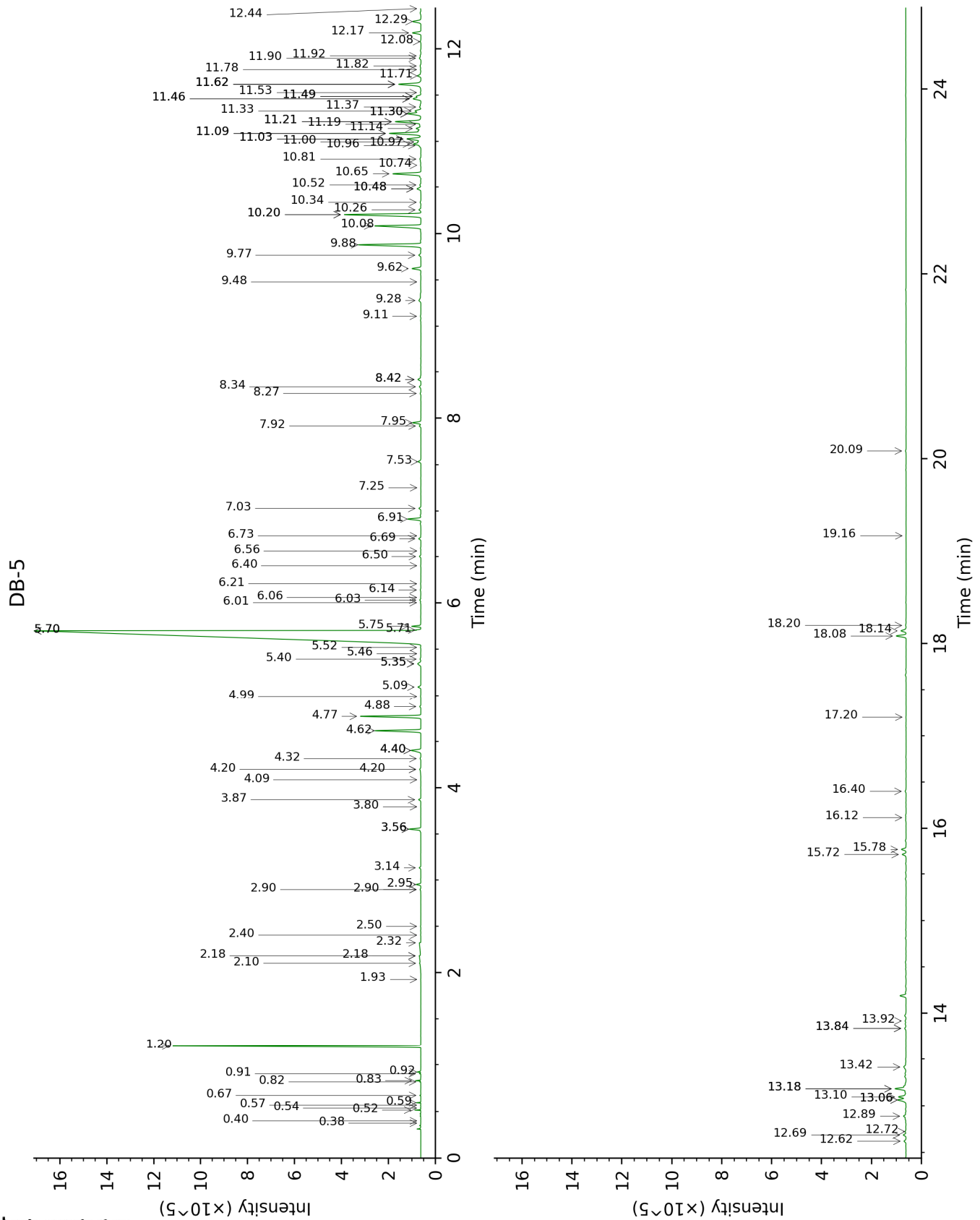
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

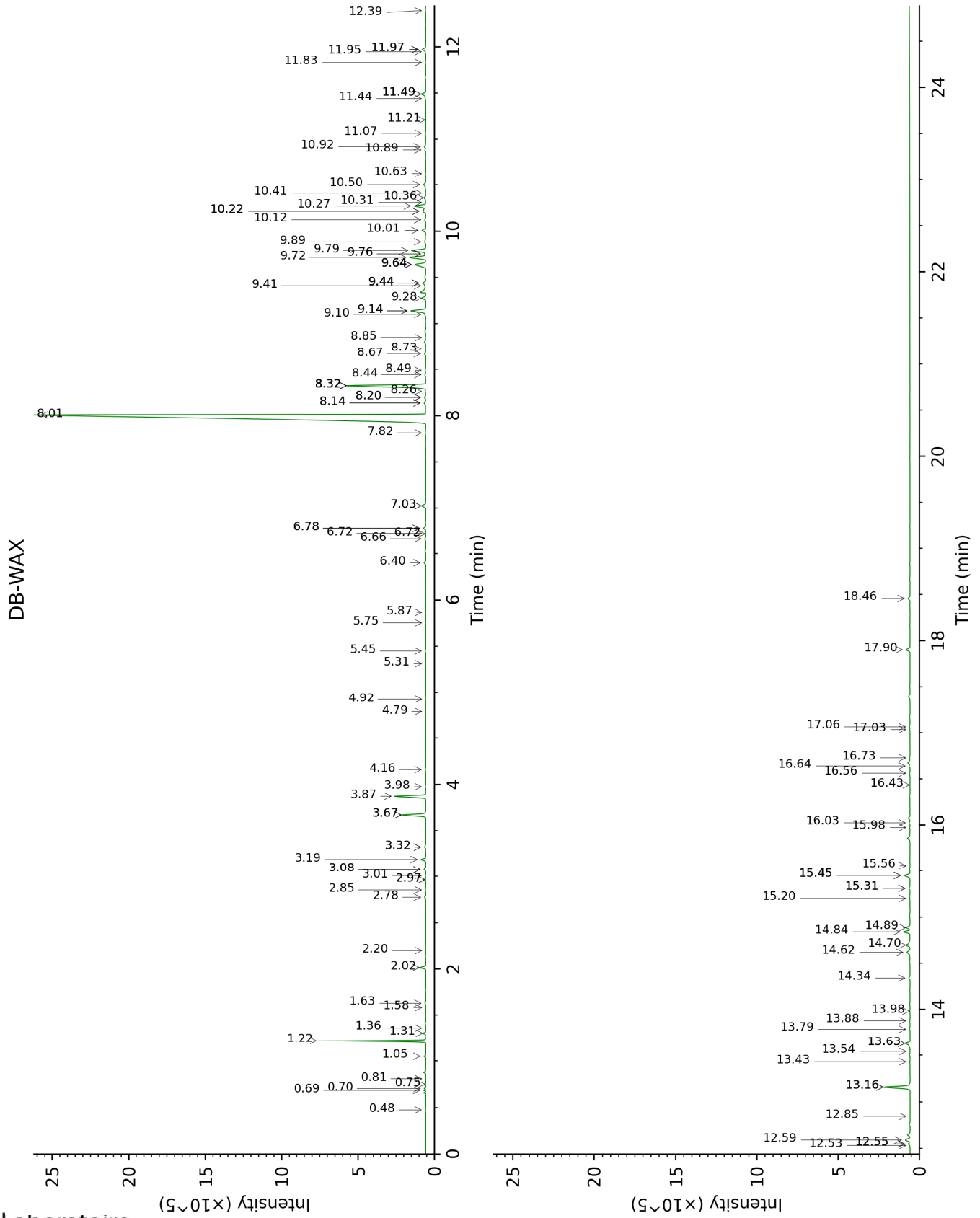
Note: no correction factor was applied

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	%
Ethanol	0.38	513	tr	0.81	908	tr
Isobutyral	0.40	536	tr	0.48	784	0.02
Methyl propionate	0.52	620	0.06	0.69	872	0.05
1,3-Cyclohexadiene	0.54	628	tr			
Isovaleral	0.57	640	tr			
2-Methylbutyral	0.59	650	0.05	0.70	879	0.04
Methyl isobutyrate	0.67	680	0.01	0.75	897	0.01
2-Methylbutanenitrile	0.82	717	0.01			
Methyl butyrate	0.83	719	0.07	1.05	949	0.08
Isoamyl alcohol	0.91	730	0.02	3.32*	1177	0.10
2-Methylbutanol	0.92	733	0.06	3.32*	1177	[0.10]
Methyl 2-methylbutyrate	1.20	775	5.67	1.22	978	5.60
Ethyl 2-methylbutyrate	1.93	850	tr	1.58	1023	tr
Methyl tiglate	2.10	865	0.10	3.08*	1158	0.12
Isovaleric acid	2.18*†	872	0.41	9.44*	1637	0.28
Hexanol	2.18*†	872	[0.41]	5.31	1323	0.01
2-Methylbutyric acid	2.32†	884	[0.41]	9.64*	1653	1.24
2-Heptanone	2.40	891	0.01	2.97*	1149	0.02
Heptanal	2.50	900	0.01	2.97*	1149	[0.02]
Methyl hexanoate	2.90*	927	0.03	3.01	1152	0.03
α-Thujene	2.90*	927	[0.03]	1.36	1001	tr
α-Pinene	2.95	931	0.14	1.31	992	0.16
Camphene	3.14	944	0.05	1.63	1028	0.05
Sabinene	3.56*	972	0.40	2.20	1085	tr
β-Pinene	3.56*	972	[0.40]	2.02	1067	0.40
6-Methyl-5-hepten-2-one	3.80	988	tr	4.92	1295	0.02
Myrcene	3.87	993	0.08	2.78	1134	0.08
(3Z)-Hexenyl acetate	4.09	1008	tr	4.79	1285	0.01
α-Terpinene	4.20*	1015	0.08	2.86	1140	0.03
Caproic acid	4.20*	1015	[0.08]	11.44	1805	0.04
para-Cymene	4.32	1022	0.03	3.98	1226	0.03
Limonene	4.40*	1028	0.46	3.08*	1158	[0.12]
1,8-Cineole	4.40*	1028	[0.46]	3.19	1167	0.34
(Z)-β-Ocimene	4.62	1041	1.68	3.67*	1204	1.69
(E)-β-Ocimene	4.77	1051	2.22	3.87	1219	2.16
γ-Terpinene	4.88	1058	0.04	3.67*	1204	[1.69]
cis-Sabinene hydrate	4.99	1065	0.01	6.78*	1430	0.18
cis-Linalool oxide (fur.)	5.09	1071	0.12	6.40	1402	0.13
trans-Linalool oxide (fur.)	5.35*	1087	0.20	6.78*	1430	[0.18]

Terpinolene	5.35*	1087	[0.20]	4.16	1240	0.04
Methyl benzoate	5.40	1090	0.03	8.49	1561	0.06
<i>trans</i> -Sabinene hydrate	5.46	1094	0.01	7.82	1508	0.06
Rosefuran	5.52	1099	0.01	5.87	1363	0.01
Hotrienol	5.70*	1110	61.72	8.67	1575	0.09
Linalool	5.70*	1110	[61.72]	8.01	1523	61.17
endo-Fenchol	5.71	1110	0.08	8.20*	1538	0.10
Phenylethyl alcohol	5.75	1113	0.26	11.97*	1852	0.31
Methyl octanoate	6.01	1130	0.02	5.76	1355	0.01
allo-Ocimene	6.03	1131	0.04	5.45	1333	0.04
(<i>Z</i>)-Myroxide	6.06	1133	0.01	6.72	1426	0.01
Camphor	6.14	1138	0.03	7.03*	1449	0.38
Camphene hydrate	6.21	1143	0.01	8.32*	1548	6.55
Nerol oxide	6.40	1155	0.01	6.72	1426	0.01
Borneol	6.50	1162	0.05	9.64*	1653	[1.24]
<i>cis</i> -Linalool oxide (pyr.)	6.56	1165	0.01	10.12	1693	0.09
Terpinen-4-ol	6.69	1174	0.08	8.44	1557	0.07
<i>trans</i> -Linalool oxide (pyr.)	6.73	1176	0.01	10.41	1717	0.02
α -Terpineol	6.91	1188	0.52	9.64*	1653	[1.24]
Methylchavicol	7.03	1195	0.08	9.14*	1612	1.29
(<i>3E,5E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.25	1210	tr	11.21	1785	tr
Nerol	7.53	1229	0.12	10.92	1760	0.11
Phenylethyl acetate	7.92	1255	0.06	10.89	1757	0.06
Geraniol	7.95	1257	0.33	11.49*	1809	0.40
Undec-(<i>5Z</i>)-en-2-one	8.27	1278	0.03	8.73	1579	0.03
Safrole	8.34	1283	0.07	11.49*	1809	[0.40]
Indole	8.42*	1288	0.14	17.06	2354	0.06
1-Nitro-2-phenylethane	8.42*	1288	[0.14]	13.98	2039	0.03
Methyl anthranilate	9.11	1336	0.02	15.20	2159	0.04
α -Cubebene	9.28	1348	0.13	6.66	1422	0.08
Hodiendiol derivative III	9.48	1362	0.02	12.55*	1904	0.13
α -Copaene	9.62	1373	0.37	7.03*	1449	[0.38]
<i>cis</i> - β -Elemene	9.77	1383	0.10	8.20*	1538	[0.10]
β -Elemene	9.88	1391	2.85	8.32*	1548	[6.55]
Methyleugenol	10.08	1405	2.10	13.16*	1961	2.08
β -Caryophyllene	10.20*	1414	3.59	8.32*	1548	[6.55]
<i>cis</i> - α -Bergamotene	10.20*	1414	[3.59]	8.14*	1534	0.16
α -Santalene	10.26	1418	0.08	8.14*	1534	[0.16]
β -Copaene	10.34	1424	0.04	8.26	1543	0.04
α -Guaiene	10.48*	1435	0.20	8.32*	1548	[6.55]
<i>trans</i> - α -Bergamotene	10.48*	1435	[0.20]	8.32*	1548	[6.55]
Phenylethyl butyrate	10.52	1438	0.05	12.55*	1904	[0.13]

α-Humulene	10.65	1448	1.27	9.14*	1612	[1.29]
allo-Aromadendrene	10.74	1455	0.02	8.85	1589	0.03
(E)-β-Farnesene	10.81	1460	0.05	9.41	1634	0.08
trans-Cadina-1(6),4-diene	10.96	1471	0.06	9.10	1609	0.06
Selina-4,11-diene	10.97	1472	0.36	9.28	1624	0.34
γ-Murolene	11.00	1474	0.09	9.44*	1637	[0.28]
Germacrene D	11.03*	1476	0.68	9.64*	1653	[1.24]
α-Amorphene	11.03*	1476	[0.68]	9.44*	1637	[0.28]
Unknown [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	11.09*	1480	1.42	9.44*	1637	[0.28]
β-Selinene	11.09*	1480	[1.42]	9.72	1660	1.39
Phenylethyl isovalerate	11.14	1484	0.20	12.85	1932	0.01
Valencene	11.19	1488	0.05	9.76*	1663	0.06
α-Selinene	11.21*	1490	1.20	9.79	1666	1.20
epi-Cubebol	11.21*	1490	[1.20]	11.83	1840	0.03
α-Murolene	11.30*	1496	0.62	9.89	1673	0.12
Methyl (E)-isoeugenol	11.30*	1496	[0.62]	14.84	2123	0.49
Germacrene A	11.33	1498	0.29	10.22*	1700	0.36
δ-Guaiene	11.37	1502	0.05	9.76*	1663	[0.06]
β-Bisabolene	11.46*	1508	0.38	10.01	1683	0.30
γ-Cadinene	11.46*	1508	[0.38]	10.22*	1700	[0.36]
Cubebol	11.49*	1510	0.20	12.39	1890	0.04
(3E,6E)-α-Farnesene	11.49*	1510	[0.20]	10.36	1713	0.14
Unknown [m/z 161, 81 (93), 105 (66), 93 (60), 119 (60), 204 (54)...]	11.53	1514	0.02			
trans-Calamenene	11.62*	1521	1.13	11.07	1773	0.04
δ-Cadinene	11.62*	1521	[1.13]	10.27	1705	0.97
Zonarene	11.62*	1521	[1.13]	10.31	1708	0.01
trans-Cadina-1,4-diene	11.71	1528	0.18	10.50	1725	0.18
α-Cadinene	11.78	1533	0.03	10.63	1736	0.02
α-Calacorene	11.82	1536	0.05	11.95	1850	0.03
Isocaryophyllene epoxide B	11.90	1543	0.07	11.97*	1852	[0.31]
α-Elemol	11.92	1545	0.04	13.88	2029	0.05
Elemicin	12.08	1557	0.03	15.31*	2170	0.10
(E)-Nerolidol	12.17	1564	0.37	13.63*	2004	0.37
Caryophyllene oxide	12.29	1574	0.40	12.59	1908	0.43
Viridiflorol	12.44	1585	0.02	13.79	2020	0.05
Humulene epoxide II	12.62	1600	0.10	13.16*	1961	[2.08]
Unknown [m/z 43, 81 (97), 135 (71), 95	12.69	1605	0.12	14.34	2073	0.10

(62), 204 (61), 71 (59), 207 (56)... 222 (3)]						
Junenol	12.72	1608	0.04	13.43	1986	0.03
1-epi-Cubenol	12.89	1622	0.12	13.63*	2004	[0.37]
τ-Muurolol	13.06*	1636	0.40	14.89	2127	0.30
τ-Cadinol	13.06*	1636	[0.40]	14.70	2108	0.33
Phenylethyl hexanoate	13.10	1639	0.32			
Selin-11-en-4α-ol	13.18*	1646	0.48	15.45*	2184	0.50
α-Cadinol	13.18*	1646	[0.48]	15.31*	2170	[0.10]
(3Z)-Caryophylla- 3,8(13)-dien-5β-ol	13.42	1666	0.16	16.64	2308	0.08
Germacra- 4(15),5,10(14)-trien- 1β-ol?	13.84*	1700	0.07	16.44	2286	0.01
Unknown [m/z 133, 93 (97), 131 (85), 145 (83), 107 (69)...220]	13.84*	1700	[0.07]	16.73	2317	0.05
Unknown [m/z 93, 81 (90), 95 (86), 91 (83), 41 (83), 107 (81)... 220 (29), 238? (4)]	13.92	1707	0.04	17.03	2350	0.03
Unknown [m/z 43, 67 (85), 81 (70), 79 (53), 95 (46), 55 (39), 41 (37)...]	15.72	1867	0.17	15.98	2238	0.03
Unknown [m/z 79, 43 (84), 67 (55), 93 (50), 95 (41), 80 (35)...]	15.78	1872	0.21	16.03	2244	0.07
Nonadecane	16.12	1903	0.02	12.53	1902	0.03
Methyl palmitate	16.40	1930	0.04	15.45*	2184	[0.50]
Eicosane	17.20	2006	0.01	13.54	1996	0.01
Methyl linoleate	18.08	2094	0.43	17.90	2446	0.33
Methyl α-linolenate	18.14	2100	0.25	18.46	2509	0.17
Heneicosane	18.20	2106	0.03	14.62	2100	0.36
Docosane	19.16	2206	0.01	15.56	2195	0.01
Tricosane	20.09	2306	0.03	16.56	2300	0.05
Total identified		97.11%			95.58%	
Total reported		97.68%			95.86%	

*: 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