Date : February 04, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22A24-PTH01
Customer identification : Jasmine Sambac Absolute - India - J10111216R
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 : Seydou Ka, Ph. D.
Analysis date : February 02, 2022

Checked and approved by :

Alexis St-Gelais, Ph. D., 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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.*

Laboratoire PhytoChemia
628 Boulevard du Saguenay Ouest, Saguenay (Qc) G7J 1H4 | www.phytochemia.com

PHYSICOCHEMICAL DATA

Physical aspect: Orange brownish liquid
Refractive index: 1.5080 ± 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	3.14	0.31	Aliphatic alcohol
Hexanol	0.47	0.05	Aliphatic alcohol
(3*Z*)-Hexenyl acetate	11.06	1.11	Aliphatic ester
(2*E*)-Hexenyl acetate	0.21	0.02	Aliphatic ester
Benzyl alcohol	94.96	9.50	Simple phenolic
(*E*)-β-Ocimene	0.67	0.07	Monoterpene
cis-Linalool oxide (fur.)	0.22	0.02	Monoterpenic alcohol
Benzyl formate	0.25	0.03	Phenolic ester
trans-Linalool oxide (fur.)	1.61	0.16	Monoterpenic alcohol
Methyl benzoate	4.70	0.47	Phenolic ester
Linalool	73.95	7.40	Monoterpenic alcohol
Phenylethyl alcohol	9.66	0.97	Simple phenolic
Benzeneacetonitrile	13.72	1.37	Simple phenolic
Benzyl acetate	78.18	7.82	Phenolic ester
Ethyl benzoate	0.87	0.09	Phenolic ester
Unknown	4.50	0.45	Unknown
trans-Linalool oxide (pyr.)	0.94	0.09	Monoterpenic alcohol
(3*Z*)-Hexenyl butyrate	0.52	0.05	Aliphatic ester
Methyl salicylate	1.78	0.18	Phenolic ester
(3*Z*)-Hexenyl 2-methylbutyrate	0.14	0.01	Aliphatic ester
(3*Z*)-Hexenyl isovalerate	0.07	0.01	Aliphatic ester
Phenylethyl acetate	2.97	0.30	Phenolic ester
Geraniol	1.49	0.15	Monoterpenic alcohol
Ethyl salicylate	0.32	0.03	Phenolic ester
Phenylacetic acid?	0.32	0.03	Phenolic acid
Unknown	1.55	0.16	Unknown
Indole	7.97	0.80	Indole
1-Nitro-2-phenylethane	2.46	0.25	Simple phenolic
(*E*)-Cinnamyl alcohol	1.28	0.13	Phenylpropanoid
Methyl anthranilate	66.24	6.62	Phenolic ester
Eugenol	0.16	0.02	Phenylpropanoid
8-Hydroxylinalool isomer	1.78	0.18	Monoterpenic alcohol
Neryl acetate	1.11	0.11	Monoterpenic ester
Butyl benzoate	0.32	0.03	Phenolic ester
Methyl (*E*)-cinnamate	0.31	0.03	Phenylpropanoid ester
(3*Z*)-Hexenyl (3*Z*)-hexenoate	0.36	0.04	Aliphatic ester
(3*Z*)-Hexenyl hexanoate?	1.09	0.11	Aliphatic ester
β-Elemene	1.01	0.10	Sesquiterpene
(*Z*)-Jasmone	0.30	0.03	Jasmonate
Dimethyl anthranilate	0.24	0.02	Phenolic ester
β-Caryophyllene	0.44	0.04	Sesquiterpene
(*E*)-Cinnamyl acetate	0.21	0.02	Phenylpropanoid ester
α-Humulene	0.76	0.08	Sesquiterpene
(*E*)-β-Farnesene	0.30	0.03	Sesquiterpene
γ-Muurolene	0.60	0.06	Sesquiterpene
Germacrene D	3.12	0.31	Sesquiterpene
Bicyclogermacrene	1.57	0.16	Sesquiterpene
epi-Cubebol	0.43	0.04	Sesquiterpenic alcohol

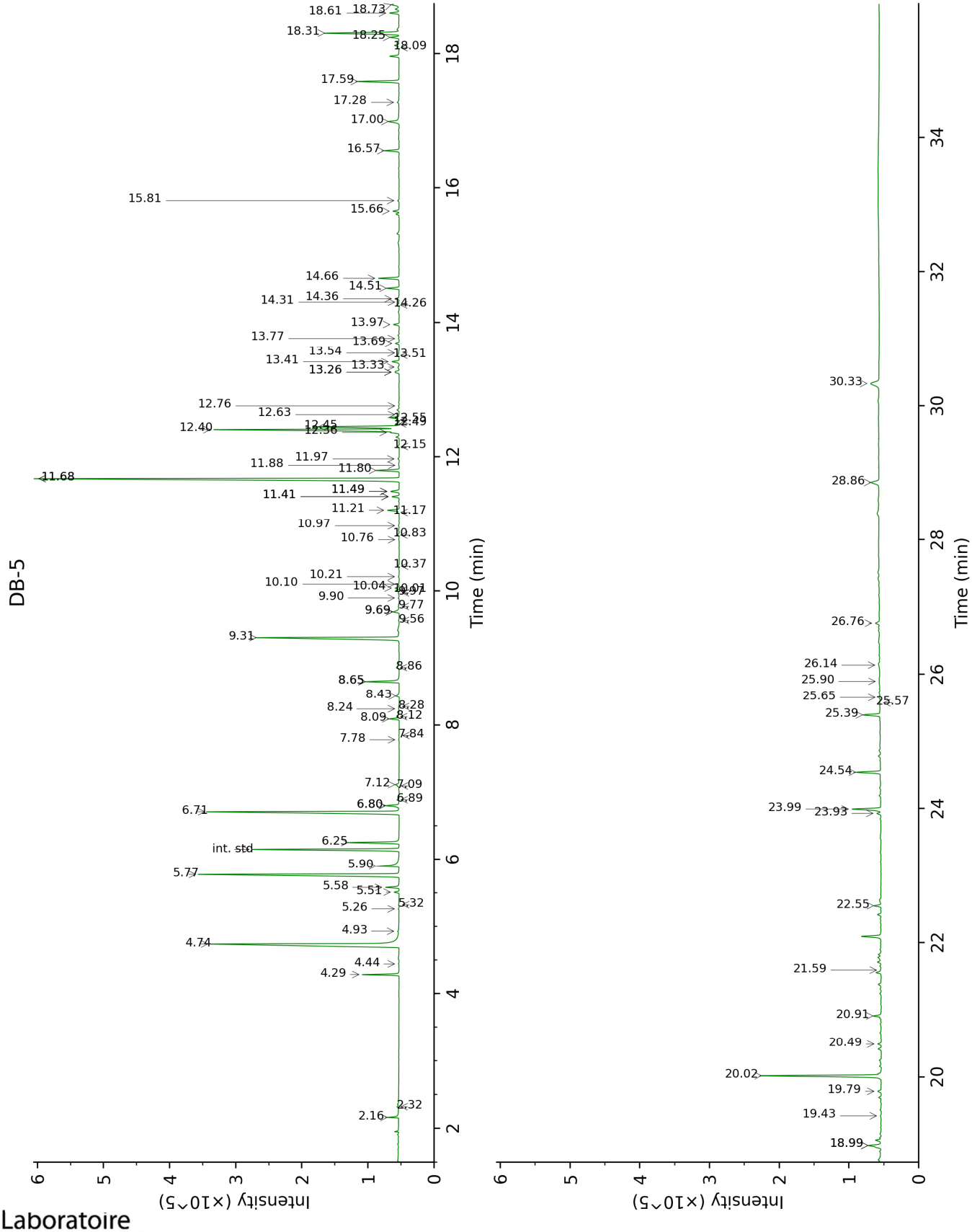
α-Muurolene	1.01	0.10	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	1.67	0.17	Sesquiterpene
γ-Cadinene	1.21	0.12	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	112.86	11.29	Sesquiterpene
δ-Cadinene	5.94	0.59	Sesquiterpene
10-epi-Cubebol?	0.14	0.01	Sesquiterpenic alcohol
α-Cadinene	0.39	0.04	Sesquiterpene
Methyl N-formylanthranilate	1.08	0.11	Phenolic ester
(*E*)-Nerolidol	2.14	0.21	Sesquiterpenic alcohol
(3*Z*)-Hexenyl benzoate	59.84	5.98	Phenolic ester
Germacrene D-4-ol	26.95	2.70	Sesquiterpenic alcohol
Hexyl benzoate	1.20	0.12	Phenolic ester
(2*E*)-Hexenyl benzoate	1.01	0.10	Phenolic ester
Methyl N-acetylanthranilate	0.30	0.03	Phenolic ester
Ledol	0.25	0.03	Sesquiterpenic alcohol
τ-Cadinol	1.13	0.11	Sesquiterpenic alcohol
τ-Muurolol	1.02	0.10	Sesquiterpenic alcohol
α-Muurolol	0.58	0.06	Sesquiterpenic alcohol
α-Cadinol	2.31	0.23	Sesquiterpenic alcohol
Unknown	0.97	0.10	Unknown
(3*E*,5*E*)-7-Hydroxyfarnesene	0.22	0.02	Sesquiterpenic alcohol
Methyl *trans*-jasmonate	1.37	0.14	Jasmonate
Shyobunol	0.25	0.03	Sesquiterpenic alcohol
Unknown	2.05	0.21	Unknown
(2*E*,6*E*)-Farnesol	0.92	0.09	Sesquiterpenic alcohol
Oplopanone	0.22	0.02	Sesquiterpenic alcohol
(*E*)-Coniferyl alcohol	1.52	0.15	Phenylpropanoid
Unknown	4.30	0.43	Unknown
Benzyl benzoate	6.18	0.62	Phenolic ester
Phenylethyl benzoate	1.91	0.19	Phenolic ester
Benzyl salicylate	0.46	0.05	Phenolic ester
Methyl palmitate	4.42	0.44	Aliphatic ester
Palmitic acid	5.04	0.50	Aliphatic acid
Ethyl palmitate	0.60	0.06	Aliphatic ester
(*E*,*E*)-Geranyllinalool	11.64	1.16	Diterpenic alcohol
(*E*)-Cinnamyl benzoate	0.65	0.07	Phenylpropanoid ester
Methyl linoleate	2.77	0.28	Aliphatic ester
Methyl α-linolenate	24.97	2.50	Aliphatic ester
Methyl stearate	2.83	0.28	Aliphatic ester
α-Linolenic acid	3.33	0.33	Aliphatic acid
Docosene isomer	1.55	0.16	Alkene
Ethyl α-linolenate	1.22	0.12	Aliphatic ester
Unknown	0.34	0.03	Unknown
(9*Z*)-Eicosenol?	1.06	0.11	Aliphatic alcohol
(9*Z*)-Tricosene	31.06	3.11	Alkene
Methyl arachidate	1.16	0.12	Aliphatic ester
Tetracosene isomer	2.40	0.24	Alkene
Unknown	0.34	0.03	Unknown
Benzyl palmitate	2.15	0.22	Phenolic ester
Benzyl oleate	1.27	0.13	Phenolic ester
Benzyl α-linolenate	9.70	0.97	Phenolic ester
Squalene	6.79	0.68	Triterpene

2,3-Oxidosqualene	5.11	0.51	Triterpenic ether
2,3-Dihydro-3-oxosqualene?	0.05	0.01	Triterpenic ketone
Benzyl arachidate	0.35	0.04	Phenolic ester
2,6,10,15,19,23-Hexamethyl-(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol	0.15	0.02	Triterpenic alcohol
Unknown	0.40	0.04	Triterpenic alcohol
α-Tocopherol	1.40	0.14	Tocopherol
Unknown	5.11	0.51	Unknown
Unknown	7.65	0.77	Unknown
Consolidated total	**777.25 mg/g**	**77.73%**	

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
Intensity (×10^5)
Time (min)
18.61
18.73
18.31
18.25
18.09
17.59
17.28
17.00
16.57
15.81
15.66
14.66
14.51
14.31
14.36
14.26
13.97
13.77
13.69
13.54
13.51
13.41
13.33
13.26
12.76
12.63
12.55
12.45
12.40
12.36
12.15
11.97
11.88
11.80
11.68
11.49
11.41
11.21
11.17
10.97
10.83
10.76
10.37
10.21
10.10
10.04
9.90
9.77
9.69
9.56
9.31
8.86
8.65
8.43
8.28
8.24
8.12
8.09
7.84
7.78
7.12
7.09
6.89
6.80
6.71
6.25
int. std
5.90
5.77
5.58
5.51
5.32
5.26
4.93
4.74
4.44
4.29
2.32
2.16
30.33
28.86
26.76
26.14
25.90
25.65
25.57
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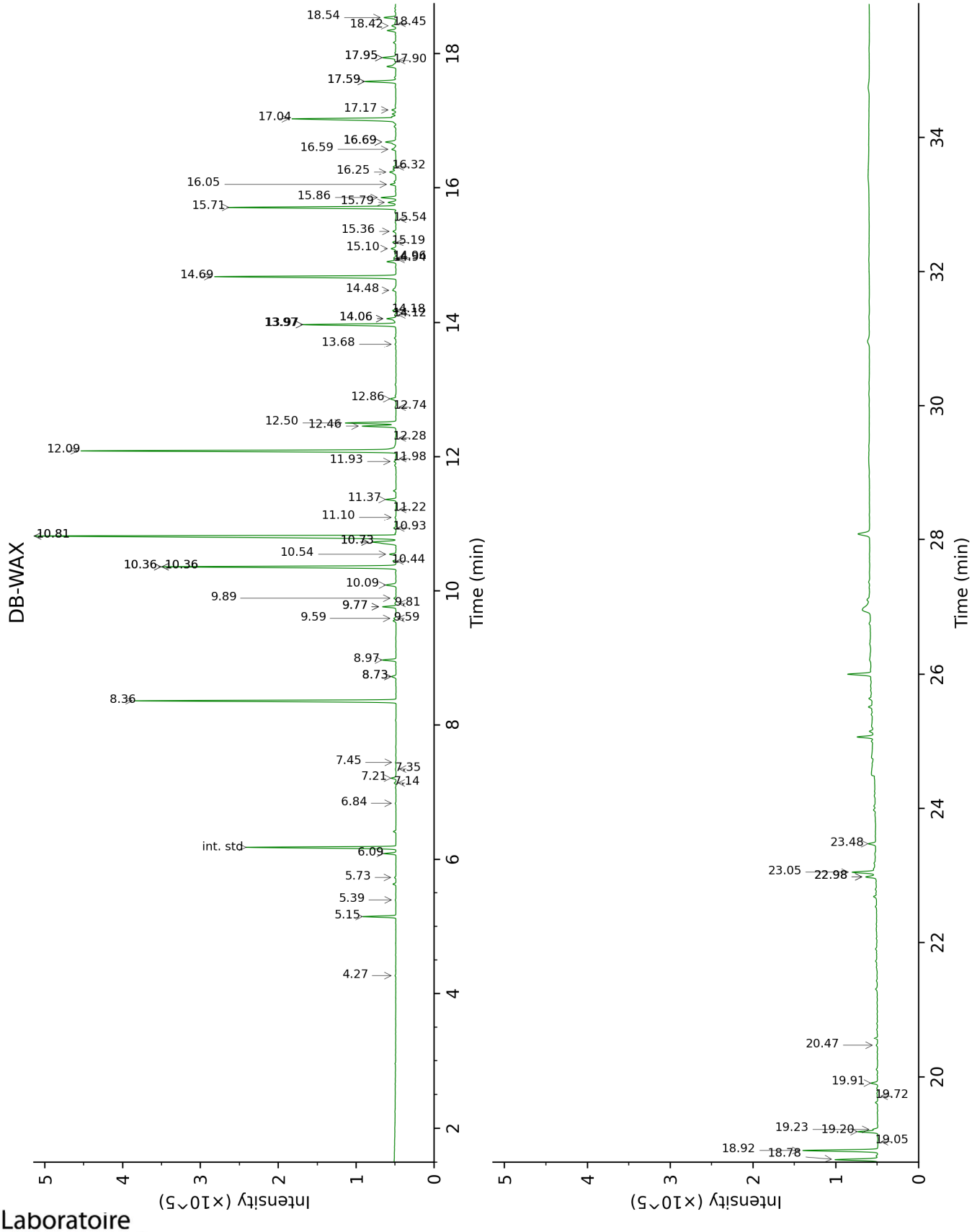
20.91
20.49
20.02
19.79
19.43
18.99


DB-WAX
Intensity (×10^5)
Time (min)
18.54
18.42
18.45
17.95
17.90
17.59
17.17
17.04
16.69
16.59
16.25
16.32
16.05
15.86
15.79
15.71
15.54
15.36
15.19
15.10
14.69
14.48
14.06
13.97
13.68
12.86
12.74
12.50
12.46
12.28
12.09
11.93
11.98
11.37
11.22
11.10
10.93
10.81
10.73
10.54
10.44
10.36
10.36
10.09
9.89
9.77
9.81
9.59
9.59
8.97
8.73
8.36
7.45
7.35
7.21
7.14
6.84
int. std
6.09
5.73
5.39
5.15
4.27
23.48
23.05
22.98
20.47
19.91
19.72
19.23
19.20
19.05
18.92
18.78

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	2.16	861	3.14	6.09	1349	3.68
Hexanol	2.32	874	0.47	5.73	1323	0.49
(3*Z*)-Hexenyl acetate	4.29	1011	11.06	5.15	1282	10.90
(2*E*)-Hexenyl acetate	4.44	1021	0.21	5.39	1299	0.26
Benzyl alcohol	4.74	1039	94.96	12.09	1820	97.97
(*E*)-β-Ocimene	4.93	1051	0.67	4.27	1219	0.18
cis-Linalool oxide (fur.)	5.26	1072	0.22	6.84	1403	0.29
Benzyl formate	5.32	1076	0.25	9.77*	1626	4.83
trans-Linalool oxide (fur.)	5.51	1088	1.61	7.21	1430	1.71
Methyl benzoate	5.58	1092	4.70	8.98	1564	4.78
Linalool	5.77	1104	73.95	8.36	1516	75.19
Phenylethyl alcohol	5.90	1112	9.66	12.46	1852	10.25
Benzeneacetonitrile	6.26	1135	13.72	12.50	1856	14.86
Benzyl acetate	6.71	1164	78.18	10.36*	1674	82.13
Ethyl benzoate	6.80*	1170	5.28	9.59*	1612	0.83
Unknown [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	6.80*	1170	[5.39]	9.77*	1626	[4.74]
trans-Linalool oxide (pyr.)	6.89	1176	0.94	10.93	1722	0.75
(3*Z*)-Hexenyl butyrate	7.10	1189	0.52	7.14	1425	0.64
Methyl salicylate	7.12	1190	1.78	10.82*	1712	181.97
(3*Z*)-Hexenyl 2-methylbutyrate	7.78	1234	0.14	7.35	1440	0.25
(3*Z*)-Hexenyl isovalerate	7.84	1238	0.07	7.45	1448	0.22
Phenylethyl acetate	8.09	1255	2.97	11.37	1758	3.37
Geraniol	8.12	1257	1.49	11.93	1806	0.61
Ethyl salicylate	8.24	1265	0.32	11.22	1746	0.25
Phenylacetic acid?	8.28	1267	0.32	17.95*	2390	5.57
Unknown [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]	8.43	1278	1.55			
Indole	8.65*	1292	9.78	17.59*	2352	9.77
1-Nitro-2-phenylethane	8.65*	1292	[13.27]	14.48	2038	2.46
(*E*)-Cinnamyl alcohol	8.86	1306	1.28	16.25	2212	2.21
Methyl anthranilate	9.31	1338	66.24	15.71	2158	68.63
Eugenol	9.56	1356	0.16	15.10	2097	1.84

8-Hydroxylinalool isomer	9.69*	1365	2.94	16.69*	2257	5.20
Neryl acetate	9.69*	1365	[2.82]	10.44	1681	1.11
Butyl benzoate	9.77	1371	0.32	11.98	1810	0.20
Methyl (*E*)-cinnamate	9.90	1380	0.31	14.12	2003	0.63
(3*Z*)-Hexenyl (3*Z*)-hexenoate	9.97	1385	0.36	10.36*	1674	[80.30]
(3*Z*)-Hexenyl hexanoate?	10.01	1387	1.09			
β-Elemene	10.04	1390	1.01	8.73*	1545	1.38
(*Z*)-Jasmone	10.10	1394	0.30	12.74	1877	0.41
Dimethyl anthranilate	10.21	1402	0.24	13.97*	1990	36.22
β-Caryophyllene	10.37	1413	0.44	8.73*	1545	[1.38]
(*E*)-Cinnamyl acetate	10.76	1443	0.21	14.96	2084	0.86
α-Humulene	10.83	1448	0.76	9.59*	1612	[0.64]
(*E*)-β-Farnesene	10.97	1458	0.30	9.89	1636	0.63
γ-Muurolene	11.17	1473	0.60	9.81	1630	0.42
Germacrene D	11.21	1476	3.12	10.09	1652	3.27
Bicyclogermacrene	11.41*	1491	1.96	10.36*	1674	[63.00]
epi-Cubebol	11.41*	1491	[2.13]	12.28	1837	0.43
α-Muurolene	11.49*	1497	2.68	10.36*	1674	[63.00]
(3*Z*,6*E*)-α-Farnesene	11.49*	1497	[2.68]	10.54	1689	1.67
γ-Cadinene	11.68*	1511	114.06	10.73*	1704	9.65
(3*E*,6*E*)-α-Farnesene	11.68*	1511	[114.06]	10.82*	1712	[113.97]
δ-Cadinene	11.80	1521	5.94	10.73*	1704	[9.65]
10-epi-Cubebol?	11.88	1527	0.14	14.06*	1998	3.60
α-Cadinene	11.97	1534	0.39	11.10	1736	0.32
Methyl N-formylanthranilate	12.15	1549	1.08	19.05	2512	0.21
(*E*)-Nerolidol	12.36	1565	2.14	14.06*	1998	[3.60]
(3*Z*)-Hexenyl benzoate	12.40	1568	59.84	14.68	2057	61.72
Germacrene D-4-ol	12.45	1572	26.95	13.97*	1990	[28.26]
Hexyl benzoate	12.49	1575	1.20	14.18	2010	1.13
(2*E*)-Hexenyl benzoate	12.55	1580	1.01	14.94	2082	0.46
Methyl N-acetylanthranilate	12.63	1586	0.30	17.90	2385	0.56
Ledol	12.76	1596	0.25	13.68	1963	0.34
τ-Cadinol	13.26*	1637	1.82	15.19	2106	1.13
τ-Muurolol	13.26*	1637	[1.82]	15.36	2122	1.02
α-Muurolol	13.33	1643	0.58	15.54	2140	0.06
α-Cadinol	13.41	1650	2.31	15.79	2165	2.73
Unknown [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]	13.51	1658	0.97			
(3*E*,5*E*)-7-Hydroxyfarnesene	13.54	1661	0.22	16.58	2246	1.62

Methyl *trans*-jasmonate	13.69	1673	1.37	17.59*	2352	[12.72]
Shyobunol	13.76	1679	0.25	16.69*	2257	[4.28]
Unknown [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	13.97	1696	2.05	12.86	1888	2.48
(2*E*,6*E*)-Farnesol	14.26	1721	0.92	17.17	2307	1.36
Oplopanone	14.31	1725	0.22	18.45	2446	0.27
(*E*)-Coniferyl alcohol	14.36	1729	1.52	23.48	3056	3.16
Unknown [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16)...]	14.51	1743	4.30	18.54	2455	4.60
Benzyl benzoate	14.66	1756	6.18	19.20	2528	6.50
Phenylethyl benzoate	15.66	1844	1.91	19.91	2611	2.27
Benzyl salicylate	15.81	1858	0.46	20.47	2677	0.52
Methyl palmitate	16.56	1928	4.42	15.86	2172	4.64
Palmitic acid	17.00	1969	5.04	22.98*	2990	4.00
Ethyl palmitate	17.28	1996	0.60	16.32	2220	0.82
(*E*,*E*)-Geranyllinalool	17.59	2026	11.64	18.78	2482	12.37
(*E*)-Cinnamyl benzoate	18.09	2076	0.65	22.98*	2990	[3.89]
Methyl linoleate	18.25	2092	2.77	18.42	2442	1.45
Methyl α-linolenate	18.31	2098	24.97	18.92	2497	23.76
Methyl stearate	18.61	2128	2.83	17.95*	2390	[4.57]
α-Linolenic acid	18.73	2141	3.33			
Docosene isomer	18.99*	2168	5.31	16.05	2192	1.55
Ethyl α-linolenate	18.99*	2168	[6.32]	19.23	2532	1.22
Unknown [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]	19.43	2214	0.34			
(9*Z*)-Eicosenol?	19.79	2253	1.06			
(9*Z*)-Tricosene	20.02	2278	31.06	17.04	2293	32.60
Methyl arachidate	20.49	2329	1.16	19.72	2588	0.23
Tetracosene isomer	20.91	2377	2.40			
Unknown [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]	21.59	2455	0.34			
Benzyl palmitate	22.55	2569	2.15			
Benzyl oleate	23.93	2742	1.27			
Benzyl α-linolenate	23.99	2750	9.70			
Squalene	24.54	2822	6.79	23.05	2999	7.90
2,3-Oxidosqualene	25.39	2937	5.11			
2,3-Dihydro-3-oxosqualene?	25.57	2962	0.05			
Benzyl arachidate	25.65	2973	0.35			
2,6,10,15,19,23-Hexamethyl-	25.90	3007	0.15			

(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol				
Unknown [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]	26.14	3039	0.40	
α-Tocopherol	26.76	3118	1.40	
Unknown [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]	28.86	3313	5.11	
Unknown [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]	30.33	3412	7.65	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

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