

Date : December 17, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20L03-PSC03

Customer identification : Rough Lemon Petitgrain - CIJA-2020-01

Type : Essential oil

Source : *Citrus jambhiri*

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 : December 08, 2020

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: 1.4731 ± 0.0003 (20 °C; method PC-MAT-016)

Optical rotation: $+66.2^\circ$ (20 °C, acetone, $c = 1.8$)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. Literature suggests that rough lemon petitgrain (leaf) oil composition is quite variable¹⁻⁴, precluding a definitive conclusion as per sample's botanical identity, but the sample features reasonable similarities with the results from Lota *et al* 2002.³

REFERENCES

- (1) Kasali, A. A.; Olaniyan, A. A. Citrus Essential Oil of Nigeria Part III Volatile Constituents of Citrus Jambhiri Lush Leaf Oil. *J. Essent. Oil-Bearing Plants* **2009**, *12* (6), 690–693. <https://doi.org/10.1080/0972060X.2009.10643776>.
- (2) Agarwal, S. G.; Lai, S.; Thappa, R. K.; Kapahi, B. K.; Sarin, Y. K. Seasonal Studies on Indian Citrus Jambhiri Lush Leaf Oil—a New Chemotype. *Flavour Fragr. J.* **1989**, *4* (1), 33–36. <https://doi.org/10.1002/ffj.2730040108>.
- (3) Lota, M. L.; De Rocca Serra, D.; Tomi, F.; Jacquemond, C.; Casanova, J. Volatile Components of Peel and Leaf Oils of Lemon and Lime Species. *J. Agric. Food Chem.* **2002**, *50* (4), 796–805. <https://doi.org/10.1021/jf010924l>.
- (4) Lund, E. D.; Shaw, P. E.; Kirkland, C. L. Composition of Rough Lemon Leaf Oil. *J. Agric. Food Chem.* **1981**, *29* (3), 490–494. <https://doi.org/10.1021/jf00105a013>.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Class
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
Toluene	tr	Simple phenolic
Unknown	tr	Unknown
(3Z)-Hexenol	tr	Aliphatic alcohol
Unknown	tr	Unknown
Unknown	tr	Unknown
Unknown	0.01	Unknown
Nonane	tr	Alkane
Heptanal	tr	Aliphatic aldehyde
Tricyclene	tr	Monoterpene
α -Thujene	0.28	Monoterpene
α -Pinene	1.36	Monoterpene
Unknown	tr	Simple phenolic
Camphene	0.04	Monoterpene
α -Fenchene	tr	Monoterpene
Sabinene	15.53	Monoterpene
β -Pinene	2.74	Monoterpene
6-Methyl-5-hepten-2-one	0.22	Aliphatic ketone
Myrcene	2.41	Monoterpene
α -Phellandrene	0.20	Monoterpene
Pseudolimonene	0.02	Monoterpene
Octanal	0.14	Aliphatic aldehyde
Δ^3 -Carene	0.10	Monoterpene
α -Terpinene	1.43	Monoterpene
para-Cymene	0.18	Monoterpene
Limonene	43.37	Monoterpene
β -Phellandrene	0.57	Monoterpene
1,8-Cineole	0.19	Monoterpenic ether
(Z)- β -Ocimene	0.76	Monoterpene
Benzeneacetaldehyde	0.01	Simple phenolic
(E)- β -Ocimene	3.59	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
γ -Terpinene	2.65	Monoterpene
cis-Sabinene hydrate	0.08	Monoterpenic alcohol
para-Mentha-3,8-diene	0.02	Monoterpene
Octanol	0.05	Aliphatic alcohol
Isoterpinolene	0.01	Monoterpene
Terpinolene	0.63	Monoterpene
para-Cymenene	0.03	Monoterpene
trans-Sabinene hydrate	0.04	Monoterpenic alcohol
Linalool	2.66	Monoterpenic alcohol
Nonanal	0.07	Aliphatic aldehyde
endo-Fenchol	0.02	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.07	Monoterpenic alcohol

<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
(<i>E</i>)-4,8-Dimethyl-1,3,7-nonatriene	0.03	Monoterpene
allo-Ocimene	0.02	Monoterpene
<i>cis</i> -Limonene oxide	0.01	Monoterpenic ether
<i>cis</i> -para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
<i>trans</i> -Limonene oxide	0.01	Monoterpenic ether
Menthatriene isomer III	0.01	Monoterpene
<i>trans</i> -para-Menth-2-en-1-ol	0.07	Monoterpenic alcohol
Isopulegol	0.16	Monoterpenic alcohol
<i>cis</i> - β -Terpineol	0.02	Monoterpenic alcohol
Citronellal	2.96	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Isoneral	0.05	Monoterpenic aldehyde
α -Phellandren-8-ol	0.01	Monoterpenic alcohol
Terpinen-4-ol	3.00	Monoterpenic alcohol
Isogeranial	0.04	Monoterpenic aldehyde
para-Cymen-8-ol	0.01	Monoterpenic alcohol
α -Terpineol	0.56	Monoterpenic alcohol
<i>cis</i> -Piperitol	0.03	Monoterpenic alcohol
Unknown	0.05	Unknown
Decanal	0.12	Aliphatic aldehyde
<i>trans</i> -Piperitol	0.03	Monoterpenic alcohol
(3 <i>E</i> ,5 <i>E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.01	Monoterpenic alcohol
Octyl acetate	0.01	Aliphatic ester
<i>trans</i> -Carveol	0.01	Monoterpenic alcohol
Nerol	0.25	Monoterpenic alcohol
<i>cis</i> -Carveol	0.01	Monoterpenic alcohol
Citronellol	1.27	Monoterpenic alcohol
Neral	0.63	Monoterpenic aldehyde
(<i>Z</i>)-Isogeraniol	0.02	Monoterpenic alcohol
Geraniol	0.18	Monoterpenic alcohol
Geranial	0.80	Monoterpenic aldehyde
Citronellyl formate	0.03	Monoterpenic ester
Limonen-10-ol	0.01	Monoterpenic alcohol
Thymol	0.01	Monoterpenic alcohol
Undecanal	0.03	Aliphatic aldehyde
4-Vinylguaiacol	0.09	Simple phenolic
Citronellic acid	0.03	Monoterpenic acid
δ -Elemene	0.48	Sesquiterpene
δ -Elemene isomer	0.03	Sesquiterpene
α -Cubebene	0.01	Sesquiterpene
Citronellyl acetate	0.42	Monoterpenic ester
Neryl acetate	0.57	Monoterpenic ester
α -Copaene	0.02	Sesquiterpene
<i>cis</i> - β -Elemene	tr	Sesquiterpene
Geranyl acetate	0.21	Monoterpenic ester
β -Elemene	0.19	Sesquiterpene
Unknown	0.01	Sesquiterpene
Dodecanal	0.04	Aliphatic aldehyde
β -Caryophyllene	2.50	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
γ -Elemene	0.06	Sesquiterpene

<i>trans</i> - α -Bergamotene	0.28	Sesquiterpene
α -Humulene	0.25	Sesquiterpene
β -Santalene	0.03	Sesquiterpene
9- <i>epi</i> - β -Caryophyllene	0.01	Sesquiterpene
γ -Muurolene	0.01	Sesquiterpene
Germacrene D	0.24	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.03	Sesquiterpene
δ -Selinene	0.03	Sesquiterpene
Viridiflorene	0.06	Sesquiterpene
Bicyclogermacrene	0.39	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	tr	Sesquiterpene
α -Muurolene	0.04	Sesquiterpene
β -Bisabolene	0.40	Sesquiterpene
γ -Cadinene	0.06	Sesquiterpene
(<i>Z</i>)- γ -Bisabolene	0.01	Sesquiterpene
δ -Cadinene	0.09	Sesquiterpene
Unknown	0.02	Sesquiterpene
Selina-3,7(11)-diene	0.01	Sesquiterpene
Unknown	0.03	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.02	Sesquiterpene
α -Elemol	0.01	Sesquiterpenic alcohol
Germacrene B	0.47	Sesquiterpene
(<i>E</i>)-Nerolidol	0.03	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Globulol	0.03	Sesquiterpenic alcohol
Viridiflorol	0.03	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.02	Sesquiterpenic alcohol
<i>cis</i> -Zingiberenol	0.03	Sesquiterpenic alcohol
Selin-6-en-4 α -ol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Alismol	0.05	Sesquiterpenic alcohol
τ -Cadinol	0.04	Sesquiterpenic alcohol
Unknown	0.01	Sesquiterpenic alcohol
α -Cadinol	0.07	Sesquiterpenic alcohol
Unknown	0.03	Oxygenated sesquiterpene
α -Bisabolol	0.07	Sesquiterpenic alcohol
Juniper camphor	0.01	Sesquiterpenic alcohol
β -Sinensal	0.03	Sesquiterpenic aldehyde
α -Sinensal	0.01	Sesquiterpenic aldehyde
β -Bisabolenal?	0.02	Sesquiterpenic aldehyde
Unknown	0.01	Unknown
Isophytol	0.01	Diterpenic alcohol
para-Camphorene	0.01	Diterpene
Phytol	0.23	Diterpenic alcohol
Consolidated total	97.98%	

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

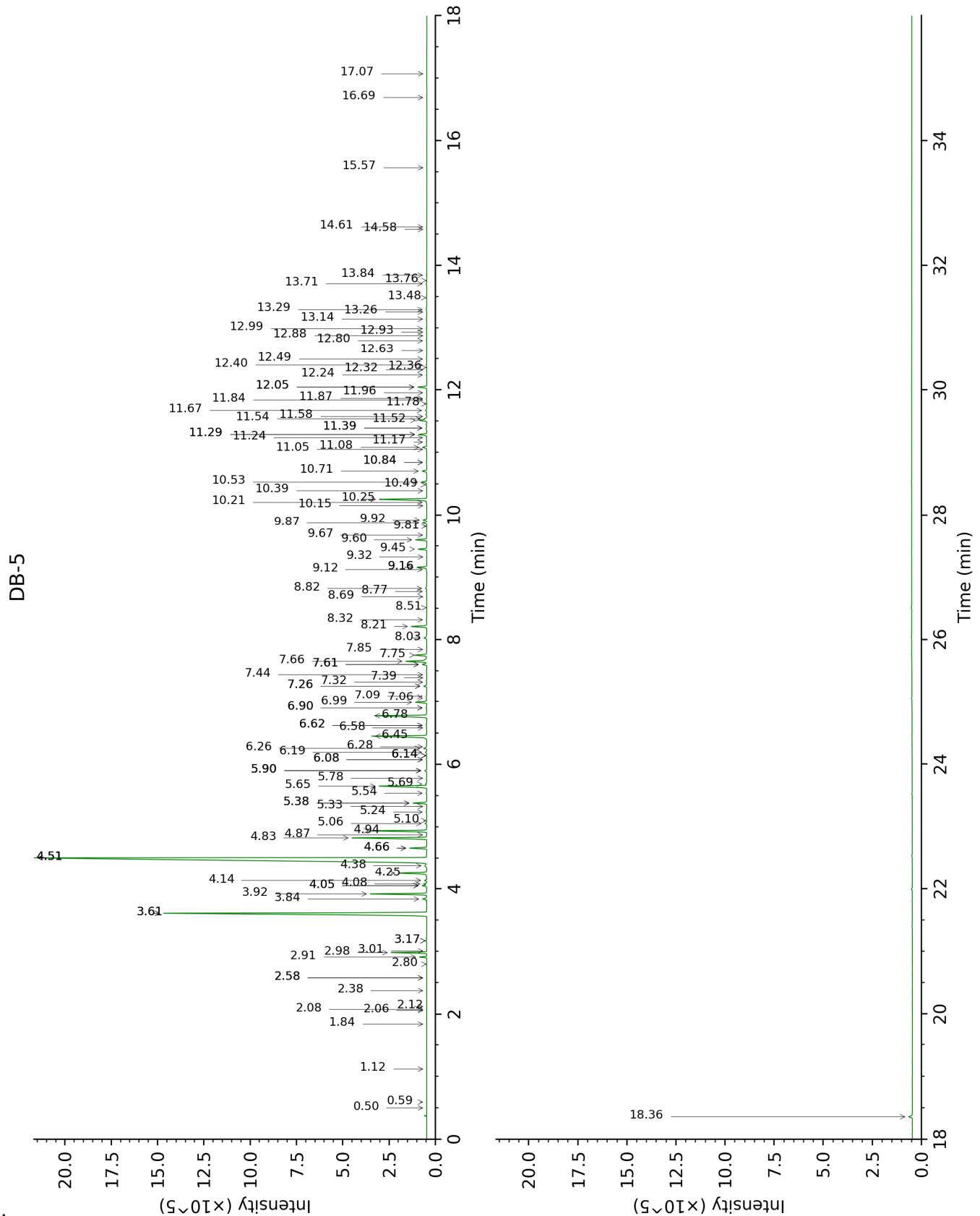
Note: no correction factor was applied

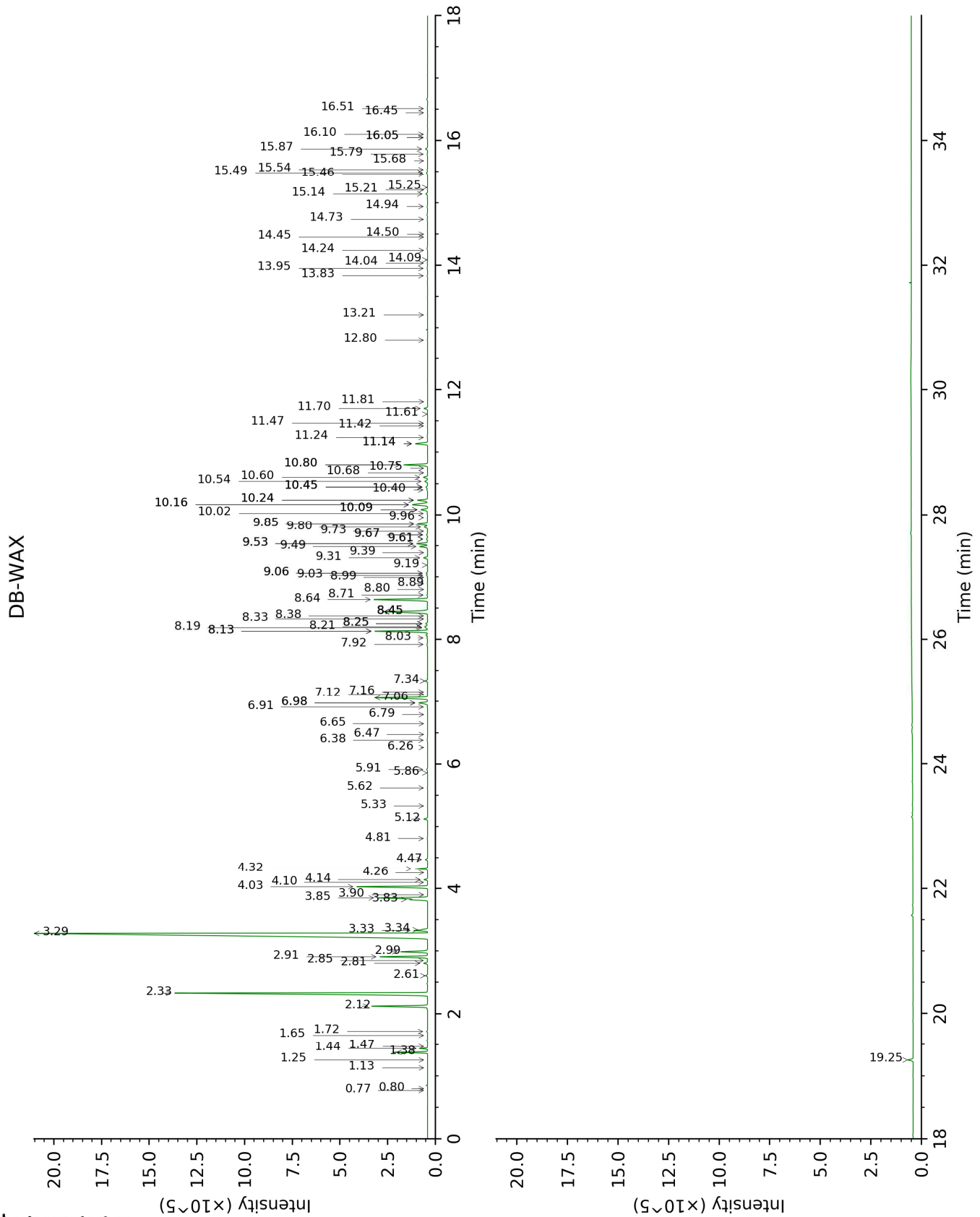
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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	%
2-Methyl-3-buten-2-ol	0.50	588	tr			
Isovaleral	0.59	638	tr	0.77	887	tr
Toluene	1.12	763	tr	1.47	1000	tr
Unknown [m/z 107, 91 (66), 122 (38), 105 (23), 79 (18), 41 (13)...]	1.84	842	tr	1.13	949	tr
(3Z)-Hexenol	2.06	860	tr	5.86	1350	0.01
Unknown [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	2.08	862	tr			
Unknown [m/z 55, 83 (79), 67 (65), 41 (63), 82 (60), 69 (58)... 111 (27), 126 (9)]	2.12	866	tr			
Unknown [m/z 69, 41 (57), 81 (57), 80 (18), 79 (18), 67 (17)...]	2.38	887	0.01			
Nonane	2.58*	904	tr	0.80	895	tr
Heptanal	2.58*	904	[tr]			
Tricyclene	2.80	918	tr	1.25	970	tr
α -Thujene	2.91	926	0.28	1.44	997	0.28
α -Pinene	2.98	930	1.36	1.38	990	1.34
Unknown [m/z 122, 121 (36), 107 (33), 79 (27), 93 (25), 77 (25), 43 (20)]	3.01	932	tr	3.90	1210	0.01
Camphene	3.17*	943	0.05	1.72	1025	0.04
α -Fenchene	3.17*	943	[0.05]	1.65	1019	tr
Sabinene	3.61*	972	18.46	2.33	1087	15.53
β -Pinene	3.61*	972	[18.46]	2.12	1066	2.74
6-Methyl-5-hepten-2-one	3.84	987	0.22	5.12	1297	0.19
Myrcene	3.92	992	2.41	2.91	1133	2.38
α -Phellandrene	4.05*	1001	0.22	2.81	1125	0.20
Pseudolimonene	4.05*	1001	[0.22]	2.85	1129	0.02
Octanal	4.08	1003	0.14	4.47	1251	0.11
Δ 3-Carene	4.14	1007	0.10	2.61	1110	0.10
α -Terpinene	4.25	1014	1.43	2.99	1140	1.42
para-Cymene	4.38	1022	0.18	4.14	1227	0.18
Limonene	4.51*	1030	44.70	3.28	1163	43.37
β -Phellandrene	4.51*	1030	[44.70]	3.33	1166	0.57
1,8-Cineole	4.51*	1030	[44.70]	3.34	1167	0.19
(Z)- β -Ocimene	4.66*	1040	0.75	3.82	1204	0.76
Benzeneacetaldehyde	4.66*	1040	[0.75]	8.80	1570	0.01
(E)- β -Ocimene	4.83	1050	3.59	4.03	1219	3.58

2,6-Dimethyl-5-heptenal (melonal)	4.87	1053	0.02	5.33	1312	0.01
γ-Terpinene	4.94	1057	2.65	3.85	1206	2.60
cis-Sabinene hydrate	5.06	1064	0.08	6.98*	1432	0.56
para-Mentha-3,8-diene	5.10	1067	0.02	4.10	1224	0.01
Octanol	5.24	1076	0.05	8.25*	1528	0.12
Isoterpinolene	5.33	1081	0.01	4.26	1236	0.01
Terpinolene	5.38*	1085	0.66	4.32	1240	0.63
para-Cymenene	5.38*	1085	[0.66]	6.38	1388	0.03
trans-Sabinene hydrate	5.54	1095	0.04	8.03	1510	0.05
Linalool	5.65	1102	2.66	8.13*	1518	2.67
Nonanal	5.69	1104	0.07	5.91	1354	0.06
endo-Fenchol	5.78	1110	0.02	8.38	1537	0.02
cis-para-Menth-2-en-1-ol	5.90*	1118	0.11	8.19†	1523	0.25
trans-para-Mentha-2,8-dien-1-ol	5.90*	1118	[0.11]	8.99	1585	0.01
(E)-4,8-Dimethyl-1,3,7-nonatriene	5.90*	1118	[0.11]	4.81	1276	0.03
allo-Ocimene	6.08*	1129	0.03	5.62	1333	0.02
cis-Limonene oxide	6.08*	1129	[0.03]	6.47	1394	0.01
cis-para-Mentha-2,8-dien-1-ol	6.14*	1133	0.03	9.53*	1628	0.62
trans-Limonene oxide	6.14*	1133	[0.03]	6.65	1407	0.01
Menthatriene isomer III	6.14*	1133	[0.03]	6.26	1379	0.01
trans-para-Menth-2-en-1-ol	6.19	1137	0.07	9.02	1587	0.06
Isopulegol	6.26	1141	0.16	8.20†	1524	[0.25]
cis-β-Terpineol	6.28	1142	0.02	9.06*	1590	0.08
Citronellal	6.45	1154	2.96	7.06	1438	2.87
Borneol	6.58	1162	0.01	9.85*	1653	0.57
Isoneral	6.62*	1165	0.05	7.92	1502	0.05
α-Phellandren-8-ol	6.62*	1165	[0.05]	10.24*	1684	0.60
Terpinen-4-ol	6.78	1175	3.00	8.64	1557	2.97
Isogeranial	6.90*	1183	0.05	8.25*	1528	[0.12]
para-Cymen-8-ol	6.90*	1183	[0.05]	11.61	1800	0.01
α-Terpineol	6.99	1189	0.56	9.85*	1653	[0.57]
cis-Piperitol	7.06	1193	0.03	9.60*	1634	0.07
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	7.09	1195	0.05	8.13*	1518	[2.67]
Decanal	7.26*	1206	0.16	7.34	1458	0.12
trans-Piperitol	7.26*	1206	[0.16]	10.45*	1702	0.12
(3E,5E)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.32	1210	0.01	11.42	1784	0.02
Octyl acetate	7.39	1215	0.01	7.12	1442	0.01
trans-Carveol	7.44	1219	0.01	11.47	1788	0.02
Nerol	7.61*	1230	0.26	11.14*	1760	0.79

<i>cis</i> -Carveol	7.61*	1230	[0.26]	11.81	1818	0.01
Citronellol	7.66	1233	1.27	10.80*	1732	1.28
Neral	7.76	1240	0.63	9.53*	1628	[0.62]
(<i>Z</i>)-Isogeraniol	7.85	1246	0.02	11.24	1769	0.03
Geraniol	8.03	1259	0.18	11.70	1808	0.20
Geranial	8.21	1271	0.80	10.16*	1679	1.20
Citronellyl formate	8.32	1279	0.03	8.89	1577	0.03
Limonen-10-ol	8.51	1292	0.01	13.21	1943	0.02
Thymol	8.69	1304	0.01	15.21	2134	0.02
Undecanal	8.77	1305	0.03	8.71	1563	0.04
4-Vinylguaiaicol	8.82	1309	0.09	15.14	2127	0.10
Citronellic acid	9.12	1330	0.03	16.10	2224	0.02
δ -Elemene	9.16*	1333	0.51	6.98*	1432	[0.56]
δ -Elemene isomer	9.16*	1333	[0.51]	6.91	1427	0.03
α -Cubebene	9.32	1344	0.01	6.79	1418	0.01
Citronellyl acetate	9.45	1353	0.42	9.49	1624	0.45
Neryl acetate	9.60	1364	0.57	10.24*	1684	[0.60]
α -Copaene	9.67	1369	0.02	7.16	1445	0.02
<i>cis</i> - β -Elemene	9.81	1380	tr	8.33	1533	0.01
Geranyl acetate	9.87	1383	0.21	10.60	1715	0.24
β -Elemene	9.92	1387	0.19	8.44*	1542	2.86
Unknown [m/z 106, 119 (99), 43 (78), 91 (74), 105 (60), 134 (55)... 204 (19)]	10.15	1404	0.01			
Dodecanal	10.20	1408	0.04	10.02	1667	0.04
β -Caryophyllene	10.25	1411	2.50	8.44*	1542	[2.86]
β -Copaene	10.39	1421	0.02	8.44*	1542	[2.86]
γ -Elemene	10.49	1429	0.06	9.06*	1590	[0.08]
<i>trans</i> - α -Bergamotene	10.53	1432	0.28	8.44*	1542	[2.86]
α -Humulene	10.70	1445	0.25	9.31	1610	0.24
β -Santalene	10.84*	1455	0.04	9.19	1600	0.03
9-epi- β -Caryophyllene	10.84*	1455	[0.04]	9.39	1616	0.01
γ -Muurolole	11.05	1471	0.01	9.67*	1639	0.07
Germacrene D	11.08	1473	0.24	9.80	1649	0.24
<i>trans</i> - β -Bergamotene	11.17	1480	0.03	9.60*	1634	[0.07]
δ -Selinene	11.24	1485	0.03	9.73	1644	0.02
Viridiflorene	11.29*	1489	0.45	9.67*	1639	[0.07]
Bicyclogermacrene	11.29*	1489	[0.45]	10.08*	1672	0.43
(<i>Z</i>)- α -Bisabolene	11.39*	1496	0.05	10.45*	1702	[0.12]
α -Muurolole	11.39*	1496	[0.05]	10.08*	1672	[0.43]
β -Bisabolene	11.52†	1506	0.54	10.16*	1679	[1.20]
γ -Cadinene	11.54†	1508	[0.54]	10.40	1698	0.06
(<i>Z</i>)- γ -Bisabolene	11.58	1511	0.01	9.96	1662	0.03
δ -Cadinene	11.67	1518	0.09	10.45*	1702	[0.12]
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	11.78	1527	0.02	10.80*	1732	[1.28]
Selina-3,7(11)-diene	11.84	1532	0.01	10.68	1721	0.02

Unknown [m/z 189, 204 (92), 161 (65), 133 (51), 105 (51), 91 (51), 119 (45)]	11.86	1534	0.03	10.54	1710	0.21
(E)- α -Bisabolene	11.96	1541	0.02	10.75	1727	0.01
α -Elemol	12.05*	1548	0.49	14.09	2025	0.01
Germacrene B	12.05*	1548	[0.49]	11.14*	1760	[0.79]
(E)-Nerolidol	12.24	1563	0.03	13.83	2001	0.03
Spathulenol	12.32	1570	0.02	14.45	2060	0.02
Caryophyllene oxide	12.36	1572	0.02	12.80	1906	0.02
Globulol	12.40	1576	0.03	13.95	2012	0.05
Viridiflorol	12.50	1583	0.03	14.04	2020	0.03
Eudesm-5-en-11-ol analog	12.63	1594	0.02	14.24	2040	0.01
cis-Zingiberenol	12.80	1607	0.03	14.50	2064	0.01
Selin-6-en-4 α -ol	12.88	1614	0.01	15.68	2180	0.01
Unknown [m/z 161, 43 (74), 105 (57), 121 (45), 81 (43)... 204 (31)...]	12.93	1619	0.02	14.73	2087	0.04
Alismol	12.99	1623	0.05	15.79	2191	0.04
τ -Cadinol	13.14	1636	0.04	14.94	2107	0.04
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.26	1645	0.01	15.25	2138	0.01
α -Cadinol	13.30	1648	0.07	15.54	2166	0.03
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.48	1664	0.03	16.05*	2219	0.03
α -Bisabolol	13.71	1683	0.07	15.49	2161	0.07
Juniper camphor	13.76	1687	0.01	16.05*	2219	[0.03]
β -Sinensal	13.84	1694	0.03	15.46	2158	0.02
α -Sinensal	14.58	1757	0.01	16.45	2259	0.01
β -Bisabolenal?	14.61	1760	0.02			
Unknown [m/z 69, 43 (73), 41 (41), 81 (39), 58 (38), 93 (30), 68 (26)...]	15.57	1845	0.01			
Isophytol	16.69	1948	0.01	16.51	2266	0.02
para-Camphorene	17.07	1984	0.01	15.87	2200	0.13
Phytol	18.36	2110	0.23	19.25	2567	0.30
Total identified		98.66%			97.78%	
Total reported		98.84%			98.05%	

*: 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