

Date : August 10, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20G27-PSC03

Customer identification : Geranium - Rwanda - G0010122019GHR

Type : Essential oil

Source : *Pelargonium graveolens*

Customer : Pacha Soap Co.

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 : July 29, 2020

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light green liquid

Refractive index: 1.4671 ± 0.0003 (20 °C; method PC-MAT-016)

Optical rotation: -11.7° (c = 5.3, methanol, 25 °C)

ISO 4731:2012 - OIL OF GERANIUM - MADAGASCAR

Compound	Min. %	Max. %	Observed %	Complies?
Phenylethyl tiglate	0.4	1.0	0.6	Yes
Geranyl tiglate	0.7	2.0	1.4	Yes
Geranyl butyrate	0.7	1.7	0.9	Yes
Geraniol	10.0	20.0	14.4	Yes
Citronellol	18.0	26.0	24.5	Yes
Geranyl formate	3.8	7.0	5.5	Yes
α-Terpineol	0.3	1.0	0.3	Yes
Citronellyl formate	6.5	11.0	11.1	No
6,9-Guaiadiene	5.0	9.0	7.6	Yes
Linalool	4.0	10.0	4.3	Yes
Isomenthone	5.0	10.0	2.3	No
Menthone		2.0	0.2	Yes
trans-Rose oxide	0.1	0.6	0.4	Yes
cis-Rose oxide	0.4	1.4	0.9	Yes
Optical rotation	-17.0°	-9.0°	-11.7°	Yes
Refractive index	1.4620	1.4710	1.4671	Yes

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. The oil slightly deviates from the ISO standard for Madagascar geranium oil, which was used as the closest available standard for Rwandese geranium oil.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Isobutyral	tr	Aliphatic aldehyde
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
Toluene	tr	Simple phenolic
Isoamyl formate	tr	Aliphatic ester
Dimethyl sulfoxide	0.02	Aliphatic sulfoxide
3-Methylpentanol	0.03	Aliphatic alcohol
Unknown	0.01	Unknown
(3Z)-Hexenol	0.01	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	0.01	Aliphatic ketone
3-Methylpentyl formate?	0.02	Aliphatic ester
Tricyclene	0.01	Monoterpene
α -Thujene	0.01	Monoterpene
α -Pinene	0.34	Monoterpene
Camphene	tr	Monoterpene
α -Fenchene	tr	Monoterpene
Geranic oxide	0.03	Monoterpenic ether
β -Pinene	0.01	Monoterpene
Sabinene	tr	Monoterpene
Octen-3-ol	0.03	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.05	Aliphatic ketone
Myrcene	0.12	Monoterpene
<i>trans</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
α -Phellandrene	0.04	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
Δ^3 -Carene	0.02	Monoterpene
para-Cymene	0.04	Monoterpene
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Limonene	0.08	Monoterpene
β -Phellandrene	0.04	Monoterpene
1,8-Cineole	0.05	Monoterpenic ether
(Z)- β -Ocimene	0.12	Monoterpene
(E)- β -Ocimene	0.12	Monoterpene
Unknown	0.01	Unknown
Isobutyl angelate	0.01	Aliphatic ester
Unknown	0.01	Oxygenated monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.12	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Fenchone	0.01	Monoterpenic ketone
Terpinolene	0.03	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.05	Monoterpenic alcohol
Rosefuran	0.01	Monoterpenic ether
Linalool	4.26	Monoterpenic alcohol

(Z)-6-Methyl-3,5-heptadien-2-one	0.08	Aliphatic ketone
cis-Rose oxide	0.88	Monoterpenic ether
trans-Rose oxide	0.37	Monoterpenic ether
Unknown	0.04	Unknown
Unknown	0.03	Oxygenated normonoterpene
Unknown	0.05	Oxygenated monoterpene
Menthone	0.17	Monoterpenic ketone
Citronellal	0.12	Monoterpenic aldehyde
Isomenthone	2.28	Monoterpenic ketone
neo-Menthol	0.06	Monoterpenic alcohol
Terpinen-4-ol	0.03	Monoterpenic alcohol
Menthol	0.02	Monoterpenic alcohol
Isomenthol	0.08	Monoterpenic alcohol
para-Cymen-8-ol	0.04	Monoterpenic alcohol
α-Terpineol	0.28	Monoterpenic alcohol
Myrtenol	0.04	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Nerol	0.51	Monoterpenic alcohol
Citronellol	24.49	Monoterpenic alcohol
Neral	0.61	Monoterpenic aldehyde
Piperitone	0.07	Monoterpenic ketone
Geraniol	14.39	Monoterpenic alcohol
Geranial	0.86	Monoterpenic aldehyde
Citronellyl formate	11.10	Monoterpenic ester
Neryl formate	0.32	Monoterpenic ester
Geranyl formate	5.54	Monoterpenic ester
(3Z)-Hexenyl tiglate	0.01	Aliphatic ester
Methyl geranate	0.08	Monoterpenic ester
α-Cubebene	0.16	Sesquiterpene
Unknown	0.02	Sesquiterpene
Citronellyl acetate	0.32	Monoterpenic ester
Geranic acid	0.30	Aliphatic acid
α-Copaene	0.39	Sesquiterpene
β-Bourbonene	0.99	Sesquiterpene
1,5-diepi-β-Bourbonene	0.08	Sesquiterpene
Geranyl acetate	0.36	Monoterpenic ester
β-Elemene	0.18	Sesquiterpene
Phenylethyl isobutyrate	0.07	Phenolic ester
α-Gurjunene	0.04	Sesquiterpene
β-Caryophyllene	1.91	Sesquiterpene
Thymohydroquinone dimethyl ether	0.05	Monoterpenic ether
β-Copaene	0.12	Sesquiterpene
Heptyl tiglate	0.03	Aliphatic ester
Aromadendrene	0.01	Sesquiterpene
α-Guaiene	0.49	Sesquiterpene
Isogermaacrene D	0.16	Sesquiterpene
6,9-Guaiadiene	7.57	Sesquiterpene
Unknown	0.55	Sesquiterpene
Citronellyl propionate	0.51	Monoterpenic ester
α-Humulene	0.43	Sesquiterpene
allo-Aromadendrene	0.18	Sesquiterpene
trans-Cadina-1(6),4-diene	0.22	Sesquiterpene

γ -Murolene	0.15	Sesquiterpene
Germacrene D	1.79	Sesquiterpene
Geranyl propionate	0.85	Monoterpenic ester
β -Selinene	0.23	Sesquiterpene
γ -Amorphene	0.45	Sesquiterpene
Phenylethyl isovalerate	0.07	Phenolic ester
Bicyclogermacrene	0.14	Sesquiterpene
Viridiflorene	0.09	Sesquiterpene
4-epi- <i>cis</i> -Dihydroagarofuran	0.11	Sesquiterpenic ether
α -Murolene	0.34	Sesquiterpene
γ -Cadinene	0.35	Sesquiterpene
Geranyl isobutyrate	0.19	Monoterpenic ester
δ -Cadinene	0.65	Sesquiterpene
<i>trans</i> -Calamenene	0.16	Sesquiterpene
Citronellyl butyrate	0.42	Monoterpenic ester
Phenylethyl angelate?	0.11	Phenolic ester
α -Cadinene	0.07	Sesquiterpene
α -Agarofuran	0.18	Sesquiterpenic ether
Furopelargone isomer	0.12	Sesquiterpenic ketone
1-nor-Bourbonanone	0.05	Norsesquiterpenic ketone
Geranyl butyrate	0.91	Monoterpenic ester
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.35	Sesquiterpenic ether
Globulol	0.09	Sesquiterpenic alcohol
Phenylethyl tiglate	0.64	Phenolic ester
Furopelargone A	0.20	Sesquiterpenic ketone
Geranyl 2-methylbutyrate?	0.08	Monoterpenic ester
Geranyl isovalerate	0.26	Monoterpenic ester
10-epi- γ -Eudesmol	0.34	Sesquiterpenic alcohol
1-epi-Cubenol	0.17	Sesquiterpenic alcohol
Unknown	0.10	Oxygenated sesquiterpene
γ -Eudesmol	0.03	Sesquiterpenic alcohol
Citronellyl valerate?	0.01	Monoterpenic ester
Cubenol	0.18	Sesquiterpenic alcohol
β -Eudesmol	0.18	Sesquiterpenic alcohol
α -Eudesmol	0.12	Sesquiterpenic alcohol
α -Cadinol	0.10	Sesquiterpenic alcohol
Valerianol	0.08	Sesquiterpenic alcohol
<i>cis</i> -Calamenen-10-ol	0.05	Sesquiterpenic alcohol
Geranyl valerate	0.11	Monoterpenic ester
Citronellyl tiglate	0.43	Monoterpenic ester
Citronellyl 4-methylvalerate	0.09	Monoterpenic ester
3 β ,4 β -Oxidoagarofuran?	0.05	Sesquiterpenic ether
Geranyl tiglate	1.43	Monoterpenic ester
Geranyl 4-methylvalerate?	0.16	Monoterpenic ester
Citronellyl caproate	0.04	Monoterpenic ester
Geranyl caproate	0.09	Monoterpenic ester
Citronellyl heptanoate	0.05	Monoterpenic ester
Phytone	0.02	Terpenic ketone
Geranyl heptanoate	0.06	Monoterpenic ester
Citronellyl caprylate	0.04	Monoterpenic ester
Geranyl caprylate	0.06	Monoterpenic ester

Consolidated total	96.62%
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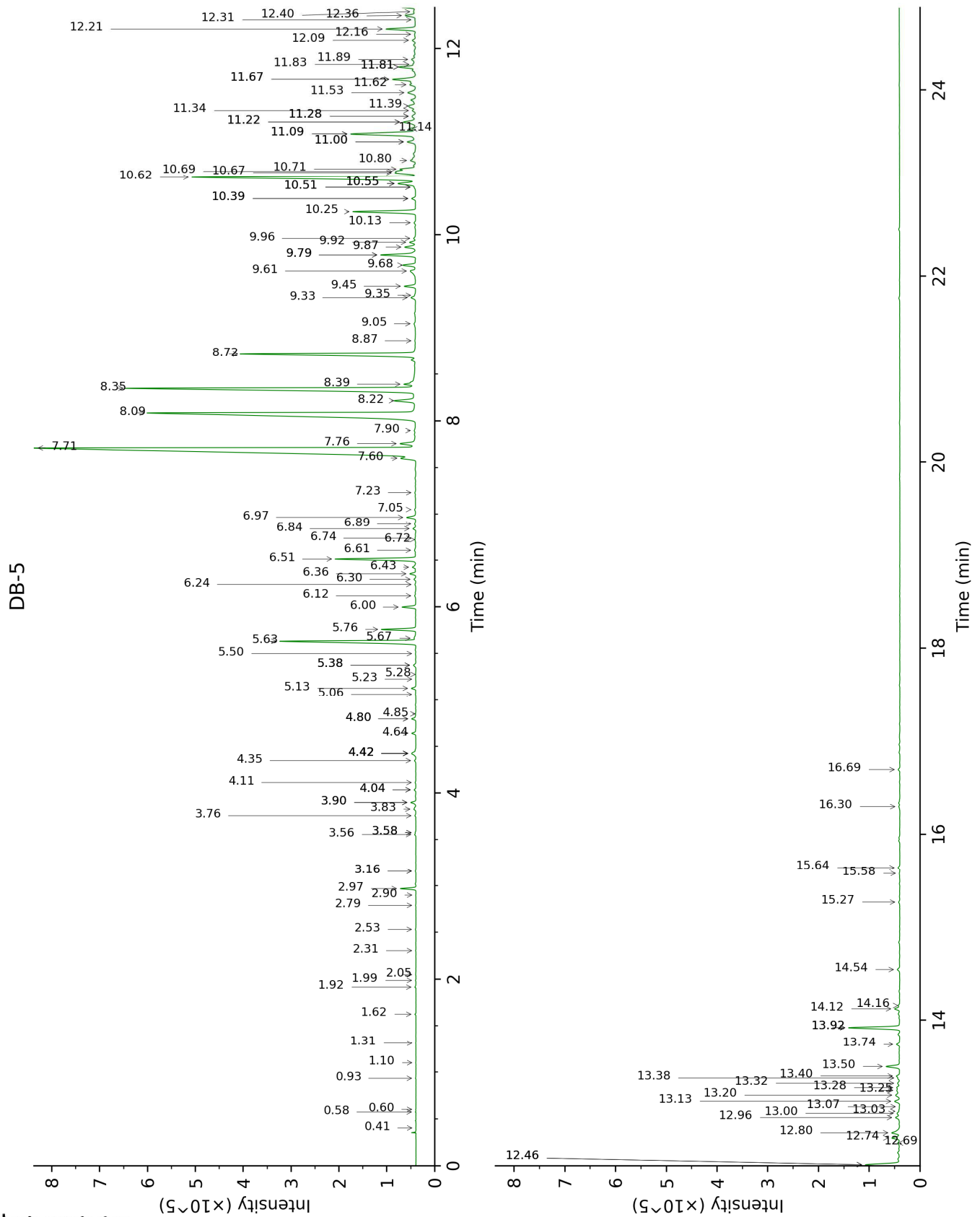
tr: The compound has been detected below 0.005% of total signal.

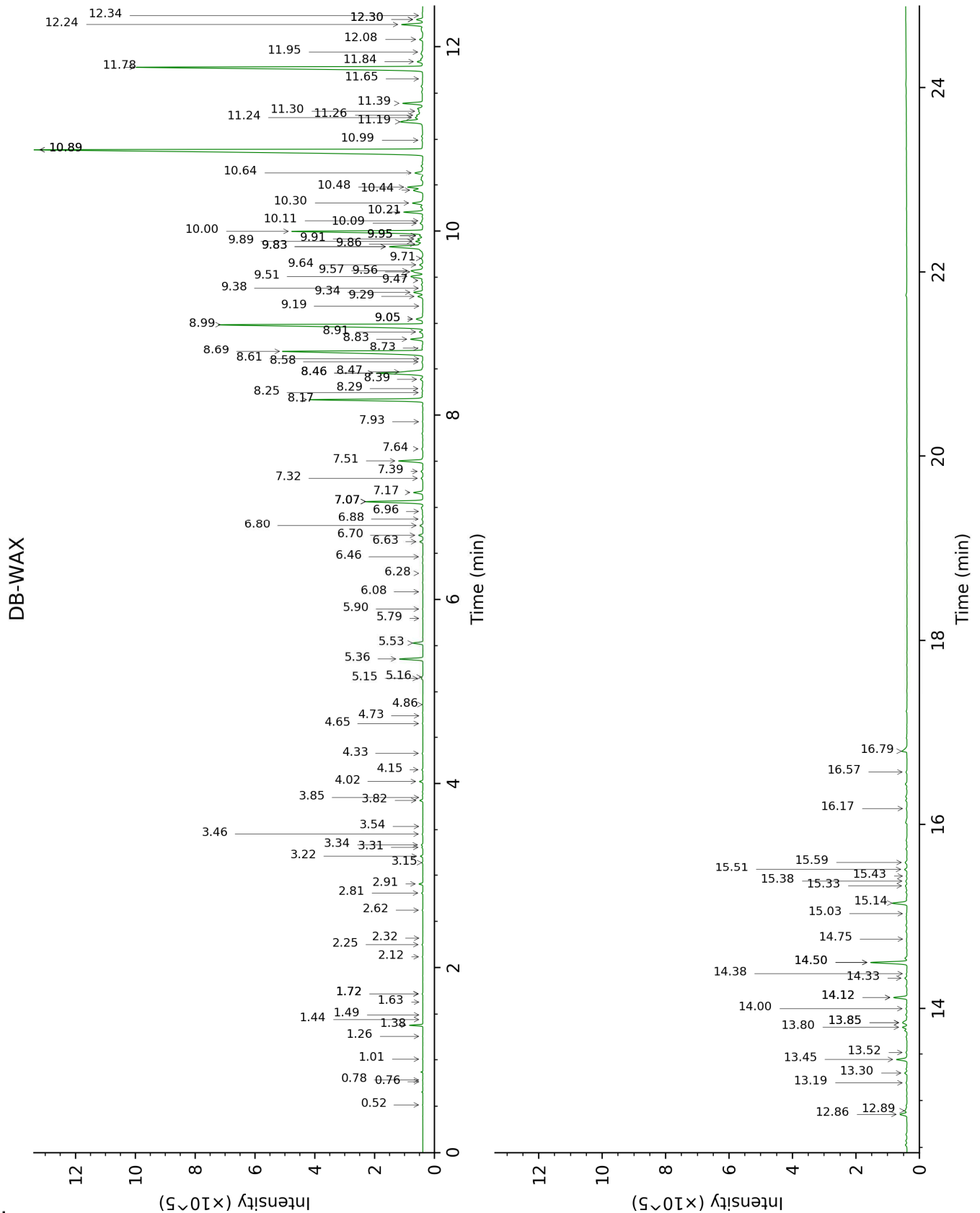
Note: no correction factor was applied

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	%
Isobutyral	0.41	539	tr	0.52	782	0.01
Isovaleral	0.58	642	0.01	0.78	887	0.01
2-Methylbutyral	0.60	653	tr	0.76	880	tr
Isoamyl alcohol	0.93	734	0.01	3.54	1181	0.02
Toluene	1.10	758	tr	1.49	1001	tr
Isoamyl formate	1.31	789	tr	1.72*	1024	0.02
Dimethyl sulfoxide	1.62	822	0.02	7.93	1501	0.02
3-Methylpentanol	1.92	847	0.03	5.16†	1299	[0.09]
Unknown [m/z 109, 43 (28), 124 (28), 41 (14), 55 (11), 79 (9), 81 (8)...]	1.99	853	0.01	1.72*	1024	[0.02]
(3Z)-Hexenol	2.05	858	0.01	5.90	1351	0.02
3-Acetyl-3-methylcyclopentene	2.31	880	0.01	1.01	927	0.01
3-Methylpentyl formate?	2.53	899	0.02	3.15	1151	0.02
Tricyclene	2.79	917	0.01	1.26	969	tr
α-Thujene	2.90	925	0.01	1.44	996	tr
α-Pinene	2.97	929	0.34	1.38	989	0.33
Camphene	3.16*	942	0.02	1.72*	1024	[0.02]
α-Fenchene	3.16*	942	[0.02]	1.63	1015	tr
Geranic oxide	3.56	969	0.03	2.25	1078	0.03
β-Pinene	3.58*	970	0.02	2.12	1064	0.01
Sabinene	3.58*	970	[0.02]	2.32	1085	tr
Octen-3-ol	3.76	982	0.03	6.88	1422	0.05
6-Methyl-5-hepten-2-one	3.83	987	0.05	5.15†	1298	0.09
Myrcene	3.90*	992	0.15	2.91	1132	0.12
<i>trans</i> -Dehydroxylinalool oxide	3.90*	992	[0.15]	3.46	1175	0.03
α-Phellandrene	4.04*	1001	0.05	2.81	1124	0.04
<i>cis</i> -Dehydroxylinalool oxide	4.04*	1001	[0.05]	3.85	1205	0.01
Δ3-Carene	4.11	1006	0.02	2.62	1110	0.02
para-Cymene	4.35	1021	0.04	4.15	1226	0.04
Unknown [m/z 59, 43 (11), 109 (10), 41 (10), 127 (8)...]	4.42*†	1026	0.20	6.28	1379	0.02
Unknown [m/z 59, 43 (12), 109 (11), 41 (10), 127 (8)...]	4.42*†	1026	[0.20]	6.46	1392	0.02
Limonene	4.42*†	1026	[0.20]	3.22	1156	0.08
β-Phellandrene	4.42*†	1026	[0.20]	3.31	1164	0.04
1,8-Cineole	4.42*†	1026	[0.20]	3.34	1166	0.05
(Z)-β-Ocimene	4.64	1039	0.12	3.82	1202	0.11

(E)- β -Ocimene	4.80*	1049	0.13	4.02	1217	0.12
Unknown [m/z 125, 69 (75), 41 (34), 55 (25), 93 (22)... 140 (3)]	4.80*	1049	[0.13]	4.73	1268	0.01
Isobutyl angelate	4.85	1053	0.01	4.65	1262	0.02
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.06	1066	0.01	4.86	1277	0.01
cis-Linalool oxide (fur.)	5.13	1070	0.12	6.63	1404	0.12
Octanol	5.23	1077	0.01	8.29	1529	0.06
Fenchone	5.28	1080	0.01	5.80	1344	0.01
Terpinolene	5.38*	1086	0.08	4.33	1239	0.03
trans-Linalool oxide (fur.)	5.38*	1086	[0.08]	7.07*	1436	2.38
Rosefuran	5.50	1094	0.01	6.08	1364	0.02
Linalool	5.63	1102	4.26	8.17	1520	4.32
(Z)-6-Methyl-3,5-heptadien-2-one	5.67	1105	0.08	8.25	1525	0.04
cis-Rose oxide	5.76	1111	0.88	5.36	1313	0.86
trans-Rose oxide	6.00	1126	0.37	5.53	1325	0.36
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.12	1134	0.04			
Unknown [m/z 41, 69 (87), 82 (66), 67 (55), 109 (46)... 142 (18)]	6.24	1142	0.03	9.38	1614	0.03
Unknown [m/z 123, 81 (60), 67 (49), 95 (36), 41 (29), 68 (25)...152 (2)]	6.30	1146	0.05	7.32	1454	0.07
Menthone	6.36	1149	0.17	6.70	1408	0.17
Citronellal	6.43	1154	0.12	7.07*	1436	[2.38]
Isomenthone	6.52	1160	2.28	7.07*	1436	[2.38]
neo-Menthol	6.61	1166	0.06	8.58	1551	0.05
Terpinen-4-ol	6.72	1173	0.03	8.73	1562	0.04
Menthol	6.74	1174	0.02	9.19	1598	0.01
Isomenthol	6.84	1181	0.08	8.91	1576	0.16
para-Cymen-8-ol	6.89	1184	0.04	11.66	1801	0.03
α -Terpineol	6.97	1189	0.28	9.89†	1654	0.49
Myrtenol	7.05	1194	0.04	10.99	1745	0.06
Unknown [m/z 123, 81 (40), 67 (29), 79 (29), 93 (26), 121 (25), 41 (24), 55 (18), 69 (15)...]	7.23	1206	0.03			
Nerol	7.60	1229	0.51	11.19	1762	1.41
Citronellol	7.71	1236	24.49	10.89*	1736	24.21
Neral	7.76	1240	0.61	9.57†	1629	[0.75]
Piperitone	7.90	1249	0.07	9.95*	1659	0.13
Geraniol	8.09	1262	14.39	11.78	1812	13.85

Geranial	8.22	1270	0.86	10.21	1680	0.73
Citronellyl formate	8.35	1279	11.10	8.99	1582	10.57
Neryl formate	8.39	1282	0.32	9.56†	1628	0.75
Geranyl formate	8.72	1304	5.54	10.00	1663	5.59
(3Z)-Hexenyl tiglate	8.87	1314	0.01	9.47	1620	0.06
Methyl geranate	9.05	1327	0.08	9.86	1652	0.09
α-Cubebene	9.33	1347	0.16	6.80	1416	0.12
Unknown [m/z 95, 147 (61), 96 (39), 93 (37), 94 (37)... 204 (4)]	9.35	1349	0.02	6.96	1428	0.02
Citronellyl acetate	9.45	1356	0.32	9.51	1624	0.66
Geranic acid	9.61	1367	0.30	16.79	2289	0.32
α-Copaene	9.68	1372	0.39	7.17	1443	0.40
β-Bourbonene	9.79*	1379	1.11	7.51	1468	0.99
1,5-diepi-β-Bourbonene	9.79*	1379	[1.11]	7.39	1460	0.08
Geranyl acetate	9.87	1385	0.36	10.64	1715	0.38
β-Elemene	9.92	1389	0.18	8.46*†	1542	2.58
Phenylethyl isobutyrate	9.96	1392	0.07	12.08	1838	0.17
α-Gurjunene	10.13	1404	0.04	7.64	1477	0.05
β-Caryophyllene	10.25	1412	1.91	8.46*†	1542	[2.58]
Thymohydroquinone dimethyl ether	10.39*	1423	0.12	11.94	1826	0.05
β-Copaene	10.39*	1423	[0.12]	8.39	1536	0.12
Heptyl tiglate	10.51*	1432	0.04			
Aromadendrene	10.51*	1432	[0.04]	8.61	1554	0.01
α-Guaiene	10.55*	1435	0.69	8.47†	1543	[2.58]
Isogermacrene D	10.55*	1435	[0.69]	9.05*	1587	0.34
6,9-Guaiadiene	10.62	1440	7.57	8.69	1560	7.34
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.67	1444	0.55	8.83	1570	0.49
Citronellyl propionate	10.69	1445	0.51	10.30	1687	0.48
α-Humulene	10.71	1447	0.43	9.34	1610	0.42
allo-Aromadendrene	10.80	1454	0.18	9.05*	1587	[0.34]
trans-Cadina-1(6),4-diene	11.00*	1468	0.32	9.29	1606	0.22
γ-Murolene	11.00*	1468	[0.32]	9.64	1634	0.15
Germacrene D	11.09*	1475	2.63	9.83*	1650	1.86
Geranyl propionate	11.09*	1475	[2.63]	11.39	1778	0.85
β-Selinene	11.14	1479	0.23	9.92†	1656	[0.49]
γ-Amorphene	11.22*	1484	0.52	9.83*	1650	[1.86]
Phenylethyl isovalerate	11.22*	1484	[0.52]	13.19	1937	0.07
Bicyclgermacrene	11.28*	1489	0.17	10.09	1670	0.14
Viridiflorene	11.28*	1489	[0.17]	9.71	1639	0.09
4-epi-cis-Dihydroagarofuran	11.34	1493	0.11	9.95*	1659	[0.13]
α-Murolene	11.39	1497	0.34	10.11	1672	0.04

γ -Cadinene	11.53	1508	0.35	10.44	1699	0.53
Geranyl isobutyrate	11.62	1515	0.19	11.30†	1771	[1.25]
δ -Cadinene	11.67*	1519	0.81	10.48	1702	0.65
<i>trans</i> -Calamenene	11.67*	1519	[0.81]	11.26†	1768	[1.25]
Citronellyl butyrate	11.81*	1530	0.52	11.24†	1765	1.25
Phenylethyl angelate?	11.81*	1530	[0.52]	14.33	2043	0.11
α -Cadinene	11.83	1532	0.07	10.89*	1736	[24.21]
α -Agarofuran	11.89	1536	0.18	11.84	1817	0.25
Furopelargone isomer	12.09	1552	0.12	12.89	1910	0.11
1-nor-Bourbonanone	12.16	1557	0.05	13.52	1967	0.05
Geranyl butyrate	12.21	1561	0.91	12.24	1852	0.89
Spathulenol	12.31	1569	0.03	14.50*	2059	1.48
Caryophyllene oxide	12.36	1573	0.35	12.86	1907	0.33
Globulol	12.40	1576	0.09	14.00	2012	0.06
Phenylethyl tiglate	12.46*	1580	1.17	15.14	2122	0.64
Furopelargone A	12.46*	1580	[1.17]	14.12*	2024	0.55
Geranyl 2-methylbutyrate?	12.69	1599	0.08	12.30*	1857	0.28
Geranyl isovalerate	12.74	1603	0.26	12.30*	1857	[0.28]
10-epi- γ -Eudesmol	12.80	1607	0.34	14.12*	2024	[0.55]
1-epi-Cubenol	12.96	1621	0.17	13.85*	1998	0.28
Unknown [m/z 147, 162 (79), 43 (64), 59 (64), 95 (47), 91 (44), 105 (43)... 238 (13)]	13.00	1624	0.10	15.33	2140	0.08
γ -Eudesmol	13.02	1626	0.03	15.03	2110	0.04
Citronellyl valerate?	13.07	1630	0.01	12.34	1861	0.01
Cubenol	13.13	1635	0.18	13.80	1993	0.19
β -Eudesmol	13.20	1640	0.18	15.51	2158	0.11
α -Eudesmol	13.25	1645	0.12	15.43	2151	0.04
α -Cadinol	13.28	1647	0.10	15.59	2166	0.10
Valerianol	13.32	1651	0.08	15.38	2145	0.07
<i>cis</i> -Calamenen-10-ol	13.38	1656	0.05	16.57	2266	0.06
Geranyl valerate	13.40	1657	0.11	13.30	1947	0.10
Citronellyl tiglate	13.50	1666	0.43	13.44	1960	0.47
Citronellyl 4-methylvalerate	13.74	1685	0.09			
3 β ,4 β -Oxidoagarofuran?	13.92*	1700	1.47	16.17	2225	0.05
Geranyl tiglate	13.92*	1700	[1.47]	14.50*	2059	[1.48]
Geranyl 4-methylvalerate?	14.12	1718	0.16	13.85*	1998	[0.28]
Citronellyl caproate	14.16	1721	0.04			
Geranyl caproate	14.54	1754	0.09	14.38	2048	0.04
Citronellyl heptanoate	15.27	1818	0.05			
Phytone	15.58	1846	0.02	14.75	2083	0.03
Geranyl heptanoate	15.64	1851	0.06			
Citronellyl caprylate	16.30	1912	0.04			
Geranyl caprylate	16.69	1949	0.06			

Total identified	96.02%	94.57%
Total reported	96.88%	95.33%

*: 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