Date : May 04, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21D20-PTH12
Customer identification : Jasmine Sambac Absolute - India - J10109212R
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 : Sylvain Mercier, M. Sc., Chimiste
Analysis date : April 21, 2021

Checked and approved by :

Sylvain Mercier, M. Sc., chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 of the version first issued on April 21, 2021 to correct a mistake in the lot number.

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 viscous liquid
Refractive index: 1.5053 ± 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	3.67	0.37	Aliphatic alcohol
Hexanol	0.73	0.07	Aliphatic alcohol
(3*Z*)-Hexenyl formate	0.06	0.01	Aliphatic ester
6-Methyl-5-hepten-2-one	0.19	0.02	Aliphatic ketone
(3*Z*)-Hexenyl acetate	14.64	1.46	Aliphatic ester
Hexyl acetate	0.18	0.02	Aliphatic ester
(2*E*)-Hexenyl acetate	0.35	0.04	Aliphatic ester
Unknown	0.55	0.06	Unknown
Benzyl alcohol	67.20	6.72	Simple phenolic
(*E*)-β-Ocimene	0.19	0.02	Monoterpene
cis-Linalool oxide (fur.)	0.23	0.02	Monoterpenic alcohol
Benzyl formate	0.49	0.05	Phenolic ester
trans-Linalool oxide (fur.)	1.55	0.16	Monoterpenic alcohol
Methyl benzoate	5.98	0.60	Phenolic ester
Linalool	73.14	7.31	Monoterpenic alcohol
Phenylethyl alcohol	13.25	1.33	Simple phenolic
Benzeneacetonitrile	10.40	1.04	Simple phenolic
Benzyl acetate	87.68	8.77	Phenolic ester
Ethyl benzoate	0.63	0.06	Phenolic ester
Unknown	4.36	0.44	Unknown
trans-Linalool oxide (pyr.)	1.12	0.11	Monoterpenic alcohol
Methyl salicylate	2.89	0.29	Phenolic ester
Unknown	1.93	0.19	Unknown
Phenylethyl acetate	4.81	0.48	Phenolic ester
Geraniol	0.53	0.05	Monoterpenic alcohol
Ethyl salicylate	0.20	0.02	Phenolic ester
Unknown	3.01	0.30	Unknown
2,6-Dimethyl-1,7-octadiene-3,6-diol	0.22	0.02	Monoterpenic alcohol
1-Nitro-2-phenylethane	2.07	0.21	Simple phenolic
Indole	0.91	0.09	Indole
(*E*)-Cinnamyl alcohol	1.18	0.12	Phenylpropanoid
Methyl anthranilate	61.15	6.12	Phenolic ester
Eugenol	0.86	0.09	Phenylpropanoid
8-Hydroxylinalool isomer	1.25	0.13	Monoterpenic alcohol
Butyl benzoate	0.33	0.03	Phenolic ester
Methyl (*E*)-cinnamate	0.48	0.05	Phenylpropanoid ester
(3*Z*)-Hexenyl (3*Z*)-hexenoate	0.16	0.02	Aliphatic ester
(3*Z*)-Hexenyl hexanoate?	0.64	0.06	Aliphatic ester
β-Elemene	0.82	0.08	Sesquiterpene
(*Z*)-Jasmone	0.34	0.03	Jasmonate
Dimethyl anthranilate	0.37	0.04	Phenolic ester
β-Caryophyllene	0.40	0.04	Sesquiterpene
(*E*)-Cinnamyl acetate	0.28	0.03	Phenylpropanoid ester
α-Humulene	0.58	0.06	Sesquiterpene
(*E*)-β-Farnesene	0.21	0.02	Sesquiterpene
γ-Muurolene	0.27	0.03	Sesquiterpene
Germacrene D	2.82	0.28	Sesquiterpene
epi-Cubebol	0.19	0.02	Sesquiterpenic alcohol

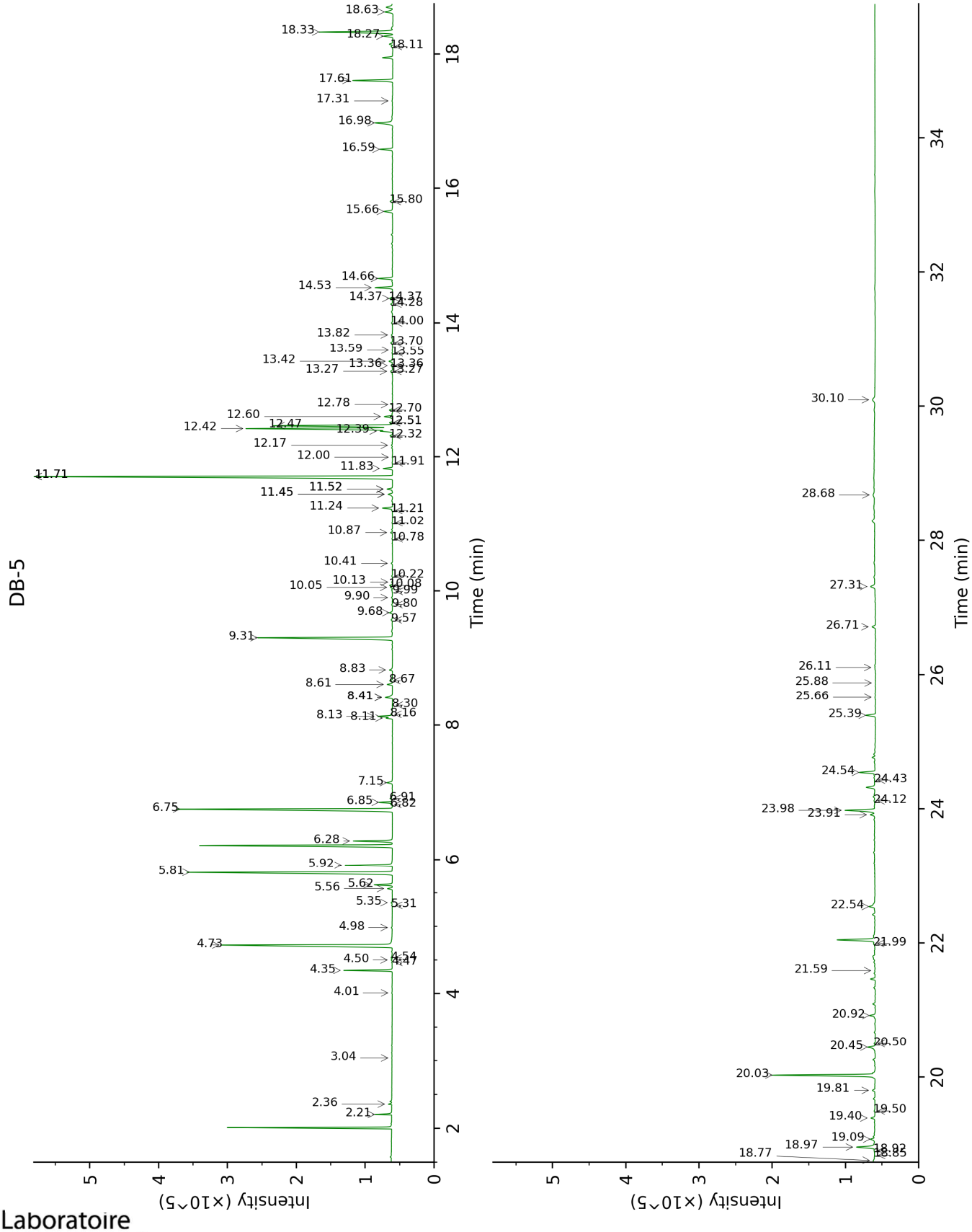
Bicyclogermacrene	1.37	0.14	Sesquiterpene
α-Muurolene	0.41	0.04	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	1.20	0.12	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	112.26	11.23	Sesquiterpene
γ-Cadinene	0.25	0.03	Sesquiterpene
δ-Cadinene	2.61	0.26	Sesquiterpene
10-epi-Cubebol?	0.27	0.03	Sesquiterpenic alcohol
α-Cadinene	0.12	0.01	Sesquiterpene
Methyl N-formylanthranilate	0.56	0.06	Phenolic ester
Hexenyl benzoate isomer	0.93	0.09	Phenolic ester
(*E*)-Nerolidol	3.14	0.31	Sesquiterpenic alcohol
(3*Z*)-Hexenyl benzoate	47.67	4.77	Phenolic ester
Germacrene D-4-ol	37.17	3.72	Sesquiterpenic alcohol
Hexyl benzoate	1.10	0.11	Phenolic ester
Caryophyllene oxide	0.16	0.02	Sesquiterpenic ether
(2*E*)-Hexenyl benzoate	3.27	0.33	Phenolic ester
Methyl N-acetylanthranilate	1.62	0.16	Phenolic ester
Ledol	0.29	0.03	Sesquiterpenic alcohol
τ-Muurolol	0.56	0.06	Sesquiterpenic alcohol
τ-Cadinol	0.59	0.06	Sesquiterpenic alcohol
α-Muurolol	0.26	0.03	Sesquiterpenic alcohol
Methyl *cis*-jasmonate	0.54	0.05	Jasmonate
α-Cadinol	1.09	0.11	Sesquiterpenic alcohol
Unknown	0.27	0.03	Unknown
(3*E*,5*E*)-7-Hydroxyfarnesene	0.15	0.02	Sesquiterpenic alcohol
Methyl *trans*-jasmonate	0.85	0.09	Jasmonate
Shyobunol	0.42	0.04	Sesquiterpenic alcohol
Unknown	0.51	0.05	Unknown
(2*E*,6*E*)-Farnesol	0.61	0.06	Sesquiterpenic alcohol
Oplopanone	0.98	0.10	Sesquiterpenic alcohol
(*E*)-Coniferyl alcohol	0.29	0.03	Phenylpropanoid
Unknown	6.51	0.65	Unknown
Benzyl benzoate	4.46	0.45	Phenolic ester
Phenylethyl benzoate	3.08	0.31	Phenolic ester
Benzyl salicylate	0.96	0.10	Phenolic ester
Methyl palmitate	4.13	0.41	Aliphatic ester
Palmitic acid	8.09	0.81	Aliphatic acid
Ethyl palmitate	0.18	0.02	Aliphatic ester
(*E*,*E*)-Geranyllinalool	11.59	1.16	Diterpenic alcohol
(*E*)-Cinnamyl benzoate	0.66	0.07	Phenylpropanoid ester
Methyl linoleate	3.07	0.31	Aliphatic ester
Methyl α-linolenate	26.38	2.64	Aliphatic ester
Methyl stearate	3.74	0.37	Aliphatic ester
α-Linolenic acid	1.15	0.12	Aliphatic acid
Ethyl linoleate	0.24	0.02	Aliphatic ester
Ethyl α-linolenate	0.32	0.03	Aliphatic ester
Stearic acid	7.49	0.75	Aliphatic acid
Methyl (*E*)-phytenate	1.80	0.18	Diterpenic ester
Unknown	1.75	0.18	Unknown
(*E*)-Phytyl acetate	0.31	0.03	Diterpenic ester
(9*Z*)-Tricosene	0.86	0.09	Alkene
(9*E*)-Tricosene?	27.68	2.77	Alkene

Methyl arachidate	3.31	0.33	Aliphatic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.41	0.04	Terpenic lactone
Tetracosene isomer	1.82	0.18	Alkene
Unknown	0.27	0.03	Unknown
2-Monopalmitin	1.02	0.10	Glyceride
Benzyl palmitate	2.71	0.27	Phenolic ester
Benzyl oleate	1.48	0.15	Phenolic ester
Benzyl α-linolenate	10.47	1.05	Phenolic ester
Benzyl stearate	0.27	0.03	Phenolic ester
(*E*)-Phytyl benzoate?	0.18	0.02	Phenolic ester
Squalene	4.52	0.45	Triterpene
2,3-Oxidosqualene	3.06	0.31	Triterpenic ether
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	0.14	0.01	Triterpenic alcohol
Unknown	0.47	0.05	Triterpenic alcohol
α-Tocopherol	1.44	0.14	Tocopherol
Benzyl behenate	2.06	0.21	Phenolic ester
Unknown	0.94	0.09	Unknown
Unknown	1.99	0.20	Unknown
Docosene isomer	0.21	0.02	Alkene
Consolidated total	**748.61 mg/g**	**74.86%**	

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)
18.63
18.33
18.27
18.11
17.61
17.31
16.98
16.59
15.80
15.66
14.66
14.53
14.37
14.28
14.00
13.82
13.70
13.59
13.55
13.42
13.36
13.27
12.78
12.70
12.60
12.51
12.47
12.42
12.39
12.32
12.17
12.00
11.91
11.83
11.71
11.52
11.45
11.24
11.21
11.02
10.87
10.78
10.41
10.22
10.13
10.08
10.05
9.99
9.90
9.80
9.68
9.57
9.31
8.83
8.67
8.61
8.41
8.30
8.16
8.13
8.11
7.15
6.91
6.85
6.82
6.75
6.28
5.92
5.81
5.62
5.56
5.35
5.31
4.98
4.73
4.54
4.50
4.47
4.35
4.01
3.04
2.36
2.21
30.10
28.68
27.31
26.71
26.11
25.88
25.66
25.39
24.54
24.43
24.12
23.98
23.91
22.54
21.99
21.59
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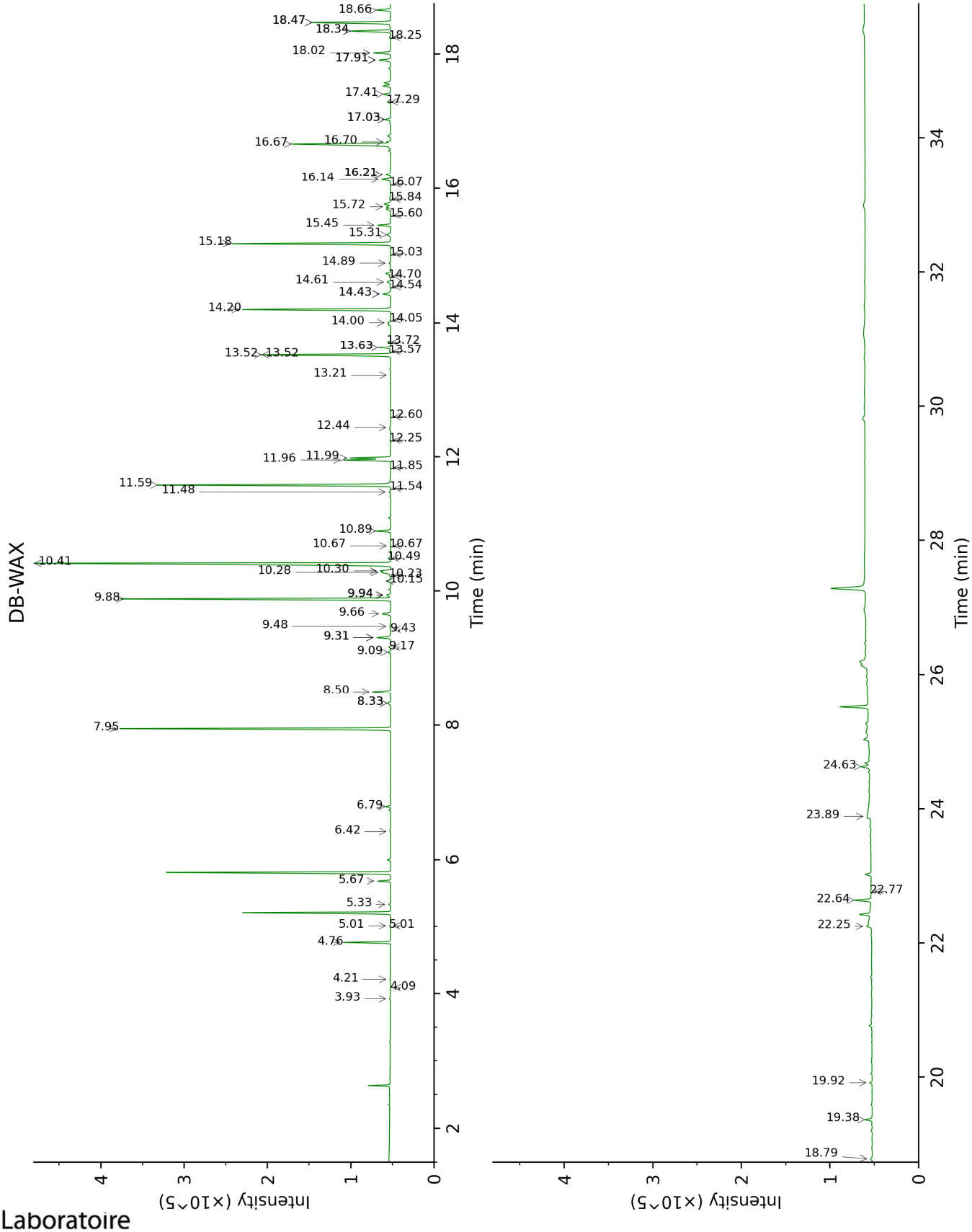
19.40
19.09
18.97
18.92
18.85
18.77


DB-WAX
Intensity (×10^5)
Time (min)
18.66
18.47
18.34
18.25
18.02
17.91
17.41
17.29
17.03
16.67
16.70
16.14
16.21
16.07
15.84
15.72
15.60
15.45
15.31
15.18
15.03
14.89
14.70
14.61
14.54
14.43
14.20
14.05
14.00
13.72
13.63
13.57
13.52
13.52
13.21
12.60
12.44
12.25
11.96
11.99
11.85
11.59
11.54
11.48
10.89
10.67
10.67
10.49
10.41
10.30
10.23
10.28
10.15
9.94
9.88
9.66
9.48
9.43
9.31
9.17
9.09
8.50
8.33
7.95
6.79
6.42
5.67
5.33
5.01
5.01
4.76
4.21
4.09
3.93
24.63
23.89
22.77
22.64
22.25
19.92
19.38
18.79

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	2.21	859	3.67	5.67	1347	3.97
Hexanol	2.36	872	0.73	5.33	1322	0.60
(3*Z*)-Hexenyl formate	3.04	923	0.06	4.09	1235	0.23
6-Methyl-5-hepten-2-one	4.01	988	0.19	5.01*	1299	0.39
(3*Z*)-Hexenyl acetate	4.35	1010	14.64	4.76	1285	14.75
Hexyl acetate	4.47	1018	0.18	4.22	1244	0.35
(2*E*)-Hexenyl acetate	4.50	1020	0.35	5.01*	1299	[0.46]
Unknown [m/z 41, 57 (55), 85 (47), 59 (45), 43 (41)...]	4.54	1022	0.55			
Benzyl alcohol	4.73	1034	67.20	11.58	1816	66.97
(*E*)-β-Ocimene	4.98	1051	0.19	3.93	1222	0.30
cis-Linalool oxide (fur.)	5.31	1072	0.23	6.42	1401	0.26
Benzyl formate	5.35	1074	0.49	9.31*	1624	4.96
trans-Linalool oxide (fur.)	5.56	1088	1.55	6.79	1429	1.62
Methyl benzoate	5.62	1091	5.98	8.50	1560	6.03
Linalool	5.81	1103	73.14	7.95	1516	73.74
Phenylethyl alcohol	5.92	1110	13.25	11.99	1852	11.38
Benzeneacetonitrile	6.28	1134	10.40	11.96	1849	12.47
Benzyl acetate	6.75	1164	87.68	9.88†	1671	89.45
Ethyl benzoate	6.82	1169	0.63	9.17	1612	0.60
Unknown [m/z 43, 69 (35), 41 (26), 83 (25), 57 (22)... 150 (1)]	6.85	1171	4.36	9.31*	1624	[4.86]
trans-Linalool oxide (pyr.)	6.91	1175	1.12	10.49	1721	0.91
Methyl salicylate	7.15	1190	2.89	10.30	1705	4.60
Unknown [m/z 91, 117 (80), 90 (42), 118 (29)... 136 (5)]	8.10	1254	1.93	16.21*	2261	1.95
Phenylethyl acetate	8.13	1256	4.81	10.89	1756	4.62
Geraniol	8.16	1258	0.53	11.48	1806	0.60
Ethyl salicylate	8.30	1268	0.20	10.67*	1737	0.29
Unknown [m/z 91, 117 (98), 90 (65), 89 (29), 65 (29), 118 (26), 135 (23)]	8.41*	1275	3.22			
2,6-Dimethyl-1,7-octadiene-3,6-diol	8.41*	1275	[3.21]	14.54	2091	0.22
1-Nitro-2-phenylethane	8.61	1289	2.07	14.00	2039	1.07
Indole	8.67	1293	0.91	17.03*	2349	1.75
(*E*)-Cinnamyl alcohol	8.83	1304	1.18	15.72	2210	1.48
Methyl anthranilate	9.31	1334	61.15	15.18	2155	61.40
Eugenol	9.57	1353	0.86	14.61	2097	1.61
8-Hydroxylinalool isomer	9.68	1361	1.25	16.21*	2261	[1.94]
Butyl benzoate	9.80	1369	0.33	11.54	1811	0.21
Methyl (*E*)-cinnamate	9.90	1377	0.48	13.63*	2003	4.57

(3*Z*)-Hexenyl (3*Z*)-hexenoate	9.99	1383	0.16	9.94*†	1675	[87.46]
(3*Z*)-Hexenyl hexanoate?	10.06	1388	0.64			
β-Elemene	10.08	1390	0.82	8.33*	1546	1.18
(*Z*)-Jasmone	10.13	1393	0.34	12.25	1875	0.26
Dimethyl anthranilate	10.22	1400	0.37	13.52*	1992	48.43
β-Caryophyllene	10.41	1413	0.40	8.33*	1546	[1.18]
(*E*)-Cinnamyl acetate	10.78	1441	0.28	14.43*	2080	3.35
α-Humulene	10.87	1448	0.58	9.09	1606	0.71
(*E*)-β-Farnesene	11.02	1458	0.21	9.43	1634	0.14
γ-Muurolene	11.21	1473	0.27	9.48	1638	0.29
Germacrene D	11.24	1476	2.82	9.66	1653	2.85
epi-Cubebol	11.45*	1491	1.68	11.84	1839	0.19
Bicyclogermacrene	11.45*	1491	[1.54]	9.94*†	1675	[68.61]
α-Muurolene	11.52*	1497	1.61	9.94*†	1675	[68.61]
(3*Z*,6*E*)-α-Farnesene	11.52*	1497	[1.61]	10.15	1692	1.20
(3*E*,6*E*)-α-Farnesene	11.71*	1511	112.20	10.41	1715	112.26
γ-Cadinene	11.71*	1511	[112.20]	10.23	1699	0.25
δ-Cadinene	11.83	1520	2.61	10.28	1703	2.89
10-epi-Cubebol?	11.91	1527	0.27	13.57	1997	0.43
α-Cadinene	12.00	1534	0.12	10.67*	1737	[0.19]
Methyl N-formylanthranilate	12.17	1548	0.56	18.47*	2510	37.16
Hexenyl benzoate isomer	12.32	1559	0.93	14.05	2043	0.24
(*E*)-Nerolidol	12.39	1564	3.14	13.63*	2003	[3.86]
(3*Z*)-Hexenyl benzoate	12.42	1567	47.67	14.20	2058	47.68
Germacrene D-4-ol	12.47	1570	37.17	13.52*	1992	[37.79]
Hexyl benzoate	12.51*	1574	1.03	13.72	2011	1.10
Caryophyllene oxide	12.51*	1574	[0.97]	12.60	1906	0.16
(2*E*)-Hexenyl benzoate	12.60	1581	3.27	14.43*	2080	[3.20]
Methyl N-acetylanthranilate	12.70	1589	1.62	17.29	2378	1.80
Ledol	12.78	1595	0.29	13.21	1964	0.27
τ-Muurolol	13.27*	1636	0.90	14.89	2126	0.56
τ-Cadinol	13.27*	1636	[0.90]	14.70	2106	0.59
α-Muurolol	13.36*	1643	0.67	15.03	2140	0.26
Methyl *cis*-jasmonate	13.36*	1643	[0.87]	16.21*	2261	[2.06]
α-Cadinol	13.42	1648	1.09	15.31	2168	1.79
Unknown [m/z 99, 161 (100), 43 (92), 204 (74), 71 (73), 121 (65)...]	13.55	1659	0.27			
(3*E*,5*E*)-7-Hydroxyfarnesene	13.59	1662	0.15	16.07	2246	0.18
Methyl *trans*-jasmonate	13.70	1672	0.85	17.03*	2349	[2.28]
Shyobunol	13.82	1682	0.42	16.14	2253	2.98
Unknown [m/z 99, 43 (47), 161 (42), 71 (39), 204 (31), 121 (28)...]	14.00	1696	0.51	12.44	1892	0.45
(2*E*,6*E*)-Farnesol	14.28	1720	0.61	16.67	2309	34.52
Oplopanone	14.36*	1728	1.23	17.91*	2447	4.51
(*E*)-Coniferyl alcohol	14.36*	1728	[1.47]	22.77	3048	0.29

Unknown [m/z 105, 77 (42), 69 (29), 161 (19), 83 (16)...]	14.52	1742	6.51	18.02	2459	6.46
Benzyl benzoate	14.66	1754	4.46	18.66	2531	4.56
Phenylethyl benzoate	15.66	1842	3.08	19.38	2616	2.41
Benzyl salicylate	15.80	1856	0.96	19.92	2681	0.91
Methyl palmitate	16.59	1929	4.13	15.45	2182	4.08
Palmitic acid	16.98	1966	8.09	22.25	2978	6.02
Ethyl palmitate	17.31	1997	0.18	15.84	2223	0.64
(*E*,*E*)-Geranyllinalool	17.61	2028	11.59	18.34*	2495	12.04
(*E*)-Cinnamyl benzoate	18.12	2078	0.66			
Methyl linoleate	18.27	2093	3.07	17.91*	2447	[4.28]
Methyl α-linolenate	18.33	2099	26.38	18.47*	2510	[25.93]
Methyl stearate	18.63	2130	3.74	17.41	2390	2.39
α-Linolenic acid	18.77	2145	1.15			
Ethyl linoleate	18.85	2153	0.24	18.25	2485	0.43
Ethyl α-linolenate	18.92	2160	0.32	18.79	2547	0.76
Stearic acid	18.97	2166	7.49	23.89	3204	7.53
Methyl (*E*)-phytenate	19.09	2178	1.80	17.91*	2447	[4.16]
Unknown [m/z 190, 158 (100), 253 (68), 193 (58), 220 (51)]	19.40	2211	1.75			
(*E*)-Phytyl acetate	19.50	2222	0.31	18.34*	2495	[12.48]
(9*Z*)-Tricosene	19.81	2255	0.86	16.70	2313	0.90
(9*E*)-Tricosene?	20.03	2279	27.68			
Methyl arachidate	20.45	2325	3.31			
4,8,12,16-Tetramethylheptadecan-4-olide?	20.50	2331	0.41			
Tetracosene isomer	20.92	2379	1.82			
Unknown [m/z 219, 218 (99), 217 (50), 108 (31), 220 (17), 216 (14)]	21.59	2456	0.27			
2-Monopalmitin	21.99	2503	1.02			
Benzyl palmitate	22.54	2570	2.71			
Benzyl oleate	23.92	2743	1.48			
Benzyl α-linolenate	23.98	2751	10.47			
Benzyl stearate	24.12	2769	0.27			
(*E*)-Phytyl benzoate?	24.43	2810	0.18			
Squalene	24.54	2825	4.52	22.64	3030	5.05
2,3-Oxidosqualene	25.39	2940	3.06	24.63	3311	2.98
Benzyl arachidate	25.66	2977	0.35			
2,6,10,15,19,23-Hexamethyl-(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol	25.88	3008	0.14			
Unknown [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]	26.11	3038	0.47			
α-Tocopherol	26.72	3116	1.44			
Benzyl behenate	27.31	3182	2.06			

Unknown [m/z 322, 245 (66), 122 (37), 204 (34), 321 (30), 323 (26)...]	28.68	3306	0.94			
Unknown [m/z 245, 246 (20), 243 (14), 217 (12), 218 (9), 91 (7), 244 (6)]	30.10	3404	1.99			
Docosene isomer				15.60	2197	0.21

*: 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