

Date : January 07, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21A05-PTH04


Customer identification : Geranium - Egypt - G30107206R

Type : Essential oil

Source : *Pelargonium graveolens* ct. Egyptian

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 : Benoit Roger, Ph. D.

Analysis date : January 07, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.4683 ± 0.0003 (20 °C; method PC-MAT-016)

ISO 4731:2012 - OIL OF GERANIUM - NORTH AFRICA

Compound	Min. %	Max. %	Observed %	Complies?
Phenylethyl tiglate	0.5	1.2	0.9	Yes
Geranyl tiglate	0.9	2.0	1.1	Yes
10-epi- γ -Eudesmol	3.0	6.2	4.9	Yes
Geranyl butyrate	0.7	2.0	1.0	Yes
Geraniol	10.0	18.0	13.7	Yes
Citronellol	25.0	36.0	31.1	Yes
Geranyl formate	2.0	7.0	2.5	Yes
α -Terpineol	0.3	0.6	0.3	Yes
Citronellyl formate	4.0	8.0	6.4	Yes
6,9-Guaiadiene		0.5	0.3	Yes
Linalool	4.0	8.5	3.8	No
Isomenthone	4.0	8.0	5.8	Yes
Menthone		2.1	0.6	Yes
trans-Rose oxide	0.3	0.6	0.5	Yes
cis-Rose oxide	0.7	1.5	1.2	Yes
Refractive index	1.4610	1.4750	1.4683	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
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Methylbutanol	0.01	Aliphatic alcohol
Dimethyl sulfoxide	0.01	Aliphatic sulfoxide
3-Methylpentanol	0.03	Aliphatic alcohol
α -Pinene	0.42	Monoterpene
Geranic oxide	0.04	Monoterpenic ether
Octen-3-ol	0.01	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.04	Monoterpenic ether
Myrcene	0.08	Monoterpene
α -Phellandrene	0.07	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
α -Terpinene	0.01	Monoterpene
para-Cymene	0.07	Monoterpene
Limonene	0.14	Monoterpene
Unknown	0.04	Unknown
Unknown	0.03	Unknown
β -Phellandrene	0.02	Monoterpene
1,8-Cineole	0.03	Monoterpenic ether
(<i>Z</i>)- β -Ocimene	0.09	Monoterpene
Unknown	0.02	Unknown
(<i>E</i>)- β -Ocimene	0.08	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.05	Aliphatic aldehyde
γ -Terpinene	0.03	Monoterpene
<i>cis</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.20	Monoterpenic alcohol
Fenchone	0.01	Monoterpenic ketone
Terpinolene	0.02	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.11	Monoterpenic alcohol
Linalool	3.83	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.11	Aliphatic ketone
<i>cis</i> -Rose oxide	1.17	Monoterpenic ether
Phenylethyl alcohol	0.02	Simple phenolic
<i>trans</i> -Rose oxide	0.50	Monoterpenic ether
Unknown	0.05	Unknown
Unknown	0.08	Oxygenated normonoterpene
Isopulegol	0.04	Monoterpenic alcohol
Menthone	0.62	Monoterpenic ketone
Unknown	0.05	Unknown
Citronellal	0.18	Monoterpenic aldehyde
iso-Isopulegol	0.02	Monoterpenic alcohol
Isomenthone	5.85	Monoterpenic ketone
neo-Menthol	0.02	Monoterpenic alcohol

Terpinen-4-ol	0.08	Monoterpenic alcohol
Menthol	0.02	Monoterpenic alcohol
Isomenthol	0.18	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
α -Terpineol	0.29	Monoterpenic alcohol
Unknown	0.02	Unknown
Unknown	0.04	Oxygenated monoterpene
β -Cyclocitral	0.03	Monoterpenic aldehyde
Nerol	0.21	Monoterpenic alcohol
Citronellol	31.06	Monoterpenic alcohol
Neral	0.29	Monoterpenic aldehyde
Piperitone	0.15	Monoterpenic ketone
Geraniol	13.71	Monoterpenic alcohol
Geranial	0.90	Monoterpenic aldehyde
Citronellyl formate	6.45	Monoterpenic ester
Neryl formate	0.10	Monoterpenic ester
Geranyl formate	2.54	Monoterpenic ester
(3Z)-Hexenyl tiglate	0.03	Aliphatic ester
Methyl geranate	0.02	Monoterpenic ester
α -Cubebene	0.23	Sesquiterpene
Citronellyl acetate	0.24	Monoterpenic ester
Phenylethyl propionate	0.04	Phenolic ester
Neryl acetate	0.08	Monoterpenic ester
α -Copaene	0.53	Sesquiterpene
Geranic acid	0.13	Aliphatic acid
β -Bourbonene	1.05	Sesquiterpene
1,5-diepi- β -Bourbonene	0.09	Sesquiterpene
Geranyl acetate	0.43	Monoterpenic ester
Phenylethyl isobutyrate	0.05	Phenolic ester
Isocaryophyllene	0.17	Sesquiterpene
α -Gurjunene	0.02	Sesquiterpene
β -Caryophyllene	1.25	Sesquiterpene
β -Copaene	0.13	Sesquiterpene
Heptyl tiglate	0.09	Aliphatic ester
6,9-Guaiadiene	0.29	Sesquiterpene
Aromadendrene	0.09	Sesquiterpene
Unknown	0.33	Sesquiterpene
Isogermacrene D	0.20	Sesquiterpene
Citronellyl propionate	0.41	Monoterpenic ester
α -Humulene	0.27	Sesquiterpene
allo-Aromadendrene	0.20	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.24	Sesquiterpene
Germacrene D	1.70	Sesquiterpene
γ -Murolene	0.70*	Sesquiterpene
α -Amorphene	[0.70]*	Sesquiterpene
Geranyl propionate	0.14	Monoterpenic ester
γ -Amorphene	0.21	Sesquiterpene
Bicyclogermacrene	0.67	Sesquiterpene
Viridiflorene	0.16	Sesquiterpene
4-epi- <i>cis</i> -Dihydroagarofuran	0.09	Sesquiterpenic ether
α -Murolene	0.21	Sesquiterpene
γ -Cadinene	0.35	Sesquiterpene

7-epi- α -Selinene	0.09	Sesquiterpene
δ -Cadinene	0.87	Sesquiterpene
<i>trans</i> -Calamenene	0.27	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.14	Sesquiterpene
Citronellyl butyrate	0.46	Monoterpenic ester
Phenylethyl angelate?	0.12	Phenolic ester
α -Agarofuran	0.39	Sesquiterpenic ether
1-nor-Bourbonanone	0.06	Norsesquiterpenic ketone
Geranyl butyrate	0.96	Monoterpenic ester
Spathulenol	0.27	Sesquiterpenic alcohol
Caryophyllene oxide	0.18	Sesquiterpenic ether
Globulol	0.12	Sesquiterpenic alcohol
Phenylethyl tiglate	0.94	Phenolic ester
Viridiflorol	0.10	Sesquiterpenic alcohol
Geranyl 2-methylbutyrate?	0.11	Monoterpenic ester
Geranyl isovalerate	0.11	Monoterpenic ester
10-epi- γ -Eudesmol	4.94	Sesquiterpenic alcohol
1,10-diepi-Cubenol	0.02	Sesquiterpenic alcohol
Unknown	0.19	Oxygenated sesquiterpene
γ -Eudesmol	0.26	Sesquiterpenic alcohol
Citronellyl valerate?	0.11	Monoterpenic ester
Cubenol	0.20	Sesquiterpenic alcohol
τ -Muurolol	0.16	Sesquiterpenic alcohol
τ -Cadinol	0.11	Sesquiterpenic alcohol
β -Eudesmol	0.31	Sesquiterpenic alcohol
α -Eudesmol	0.32	Sesquiterpenic alcohol
α -Cadinol	0.16	Sesquiterpenic alcohol
Valerianol	0.04	Sesquiterpenic alcohol
Geranyl valerate	0.21	Monoterpenic ester
Citronellyl tiglate	0.34	Monoterpenic ester
Citronellyl 4-methylvalerate	0.11	Monoterpenic ester
Geranyl tiglate	1.15	Monoterpenic ester
Geranyl 4-methylvalerate?	0.19	Monoterpenic ester
Citronellyl caproate	0.05	Monoterpenic ester
Geranyl caproate	0.10	Monoterpenic ester
Citronellyl heptanoate	0.07	Monoterpenic ester
Phytone	0.05	Terpenic ketone
Geranyl heptanoate	0.11	Monoterpenic ester
Citronellyl caprylate	0.03	Monoterpenic ester
Geranyl caprylate	0.05	Monoterpenic ester
Consolidated total	95.79%	

*: 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

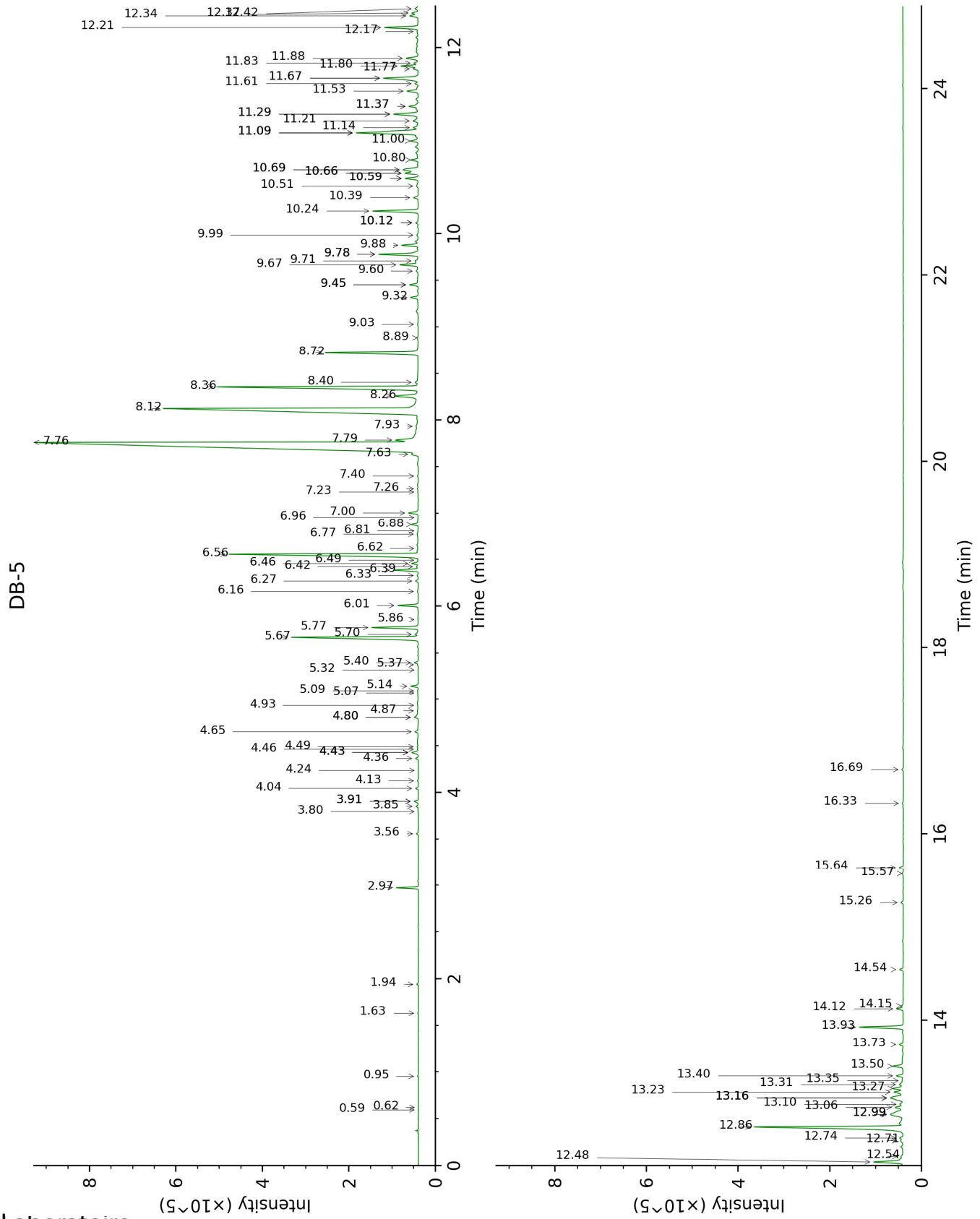
tr: The compound has been detected below 0.005% of total signal.

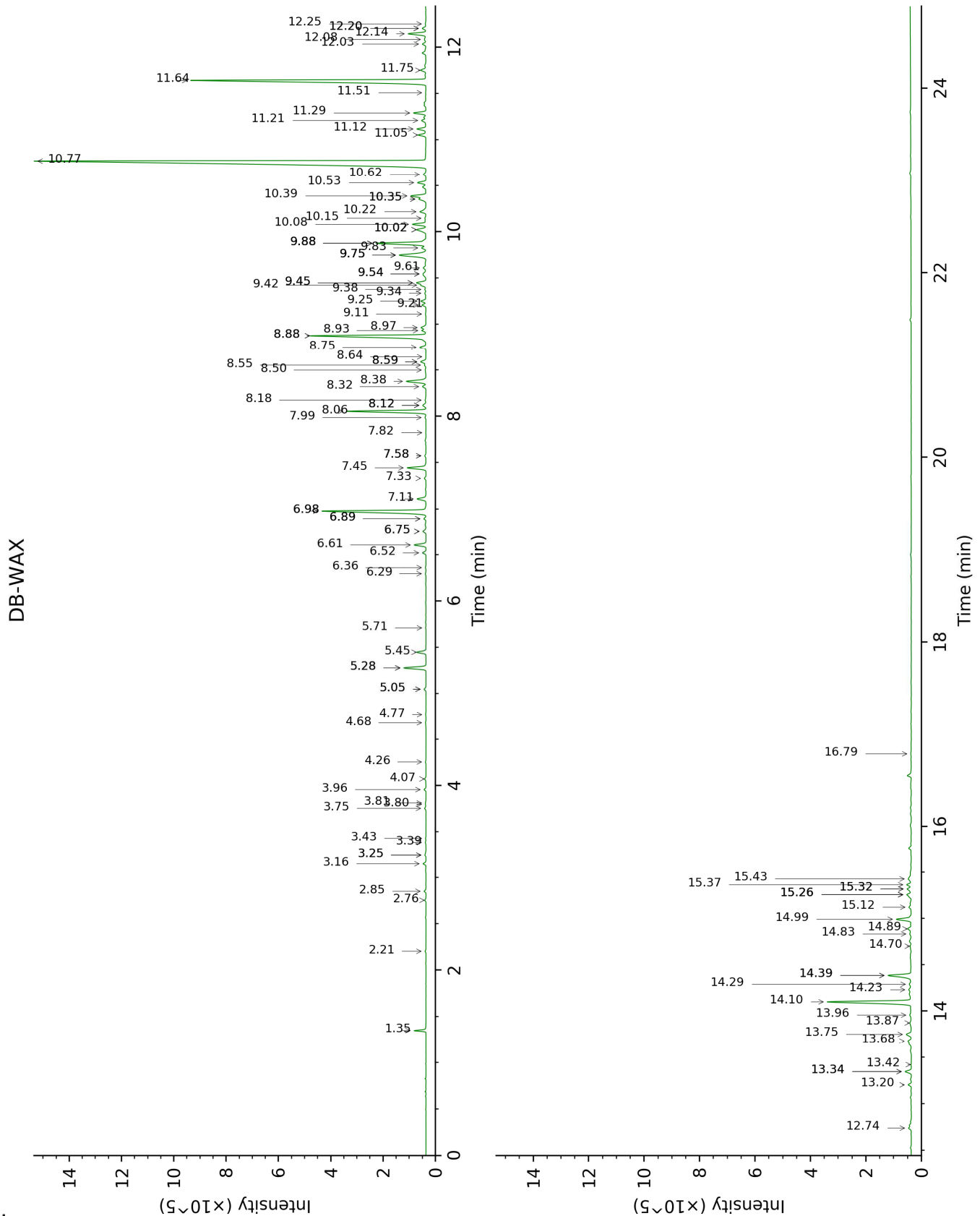
Note: no correction factor was applied

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.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isovaleral	0.59	639	tr			
2-Methylbutyral	0.62	651	tr			
2-Methylbutanol	0.95	740	0.01	3.43	1178	0.02
Dimethyl sulfoxide	1.63	825	0.01	7.82	1498	0.01
3-Methylpentanol	1.94	850	0.03	5.05*	1299	0.10
α -Pinene	2.97	930	0.42	1.35	989	0.41
Geranic oxide	3.56	969	0.04	2.20	1077	0.04
Octen-3-ol	3.80	984	0.01	6.75*	1418	0.19
6-Methyl-5-hepten-2-one	3.85	988	0.06	5.05*	1299	[0.10]
<i>trans</i> -Dehydroxylinalool oxide	3.91*	992	0.12	3.39	1174	0.04
Myrcene	3.91*	992	[0.12]	2.85	1132	0.08
α -Phellandrene	4.04	1001	0.07	2.76	1124	0.06
<i>cis</i> -Dehydroxylinalool oxide	4.13	1006	0.03	3.81	1207	0.02
α -Terpinene	4.24	1013	0.01			
para-Cymene	4.36	1021	0.07	4.07	1226	0.07
Limonene	4.43*	1025	0.21	3.16	1156	0.14
Unknown [m/z 59, 43 (11), 109 (10), 41 (10), 127 (8)...]	4.43*	1025	[0.21]	6.30	1385	0.04
Unknown [m/z 59, 43 (12), 109 (11), 41 (10), 127 (8)...]	4.43*	1025	[0.21]	6.36	1389	0.03
β -Phellandrene	4.46	1027	0.02	3.25*	1163	0.05
1,8-Cineole	4.49	1029	0.03	3.25*	1163	[0.05]
(Z)- β -Ocimene	4.65	1039	0.09	3.76	1203	0.07
Unknown [m/z 125, 69 (75), 41 (34), 55 (25), 93 (22)... 140 (3)]	4.80*	1048	0.11	4.68	1271	0.02
(E)- β -Ocimene	4.80*	1048	[0.11]	3.96	1218	0.08
2,6-Dimethyl-5-heptenal (melonal)	4.87	1053	0.05	5.28*	1312	1.16
γ -Terpinene	4.93	1056	0.03	3.80	1206	0.03
<i>cis</i> -Sabinene hydrate	5.07	1065	0.02	6.90*	1429	0.11
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.10	1067	0.03	4.77	1278	0.02
<i>cis</i> -Linalool oxide (fur.)	5.14	1070	0.20	6.52	1401	0.18
Fenchone	5.32	1081	0.01	5.71	1342	0.02

Terpinolene	5.37	1084	0.02	4.26	1240	0.03
<i>trans</i> -Linalool oxide (fur.)	5.40	1086	0.11	6.90*	1429	[0.11]
Linalool	5.67	1103	3.83	8.06	1516	3.83
(<i>Z</i>)-6-Methyl-3,5- heptadien-2-one	5.70	1105	0.11	8.18	1525	0.06
<i>cis</i> -Rose oxide	5.77	1110	1.17	5.28*	1312	[1.16]
Phenylethyl alcohol	5.86	1115	0.02	12.08	1847	0.12
<i>trans</i> -Rose oxide	6.01	1125	0.50	5.45	1324	0.48
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.16	1134	0.05	7.58*	1479	0.07
Unknown [m/z 41, 69 (87), 82 (66), 67 (55), 109 (46)... 142 (18)]	6.27	1141	0.08	9.38	1619	0.06
Isopulegol	6.33	1145	0.04	8.12*	1521	0.21
Menthone	6.39	1149	0.62	6.60	1407	0.63
Unknown [m/z 43, 141 (51), 55 (36), 69 (31), 41 (29)... 156 (4)]	6.42	1151	0.05	8.50	1550	0.07
Citronellal	6.46	1154	0.18	6.98*	1435	5.95
iso-Isopulegol	6.49	1156	0.02	7.99	1510	0.05
Isomenthone	6.56	1160	5.85	6.98*	1435	[5.95]
neo-Menthol	6.62	1164	0.02	8.64	1561	0.01
Terpinen-4-ol	6.77	1174	0.08	8.55	1554	0.08
Menthol	6.81	1176	0.02	9.11	1598	0.03
Isomenthol	6.88	1180	0.18	8.88*	1579	6.50
para-Cymen-8-ol	6.96	1186	0.02	11.51	1796	0.02
α -Terpineol	7.00	1189	0.29	9.75*	1649	2.02
Unknown [m/z 43, 99 (84), 81 (46), 986 (43), 126 (36), 71 (28)... 170 (12)]	7.23	1203	0.02			
Unknown [m/z 123, 81 (40), 67 (29), 79 (29), 93 (26), 121 (25), 41 (24), 55 (18), 69 (15)...]	7.26	1206	0.04			
β -Cyclocitral	7.40	1215	0.03	8.59*	1557	0.32
Nerol	7.63	1231	0.21	11.05	1757	0.40
Citronellol	7.76†	1239	31.36	10.77	1734	31.06
Neral	7.79†	1241	[31.36]	9.45*	1625	0.56
Piperitone	7.93	1251	0.15	9.88*	1659	2.78
Geraniol	8.12	1264	13.71	11.64	1808	13.79
Geranial	8.26	1273	0.90	10.08	1676	0.70
Citronellyl formate	8.36	1280	6.45	8.88*	1579	[6.50]
Neryl formate	8.40	1283	0.10	9.45*	1625	[0.56]
Geranyl formate	8.72	1300	2.54	9.88*	1659	[2.78]

(3Z)-Hexenyl tiglate	8.89	1312	0.03	9.34	1616	0.06
Methyl geranate	9.03	1323	0.02	9.75*	1649	[2.02]
α-Cubebene	9.32	1343	0.23	6.75*	1418	[0.19]
Citronellyl acetate	9.45*	1353	0.28	9.42	1623	0.24
Phenylethyl propionate	9.45*	1353	[0.28]			
Neryl acetate	9.60	1363	0.08	10.15	1681	0.06
α-Copaene	9.67	1368	0.53	7.11	1445	0.52
Geranic acid	9.71	1371	0.13	16.79	2303	0.05
β-Bourbonene	9.78*	1376	1.12	7.44	1470	1.05
1,5-diepi-β-Bourbonene	9.78*	1376	[1.12]	7.33	1461	0.09
Geranyl acetate	9.88	1383	0.43	10.53	1713	0.45
Phenylethyl isobutyrate	9.99	1391	0.05	12.03	1842	0.19
Isocaryophyllene	10.12*	1400	0.07	8.12*	1521	[0.21]
α-Gurjunene	10.12*	1400	[0.07]	7.58*	1479	[0.07]
β-Caryophyllene	10.24	1410	1.25	8.38	1541	1.20
β-Copaene	10.39	1421	0.13	8.32	1536	0.20
Heptyl tiglate	10.51	1430	0.09			
6,9-Guaiadiene	10.59*	1436	0.38	8.59*	1557	[0.32]
Aromadendrene	10.59*	1436	[0.38]			
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.66*	1441	0.41	8.75	1570	0.33
Isogermacrene D	10.66*	1441	[0.41]	8.93	1584	0.20
Citronellyl propionate	10.69*	1444	0.63	10.22	1687	0.41
α-Humulene	10.69*	1444	[0.63]	9.25	1609	0.27
allo-Aromadendrene	10.80	1452	0.20	8.97	1586	0.29
trans-Cadina-1(6),4-diene	11.00	1467	0.24	9.21	1606	0.20
Germacrene D	11.09*	1473	2.40	9.75*	1649	[2.02]
γ-Murolene	11.09*	1473	[2.40]	9.54*	1633	0.29
α-Amorphene	11.09*	1473	[2.40]	9.54*	1633	[0.29]
Geranyl propionate	11.14	1478	0.14	11.29	1778	0.63
γ-Amorphene	11.22	1483	0.21	9.83	1655	0.23
Bicyclogermacrene	11.29*	1488	0.84	10.02*	1671	0.67
Viridiflorene	11.29*	1488	[0.84]	9.61	1638	0.16
4-epi-cis-Dihydroagarofuran	11.37*	1495	0.30	9.88*	1659	[2.78]
α-Murolene	11.37*	1495	[0.30]	10.02*	1671	[0.67]
γ-Cadinene	11.53	1507	0.35	10.35*	1698	0.42
7-epi-α-Selinene	11.61	1513	0.09	10.35*	1698	[0.42]
δ-Cadinene	11.67*	1518	1.27	10.39	1701	0.87
trans-Calamenene	11.67*	1518	[1.27]	11.21	1771	0.27
trans-Cadina-1,4-diene	11.77	1526	0.14	10.62	1721	0.16

Citronellyl butyrate	11.80	1528	0.46	11.12	1763	0.48
Phenylethyl angelate?	11.83	1531	0.12	14.23	2045	0.20
α -Agarofuran	11.88	1535	0.39	11.75	1818	0.32
1-nor-Bourbonanone	12.17	1558	0.06	13.42	1968	0.02
Geranyl butyrate	12.21	1561	0.96	12.14	1852	0.94
Spathulenol	12.34	1571	0.27	14.39*	2060	1.52
Caryophyllene oxide	12.37	1573	0.18	12.74	1905	0.16
Globulol	12.42	1577	0.12	13.87	2011	0.14
Phenylethyl tiglate	12.48	1582	0.94	14.99	2119	0.90
Viridiflorol	12.54	1587	0.10	13.96	2019	0.17
Geranyl 2-methylbutyrate?	12.71	1600	0.11	12.20*	1857	0.20
Geranyl isovalerate	12.74	1602	0.11	12.20*	1857	[0.20]
10-epi- γ -Eudesmol	12.86	1612	4.94	14.10	2032	4.75
1,10-diepi-Cubenol	12.99*	1623	0.84	13.34*	1961	0.36
Unknown [m/z 147, 162 (79), 43 (64), 59 (64), 95 (47), 91 (44), 105 (43)... 238 (13)]	12.99*	1623	[0.84]	15.26*	2146	0.34
γ -Eudesmol	13.06	1629	0.26	14.89	2109	0.25
Citronellyl valerate?	13.10	1632	0.11	12.25	1862	0.04
Cubenol	13.16*	1637	0.69	13.68	1992	0.20
τ -Muurolol	13.16*	1637	[0.69]	15.12	2132	0.16
τ -Cadinol	13.16*	1637	[0.69]	14.83	2103	0.11
β -Eudesmol	13.23	1643	0.31	15.37	2156	0.26
α -Eudesmol	13.26	1646	0.32	15.32*	2152	0.29
α -Cadinol	13.31	1649	0.16	15.43	2163	0.30
Valerianol	13.35	1653	0.04	15.32*	2152	[0.29]
Geranyl valerate	13.40	1657	0.21	13.20	1948	0.16
Citronellyl tiglate	13.50	1665	0.34	13.34*	1961	[0.36]
Citronellyl 4-methylvalerate	13.73	1684	0.11			
Geranyl tiglate	13.92	1700	1.15	14.39*	2060	[1.52]
Geranyl 4-methylvalerate?	14.12	1717	0.19	13.75	1999	0.36
Citronellyl caproate	14.15	1720	0.05			
Geranyl caproate	14.54	1754	0.10	14.29	2051	0.15
Citronellyl heptanoate	15.26	1816	0.07			
Phytone	15.57	1844	0.05	14.70	2090	0.07
Geranyl heptanoate	15.64	1850	0.11	15.26*	2146	[0.34]
Citronellyl caprylate	16.33	1913	0.03			

Geranyl caprylate	16.69	1947	0.05	15.26*	2146	[0.34]
Total identified	96.21%			94.60%		
Total reported	96.48%			95.17%		

*: 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