

Date : 2024-04-18

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24D04-PTH05

Customer Identification : Jasmine Sambac Absolute - India - J10115R

Type : Absolute

Source : *Jasminum sambac*

Customer : Plant Therapy

Checked and approved by:

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-004 - Terpenes and volatiles profiling by response factor

Results : See analysis summary (next page)

Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005

Date : 2024-04-10

PHYSICOCHEMICAL DATA

CONCLUSION

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

ANALYSIS SUMMARY

Identification	mg/g	% m/m	Class
Hexan-2-ol	0.07	0.01	Aliphatic alcohol
(3E)-Hexenol	0.21	0.02	Aliphatic alcohol
(3Z)-Hexenol	3.19	0.32	Aliphatic alcohol
Hexanol	0.78	0.08	Aliphatic alcohol
Prenyl acetate	0.02	0.0	Aliphatic ester
6-Methyl-5-hepten-2-one	0.16	0.02	Aliphatic ketone
(3Z)-Hexenyl acetate	20.26	2.03	Aliphatic ester
(2E)-Hexenyl acetate	0.16	0.02	Aliphatic ester
Caproic acid	1.10	0.11	Aliphatic acid
Benzyl alcohol	91.25	9.12	Simple phenolic
(Z)- β -Ocimene	0.02	0.0	Monoterpene
(E)- β -Ocimene	0.83	0.08	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.18	0.02	Monoterpenic alcohol
Benzyl formate	0.25	0.03	Phenolic ester
<i>trans</i> -Linalool oxide (fur.)	1.12	0.11	Monoterpenic alcohol
Methyl benzoate	4.87	0.49	Phenolic ester
Linalool	63.80	6.38	Monoterpenic alcohol
Phenylethyl alcohol	10.93	1.09	Simple phenolic
Benzeneacetonitrile	16.23	1.62	Simple phenolic
<i>para</i> -Vinylanisole	0.11	0.01	Simple phenolic
Benzyl acetate	106.57	10.66	Phenolic ester
Ethyl benzoate	1.12	0.11	Phenolic ester
Unknown	8.20	0.82	Unknown
<i>trans</i> -Linalool oxide (pyr.)	0.95	0.1	Monoterpenic alcohol
(3Z)-Hexenyl butyrate	0.14	0.01	Aliphatic ester
Methyl salicylate	2.67	0.27	Phenolic ester
(3Z)-Hexenyl isovalerate	0.24	0.02	Aliphatic ester
Geraniol	0.13	0.01	Monoterpenic alcohol
Phenylethyl acetate	4.67	0.47	Phenolic ester
Unknown	6.17	0.62	Unknown
Ethyl salicylate	0.08	0.01	Phenolic ester
Phenylacetic acid?	0.51	0.05	Phenolic acid
Unknown	5.42	0.54	Unknown
2,6-Dimethyl-1,7-octadiene-3,6-diol	1.63	0.16	Monoterpenic alcohol
Indole	16.37	1.64	Indole
1-Nitro-2-phenylethane	1.10	0.11	Simple phenolic
(E)-Cinnamyl alcohol	1.68	0.17	Phenylpropanoid
Methyl anthranilate	85.89	8.59	Phenolic ester
Eugenol	0.23	0.02	Phenylpropanoid
8-Hydroxylinalool isomer	0.13	0.01	Monoterpenic alcohol
Neryl acetate	1.78	0.18	Monoterpenic ester

Butyl benzoate	0.63	0.06	Phenolic ester
Methyl (<i>E</i>)-cinnamate	0.36	0.04	Phenylpropanoid ester
(3 <i>Z</i>)-Hexenyl (3 <i>Z</i>)-hexenoate	0.11	0.01	Aliphatic ester
β -Cubebene	0.13	0.01	Sesquiterpene
(3 <i>Z</i>)-Hexenyl hexanoate?	0.42	0.04	Aliphatic ester
β -Elemene	1.54	0.15	Sesquiterpene
(<i>Z</i>)-Jasmone	0.12	0.01	Jasmonate
Dimethyl anthranilate	0.31	0.03	Phenolic ester
β -Caryophyllene	0.55	0.06	Sesquiterpene
(<i>E</i>)-Cinnamyl acetate	0.18	0.02	Phenylpropanoid ester
α -Humulene	0.55	0.06	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.18	0.02	Sesquiterpene
Oxindole?	0.10	0.01	Indole
γ -Muurolene	0.24	0.02	Sesquiterpene
Germacrene D	2.85	0.29	Sesquiterpene
(<i>Z</i>)-Jasmin lactone	0.10	0.01	Aliphatic lactone
Bicyclogermacrene	1.67	0.17	Sesquiterpene
epi-Cubebol	0.16	0.02	Sesquiterpenic alcohol
(3 <i>Z</i> ,6 <i>E</i>)- α -Farnesene	2.56	0.26	Sesquiterpene
γ -Cadinene	0.20	0.02	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	99.45	9.95	Sesquiterpene
δ -Cadinene	2.72	0.27	Sesquiterpene
10-epi-Cubebol?	0.10	0.01	Sesquiterpenic alcohol
α -Cadinene	0.15	0.01	Sesquiterpene
Methyl N-formylanthranilate	0.81	0.08	Phenolic ester
Hexenyl benzoate isomer	0.02	0.0	Phenolic ester
(<i>E</i>)-Nerolidol	3.45	0.35	Sesquiterpenic alcohol
(3 <i>Z</i>)-Hexenyl benzoate	49.35	4.94	Phenolic ester
Germacrene D-4-ol	38.68	3.87	Sesquiterpenic alcohol
Hexyl benzoate	1.01	0.1	Phenolic ester
(2 <i>E</i>)-Hexenyl benzoate	1.24	0.12	Phenolic ester
Methyl N-acetylanthranilate	3.25	0.33	Phenolic ester
Ledol	0.22	0.02	Sesquiterpenic alcohol
τ -Cadinol	0.53	0.05	Sesquiterpenic alcohol
τ -Muurolol	0.69	0.07	Sesquiterpenic alcohol
α -Muurolol	0.19	0.02	Sesquiterpenic alcohol
α -Cadinol	1.52	0.15	Sesquiterpenic alcohol
Unknown	0.33	0.03	Unknown
(3 <i>E</i> ,5 <i>E</i>)-7-Hydroxyfarnesene	0.19	0.02	Sesquiterpenic alcohol
Methyl <i>trans</i> -jasmonate	1.11	0.11	Jasmonate
Shyobunol	0.60	0.06	Sesquiterpenic alcohol
Unknown	0.47	0.05	Unknown
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	1.31	0.13	Sesquiterpenic alcohol
Oplopanone	0.93	0.09	Sesquiterpenic alcohol
Unknown	5.87	0.59	Unknown

Benzyl benzoate	4.52	0.45	Phenolic ester
Unknown	0.17	0.02	Unknown
(2E,6E)-Farnesyl acetate	0.93	0.09	Sesquiterpenic ester
Phenylethyl benzoate	2.00	0.2	Phenolic ester
Phytadiene isomer I	0.18	0.02	Diterpene
Benzyl salicylate	0.61	0.06	Phenolic ester
Methyl palmitate	5.12	0.51	Aliphatic ester
Palmitic acid	4.88	0.49	Aliphatic acid
Ethyl palmitate	0.47	0.05	Aliphatic ester
(E,E)-Geranylinalool	10.20	1.02	Diterpenic alcohol
(E)-Cinnamyl benzoate	0.55	0.06	Phenylpropanoid ester
Methyl linoleate	3.18	0.32	Aliphatic ester
Methyl α -linolenate	28.05	2.81	Aliphatic ester
Methyl stearate	3.14	0.31	Aliphatic ester
α -Linolenic acid	3.49	0.35	Aliphatic acid
Ethyl linoleate	0.28	0.03	Aliphatic ester
Ethyl α -linolenate	0.71	0.07	Aliphatic ester
Stearic acid	1.62	0.16	Aliphatic acid
Methyl (E)-phytenate	1.95	0.2	Diterpenic ester
Unknown	1.49	0.15	Unknown
(9Z)-Eicosenol?	1.17	0.12	Aliphatic alcohol
(9Z)-Tricosene	0.13	0.01	Alkene
(9E)-Tricosene?	27.94	2.79	Alkene
Methyl arachidate	1.18	0.12	Aliphatic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.54	0.05	Terpenic lactone
Tetracosene isomer	2.00	0.2	Alkene
Unknown	3.29	0.33	Unknown
2-Monopalmitin	0.24	0.02	Glyceride
Benzyl palmitate	1.73	0.17	Phenolic ester
Benzyl oleate	1.00	0.1	Phenolic ester
Benzyl α -linolenate	8.04	0.8	Phenolic ester
Benzyl stearate	0.50	0.05	Phenolic ester
Squalene	5.76	0.58	Triterpene
2,3-Oxidosqualene	5.39	0.54	Triterpenic ether
Benzyl arachidate	0.20	0.02	Phenolic ester
2,6,10,15,19,23-Hexamethyl-(6E,10E,14E,18E)-1,6,10,14,18,22-tetracosahexaen-3-ol	0.24	0.02	Triterpenic alcohol
Unknown	0.54	0.05	Triterpenic alcohol
α -Tocopherol	1.82	0.18	Tocopherol
Unknown	0.13	0.01	Unknown
Benzyl behenate	0.20	0.02	Phenolic ester
Unknown	4.11	0.41	Unknown
β -Amyrin	0.04	0.01	Triterpenic alcohol
α -Amyrin	0.40	0.04	Triterpenic alcohol

Unknown	9.87	0.99	Unknown
Consolidated total	838.37	83.84	

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

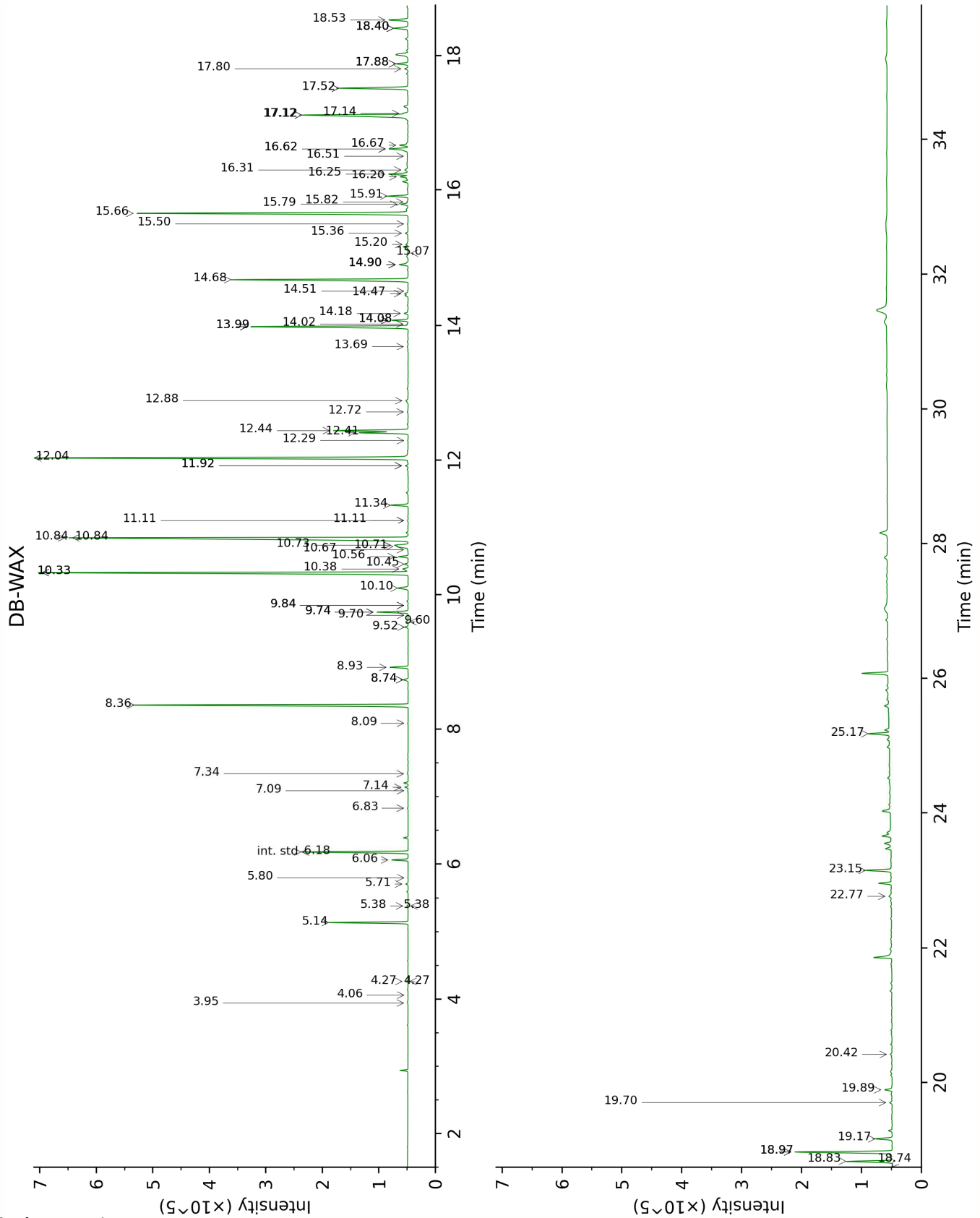
Note: Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).

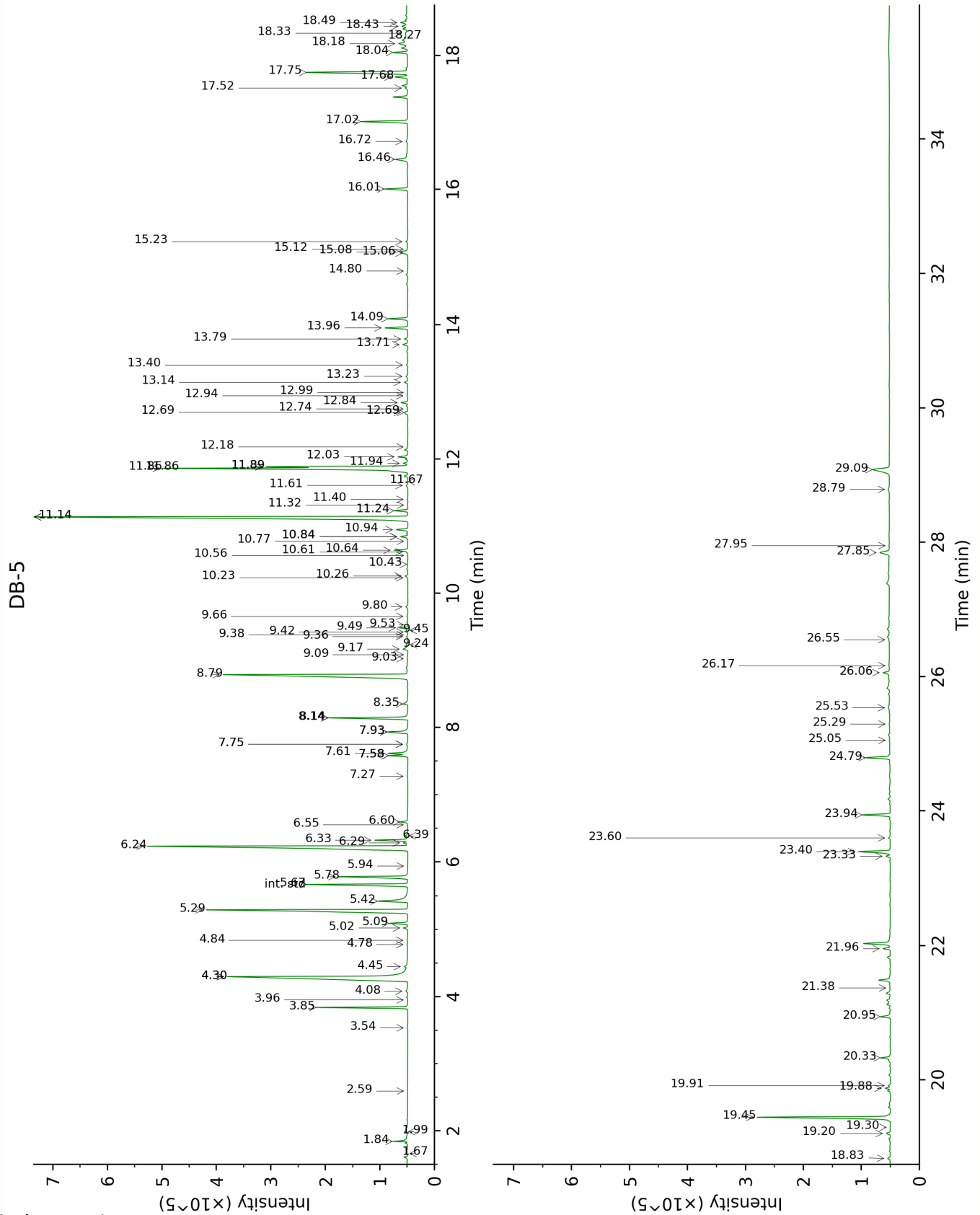
Unknown compounds are expressed in equivalents of internal standard without correction.

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: The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.





FULL ANALYSIS DATA

Hexan-2-ol	Column DB-WAX			Column DB-5		
	3.95	1196.0	0.02	1.23	803.8	0.01
(3E)-Hexenol	5.80	1329.0	0.01	1.67	844.4	0.02
(3Z)-Hexenol	6.06	1347.9	0.39	1.84	861.1	0.31
Hexanol	5.71	1322.4	0.06	1.99	874.6	0.08
Prenyl acetate	4.27*	1218.6	[0.05]	2.59	924.2	tr
6-Methyl-5-hepten-2-one	5.38*	1299.1	[0.03]	3.54	990.9	0.02
(3Z)-Hexenyl acetate	5.14	1280.0	1.79	3.84	1011.5	1.77
(2E)-Hexenyl acetate	5.38*	1299.1	[0.03]	3.96	1018.7	0.01
Caproic acid				4.08	1027.1	0.09
Benzyl alcohol	12.04	1816.6	10.12	4.30*	1041.1	[9.60]
(Z)- β -Ocimene	4.06	1204.4	tr	4.30*	1041.1	[9.60]
(E)- β -Ocimene	4.27*	1218.6	[0.05]	4.45	1050.6	0.10
<i>cis</i> -Linalool oxide (fur.)	6.83	1403.0	0.02	4.78	1071.8	0.02
Benzyl formate	9.74*	1625.2	[0.82]	4.84	1075.9	0.02
<i>trans</i> -Linalool oxide (fur.)	7.14	1425.9	0.08	5.02	1087.7	0.11
Methyl benzoate	8.93	1560.9	0.47	5.09	1092.1	0.45
Linalool	8.36	1516.8	7.07	5.29	1105.1	6.96
Phenylethyl alcohol	12.44*†	1852.4	[2.00]	5.42	1113.5	1.24
Benzeneacetonitrile	12.41*†	1849.6	[1.28]	5.78	1137.1	1.90
<i>para</i> -Vinylanisole	9.70	1621.5	0.01	5.94	1147.4	0.01
Benzyl acetate	10.33*	1672.5	[10.52]	6.24	1166.5	10.32
Ethyl benzoate	9.60	1613.8	0.06	6.29	1169.7	0.11
Unknown JASA I [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	9.74*	1625.2	[0.82]	6.33	1172.3	0.78
<i>trans</i> -Linalool oxide (pyr.)	10.84*	1714.9	[12.50]	6.39	1176.5	0.09
(3Z)-Hexenyl butyrate	7.09	1422.2	0.02	6.56	1187.3	0.01
Methyl salicylate	10.73	1705.6	0.42	6.60	1190.0	0.21
(3Z)-Hexenyl isovalerate	7.34	1440.7	0.03	7.27	1235.2	0.02
Geraniol	11.92*	1806.5	[0.08]	7.58*†	1255.9	[0.42]
Phenylethyl acetate	11.34	1756.7	0.47	7.58*†	1255.9	[0.42]
Unknown JASA II [m/z 91, 117 (80), 90 (42), 118 (29)... 136 (5)]	16.62*	2254.0	[0.66]	7.61*†	1258.2	[0.61]
Ethyl salicylate	11.11*	1737.4	[0.03]	7.75*	1267.4	[0.05]
Phenylacetic acid?	17.88*	2388.2	[0.35]	7.75*	1267.4	[0.05]
Unknown JASA III [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]				7.93*	1279.7	[0.67]
2,6-Dimethyl-1,7-	14.90*	2080.8	[0.30]	7.93*	1279.7	[0.67]

octadiene-3,6-diol						
Indole	17.52*	2349.2	[2.00]	8.14*	1293.9	[2.01]
1-Nitro-2-phenylethane	14.47	2039.7	0.10	8.14*	1293.9	[2.01]
(E)-Cinnamyl alcohol	16.20	2210.3	0.22	8.35	1308.0	0.19
Methyl anthranilate	15.66	2155.8	7.43	8.79	1339.7	7.40
Eugenol	15.07	2097.2	0.02	9.03	1356.7	0.02
8-Hydroxylinalool isomer	16.67	2259.8	0.23	9.09	1360.8	0.01
Neryl acetate	10.45	1682.7	0.10	9.17	1366.8	0.18
Butyl benzoate	11.92*	1806.5	[0.08]	9.24	1371.3	0.06
Methyl (E)-cinnamate	14.08*	2002.0	[0.44]	9.36	1379.9	0.04
(3Z)-Hexenyl (3Z)-hexenoate	10.33*	1672.5	[10.52]	9.38	1381.8	0.01
β-Cubebene	8.09	1496.2	0.02	9.42	1384.8	0.02
(3Z)-Hexenyl hexanoate?				9.45	1386.7	0.04
β-Elemene	8.74*	1546.6	[0.15]	9.49	1389.3	0.19
(Z)-Jasmone	12.72	1876.8	0.03	9.53	1392.5	0.01
Dimethyl anthranilate	13.99*	1993.1	[4.53]	9.66	1401.4	0.03
β-Caryophyllene	8.74*	1546.6	[0.15]	9.80	1411.8	0.07
(E)-Cinnamyl acetate	14.90*	2080.8	[0.30]	10.23	1444.2	0.02
α-Humulene	9.52	1607.2	0.09	10.26	1446.2	0.07
(E)-β-Farnesene	9.84*	1633.2	[0.02]	10.43	1459.2	0.02
Oxindole?				10.56	1469.0	0.01
γ-Murolene	9.84*	1633.2	[0.02]	10.61	1473.1	0.03
Germacrene D	10.10	1653.9	0.37	10.64	1474.9	0.36
(Z)-Jasmin lactone	15.82	2172.6	0.04	10.77	1484.9	0.01
Bicyclgermacrene	10.38	1676.9	0.21	10.84*	1490.0	[0.21]
epi-Cubebol	12.29	1839.4	0.02	10.84*	1490.0	[0.21]
(3Z,6E)-α-Farnesene	10.56	1691.6	0.25	10.94	1497.8	0.32
γ-Cadinene	10.67	1700.1	0.03	11.14*	1513.2	[12.58]
(3E,6E)-α-Farnesene	10.84*	1714.9	[12.50]	11.14*	1513.2	[12.58]
δ-Cadinene	10.71	1704.1	0.32	11.24	1520.5	0.34
10-epi-Cubebol?	14.02	1996.6	0.03	11.32	1527.0	0.01
α-Cadinene	11.11*	1737.4	[0.03]	11.40	1533.8	0.02
Methyl N-formylanthranilate	18.97*	2510.4	[2.84]	11.61	1550.2	0.06
Hexenyl benzoate isomer	14.51	2043.3	0.02	11.67	1554.6	tr
(E)-Nerolidol	14.08*	2002.0	[0.44]	11.86*†	1570.2	[6.77]
(3Z)-Hexenyl benzoate	14.68	2059.5	5.23	11.86*†	1570.2	[6.77]
Germacrene D-4-ol	13.99*	1993.1	[4.53]	11.89*†	1572.0	[3.16]
Hexyl benzoate	14.18	2011.8	0.11	11.89*†	1572.0	[3.16]
(2E)-Hexenyl benzoate	14.90*	2080.8	[0.30]	11.94	1576.2	0.13
Methyl N-acetylanthranilate	17.80	2380.2	0.10	12.03	1583.7	0.26

Ledol	13.69	1966.0	0.03	12.18	1595.3	0.03
τ -Cadinol	15.20	2110.1	0.06	12.69*	1637.5	[0.13]
τ -Muurolol	15.36	2126.5	0.08	12.69*	1637.5	[0.13]
α -Muurolol	15.50	2140.2	0.02	12.74	1641.7	0.02
α -Cadinol	15.79	2169.1	0.22	12.84	1649.5	0.18
Unknown JASA IV [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]				12.94	1657.9	0.03
(3E,5E)-7- Hydroxyfarnesene	16.51	2242.9	0.04	12.99	1662.0	0.02
Methyl <i>trans</i> -jasmonate	17.52*	2349.2	[2.00]	13.14	1674.5	0.10
Shyobunol	16.62*	2254.0	[0.66]	13.23	1681.9	0.07
Unknown JASA V [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]				13.40	1695.9	0.04
(2E,6E)-Farnesol	17.14	2309.0	0.11	13.71	1722.9	0.15
Oplopanone	18.40*	2446.5	[0.45]	13.79	1730.1	0.10
Unknown JASA VI [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16)...]				13.96	1744.4	0.56
Benzyl benzoate	19.17	2532.9	0.50	14.09	1756.3	0.50
Unknown JASA VII [m/z 43, 159 (79), 93 (49), 119 (48), 161 (40), 187 (36)... 238? (2)]				14.80	1818.5	0.02
(2E,6E)-Farnesyl acetate	16.25	2215.4	0.56	15.06	1842.8	0.10
Phenylethyl benzoate	19.89	2617.6	0.24	15.08	1844.4	0.23
Phytadiene isomer I				15.12	1848.2	0.02
Benzyl salicylate	20.42	2680.2	0.05	15.23	1858.3	0.06
Methyl palmitate	15.91	2181.1	0.56	16.01	1930.6	0.57
Palmitic acid				16.46	1973.6	0.54
Ethyl palmitate	16.31	2221.8	0.12	16.72	1998.8	0.05
(E,E)-Geranylinalool	18.83	2494.1	1.24	17.02	2028.1	1.22
(E)-Cinnamyl benzoate	22.77	2977.8	0.11	17.52	2077.7	0.06
Methyl linoleate	18.40*	2446.5	[0.45]	17.68	2094.1	0.35
Methyl α -linolenate	18.97*	2510.4	[2.84]	17.75	2101.0	3.08
Methyl stearate	17.88*	2388.2	[0.35]	18.04	2131.5	0.36
α -Linolenic acid				18.18	2145.4	0.38
Ethyl linoleate	18.74	2484.4	0.02	18.27	2155.5	0.03
Ethyl α -linolenate				18.33	2161.3	0.08
Stearic acid				18.43	2171.9	0.18
Methyl (E)-phytenate	18.40*	2446.5	[0.45]	18.49	2177.9	0.22
Unknown JASA VIII [m/z 190, 158 (100), 253 (68),				18.83	2214.0	0.14

193 (58), 220 (51)]						
(9Z)-Eicosenol?				19.20	2254.3	0.14
(9Z)-Tricosene	17.12*	2306.4	[3.82]	19.30	2264.1	0.02
(9E)-Tricosene?	17.12*	2306.4	[3.82]	19.44	2280.3	3.69
Methyl arachidate	19.70	2595.0	0.08	19.88	2327.9	0.14
4,8,12,16-Tetramethylheptadecan-4-olide?				19.92	2332.3	0.06
Tetracosene isomer				20.33	2378.8	0.26
Unknown JASA IX [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]				20.95	2450.6	0.31
2-Monopalmitin				21.38	2500.3	0.02
Benzyl palmitate				21.96	2570.9	0.20
Benzyl oleate				23.33	2743.2	0.12
Benzyl α -linolenate				23.40	2752.1	0.94
Benzyl stearate				23.60	2778.3	0.06
Squalene	23.15	3029.2	0.77	23.94	2823.3	0.74
2,3-Oxidosqualene	25.17	3312.4	0.64	24.79	2938.1	0.66
Benzyl arachidate				25.05	2973.9	0.02
2,6,10,15,19,23-Hexamethyl-(6E,10E,14E,18E)-1,6,10,14,18,22-tetracosahexaen-3-ol				25.29	3007.4	0.03
Unknown JAGR V [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]				25.53	3041.9	0.05
α -Tocopherol				26.06	3116.6	0.22
Unknown JAGR VI [m/z 109, 95 (52), 69 (51), 57 (47), 97 (45)... 278 (9)...]				26.17	3130.1	0.01
Benzyl behenate				26.55	3180.3	0.02
Unknown JASA X [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]				27.85	3317.2	0.39
β -Amyrin				27.95	3325.7	0.01
α -Amyrin				28.79	3396.9	0.05
Unknown JASA XI [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]				29.09	3417.7	0.94
Total reported		87.59%			92.08%	

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*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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