

Date : 2024-02-07

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 24A25-PTH02

**Customer Identification** : Jasmine Sambac Absolute - India - J10114R

**Type** : Absolute

**Source** : *Jasminum sambac*

**Customer** : Plant Therapy

Checked and approved by:

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

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This report is an update from the first version issued on 2024-01-30 to correct the customer identification.

## *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 :** 2024-01-29

## *PHYSICOCHEMICAL DATA*

## *CONCLUSION*

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

## ANALYSIS SUMMARY

Identification	mg/g	% m/m	Class
(3Z)-Hexenol	2.68	0.27	Aliphatic alcohol
Hexanol	0.87	0.09	Aliphatic alcohol
Benzaldehyde	0.31	0.03	Simple phenolic
(3Z)-Hexenyl acetate	16.02	1.6	Aliphatic ester
(2E)-Hexenyl acetate	0.33	0.03	Aliphatic ester
Unknown	0.51	0.05	Unknown
Benzyl alcohol	70.43	7.04	Simple phenolic
(E)- $\beta$ -Ocimene	0.40	0.04	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.21	0.02	Monoterpenic alcohol
Benzyl formate	0.24	0.02	Phenolic ester
<i>trans</i> -Linalool oxide (fur.)	1.42	0.14	Monoterpenic alcohol
<i>para</i> -Cresol	0.24	0.02	Simple phenolic
Methyl benzoate	5.01	0.5	Phenolic ester
Linalool	63.91	6.39	Monoterpenic alcohol
Phenylethyl alcohol	10.27	1.03	Simple phenolic
Benzeneacetonitrile	16.10	1.61	Simple phenolic
Benzyl acetate	125.04	12.5	Phenolic ester
Ethyl benzoate	0.89	0.09	Phenolic ester
Unknown	7.30	0.73	Unknown
<i>trans</i> -Linalool oxide (pyr.)	0.94	0.09	Monoterpenic alcohol
(3Z)-Hexenyl butyrate	0.76	0.08	Aliphatic ester
Methyl salicylate	1.57	0.16	Phenolic ester
(3Z)-Hexenyl 2-methylbutyrate	0.15	0.01	Aliphatic ester
(3Z)-Hexenyl isovalerate	0.14	0.01	Aliphatic ester
Phenylethyl acetate	3.59	0.36	Phenolic ester
Unknown	2.46	0.25	Unknown
Geraniol	0.29	0.03	Monoterpenic alcohol
(E)-Isogeraniol?	0.50	0.05	Monoterpenic alcohol
Phenylacetic acid?	2.82	0.28	Phenolic acid
Ethyl salicylate	0.15	0.01	Phenolic ester
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.35	0.03	Monoterpenic alcohol
Unknown	3.18	0.32	Unknown
1-Nitro-2-phenylethane	2.09	0.21	Simple phenolic
Indole	13.70	1.37	Indole
(E)-Cinnamyl alcohol	1.59	0.16	Phenylpropanoid
Methyl anthranilate	71.29	7.13	Phenolic ester
Eugenol	0.17	0.02	Phenylpropanoid
Neryl acetate	1.12	0.11	Monoterpenic ester
8-Hydroxylinalool isomer	0.31	0.03	Monoterpenic alcohol
Butyl benzoate	0.52	0.05	Phenolic ester
Methyl (E)-cinnamate	0.55	0.06	Phenylpropanoid ester

(3Z)-Hexenyl (3Z)-hexenoate	0.38	0.04	Aliphatic ester
(3Z)-Hexenyl hexanoate?	1.88	0.19	Aliphatic ester
$\beta$ -Elemene	0.09	0.01	Sesquiterpene
(Z)-Jasmone	0.24	0.02	Jasmonate
Dimethyl anthranilate	0.13	0.01	Phenolic ester
Ethyl anthranilate	0.05	0.01	Phenolic ester
$\beta$ -Caryophyllene	0.44	0.04	Sesquiterpene
(E)-Cinnamyl acetate	0.69	0.07	Phenylpropanoid ester
$\alpha$ -Humulene	0.12	0.01	Sesquiterpene
(E)- $\beta$ -Farnesene	0.17	0.02	Sesquiterpene
Oxindole?	0.80	0.08	Indole
$\gamma$ -Muurolene	0.32	0.03	Sesquiterpene
Germacrene D	2.65	0.27	Sesquiterpene
(Z)-Jasmin lactone	0.29	0.03	Aliphatic lactone
Bicyclogermacrene	1.28	0.13	Sesquiterpene
epi-Cubebol	0.21	0.02	Sesquiterpenic alcohol
(3Z,6E)- $\alpha$ -Farnesene	1.50	0.15	Sesquiterpene
$\alpha$ -Muurolene	0.55	0.06	Sesquiterpene
$\gamma$ -Cadinene	2.46	0.25	Sesquiterpene
(3E,6E)- $\alpha$ -Farnesene	91.06	9.11	Sesquiterpene
$\delta$ -Cadinene	3.66	0.37	Sesquiterpene
10-epi-Cubebol?	0.28	0.03	Sesquiterpenic alcohol
$\alpha$ -Cadinene	0.18	0.02	Sesquiterpene
Methyl N-formylanthranilate	0.67	0.07	Phenolic ester
Hexenyl benzoate isomer	1.05	0.11	Phenolic ester
(E)-Nerolidol	2.96	0.3	Sesquiterpenic alcohol
(3Z)-Hexenyl benzoate	53.23	5.32	Phenolic ester
Spathulenol	0.12	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	40.87	4.09	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.14	0.01	Sesquiterpenic ether
Hexyl benzoate	0.47	0.05	Phenolic ester
Caryophyllene oxide	0.17	0.02	Sesquiterpenic ether
(2E)-Hexenyl benzoate	0.15	0.01	Phenolic ester
Methyl N-acetylanthranilate	3.19	0.32	Phenolic ester
Ledol	0.24	0.02	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.51	0.05	Sesquiterpenic alcohol
$\tau$ -Muurolol	0.70	0.07	Sesquiterpenic alcohol
$\alpha$ -Muurolol	0.18	0.02	Sesquiterpenic alcohol
Methyl <i>cis</i> -jasmonate	0.54	0.05	Jasmonate
$\alpha$ -Cadinol	1.57	0.16	Sesquiterpenic alcohol
Unknown	0.28	0.03	Unknown
(3E,5E)-7-Hydroxyfarnesene	0.19	0.02	Sesquiterpenic alcohol
Methyl <i>trans</i> -jasmonate	0.78	0.08	Jasmonate
Shyobunol	0.64	0.06	Sesquiterpenic alcohol
Unknown	0.38	0.04	Unknown

(2E,6E)-Farnesol	1.61	0.16	Sesquiterpenic alcohol
Oplopanone	0.95	0.1	Sesquiterpenic alcohol
(E)-Coniferyl alcohol	0.08	0.01	Phenylpropanoid
Unknown	6.59	0.66	Unknown
Benzyl benzoate	4.51	0.45	Phenolic ester
Unknown	0.15	0.01	Unknown
(2E,6E)-Farnesyl acetate	0.97	0.1	Sesquiterpenic ester
Phenylethyl benzoate	1.60	0.16	Phenolic ester
Benzyl salicylate	0.72	0.07	Phenolic ester
Methyl palmitate	4.14	0.41	Aliphatic ester
Palmitic acid	2.52	0.25	Aliphatic acid
<i>para</i> -Camphorene	0.29	0.03	Diterpene
Ethyl palmitate	0.29	0.03	Aliphatic ester
(E,E)-Geranylinalool	9.71	0.97	Diterpenic alcohol
(E)-Cinnamyl benzoate	0.52	0.05	Phenylpropanoid ester
Methyl linoleate	2.81	0.28	Aliphatic ester
Methyl $\alpha$ -linolenate	25.59	2.56	Aliphatic ester
Phytol	0.54	0.05	Diterpenic alcohol
Methyl stearate	2.63	0.26	Aliphatic ester
$\alpha$ -Linolenic acid	2.63	0.26	Aliphatic acid
Ethyl linoleate	0.67	0.07	Aliphatic ester
Ethyl $\alpha$ -linolenate	1.41	0.14	Aliphatic ester
Stearic acid	1.73	0.17	Aliphatic acid
Methyl (E)-phytenate	1.95	0.2	Diterpenic ester
Unknown	0.71	0.07	Unknown
(E)-Phytyl acetate	0.25	0.03	Diterpenic ester
(9Z)-Eicosenol?	0.94	0.09	Aliphatic alcohol
(9Z)-Tricosene	26.29	2.63	Alkene
(9E)-Tricosene?	0.71	0.07	Alkene
1-Tricosene?	0.45	0.04	Alkene
Methyl arachidate	0.49	0.05	Aliphatic ester
Tetracosene isomer	1.79	0.18	Alkene
Unknown	0.31	0.03	Unknown
2-Monopalmitin	2.09	0.21	Glyceride
Benzyl palmitate	1.14	0.11	Phenolic ester
Benzyl oleate	6.99	0.7	Phenolic ester
Benzyl linoleate	0.41	0.04	Phenolic ester
Benzyl $\alpha$ -linolenate	0.58	0.06	Phenolic ester
Squalene	5.17	0.52	Triterpene
2,3-Oxidosqualene	0.21	0.02	Triterpenic ether
2,3-Dihydro-3-oxosqualene?	0.43	0.04	Triterpenic ketone
Benzyl arachidate	0.14	0.01	Phenolic ester
Unknown	0.15	0.01	Triterpenic alcohol
$\alpha$ -Tocopherol	1.63	0.16	Tocopherol
Benzyl behenate	0.37	0.04	Phenolic ester

Unknown	2.13	0.21	Unknown
Unknown	11.23	1.12	Unknown
<b>Consolidated total</b>	<b>788.10</b>	<b>78.81</b>	

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).

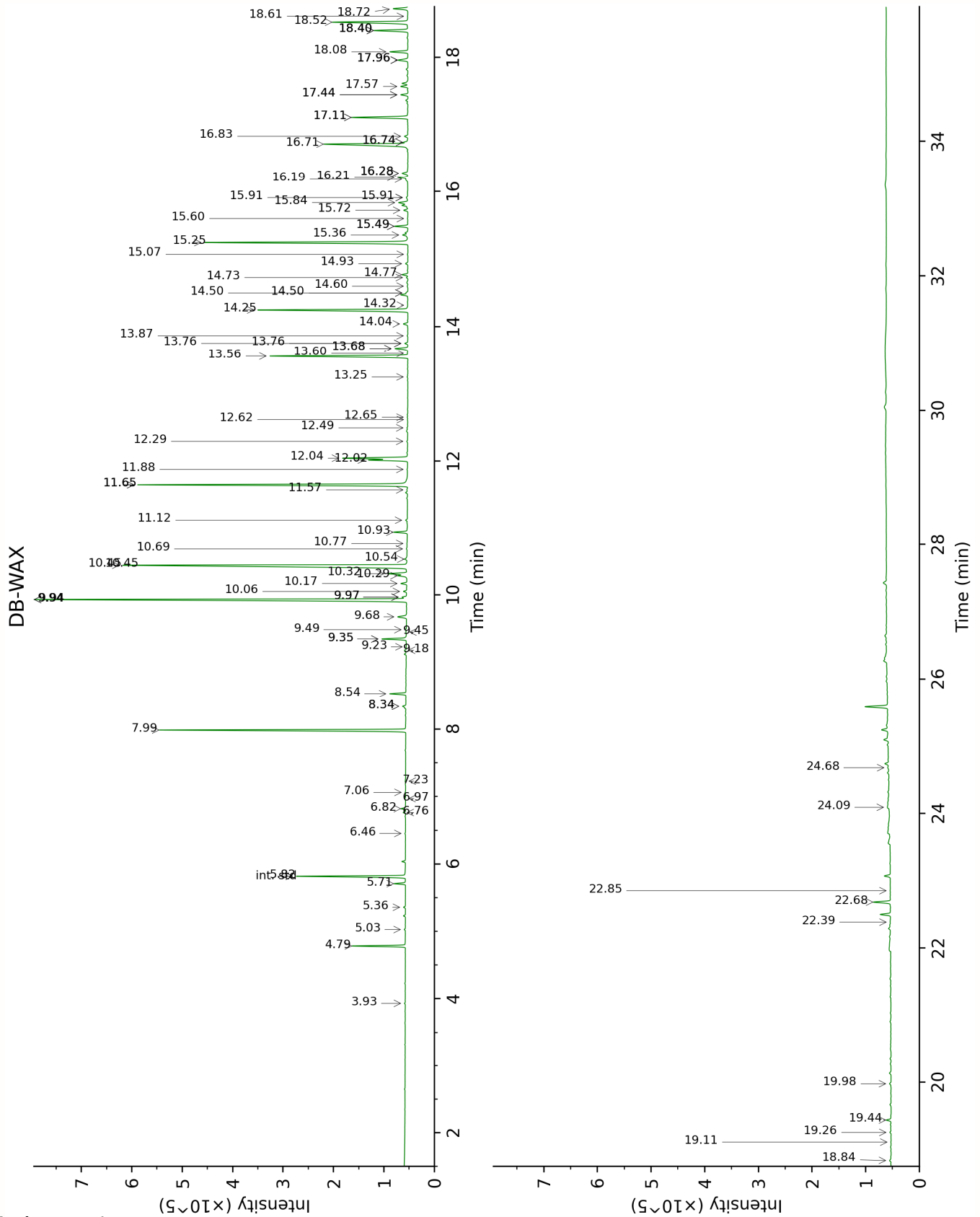
Unknown compounds are expressed in equivalents of internal standard without correction.

**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.

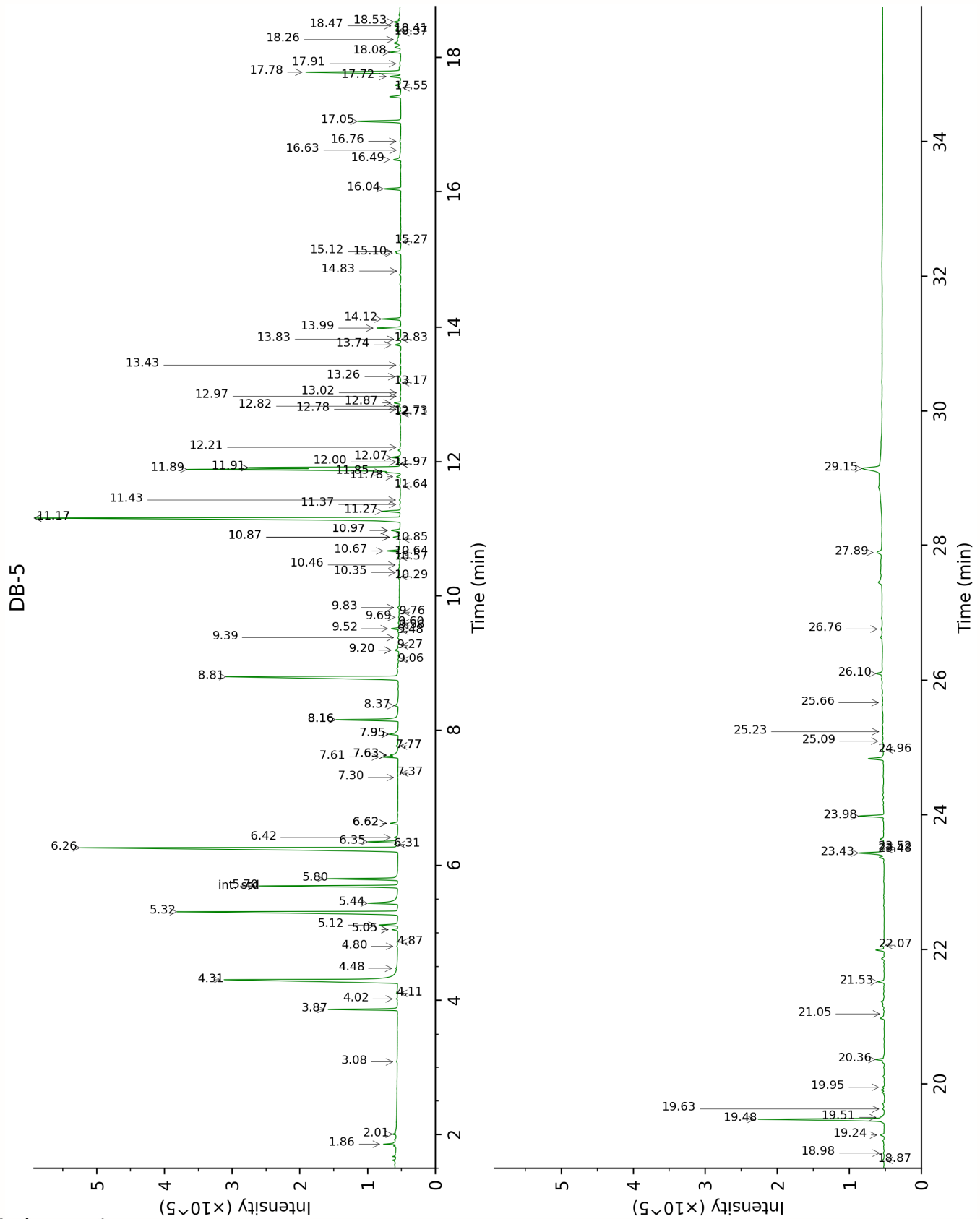
**Unknowns:** The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

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









FULL ANALYSIS DATA

(3Z)-Hexenol	Column DB-WAX			Column DB-5		
	5.71	1348.0	0.34	1.86	859.6	0.28
Hexanol	5.36	1323.0	0.06	2.01	873.6	0.09
Benzaldehyde	7.23	1458.7	0.02	3.08	956.8	0.04
(3Z)-Hexenyl acetate	4.79	1274.7	1.50	3.87	1011.7	1.50
(2E)-Hexenyl acetate	5.03	1299.3	0.04	4.02	1021.7	0.03
Unknown MISC CLXL [m/z 41, 57 (55), 85 (47), 59 (45), 43 (41)...]				4.11	1027.1	0.05
Benzyl alcohol	11.65*	1813.5	[9.07]	4.31	1040.0	8.31
(E)- $\beta$ -Ocimene	3.93	1215.8	0.02	4.48	1051.0	0.05
cis-Linalool oxide (fur.)	6.46	1401.5	0.02	4.80	1071.9	0.02
Benzyl formate	9.35*	1621.7	[0.80]	4.87	1076.0	0.02
trans-Linalool oxide (fur.)	6.82	1428.6	0.14	5.05*	1087.8	[0.14]
para-Cresol	13.87	2015.7	0.03	5.05*	1087.8	[0.14]
Methyl benzoate	8.54	1557.7	0.51	5.12	1092.1	0.50
Linalool	7.99	1515.5	7.62	5.32	1104.7	7.45
Phenylethyl alcohol	12.02*†	1845.8	[1.23]	5.44	1113.0	1.24
Benzeneacetonitrile	12.04*†	1848.3	[2.22]	5.80	1136.3	2.01
Benzyl acetate	9.94*	1668.9	[13.62]	6.26	1165.8	12.93
Ethyl benzoate	9.18	1608.3	0.06	6.31	1168.9	0.09
Unknown JASA I [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	9.35*	1621.7	[0.80]	6.35	1171.4	0.74
trans-Linalool oxide (pyr.)	10.54	1718.5	0.10	6.42	1175.6	0.10
(3Z)-Hexenyl butyrate	6.76	1424.3	0.08	6.62*	1189.0	[0.21]
Methyl salicylate	10.44*	1710.9	[12.91]	6.62*	1189.0	[0.21]
(3Z)-Hexenyl 2-methylbutyrate	6.97	1439.6	0.03	7.30	1233.5	0.02
(3Z)-Hexenyl isovalerate	7.06	1446.4	0.02	7.37	1237.8	0.02
Phenylethyl acetate	10.93	1752.2	0.46	7.61	1253.7	0.38
Unknown JASA II [m/z 91, 117 (80), 90 (42), 118 (29)... 136 (5)]	16.28*	2256.5	[0.27]	7.64*	1255.5	[0.34]

Geraniol	11.57	1806.9	0.03	7.64*	1255.5	[0.34]
(E)-Isogeraniol?	11.12	1768.1	0.06	7.64*	1255.5	[0.34]
Phenylacetic acid?	17.57	2395.1	0.28	7.77*	1264.5	[0.07]
Ethyl salicylate	10.77	1738.1	0.01	7.77*	1264.5	[0.07]
2,6-Dimethyl-1,7-octadiene-3,6-diol	14.60	2086.2	0.04	7.94*	1276.0	[0.36]
Unknown JASA III [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]				7.94*	1276.0	[0.36]
1-Nitro-2-phenylethane	14.04	2032.7	0.19	8.16*	1290.1	[1.90]
Indole	17.11*	2345.1	[2.04]	8.16*	1290.1	[1.90]
(E)-Cinnamyl alcohol	15.84	2210.7	0.42	8.37	1304.1	0.19
Methyl anthranilate	15.25	2150.7	7.02	8.81	1335.6	6.56
Eugenol	14.73	2099.0	0.05	9.06	1353.5	0.02
Neryl acetate	10.06	1678.6	0.12	9.20*	1363.8	[0.15]
8-Hydroxylinalool isomer	16.28*	2256.5	[0.27]	9.20*	1363.8	[0.15]
Butyl benzoate	11.65*	1813.5	[9.07]	9.26	1368.4	0.06
Methyl (E)-cinnamate	13.76*	2005.0	[0.11]	9.39	1377.1	0.06
(3Z)-Hexenyl (3Z)-hexenoate	9.97*	1671.7	[0.17]	9.48	1384.1	0.04
(3Z)-Hexenyl hexanoate?				9.52	1386.6	0.20
β-Elemene	8.34*	1542.7	[0.12]	9.56	1389.6	0.01
(Z)-Jasmone	12.29	1870.4	0.04	9.60	1392.7	0.03
Dimethyl anthranilate	13.60	1990.2	0.02	9.69	1398.7	0.01
Ethyl anthranilate	15.60	2186.2	0.02	9.76	1404.1	tr
β-Caryophyllene	8.34*	1542.7	[0.12]	9.83	1409.4	0.06
(E)-Cinnamyl acetate	14.50*	2076.5	[0.07]	10.29	1443.9	0.07
α-Humulene	9.23	1612.3	0.01	10.35	1448.6	0.02
(E)-β-Farnesene	9.45	1630.0	0.03	10.46	1457.0	0.02
Oxindole?				10.57	1465.0	0.08
γ-Murolene	9.49	1632.8	0.05	10.64	1470.5	0.04
Germacrene D	9.68	1648.2	0.39	10.67	1472.6	0.36
(Z)-Jasmin lactone	15.49*	2174.7	[0.48]	10.85	1485.9	0.03
Bicyclogermacrene	9.97*	1671.7	[0.17]	10.87*	1488.0	[0.20]
epi-Cubebol	11.88	1833.7	0.03	10.87*	1488.0	[0.20]
(3Z,6E)-α-Farnesene	10.17	1688.0	0.20	10.97*	1495.5	[0.28]

α-Muurolene	9.94*	1668.9	[13.62]	10.97*	1495.5	[0.28]
γ-Cadinene	10.29	1697.8	0.33	11.17*	1510.6	[12.61]
(3E,6E)-α-Farnesene	10.44*	1710.9	[12.91]	11.17*	1510.6	[12.61]
δ-Cadinene	10.32	1700.2	0.67	11.27	1518.5	0.49
10-epi-Cubebol?	13.68*	1997.5	[0.50]	11.37	1526.6	0.04
α-Cadinene	10.69	1731.3	0.03	11.43	1531.7	0.02
Methyl N-formylanthranilate	18.61	2512.7	0.02	11.64	1548.3	0.05
Hexenyl benzoate isomer				11.78	1559.3	0.12
(E)-Nerolidol	13.68*	1997.5	[0.50]	11.85	1564.6	0.37
(3Z)-Hexenyl benzoate	14.25	2052.4	5.35	11.89	1567.9	6.00
Spathulenol	14.32	2059.1	0.01	11.92*	1570.0	[3.98]
Germacrene D-4-ol	13.56	1986.3	4.97	11.92*	1570.0	[3.98]
Caryophyllene oxide isomer	12.62	1899.3	0.02	11.97*	1574.4	[0.12]
Hexyl benzoate	13.76*	2005.0	[0.11]	11.97*	1574.4	[0.12]
Caryophyllene oxide	12.65	1902.6	0.02	11.97*	1574.4	[0.12]
(2E)-Hexenyl benzoate	14.50*	2076.5	[0.07]	12.00	1576.6	0.02
Methyl N-acetylanthranilate	17.44*	2381.3	[0.26]	12.07	1582.0	0.28
Ledol	13.25	1957.6	0.02	12.21	1593.8	0.03
τ-Cadinol	14.77	2103.2	0.21	12.71	1634.7	0.06
τ-Muurolol	14.93	2119.4	0.10	12.73	1636.1	0.09
α-Muurolol	15.07	2133.3	0.02	12.78	1640.2	0.02
Methyl <i>cis</i> -jasmonate	16.28*	2256.5	[0.27]	12.82	1644.1	0.05
α-Cadinol	15.36	2161.8	0.25	12.87	1648.1	0.19
Unknown JASA IV [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]				12.97	1656.3	0.03
(3E,5E)-7-Hydroxyfarnesene	16.19	2247.0	0.11	13.02	1660.6	0.02
Methyl <i>trans</i> -jasmonate	17.11*	2345.1	[2.04]	13.17	1673.2	0.08
Shyobunol	16.21	2249.7	0.36	13.26	1680.5	0.08
Unknown JASA V [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	12.49	1888.0	0.03	13.43	1694.8	0.04
(2E,6E)-Farnesol	16.74*†	2305.1	[0.17]	13.74	1721.4	0.20

Oplopanone	17.96*	2438.9	[0.44]	13.83*	1728.7	[0.11]
(E)-Coniferyl alcohol	22.85	3046.4	0.01	13.83*	1728.7	[0.11]
Unknown JASA VI [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16)...]	18.08	2452.7	0.67	13.99	1743.0	0.67
Benzyl benzoate	18.72	2525.8	0.57	14.12	1754.7	0.54
Unknown JASA VII [m/z 43, 159 (79), 93 (49), 119 (48), 161 (40), 187 (36)... 238? (2)]				14.83	1817.1	0.02
(2E,6E)-Farnesyl acetate	15.91*	2218.5	[0.08]	15.10	1841.4	0.11
Phenylethyl benzoate	19.44	2609.9	0.19	15.12	1843.0	0.19
Benzyl salicylate	19.98	2674.8	0.07	15.27	1856.8	0.08
Methyl palmitate	15.49*	2174.7	[0.48]	16.04	1928.8	0.49
Palmitic acid				16.49	1970.9	0.30
para-Camphorene	15.72	2198.9	0.15	16.63	1984.4	0.04
Ethyl palmitate	15.91*	2218.5	[0.08]	16.76	1996.8	0.04
(E,E)-Geranylinalool	18.40*	2488.3	[1.27]	17.05	2026.0	1.24
(E)-Cinnamyl benzoate	22.39	2983.0	0.02	17.55	2075.5	0.06
Methyl linoleate	17.96*	2438.9	[0.44]	17.72	2091.9	0.33
Methyl α-linolenate	18.52	2502.6	2.94	17.78	2098.3	3.00
Phytol	19.11	2570.9	0.01	17.91	2111.1	0.07
Methyl stearate	17.44*	2381.3	[0.26]	18.08	2128.9	0.32
α-Linolenic acid	24.09	3220.3	0.27	18.26	2147.9	0.31
Ethyl linoleate	18.40*	2488.3	[1.27]	18.37	2158.4	0.08
Ethyl α-linolenate	18.84	2539.1	0.07	18.41	2162.6	0.17
Stearic acid				18.47	2169.1	0.21
Methyl (E)-phytenate	17.96*	2438.9	[0.44]	18.53	2175.0	0.24
Unknown JASA VIII [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]				18.87	2210.7	0.07
(E)-Phytyl acetate	18.40*	2488.3	[1.27]	18.98	2222.3	0.03
(9Z)-Eicosenol?				19.24	2250.9	0.12
(9Z)-Tricosene	16.74*†	2305.1	[0.17]	19.48	2276.0	3.71
(9E)-Tricosene?	16.71*†	2302.4	[3.89]	19.51	2279.0	0.10
1-Tricosene?	16.83	2314.9	0.15	19.63	2292.3	0.06

Methyl arachidate	19.26	2587.9	0.05	19.95	2327.8	0.06
Tetracosene isomer				20.36	2373.7	0.25
Unknown JASA IX [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]				21.05	2452.0	0.03
2-Monopalmitin				21.53	2507.4	0.22
Benzyl palmitate				22.07	2571.8	0.14
Benzyl oleate				23.43	2741.0	0.89
Benzyl linoleate				23.48	2747.3	0.05
Benzyl α-linolenate				23.52	2751.8	0.07
Squalene	22.68	3023.4	0.65	23.98	2811.2	0.71
2,3-Oxidosqualene	24.68	3305.9	0.05	24.96	2941.1	0.03
2,3-Dihydro-3-oxosqualene?				25.09	2959.1	0.06
Benzyl arachidate				25.23	2978.2	0.02
Unknown JAGR V [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]				25.66	3037.5	0.02
α-Tocopherol				26.10	3097.6	0.21
Benzyl behenate				26.76	3180.2	0.05
Unknown JASA X [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]				27.90	3291.8	0.22
Unknown JASA XI [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]				29.15	3389.5	1.14
Total reported	91.62%			92.78%		

\*: 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