

Date : September 20, 2019

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 19I06-PTH23-1-SCC

Customer identification : Jasmine Sambac Absolute - India - J1010796R

Type : Absolute

Source : *Jasminum sambac*

Customer : Plant Therapy

ANALYSIS

Method: Dilution of a known amount with an appropriate solvent, and addition of a methyl octanoate internal standard for quantitation. Application of a correction factor¹. Analysis with 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 : September 17, 2019

Checked and approved by :



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

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REFERENCE

- (1) Cachet, T.; Brevard, H.; Chaintreau, A.; Demyttenaere, J.; French, L.; Gassenmeier, K.; Joulain, D.; Koenig, T.; Leij, H.; Liddle, P.; et al. IOFI Recommended Practice for the Use of Predicted Relative-Response Factors for the Rapid Quantification of Volatile Flavouring Compounds by GC-FID. *Flavour Fragr. J.* 2016, 31 (3), 191–194.

PYHSICOCHEMICAL DATA

Physical aspect: Dark orange viscous liquid

Refractive index: 1.5092 ± 0.0003 (20 °C)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY

Identification	(mg/g)	% of total volatiles	Classe
Hexan-2-ol	0.07	0.01	Aliphatic alcohol
(3Z)-Hexenol	4.29	0.53	Aliphatic alcohol
(2E)-Hexenol	1.39	0.17	Aliphatic alcohol
Hexanol	0.64	0.08	Aliphatic alcohol
Prenyl acetate	0.17	0.02	Aliphatic ester
Benzaldehyde	0.12	0.01	Simple phenolic
(3Z)-Hexenyl acetate	13.87	1.73	Aliphatic ester
Hexyl acetate	0.20	0.02	Aliphatic ester
(2E)-Hexenyl acetate	0.27	0.03	Aliphatic ester
Benzyl alcohol	56.55	7.04	Simple phenolic
(E)- β -Ocimene	0.97	0.12	Monoterpene
cis-Linalool oxide (fur.)	0.34	0.04	Monoterpenic alcohol
Benzyl formate	0.20	0.03	Phenolic ester
trans-Linalool oxide (fur.)	3.20	0.40	Monoterpenic alcohol
Methyl benzoate	2.59	0.32	Phenolic ester
Linalool	63.58	7.92	Monoterpenic alcohol
Phenylethyl alcohol	15.47	1.93	Simple phenolic
Benzeneacetonitrile	11.76	1.47	Simple phenolic
Benzyl acetate	81.32	10.13	Phenolic ester
cis-Linalool oxide (pyr.)	0.22	0.03	Monoterpenic alcohol
Ethyl benzoate	0.97	0.12	Phenolic ester
Unknown	6.73	0.84	Unknown
Methyl salicylate	2.20	0.27	Phenolic ester
α -Terpineol	0.35	0.04	Monoterpenic alcohol
(3Z)-Hexenyl 2-methylbutyrate	0.12	0.01	Aliphatic ester
(3Z)-Hexenyl isovalerate	0.16	0.02	Aliphatic ester
(E)-Isogeraniol?	0.82	0.10	Monoterpenic alcohol
Phenylethyl acetate	5.36	0.67	Phenolic ester
Unknown	2.27	0.28	Unknown
Geraniol	1.15	0.14	Monoterpenic alcohol
Phenylacetic acid?	0.77	0.10	Phenolic acid
Ethyl salicylate	0.09	0.01	Phenolic ester
Unknown	7.97	0.99	Unknown
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.54	0.07	Monoterpenic alcohol
1-Nitro-2-phenylethane	1.97	0.24	Simple phenolic
Indole	32.85	4.09	Indole
(E)-Cinnamyl alcohol	1.71	0.21	Phenylpropanoid
Methyl anthranilate	75.83	9.45	Phenolic ester
Eugenol	1.28	0.16	Phenylpropanoid
8-Hydroxylinalool isomer	2.16	0.27	Monoterpenic alcohol
Butyl benzoate	0.21	0.03	Phenolic ester
Methyl (E)-cinnamate	0.35	0.04	Phenylpropanoid ester
(3Z)-Hexenyl (3Z)-hexenoate	0.20	0.03	Aliphatic ester
(3Z)-Hexenyl hexanoate?	0.25	0.03	Aliphatic ester
β -Cubebene	0.14	0.02	Sesquiterpene
β -Elemene	0.78	0.10	Sesquiterpene
(Z)-Jasmone	0.39	0.05	Jasmonate

Dimethyl anthranilate	0.52	0.06	Phenolic ester
Ethyl anthranilate	0.35	0.04	Phenolic ester
β -Caryophyllene	0.53	0.07	Sesquiterpene
(E)-Cinnamyl acetate	0.23	0.03	Phenylpropanoid ester
α -Humulene	0.65	0.08	Sesquiterpene
(E)- β -Farnesene	0.23	0.03	Sesquiterpene
Oxindole?	0.40	0.05	Indole
γ -Muurolene	0.50	0.06	Sesquiterpene
Germacrene D	2.64	0.33	Sesquiterpene
epi-Cubebol	0.29	0.04	Sesquiterpenic alcohol
Bicyclogermacrene	1.31	0.16	Sesquiterpene
α -Muurolene	0.79	0.10	Sesquiterpene
(3Z,6E)- α -Farnesene	1.63	0.20	Sesquiterpene
(3E,6E)- α -Farnesene	101.33	12.62	Sesquiterpene
δ -Cadinene	4.65	0.58	Sesquiterpene
10-epi-Cubebol?	0.34	0.04	Sesquiterpenic alcohol
α -Cadinene	0.34	0.04	Sesquiterpene
Methyl N-formylanthranilate	0.36	0.04	Phenolic ester
Hexenyl benzoate isomer	1.01	0.13	Phenolic ester
(E)-Nerolidol	0.70	0.09	Sesquiterpenic alcohol
(3Z)-Hexenyl benzoate	38.52	4.80	Phenolic ester
Germacrene D-4-ol	26.60	3.31	Sesquiterpenic alcohol
Hexyl benzoate	0.93	0.12	Phenolic ester
(2E)-Hexenyl benzoate	2.99	0.37	Phenolic ester
Methyl N-acetylanthranilate	1.49	0.19	Phenolic ester
Ledol	0.18	0.02	Sesquiterpenic alcohol
τ -Muurolol	1.40	0.17	Sesquiterpenic alcohol
τ -Cadinol	0.05	0.01	Sesquiterpenic alcohol
α -Muurolol	0.31	0.04	Sesquiterpenic alcohol
α -Cadinol	3.23	0.40	Sesquiterpenic alcohol
Unknown	0.15	0.02	Unknown
(3E,5E)-7-Hydroxyfarnesene	0.85	0.11	Sesquiterpenic alcohol
Methyl (E)-jasmonate	1.50	0.19	Jasmonate
Shyobunol	0.44	0.06	Sesquiterpenic alcohol
Unknown	2.00	0.25	Unknown
Pentadecanal	0.23	0.03	Aliphatic aldehyde
(2E,6E)-Farnesol	1.41	0.18	Sesquiterpenic alcohol
Oplopanone	1.34	0.17	Sesquiterpenic alcohol
Unknown	4.18	0.52	Unknown
Benzyl benzoate	3.38	0.42	Phenolic ester
Phenylethyl benzoate	2.03	0.25	Phenolic ester
(2E,6E)-Farnesyl acetate	0.39	0.05	Sesquiterpenic ester
Phytone	0.13	0.02	Terpenic ketone
Phytadiene isomer I	0.07	0.01	Diterpene
Benzyl salicylate	0.54	0.07	Phenolic ester
Methyl palmitate	2.57	0.32	Aliphatic ester
meta-Camphorene	0.09	0.01	Diterpene
Isophytol	0.12	0.01	Diterpenic alcohol
Palmitic acid	6.22	0.78	Aliphatic acid
para-Camphorene	0.14	0.02	Diterpene
Ethyl palmitate	0.26	0.03	Aliphatic ester
(E,E)-Geranylinalool	11.15	1.39	Diterpenic alcohol

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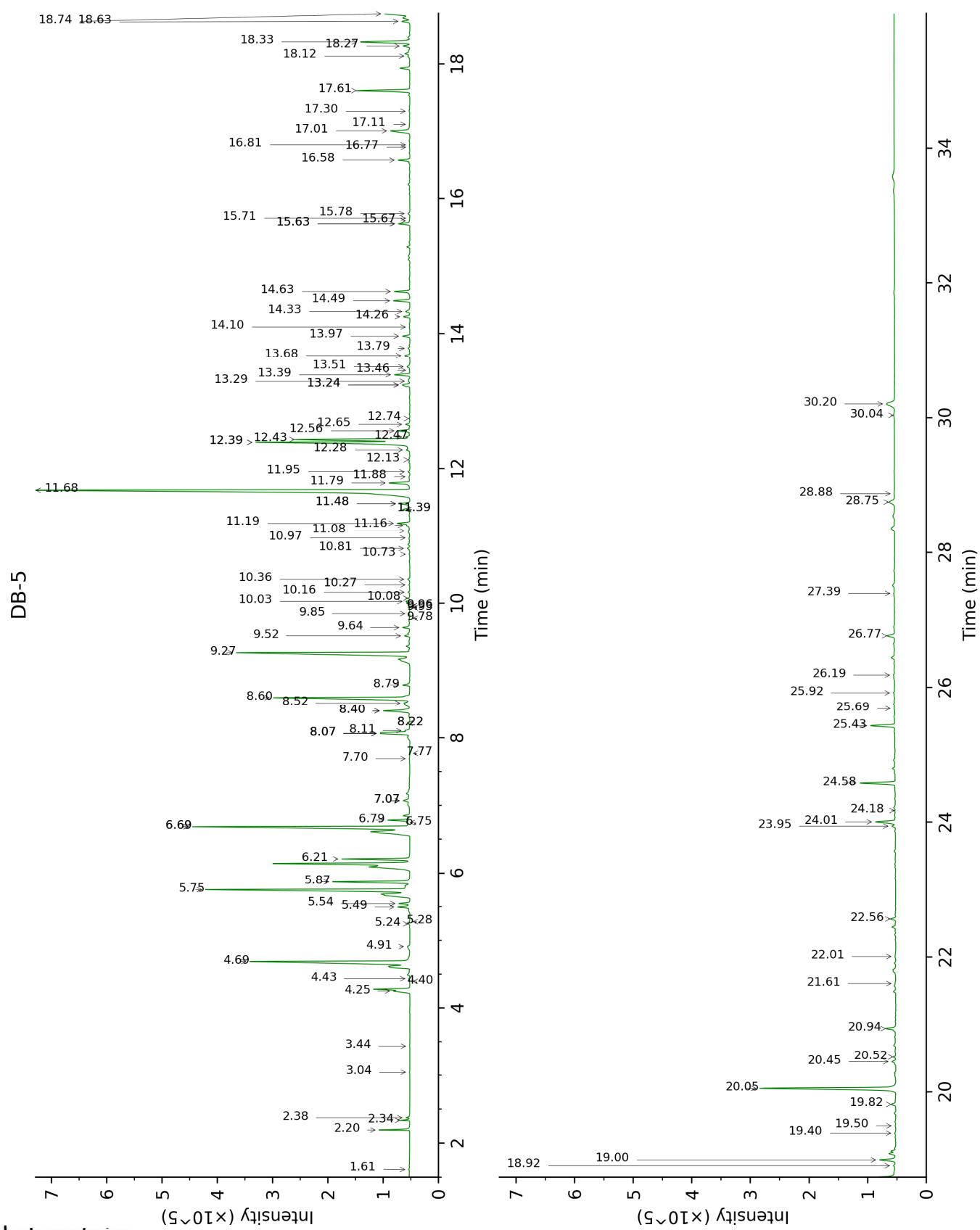
Plus que des analyses... des conseils

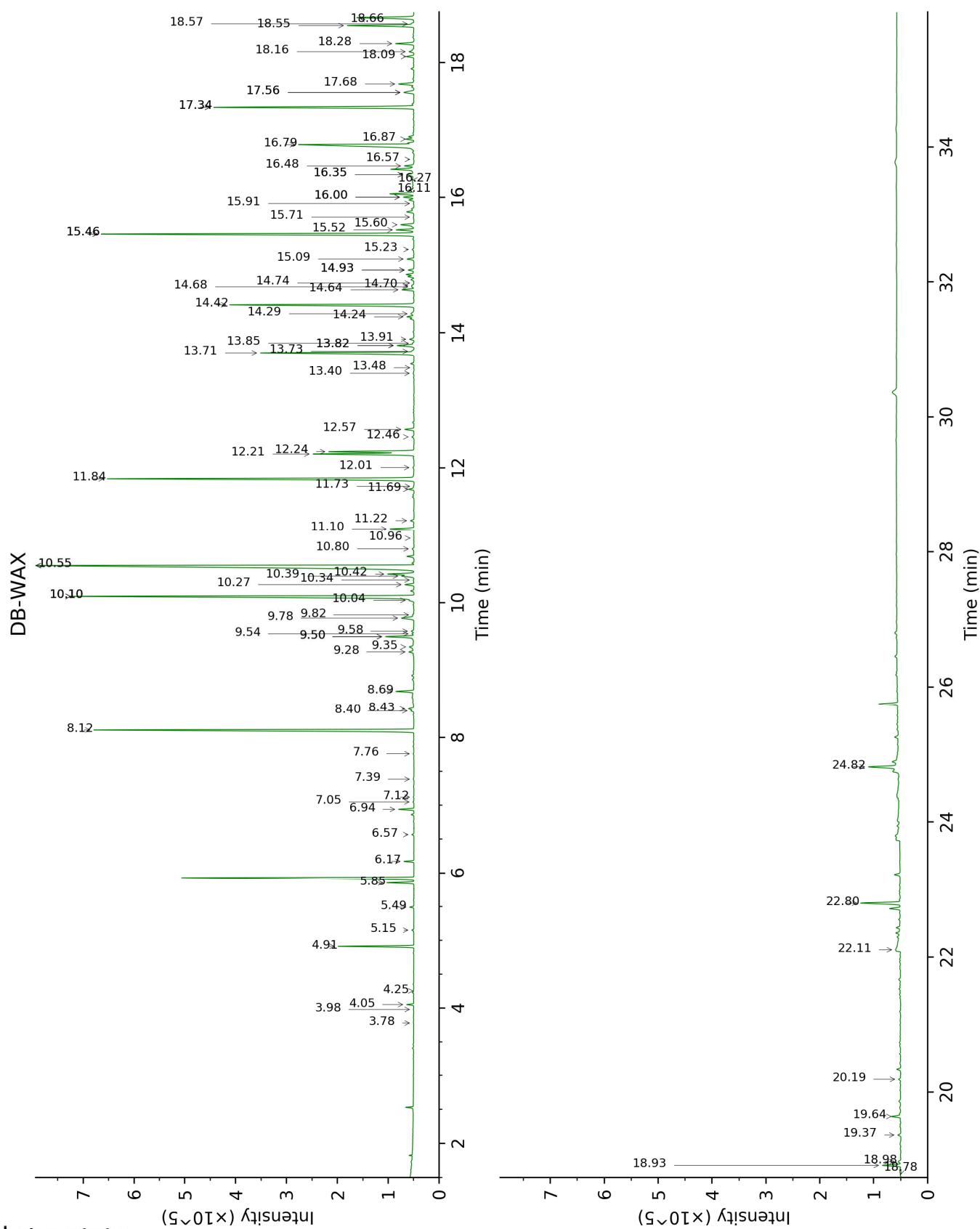
(E)-Cinnamyl benzoate	0.71	0.09	Phenylpropanoid ester
Methyl linoleate	1.58	0.20	Aliphatic ester
Methyl α-linolenate	12.87	1.60	Aliphatic ester
Methyl stearate	1.86	0.23	Aliphatic ester
α-Linolenic acid	8.99	1.12	Aliphatic acid
Ethyl α-linolenate	0.86	0.11	Aliphatic ester
Docosene isomer	3.65	0.45	Alkene
Unknown	0.37	0.05	Unknown
(E)-Phytol acetate	0.17	0.02	Diterpenic ester
(9Z)-Eicosenol?	1.04	0.13	Aliphatic alcohol
(9Z)-Tricosene	28.38	3.54	Alkene
Methyl arachidate	0.94	0.12	Aliphatic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.55	0.07	Terpenic lactone
Tetracosene isomer	2.23	0.28	Alkene
Unknown	0.28	0.04	Unknown
2-Monopalmitin	0.26	0.03	Glyceride
Benzyl palmitate	1.19	0.15	Phenolic ester
Benzyl oleate	0.76	0.09	Phenolic ester
Benzyl α-linolenate	5.25	0.65	Phenolic ester
Benzyl stearate	0.16	0.02	Phenolic ester
Squalene	6.95	0.87	Triterpene
2,3-Oxidosqualene	5.28	0.66	Triterpenic ether
Benzyl arachidate	0.29	0.04	Phenolic ester
2,6,10,15,19,23-Hexamethyl-(6E,10E,14E,18E)-1,6,10,14,18,22-tetracosahexaen-3-ol	0.30	0.04	Triterpenic alcohol
Unknown	0.38	0.05	Triterpenic alcohol
α-Tocopherol	1.86	0.23	Tocopherol
Benzyl behenate	0.18	0.02	Phenolic ester
Unknown	3.05	0.38	Unknown
β-Amyrin	0.24	0.03	Triterpenic alcohol
α-Amyrin	0.33	0.04	Triterpenic alcohol
Unknown	4.96	0.62	Unknown
γ-Cadinene	2.25	0.28	Sesquiterpene
Consolidated total	736.72 mg/g	91.79%	

Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).
Unknown compounds are expressed in equivalents of internal standard without correction.

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.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Hexan-2-ol	1.62	818	0.07	3.78	1202	0.09
(3Z)-Hexenol	2.20	865	4.29	5.85	1352	4.98
(2E)-Hexenol	2.34	877	1.39	6.18	1375	1.78
Hexanol	2.38	880	0.64	5.49	1327	0.73
Prenyl acetate	3.04	929	0.17	3.98	1217	0.12
Benzaldehyde	3.44	954	0.12	7.39	1463	0.22
(3Z)-Hexenyl acetate	4.25	1008	13.87	4.91	1284	14.83
Hexyl acetate	4.40	1017	0.20	4.25	1236	0.08
(2E)-Hexenyl acetate	4.43	1020	0.27	5.15	1303	0.42
Benzyl alcohol	4.69	1036	56.55	11.84	1819	61.48
(E)- β -Ocimene	4.91	1049	0.97	4.05	1222	0.97
cis-Linalool oxide (fur.)	5.24	1071	0.34	6.57	1404	0.44
Benzyl formate	5.28	1073	0.20	9.50*	1625	7.15
trans-Linalool oxide (fur.)	5.49	1086	3.20	6.94	1431	3.06
Methyl benzoate	5.54	1090	2.59	8.69	1562	4.33
Linalool	5.75	1103	63.58	8.12	1518	65.57
Phenylethyl alcohol	5.87	1110	15.47	12.24†	1854	[35.66]
Benzeneacetonitrile	6.21	1133	11.76	12.21†	1851	34.51
Benzyl acetate	6.69*†	1164	81.54	10.10*	1672	88.62
cis-Linalool oxide (pyr.)	6.69*†	1164	[82.90]	10.34	1692	0.22
Ethyl benzoate	6.75	1168	0.97	9.35	1613	1.82
Unknown [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	6.79	1170	6.73	9.50*	1625	[7.01]
Methyl salicylate	7.07*	1189	2.68	10.55*	1710	171.96
α -Terpineol	7.07*	1189	[1.94]	9.82	1651	0.35
(3Z)-Hexenyl 2-methylbutyrate	7.70	1231	0.12	7.05	1439	0.29
(3Z)-Hexenyl isovalerate	7.77	1236	0.16	7.12	1444	0.15
(E)-Isogeraniol?	8.07*	1256	9.97	11.22	1766	0.82
Phenylethyl acetate	8.07*	1256	[10.87]	11.10	1756	5.36
Unknown [m/z 91, 117 (80), 90 (42), 118 (29)... 136 (5)]	8.07*	1256	[11.48]	16.48	2262	2.27
Geraniol	8.11	1259	1.15	11.69	1806	1.23
Phenylacetic acid?	8.22*	1267	0.85	17.56*	2378	3.41
Ethyl salicylate	8.22*	1267	[0.95]	10.96	1744	0.09
Unknown [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]	8.40*	1280	8.51			
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.40*	1280	[8.47]	14.68	2080	0.54
1-Nitro-2-phenylethane	8.52	1288	1.97	14.24	2038	1.85
Indole	8.60	1294	32.85	17.34*	2354	37.82
(E)-Cinnamyl alcohol	8.79	1307	1.71	16.00*	2213	2.08
Methyl anthranilate	9.27	1335	75.83	15.46*	2158	79.67
Eugenol	9.52	1353	1.28	14.93*	2105	1.34
8-Hydroxylinalool	9.64	1361	2.16	16.35*	2248	2.44

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isomer						
Butyl benzoate	9.78	1371	0.21	11.73	1810	0.08
Methyl (<i>E</i>)-cinnamate	9.85	1376	0.35	13.85	2000	0.34
(3 <i>Z</i>)-Hexenyl (3 <i>Z</i>)-hexenoate	9.93	1382	0.20	10.10*	1672	[86.65]
(3 <i>Z</i>)-Hexenyl hexanoate?	9.96*	1384	0.43			
β -Cubebene	9.96*	1384	[0.34]	7.76	1491	0.14
β -Elemene	10.03	1389	0.78	8.43	1542	1.02
(<i>Z</i>)-Jasmone	10.08	1392	0.39	12.46	1873	0.58
Dimethyl anthranilate	10.16	1398	0.52	13.73	1989	0.48
Ethyl anthranilate	10.27	1406	0.35	15.71	2182	0.32
β -Caryophyllene	10.36	1412	0.53	8.40	1539	0.53
(<i>E</i>)-Cinnamyl acetate	10.73	1440	0.23	14.70	2082	0.56
α -Humulene	10.81	1447	0.65	9.28	1607	1.08
(<i>E</i>)- β -Farnesene	10.97	1458	0.23	9.54	1628	0.36
Oxindole?	11.08	1466	0.40			
γ -Muurolene	11.16	1473	0.50	9.58	1631	0.53
Germacrene D	11.19	1475	2.64	9.78	1647	3.05
epi-Cubebol	11.39*	1490	1.72	12.01	1834	0.29
Bicyclogermacrene	11.39*	1490	[1.58]	10.10*	1672	[67.98]
α -Muurolene	11.48*	1497	2.30	10.04	1668	0.79
(3 <i>Z</i> ,6 <i>E</i>)- α -Farnesene	11.48*	1497	[2.30]	10.27	1686	1.63
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	11.68	1512	101.33	10.55*	1710	[107.70]
δ -Cadinene	11.79	1521	4.65	10.42	1699	4.86
10-epi-Cubebol?	11.88	1528	0.34	13.82*	1998	3.73
α -Cadinene	11.95	1534	0.34	10.80	1730	0.43
Methyl N-formylanthranilate	12.13	1548	0.36	18.78	2515	0.27
Hexenyl benzoate isomer	12.28	1559	1.01	14.28	2042	1.17
(<i>E</i>)-Nerolidol	12.39*	1568	35.82	13.82*	1998	[3.73]
(3 <i>Z</i>)-Hexenyl benzoate	12.39*	1568	[39.29]	14.42	2055	38.52
Germacrene D-4-ol	12.43	1571	26.60	13.71	1987	29.60
Hexyl benzoate	12.47	1574	0.93	13.91	2006	0.99
(2 <i>E</i>)-Hexenyl benzoate	12.56	1581	2.99	14.64	2076	2.50
Methyl N-acetylanthranilate	12.66	1589	1.49	17.56*	2378	[3.92]
Ledol	12.74	1596	0.18	13.40	1959	0.32
τ -Muurolol	13.24*	1636	2.24	15.09	2121	1.40
τ -Cadinol	13.24*	1636	[2.24]	14.93*	2105	[1.16]
α -Muurolol	13.29	1641	0.31	15.23	2135	0.44
α -Cadinol	13.39	1649	3.23	15.52	2164	3.45
Unknown [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]	13.46	1654	0.15			
(3 <i>E</i> ,5 <i>E</i>)-7-Hydroxyfarnesene	13.51	1659	0.85	16.27	2240	1.47
Methyl (<i>E</i>)-jasmonate	13.68	1673	1.50	17.34*	2354	[49.25]
Shyobunol	13.79	1682	0.44	16.35*	2248	[2.01]
Unknown [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	13.97	1697	2.00	12.57	1883	2.32

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Pentadecanal	14.10	1708	0.23	13.48	1966	0.09
(2E,6E)-Farnesol	14.26	1721	1.41	16.87	2303	1.52
Oplopanone	14.33	1728	1.34	18.16	2444	1.12
Unknown [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16) ...]	14.49	1742	4.18	18.28	2458	4.47
Benzyl benzoate	14.63	1754	3.38	18.93	2532	3.73
Phenylethyl benzoate	15.63*	1842	2.62	19.64	2616	2.03
(2E,6E)-Farnesyl acetate	15.63*	1842	[2.76]	16.00*	2213	[2.19]
Phytone	15.67	1846	0.13	14.74	2086	0.07
Phytadiene isomer I	15.71	1850	0.07			
Benzyl salicylate	15.78	1856	0.54	20.19	2682	0.56
Methyl palmitate	16.58	1930	2.57	15.60	2171	2.99
meta-Camphorene	16.77	1948	0.09	15.46*	2158	[53.90]
Isophytol	16.81	1952	0.12	16.57	2272	0.15
Palmitic acid	17.01	1971	6.22	22.11	2926	5.34
para-Camphorene	17.11	1980	0.14	15.91	2203	0.13
Ethyl palmitate	17.30	1999	0.26	16.11	2223	1.47
(E,E)-Geranylinalool	17.61	2029	11.15	18.55	2488	12.20
(E)-Cinnamyl benzoate	18.12	2079	0.71			
Methyl linoleate	18.27	2094	1.58	18.09	2436	1.61
Methyl α-linolenate	18.33	2100	12.87	18.66	2501	12.43
Methyl stearate	18.63	2131	1.86	17.68	2391	3.59
α-Linolenic acid	18.74	2143	8.99			
Ethyl α-linolenate	18.92	2161	0.86	18.98	2538	0.80
Docosene isomer	19.00	2170	3.65			
Unknown [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]	19.40	2211	0.37			
(E)-Phytol acetate	19.50	2222	0.17	18.57	2491	0.37
(9Z)-Eicosenol?	19.82	2256	1.04			
(9Z)-Tricosene	20.06	2282	28.38	16.79	2294	28.69
Methyl arachidate	20.45	2325	0.94	19.37	2583	0.66
4,8,12,16-Tetramethylheptadecan-4-oxide?	20.52	2332	0.55			
Tetracosene isomer	20.94	2380	2.23			
Unknown [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]	21.61	2456	0.28			
2-Monopalmitin	22.01	2503	0.26			
Benzyl palmitate	22.56	2570	1.19			
Benzyl oleate	23.94	2742	0.76			
Benzyl α-linolenate	24.01	2750	5.25			
Benzyl stearate	24.18	2771	0.16			
Squalene	24.58	2824	6.95	22.80	3018	7.43
2,3-Oxidosqualene	25.43	2938	5.28	24.82	3304	9.31
Benzyl arachidate	25.69	2973	0.29			
2,6,10,15,19,23-Hexamethyl-(6E,10E,14E,18E)-1,6,10,14,18,22-	25.92	3005	0.30			

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tetracosahexaen-3-ol					
Unknown [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]	26.19	3040	0.38		
α -Tocopherol	26.77	3113	1.86		
Benzyl behenate	27.39	3178	0.18		
Unknown [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]	28.75	3298	3.05		
β -Amyrin	28.88	3308	0.24		
α -Amyrin	30.04	3385	0.33		
Unknown [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]	30.20	3396	4.96		
γ -Cadinene				10.40	1697
					2.25

*: 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

Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).

Unknown compounds are expressed in equivalents of internal standard without correction.

R.T.: Retention time (minutes)

R.I.: Retention index