Date : July 23, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21G13-PTH04
Customer identification : Jasmine Sambac Absolute - India - J10110218R
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 : Alexis St-Gelais, M. Sc., Chimiste 2013-174
Analysis date : July 20, 2021

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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: Orange brownish liquid
Refractive index: 1.5030 ± 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	5.96	0.60	Aliphatic alcohol
Hexanol	0.71	0.07	Aliphatic alcohol
(3*Z*)-Hexenyl acetate	16.05	1.61	Aliphatic ester
(2*E*)-Hexenyl acetate	0.61	0.06	Aliphatic ester
Unknown	0.77	0.08	Unknown
Benzyl alcohol	97.40	9.74	Simple phenolic
cis-Linalool oxide (fur.)	0.44	0.04	Monoterpenic alcohol
Benzyl formate	0.37	0.04	Phenolic ester
trans-Linalool oxide (fur.)	3.59	0.36	Monoterpenic alcohol
Methyl benzoate	4.55	0.46	Phenolic ester
Linalool	86.88	8.69	Monoterpenic alcohol
Phenylethyl alcohol	12.69	1.27	Simple phenolic
Benzeneacetonitrile	13.13	1.31	Simple phenolic
Benzyl acetate	64.44	6.44	Phenolic ester
cis-Linalool oxide (pyr.)	0.76	0.08	Monoterpenic alcohol
Ethyl benzoate	0.65	0.07	Phenolic ester
Unknown	3.85	0.39	Unknown
trans-Linalool oxide (pyr.)	2.04	0.20	Monoterpenic alcohol
Benzoic acid	5.30	0.53	Simple phenolic
Methyl salicylate	3.00	0.30	Phenolic ester
(3*Z*)-Hexenyl butyrate	0.41	0.04	Aliphatic ester
(3*Z*)-Hexenyl isovalerate	0.18	0.02	Aliphatic ester
Phenylethyl acetate	3.86	0.39	Phenolic ester
Geraniol	1.04	0.10	Monoterpenic alcohol
Ethyl salicylate	0.40	0.04	Phenolic ester
Unknown	1.87	0.19	Unknown
Indole	3.67	0.37	Indole
1-Nitro-2-phenylethane	1.43	0.14	Simple phenolic
(*E*)-Cinnamyl alcohol	1.59	0.16	Phenylpropanoid
Methyl anthranilate	47.85	4.79	Phenolic ester
Eugenol	0.34	0.03	Phenylpropanoid
8-Hydroxylinalool isomer	3.89	0.39	Monoterpenic alcohol
Butyl benzoate	0.23	0.02	Phenolic ester
α-Copaene	0.19	0.02	Sesquiterpene
Methyl (*E*)-cinnamate	0.53	0.05	Phenylpropanoid ester
(3*Z*)-Hexenyl (3*Z*)-hexenoate	0.71	0.07	Aliphatic ester
(3*Z*)-Hexenyl hexanoate?	1.01	0.10	Aliphatic ester
β-Elemene	0.30	0.03	Sesquiterpene
(*Z*)-Jasmone	0.10	0.01	Jasmonate
Dimethyl anthranilate	0.13	0.01	Phenolic ester
β-Caryophyllene	0.42	0.04	Sesquiterpene
(*E*)-Cinnamyl acetate	0.96	0.10	Phenylpropanoid ester
(*E*)-β-Farnesene	0.29	0.03	Sesquiterpene
γ-Muurolene	0.55	0.06	Sesquiterpene
Germacrene D	2.69	0.27	Sesquiterpene
epi-Cubebol	0.27	0.03	Sesquiterpenic alcohol
Bicyclogermacrene	1.65	0.17	Sesquiterpene
α-Muurolene	2.14	0.21	Sesquiterpene

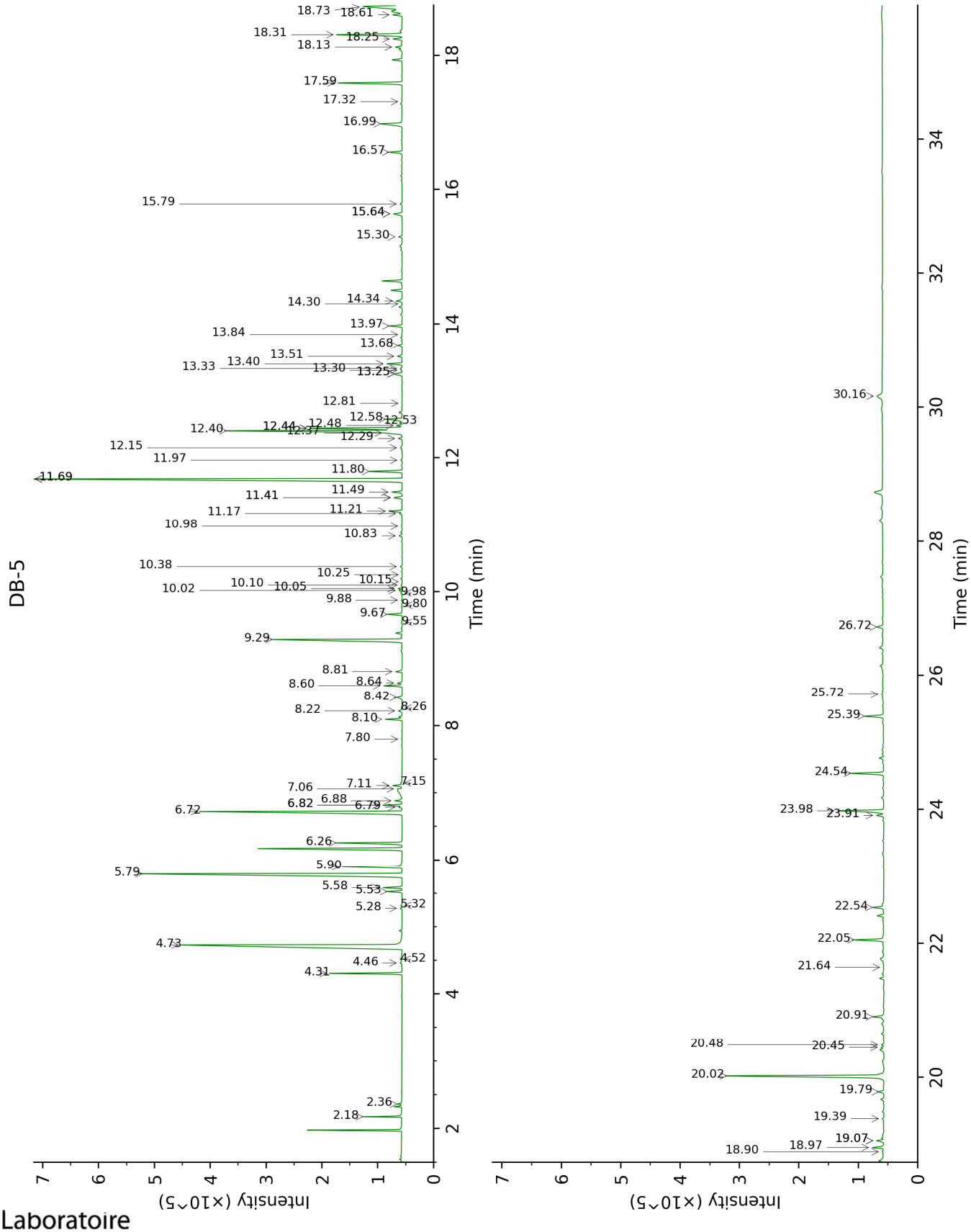
(3*E*,6*E*)-α-Farnesene	90.88	9.09	Sesquiterpene
γ-Cadinene	1.89	0.19	Sesquiterpene
δ-Cadinene	6.60	0.66	Sesquiterpene
α-Cadinene	0.36	0.04	Sesquiterpene
Methyl N-formylanthranilate	0.94	0.09	Phenolic ester
Hexenyl benzoate isomer	0.96	0.10	Phenolic ester
(*E*)-Nerolidol	2.30	0.23	Sesquiterpenic alcohol
(3*Z*)-Hexenyl benzoate	45.09	4.51	Phenolic ester
Germacrene D-4-ol	20.58	2.06	Sesquiterpenic alcohol
Hexyl benzoate	1.17	0.12	Phenolic ester
Spathulenol	1.20	0.12	Sesquiterpenic alcohol
Caryophyllene oxide	0.14	0.01	Sesquiterpenic ether
Methyl N-acetylanthranilate	4.83	0.48	Phenolic ester
Ledol	0.10	0.01	Sesquiterpenic alcohol
τ-Muurolol	1.27	0.13	Sesquiterpenic alcohol
τ-Cadinol	2.66	0.27	Sesquiterpenic alcohol
α-Muurolol	0.31	0.03	Sesquiterpenic alcohol
Methyl *cis*-jasmonate	0.65	0.07	Jasmonate
α-Cadinol	3.34	0.33	Sesquiterpenic alcohol
Unknown	1.42	0.14	Unknown
Methyl *trans*-jasmonate	1.20	0.12	Jasmonate
Shyobunol	0.16	0.02	Sesquiterpenic alcohol
Unknown	3.47	0.35	Unknown
(2*E*,6*E*)-Farnesol	0.09	0.01	Sesquiterpenic alcohol
Oplopanone	1.83	0.18	Sesquiterpenic alcohol
Unknown	1.00	0.10	Unknown
(2*E*,6*E*)-Farnesyl acetate	0.27	0.03	Sesquiterpenic ester
Phenylethyl benzoate	2.43	0.24	Phenolic ester
Benzyl salicylate	0.59	0.06	Phenolic ester
Methyl palmitate	3.14	0.31	Aliphatic ester
Palmitic acid	7.42	0.74	Aliphatic acid
Ethyl palmitate	0.11	0.01	Aliphatic ester
(*E*,*E*)-Geranyllinalool	14.09	1.41	Diterpenic alcohol
(*E*)-Cinnamyl benzoate	1.52	0.15	Phenylpropanoid ester
Methyl linoleate	2.15	0.22	Aliphatic ester
Methyl α-linolenate	17.48	1.75	Aliphatic ester
Methyl stearate	2.15	0.22	Aliphatic ester
α-Linolenic acid	15.43	1.54	Aliphatic acid
Ethyl linoleate	0.64	0.06	Aliphatic ester
Ethyl α-linolenate	2.91	0.29	Aliphatic ester
Stearic acid	2.10	0.21	Aliphatic acid
Methyl (*E*)-phytenate	tr	tr	Diterpenic ester
Unknown	0.39	0.04	Unknown
(9*Z*)-Eicosenol?	1.29	0.13	Aliphatic alcohol
(9*E*)-Tricosene?	35.21	3.52	Alkene
Methyl arachidate	0.61	0.06	Aliphatic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.55	0.06	Terpenic lactone
Tetracosene isomer	2.52	0.25	Alkene
Unknown	0.19	0.02	Unknown
2-Monopalmitin	8.16	0.82	Glyceride
Benzyl palmitate	2.57	0.26	Phenolic ester

Benzyl oleate	1.73	0.17	Phenolic ester
Benzyl α-linolenate	11.85	1.19	Phenolic ester
Squalene	6.91	0.69	Triterpene
2,3-Oxidosqualene	4.46	0.45	Triterpenic ether
Benzyl arachidate	0.25	0.03	Phenolic ester
α-Tocopherol	1.75	0.18	Tocopherol
Unknown	3.42	0.34	Unknown
Consolidated total	**750.71 mg/g**	**75.07%**	

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)
18.73
18.61
18.31
18.25
18.13
17.59
17.32
16.99
16.57
15.79
15.64
15.30
14.30
14.34
13.97
13.84
13.68
13.51
13.40
13.33
13.30
13.25
12.81
12.58
12.53
12.48
12.44
12.40
12.37
12.29
12.15
11.97
11.80
11.69
11.49
11.41
11.21
11.17
10.98
10.83
10.38
10.25
10.15
10.10
10.05
10.02
9.98
9.88
9.80
9.67
9.55
9.29
8.81
8.64
8.60
8.42
8.26
8.22
8.10
7.80
7.15
7.11
7.06
6.88
6.82
6.79
6.72
6.26
5.90
5.79
5.58
5.53
5.32
5.28
4.73
4.52
4.46
4.31
2.36
2.18
30.16
26.72
25.72
25.39
24.54
23.98
23.91
22.54
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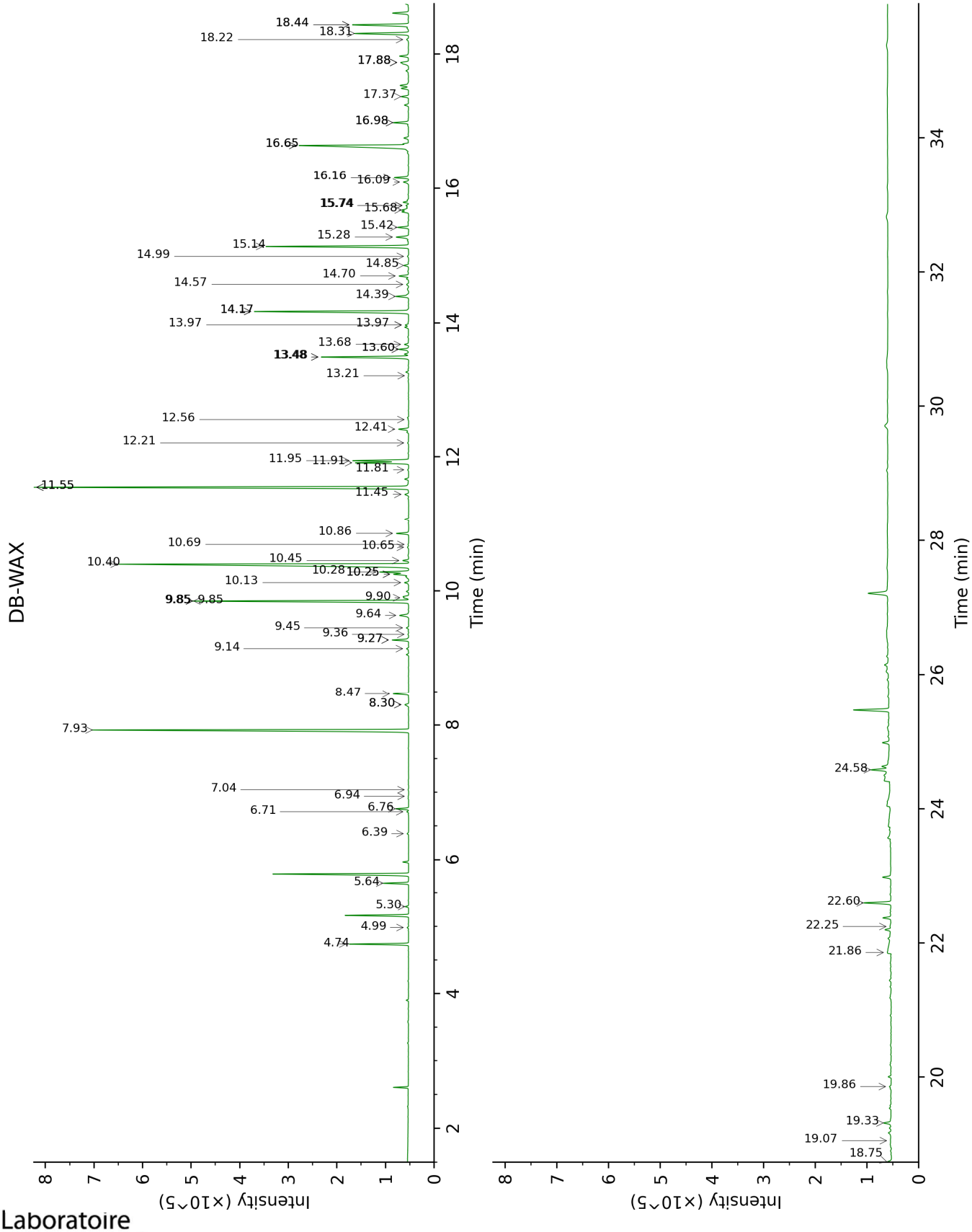
20.02
19.79
19.39
19.07
18.97
18.90


DB-WAX
Intensity (×10^5)
Time (min)
18.44
18.31
18.22
17.88
17.37
16.98
16.65
16.16
16.09
15.74
15.68
15.42
15.28
15.14
14.99
14.85
14.70
14.57
14.39
14.17
13.97
13.97
13.68
13.60
13.48
13.21
12.56
12.41
12.21
11.95
11.91
11.81
11.55
11.45
10.86
10.69
10.65
10.45
10.40
10.28
10.25
10.13
9.85
9.85
9.90
9.64
9.45
9.36
9.27
9.14
8.47
8.30
7.93
7.04
6.94
6.71
6.76
6.39
5.64
5.30
4.99
4.74
24.58
22.60
22.25
21.86
19.86
19.33
19.07
18.75

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	2.18	859	5.96	5.64	1347	6.30
Hexanol	2.36	874	0.71	5.30	1322	0.80
(3*Z*)-Hexenyl acetate	4.31	1009	16.05	4.74	1290	15.92
(2*E*)-Hexenyl acetate	4.46	1019	0.61	4.98	1299	0.41
Unknown [m/z 41, 57 (55), 85 (47), 59 (45), 43 (41)...]	4.52	1022	0.77			
Benzyl alcohol	4.73	1036	97.40	11.55*	1816	96.68
cis-Linalool oxide (fur.)	5.28	1070	0.44	6.39	1401	0.47
Benzyl formate	5.32	1073	0.37	9.27*	1624	5.11
trans-Linalool oxide (fur.)	5.53	1086	3.59	6.76	1429	3.50
Methyl benzoate	5.58	1090	4.55	8.47	1560	4.61
Linalool	5.79	1103	86.88	7.93	1518	86.44
Phenylethyl alcohol	5.90	1110	12.69	11.92	1849	12.68
Benzeneacetonitrile	6.26	1133	13.13	11.95	1852	13.28
Benzyl acetate	6.72	1163	64.44	9.85*	1671	64.44
cis-Linalool oxide (pyr.)	6.79	1167	0.76	10.13	1694	1.35
Ethyl benzoate	6.82*	1169	4.42	9.14	1614	0.65
Unknown [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	6.82*	1169	[4.51]	9.27*	1624	[5.01]
trans-Linalool oxide (pyr.)	6.88	1174	2.04	10.45	1722	1.71
Benzoic acid	7.06	1185	5.30			
Methyl salicylate	7.11	1188	3.00	10.25*	1704	6.01
(3*Z*)-Hexenyl butyrate	7.15	1191	0.41	6.71	1426	0.50
(3*Z*)-Hexenyl isovalerate	7.80	1234	0.18	6.94	1443	0.14
Phenylethyl acetate	8.10	1254	3.86	10.86	1756	3.50
Geraniol	8.22	1263	1.04	11.45	1807	1.23
Ethyl salicylate	8.26	1266	0.40	10.69	1742	0.25
Unknown [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]	8.42	1276	1.87			
Indole	8.60	1289	3.67	16.98*	2350	4.04
1-Nitro-2-phenylethane	8.64	1292	1.43	13.97*	2040	1.12
(*E*)-Cinnamyl alcohol	8.81	1303	1.59	15.68	2211	2.11
Methyl anthranilate	9.29	1333	47.85	15.14	2156	47.76
Eugenol	9.55	1352	0.34	14.57	2099	0.73
8-Hydroxylinalool isomer	9.67	1360	3.89	16.16*	2261	4.45
Butyl benzoate	9.80	1370	0.23	11.55*	1816	[103.76]
α-Copaene	9.88	1375	0.19	7.04	1450	0.14
Methyl (*E*)-cinnamate	9.98	1382	0.53	13.60*	2004	3.19
(3*Z*)-Hexenyl (3*Z*)-hexenoate	10.02	1385	0.71	9.90	1675	1.19
(3*Z*)-Hexenyl hexanoate?	10.05	1387	1.01			
β-Elemene	10.10	1391	0.30	8.30*	1547	1.12
(*Z*)-Jasmone	10.15	1394	0.10	12.21	1875	0.28

Dimethyl anthranilate	10.25	1402	0.13	13.48*	1993	28.56
β-Caryophyllene	10.38	1411	0.42	8.30*	1547	[1.12]
(*E*)-Cinnamyl acetate	10.83	1445	0.96	14.40	2081	4.37
(*E*)-β-Farnesene	10.98	1456	0.29	9.36	1631	0.17
γ-Muurolene	11.17	1470	0.55	9.45	1639	0.55
Germacrene D	11.21	1473	2.69	9.64	1654	2.79
epi-Cubebol	11.41*	1488	2.08	11.81	1840	0.27
Bicyclogermacrene	11.41*	1488	[1.91]	9.85*	1671	[49.43]
α-Muurolene	11.49	1494	2.14	9.85*	1671	[49.43]
(3*E*,6*E*)-α-Farnesene	11.69*	1509	94.76	10.40	1717	90.88
γ-Cadinene	11.69*	1509	[94.76]	10.25*	1704	[3.77]
δ-Cadinene	11.80	1518	6.60	10.28	1707	6.70
α-Cadinene	11.97	1531	0.36	10.65	1738	0.35
Methyl N-formylanthranilate	12.15	1546	0.94	18.44*	2513	23.54
Hexenyl benzoate isomer	12.29	1557	0.96	13.97*	2040	[0.92]
(*E*)-Nerolidol	12.37	1563	2.30	13.60*	2004	[2.70]
(3*Z*)-Hexenyl benzoate	12.40	1566	45.09	14.17*	2059	44.82
Germacrene D-4-ol	12.44*	1569	21.66	13.48*	1993	[22.28]
Hexyl benzoate	12.44*	1569	[23.39]	13.68	2012	1.17
Spathulenol	12.48	1572	1.20	14.17*	2059	[41.40]
Caryophyllene oxide	12.53	1576	0.14	12.56	1906	0.15
Methyl N-acetylanthranilate	12.58	1579	4.83	17.37	2392	2.85
Ledol	12.81	1598	0.10	13.21	1967	0.08
τ-Muurolol	13.25*	1634	2.47	14.85	2127	1.27
τ-Cadinol	13.25*	1634	[2.47]	14.70	2111	2.66
α-Muurolol	13.30	1638	0.31	14.99	2141	0.39
Methyl *cis*-jasmonate	13.33	1641	0.65	16.16*	2261	[4.72]
α-Cadinol	13.40	1646	3.34	15.28	2170	3.92
Unknown [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]	13.51	1656	1.42			
Methyl *trans*-jasmonate	13.68	1670	1.20	16.98*	2350	[5.26]
Shyobunol	13.84	1683	0.16	16.09	2254	1.64
Unknown [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	13.97	1694	3.47	12.41	1893	3.31
(2*E*,6*E*)-Farnesol	14.30	1722	0.09	16.65*	2313	41.81
Oplopanone	14.34	1726	1.83	17.88*	2449	3.96
Unknown [m/z 43, 159 (79), 93 (49), 119 (48), 161 (40), 187 (36)... 238? (2)]	15.30	1809	1.00			
(2*E*,6*E*)-Farnesyl acetate	15.64*	1840	2.84	15.74*	2218	0.75
Phenylethyl benzoate	15.64*	1840	[2.69]	19.33	2618	2.43
Benzyl salicylate	15.78	1853	0.59	19.86	2682	0.60
Methyl palmitate	16.56	1926	3.14	15.42	2184	2.94
Palmitic acid	16.99	1966	7.42	21.86	2936	5.54
Ethyl palmitate	17.32	1997	0.11	15.74*	2218	[0.71]
(*E*,*E*)-Geranyllinalool	17.59	2024	14.09	18.31	2498	14.07

(*E*)-Cinnamyl benzoate	18.13	2078	1.52	22.24	2987	0.45
Methyl linoleate	18.25	2090	2.15	17.88*	2449	[3.76]
Methyl α-linolenate	18.31	2096	17.48	18.44*	2513	[16.42]
Methyl stearate	18.61	2126	2.15			
α-Linolenic acid	18.73	2139	15.43			
Ethyl linoleate	18.90	2157	0.64	18.22	2487	0.66
Ethyl α-linolenate	18.97	2164	2.91	18.75	2550	1.38
Stearic acid	19.07*	2174	1.98			
Methyl (*E*)-phytenate	19.07*	2174	[1.95]	17.88*	2449	[3.66]
Unknown [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]	19.39	2208	0.39			
(9*Z*)-Eicosenol?	19.79	2251	1.29			
(9*E*)-Tricosene?	20.02	2276	35.21	16.65*	2313	[36.63]
Methyl arachidate	20.45	2323	0.61	19.07	2586	0.11
4,8,12,16-Tetramethylheptadecan-4-olide?	20.48	2327	0.55			
Tetracosene isomer	20.91	2375	2.52			
Unknown [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]	21.64	2459	0.19			
2-Monopalmitin	22.05	2507	8.16			
Benzyl palmitate	22.54	2566	2.57			
Benzyl oleate	23.91	2738	1.73			
Benzyl α-linolenate	23.98	2747	11.85			
Squalene	24.54	2819	6.91	22.60	3035	6.80
2,3-Oxidosqualene	25.39	2934	4.46	24.58	3317	5.95
Benzyl arachidate	25.72	2979	0.25			
α-Tocopherol	26.72	3110	1.75			
Unknown [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]	30.16	3399	3.42			

*: 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