Date : November 26, 2020

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 20K13-PTH02
Customer identification : Jasmine Sambac Absolute - J10108206R
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 factor[1]. Analysis with PC-MAT-004 - Terpenes and volatiles profiling by response factor (in French); identifications validated by GC-MS.
Analyst : Fanny Charlier, B. Sc., chimiste à l'entraînement
Analysis date : November 18, 2020

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

This report is an update from the first version issued on November 20, 2020, to correct an erroneously identified compound.

Reference

(1) Cachet, T.; Brevard, H.; Chaintreau, A.; Demyttenaere, J.; French, L.; Gassenmeier, K.; Joulain, D.; Koenig, T.; Leijs, 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.*

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PHYSICOCHEMICAL DATA

Physical aspect: Dark red liquid
Refractive index: 1.5063 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

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

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ANALYSIS SUMMARY

Identification	(mg/g)	% m/m	Classe
(3*Z*)-Hexenol	5.69	0.57	Aliphatic alcohol
Hexanol	0.94	0.09	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.14	0.01	Aliphatic ketone
(3*Z*)-Hexenyl acetate	14.47	1.45	Aliphatic ester
(2*E*)-Hexenyl acetate	0.30	0.03	Aliphatic ester
Unknown	1.29	0.13	Unknown
Benzyl alcohol	120.46	12.05	Simple phenolic
(*E*)-β-Ocimene	0.60	0.06	Monoterpene
cis-Linalool oxide (fur.)	0.36	0.04	Monoterpenic alcohol
Benzyl formate	0.25	0.03	Phenolic ester
trans-Linalool oxide (fur.)	2.75	0.28	Monoterpenic alcohol
Methyl benzoate	5.88	0.59	Phenolic ester
Linalool	92.48	9.25	Monoterpenic alcohol
Phenylethyl alcohol	12.68	1.27	Simple phenolic
Benzeneacetonitrile	14.02	1.40	Simple phenolic
Benzyl acetate	79.34	7.93	Phenolic ester
Ethyl benzoate	1.08	0.11	Phenolic ester
Unknown	4.81	0.48	Unknown
trans-Linalool oxide (pyr.)	0.52	0.05	Monoterpenic alcohol
(3*Z*)-Hexenyl butyrate	0.04	0.00	Aliphatic ester
α-Terpineol	0.02	0.00	Monoterpenic alcohol
Methyl salicylate	3.61	0.36	Phenolic ester
(3*Z*)-Hexenyl isovalerate	0.23	0.02	Aliphatic ester
Phenylethyl acetate	4.09	0.41	Phenolic ester
Geraniol	1.25	0.13	Monoterpenic alcohol
Ethyl salicylate	0.95	0.10	Phenolic ester
Phenylacetic acid?	0.36	0.04	Phenolic acid
Unknown	2.77	0.28	Unknown
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.44	0.04	Monoterpenic alcohol
Indole	9.36	0.94	Indole
(*E*)-Cinnamyl alcohol	1.60	0.16	Phenylpropanoid
Methyl anthranilate	58.86	5.89	Phenolic ester
Eugenol	0.57	0.06	Phenylpropanoid
8-Hydroxylinalool isomer	3.21	0.32	Monoterpenic alcohol
Butyl benzoate	0.36	0.04	Phenolic ester
Methyl (*E*)-cinnamate	0.40	0.04	Phenylpropanoid ester
(3*Z*)-Hexenyl (3*Z*)-hexenoate	0.18	0.02	Aliphatic ester
(3*Z*)-Hexenyl hexanoate?	0.35	0.04	Aliphatic ester
β-Elemene	1.58	0.16	Sesquiterpene
(*Z*)-Jasmone	0.31	0.03	Jasmonate
Dimethyl anthranilate	0.46	0.05	Phenolic ester
Ethyl anthranilate	0.21	0.02	Phenolic ester
β-Caryophyllene	0.48	0.05	Sesquiterpene
(*E*)-Cinnamyl acetate	0.22	0.02	Phenylpropanoid ester
α-Humulene	0.70	0.07	Sesquiterpene
(*E*)-β-Farnesene	0.24	0.02	Sesquiterpene
Oxindole?	0.24	0.02	Indole
Germacrene D	3.19	0.32	Sesquiterpene

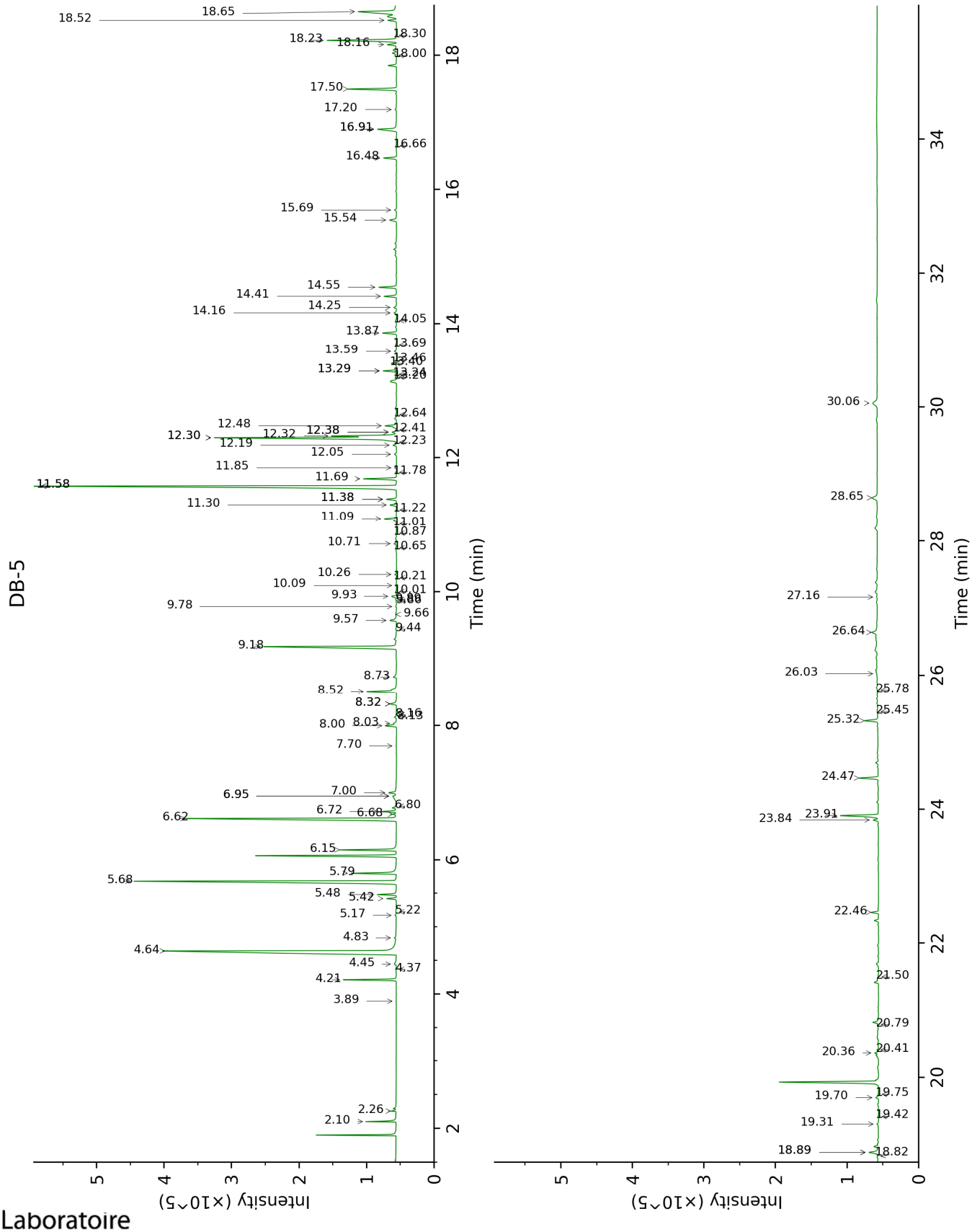
(*Z*)-Jasmin lactone	0.24	0.02	Aliphatic lactone
Bicyclogermacrene	2.00	0.20	Sesquiterpene
α-Muurolene	0.76	0.08	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	1.08	0.11	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	102.10	10.21	Sesquiterpene
γ-Cadinene	6.05	0.61	Sesquiterpene
δ-Cadinene	8.34	0.83	Sesquiterpene
10-epi-Cubebol?	0.41	0.04	Sesquiterpenic alcohol
α-Cadinene	0.50	0.05	Sesquiterpene
Methyl N-formylanthranilate	1.05	0.11	Phenolic ester
Hexenyl benzoate isomer	1.12	0.11	Phenolic ester
(*E*)-Nerolidol	0.26	0.03	Sesquiterpenic alcohol
(3*Z*)-Hexenyl benzoate	39.16	3.92	Phenolic ester
Germacrene D-4-ol	18.37	1.84	Sesquiterpenic alcohol
Spathulenol	17.71	1.77	Sesquiterpenic alcohol
Hexyl benzoate	0.91	0.09	Phenolic ester
Caryophyllene oxide	0.17	0.02	Sesquiterpenic ether
(2*E*)-Hexenyl benzoate	0.20	0.02	Phenolic ester
Methyl N-acetylanthranilate	4.77	0.48	Phenolic ester
Ledol	0.35	0.04	Sesquiterpenic alcohol
α-Muurolol	0.41	0.04	Sesquiterpenic alcohol
Methyl *cis*-jasmonate	0.60	0.06	Jasmonate
τ-Cadinol	1.04	0.10	Sesquiterpenic alcohol
τ-Muurolol	2.31	0.23	Sesquiterpenic alcohol
Unknown	2.07	0.21	Unknown
(3*E*,5*E*)-7-Hydroxyfarnesene	0.18	0.02	Sesquiterpenic alcohol
Methyl *trans*-jasmonate	0.92	0.09	Jasmonate
Shyobunol	0.39	0.04	Sesquiterpenic alcohol
Unknown	4.81	0.48	Unknown
Pentadecanal	0.54	0.05	Aliphatic aldehyde
(2*E*,6*E*)-Farnesol	0.93	0.09	Sesquiterpenic alcohol
Oplopanone	1.09	0.11	Sesquiterpenic alcohol
Unknown	4.44	0.44	Unknown
Benzyl benzoate	5.42	0.54	Phenolic ester
Phenylethyl benzoate	2.74	0.27	Phenolic ester
Benzyl salicylate	0.80	0.08	Phenolic ester
Methyl palmitate	3.89	0.39	Aliphatic ester
meta-Camphorene	0.24	0.02	Diterpene
Palmitic acid	7.33	0.73	Aliphatic acid
para-Camphorene	1.57	0.16	Diterpene
Ethyl palmitate	0.43	0.04	Aliphatic ester
(*E*,*E*)-Geranyllinalool	12.95	1.30	Diterpenic alcohol
(*E*)-Cinnamyl benzoate	0.57	0.06	Phenylpropanoid ester
Methyl linoleate	2.89	0.29	Aliphatic ester
Methyl α-linolenate	22.62	2.26	Aliphatic ester
Phytol	0.35	0.04	Diterpenic alcohol
Methyl stearate	2.47	0.25	Aliphatic ester
α-Linolenic acid	19.89	1.99	Aliphatic acid
Ethyl α-linolenate	0.83	0.08	Aliphatic ester
Docosene isomer	2.97	0.30	Alkene
Methyl (*E*)-phytenate	0.75	0.08	Diterpenic ester
Unknown	0.86	0.09	Unknown

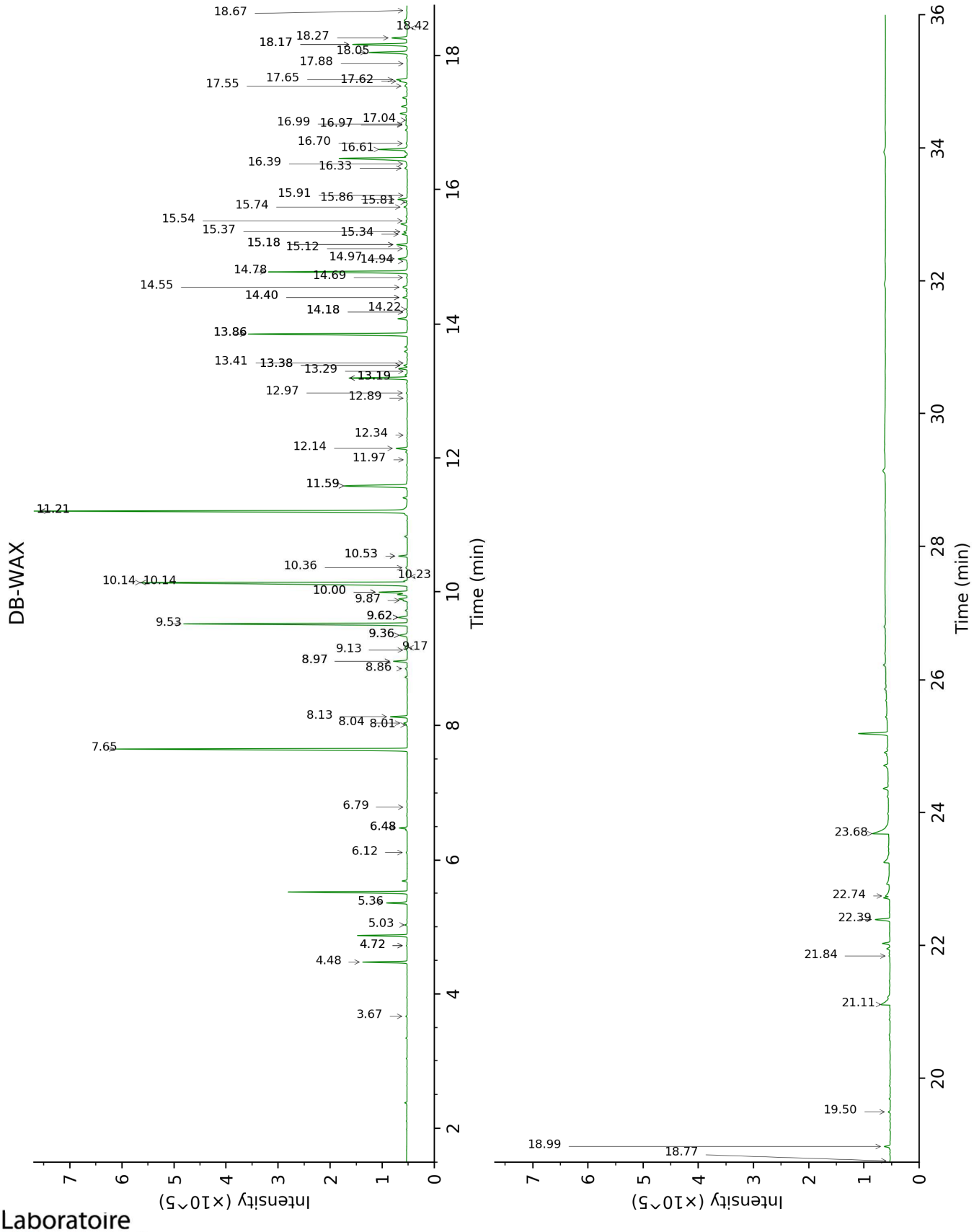
(*E*)-Phytyl acetate	0.31	0.03	Diterpenic ester
(9*Z*)-Eicosenol?	1.02	0.10	Aliphatic alcohol
(9*Z*)-Tricosene	0.17	0.02	Alkene
Methyl arachidate	1.24	0.12	Aliphatic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.56	0.06	Terpenic lactone
Tetracosene isomer	0.34	0.03	Alkene
Unknown	0.41	0.04	Unknown
Benzyl palmitate	2.16	0.22	Phenolic ester
Benzyl oleate	1.59	0.16	Phenolic ester
Benzyl α-linolenate	12.05	1.21	Phenolic ester
Squalene	4.90	0.49	Triterpene
2,3-Oxidosqualene	4.01	0.40	Triterpenic ether
2,3-Dihydro-3-oxosqualene?	0.17	0.02	Triterpenic ketone
2,6,10,15,19,23-Hexamethyl-(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol	0.19	0.02	Triterpenic alcohol
Unknown	0.41	0.04	Triterpenic alcohol
α-Tocopherol	3.23	0.32	Tocopherol
Benzyl behenate	0.33	0.03	Phenolic ester
Unknown	3.79	0.38	Unknown
Unknown	4.39	0.44	Unknown
Consolidated total	**810.50 mg/g**	**81.05%**	

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.


DB-5
Time (min)
Intensity (×10^5)
18.52
18.65
18.23
18.16
18.30
18.00
17.50
17.20
16.91
16.66
16.48
15.69
15.54
14.55
14.41
14.25
14.16
14.05
13.87
13.69
13.59
13.46
13.40
13.29
13.24
12.64
12.48
12.41
12.38
12.32
12.30
12.23
12.19
12.05
11.85
11.78
11.69
11.58
11.38
11.30
11.22
11.09
11.01
10.87
10.71
10.65
10.26
10.21
10.09
10.01
9.93
9.78
9.66
9.57
9.44
9.18
8.73
8.52
8.32
8.16
8.03
8.00
7.70
7.00
6.95
6.80
6.72
6.68
6.62
6.15
5.79
5.68
5.48
5.42
5.22
5.17
4.83
4.64
4.45
4.37
4.21
3.89
2.26
2.10
30.06
28.65
27.16
26.64
26.03
25.78
25.45
25.32
24.47
23.91
23.84
22.46
21.50
20.79
20.41
20.36
19.75
19.70
19.42
19.31
18.89
18.82


DB-WAX
Time (min)
Intensity (×10^5)
18.67
18.42
18.27
18.17
18.05
17.88
17.65
17.62
17.55
17.04
16.99
16.97
16.70
16.61
16.39
16.33
15.91
15.86
15.81
15.74
15.54
15.37
15.34
15.18
15.12
14.97
14.94
14.78
14.69
14.55
14.40
14.22
14.18
13.86
13.41
13.38
13.29
13.19
12.97
12.89
12.34
12.14
11.97
11.59
11.21
10.53
10.36
10.23
10.14
10.14
10.00
9.87
9.62
9.53
9.36
9.17
9.13
8.97
8.86
8.13
8.04
8.01
7.65
6.79
6.48
6.12
5.36
5.03
4.72
4.48
3.67
23.68
22.74
22.39
21.84
21.11
19.50
18.99
18.77

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
(3*Z*)-Hexenol	2.10	861	5.69	5.36	1344	6.69
Hexanol	2.26	874	0.94	5.03	1320	0.74
6-Methyl-5-hepten-2-one	3.89	990	0.14	4.72*	1302	0.29
(3*Z*)-Hexenyl acetate	4.21	1011	14.47	4.48	1283	14.75
(2*E*)-Hexenyl acetate	4.37	1021	0.30	4.72*	1302	[0.35]
Unknown [m/z 41, 57 (55), 85 (47), 59 (45), 43 (41)...]	4.44	1026	1.29			
Benzyl alcohol	4.64	1038	120.46	11.21*	1807	124.47
(*E*)-β-Ocimene	4.84	1050	0.60	3.67	1221	0.41
cis-Linalool oxide (fur.)	5.17	1072	0.36	6.12	1399	0.44
Benzyl formate	5.22	1075	0.25	9.14	1632	0.18
trans-Linalool oxide (fur.)	5.42	1088	2.75	6.48*	1426	2.80
Methyl benzoate	5.48	1091	5.88	8.13	1552	6.16
Linalool	5.68	1104	92.48	7.65	1515	92.12
Phenylethyl alcohol	5.80	1112	12.68	11.59*	1841	27.97
Benzeneacetonitrile	6.15	1135	14.02	11.59*	1841	[27.07]
Benzyl acetate	6.62	1165	79.34	9.53	1664	80.22
Ethyl benzoate	6.68	1169	1.08	8.86	1609	1.12
Unknown [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	6.72	1172	4.81	8.97*	1618	5.20
trans-Linalool oxide (pyr.)	6.80	1177	0.52	10.23	1722	0.36
(3*Z*)-Hexenyl butyrate	6.95*	1187	3.40	6.48*	1426	[2.80]
α-Terpineol	6.95*	1187	[2.96]	9.36*	1650	3.71
Methyl salicylate	7.00	1190	3.61	10.14*	1714	166.63
(3*Z*)-Hexenyl isovalerate	7.70	1237	0.23	6.79	1450	0.21
Phenylethyl acetate	8.00	1257	4.09	10.53*	1748	3.00
Geraniol	8.03	1259	1.25	11.21*	1807	[125.90]
Ethyl salicylate	8.13	1266	0.95	10.53*	1748	[3.58]
Phenylacetic acid?	8.16	1268	0.36	17.04	2389	0.33
Unknown [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]	8.32*	1279	3.22			
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.32*	1279	[3.21]	14.22	2090	0.44
Indole	8.52	1292	9.36	16.61	2340	9.75
(*E*)-Cinnamyl alcohol	8.73	1304	1.60	15.37	2207	1.48
Methyl anthranilate	9.18	1336	58.86	14.78	2146	58.77
Eugenol	9.44	1354	0.57	14.40*	2107	1.77
8-Hydroxylinalool isomer	9.57	1363	3.21	15.86	2259	3.74
Butyl benzoate	9.66	1370	0.36	11.21*	1807	[133.59]
Methyl (*E*)-cinnamate	9.78	1378	0.40	13.38*	2006	1.40
(3*Z*)-Hexenyl (3*Z*)-hexenoate	9.86	1384	0.18	9.62*	1672	3.71

(3*Z*)-Hexenyl hexanoate?	9.89	1386	0.35			
β-Elemene	9.93	1389	1.58	8.04	1545	1.02
(*Z*)-Jasmone	10.00	1394	0.31	11.97	1876	0.16
Dimethyl anthranilate	10.09	1400	0.46	13.19*	1989	24.00
Ethyl anthranilate	10.21	1408	0.21	15.18*	2188	4.55
β-Caryophyllene	10.26	1412	0.48	8.01	1542	0.41
(*E*)-Cinnamyl acetate	10.65	1442	0.22	14.18*	2086	0.26
α-Humulene	10.72	1446	0.70	8.97*	1618	[3.91]
(*E*)-β-Farnesene	10.87	1458	0.24	9.17	1634	0.45
Oxindole?	11.01	1469	0.24			
Germacrene D	11.09	1475	3.19	9.36*	1650	[3.21]
(*Z*)-Jasmin lactone	11.22	1484	0.24	15.12	2182	0.58
Bicyclogermacrene	11.30	1490	2.00	9.62*	1672	[2.91]
α-Muurolene	11.38*	1496	2.81	9.62*	1672	[2.91]
(3*Z*,6*E*)-α-Farnesene	11.38*	1496	[2.81]	9.87	1692	1.08
(3*E*,6*E*)-α-Farnesene	11.58*	1512	108.16	10.14*	1714	[104.36]
γ-Cadinene	11.58*	1512	[108.16]	10.00*	1702	8.32
δ-Cadinene	11.69	1520	8.34	10.00*	1702	[8.32]
10-epi-Cubebol?	11.78	1528	0.41	13.29	1998	0.19
α-Cadinene	11.85	1533	0.50	10.36	1734	0.61
Methyl N-formylanthranilate	12.05	1549	1.05	18.17*	2518	29.65
Hexenyl benzoate isomer	12.19	1560	1.12			
(*E*)-Nerolidol	12.23	1563	0.26	13.41	2010	0.15
(3*Z*)-Hexenyl benzoate	12.30*	1568	61.41	13.86*	2054	58.34
Germacrene D-4-ol	12.30*	1568	[55.99]	13.19*	1989	[18.73]
Spathulenol	12.32	1570	17.71	13.86*	2054	[53.88]
Hexyl benzoate	12.38*	1575	1.48	13.38*	2006	[1.28]
Caryophyllene oxide	12.38*	1575	[1.39]	12.34	1909	0.17
(2*E*)-Hexenyl benzoate	12.42	1577	0.20	14.18*	2086	[0.25]
Methyl N-acetylanthranilate	12.48	1582	4.77	16.99	2382	1.61
Ledol	12.64	1595	0.35	12.89	1961	0.16
α-Muurolol	13.20	1641	0.41	14.69	2137	0.39
Methyl *cis*-jasmonate	13.24	1644	0.60	15.92	2265	0.26
τ-Cadinol	13.29*	1649	3.80	14.40*	2107	[1.53]
τ-Muurolol	13.29*	1649	[3.80]	14.55	2123	2.31
Unknown [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]	13.40	1658	2.07			
(3*E*,5*E*)-7-Hydroxyfarnesene	13.46	1663	0.18	15.74	2246	1.46
Methyl *trans*-jasmonate	13.58	1673	0.92	16.70	2350	0.90
Shyobunol	13.69	1682	0.39	15.81	2254	0.47
Unknown [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	13.87	1696	4.81	12.14	1891	4.46
Pentadecanal	14.05	1712	0.54	12.97	1968	0.48
(2*E*,6*E*)-Farnesol	14.16	1722	0.93	16.33	2310	1.17
Oplopanone	14.25	1729	1.09	17.62	2455	2.78

Unknown [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16)...]	14.41	1743	4.44	17.65	2458	4.38
Benzyl benzoate	14.55	1755	5.42	18.27	2530	5.93
Phenylethyl benzoate	15.54	1844	2.74	18.99	2616	2.24
Benzyl salicylate	15.69	1857	0.80	19.50	2680	0.89
Methyl palmitate	16.48	1930	3.89	14.97	2166	3.81
meta-Camphorene	16.66	1947	0.24	14.94	2162	0.21
Palmitic acid	16.90*	1971	7.79	21.11	2889	7.33
para-Camphorene	16.90*	1971	[6.71]	15.34	2204	1.57
Ethyl palmitate	17.20	1998	0.43	15.54	2224	0.63
(*E*,*E*)-Geranyllinalool	17.50	2029	12.95	18.05	2504	12.96
(*E*)-Cinnamyl benzoate	18.00	2078	0.57	21.84	2988	0.42
Methyl linoleate	18.16	2095	2.89	17.55	2447	1.27
Methyl α-linolenate	18.22	2101	22.62	18.17*	2518	[20.69]
Phytol	18.30	2108	0.35	18.67	2579	0.37
Methyl stearate	18.52	2132	2.47	16.97	2381	0.36
α-Linolenic acid	18.65	2145	19.89	23.68	3254	15.27
Ethyl α-linolenate	18.82	2162	0.83	18.42	2548	0.12
Docosene isomer	18.89*	2170	3.62	15.18*	2188	[3.12]
Methyl (*E*)-phytenate	18.89*	2170	[4.19]			
Unknown [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]	19.31	2214	0.86			
(*E*)-Phytyl acetate	19.42	2226	0.31	17.88	2485	0.14
(9*Z*)-Eicosenol?	19.70	2256	1.02			
(9*Z*)-Tricosene	19.75	2261	0.17	16.39	2316	0.19
Methyl arachidate	20.36	2328	1.24	18.77	2590	0.32
4,8,12,16-Tetramethylheptadecan-4-olide?	20.40	2333	0.56			
Tetracosene isomer	20.79	2376	0.34			
Unknown [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]	21.50	2458	0.41			
Benzyl palmitate	22.46	2572	2.16			
Benzyl oleate	23.84	2746	1.59			
Benzyl α-linolenate	23.91	2755	12.05			
Squalene	24.47	2828	4.90	22.39	3065	4.84
2,3-Oxidosqualene	25.32	2943	4.01	22.74	3115	2.78
2,3-Dihydro-3-oxosqualene?	25.45	2962	0.17			
2,6,10,15,19,23-Hexamethyl-(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol	25.78	3007	0.19			
Unknown [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]	26.03	3040	0.41			
α-Tocopherol	26.64	3121	3.23			
Benzyl behenate	27.16	3179	0.33			

Unknown [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]	28.65	3316	3.79	
Unknown [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]	30.06	3415	4.39	

*: 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