Date : February 27, 2023

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 23B21-PTH03
Customer identification : Jasmine Grandiflorum Absolute - India - JB1100R
Type : Absolute
Source : *Jasminum grandiflorum*
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 : Amélie Simard, Analyste
Analysis date : February 27, 2023

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

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PHYSICOCHEMICAL DATA

Physical aspect: Orange yellow liquid
Refractive index: 1.5058 ± 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
Benzaldehyde	0.30	0.03	Simple phenolic
6-Methyl-5-hepten-2-one	0.11	0.01	Aliphatic ketone
(3*Z*)-Hexenyl acetate	0.12	0.01	Aliphatic ester
Limonene	0.07	0.01	Monoterpene
Benzyl alcohol	14.92	1.49	Simple phenolic
cis-Linalool oxide (fur.)	0.15	0.02	Monoterpenic alcohol
trans-Linalool oxide (fur.)	0.24	0.02	Monoterpenic alcohol
para-Cresol	3.13	0.31	Simple phenolic
Methyl benzoate	0.90	0.09	Phenolic ester
Linalool	63.68	6.37	Monoterpenic alcohol
Phenylethyl alcohol	0.19	0.02	Simple phenolic
Benzeneacetonitrile	0.12	0.01	Simple phenolic
para-Vinylanisole	0.12	0.01	Simple phenolic
Benzyl acetate	244.13	24.41	Phenolic ester
Methyl salicylate	0.47	0.05	Phenolic ester
Phenylethyl acetate	0.64	0.06	Phenolic ester
Indole	10.14	1.01	Indole
Eugenol	22.79	2.28	Phenylpropanoid
8-Hydroxylinalool isomer	0.56	0.06	Monoterpenic alcohol
Unknown	0.06	0.01	Unknown
(*Z*)-Jasmone	21.81	2.18	Jasmonate
(*E*)-Isoeugenol	0.65	0.07	Phenylpropanoid
Unknown	0.13	0.01	Unknown
(*Z*)-Jasmin lactone	2.27	0.23	Aliphatic lactone
Benzyl tiglate	0.40	0.04	Phenolic ester
(3*E*,6*E*)-α-Farnesene	3.54	0.35	Sesquiterpene
(*E*)-Nerolidol	1.92	0.19	Sesquiterpenic alcohol
Unknown	0.28	0.03	Unknown
(3*Z*)-Hexenyl benzoate	3.76	0.38	Phenolic ester
Hexyl benzoate	0.18	0.02	Phenolic ester
(2*E*)-Hexenyl benzoate	0.21	0.02	Phenolic ester
Methyl N-acetylanthranilate	0.98	0.10	Phenolic ester
Methyl *cis*-jasmonate	8.46	0.85	Jasmonate
Unknown	0.22	0.02	Unknown
Methyl *trans*-jasmonate	0.56	0.06	Jasmonate
Jasmine ketolactone	0.70	0.07	Aliphatic lactone
Pentadecanal	0.55	0.06	Aliphatic aldehyde
(*E*)-Coniferyl alcohol	0.26	0.03	Phenylpropanoid
Benzyl benzoate	202.85	20.29	Phenolic ester
Phytadiene analog?	0.06	0.01	Diterpene
Neophytadiene	0.72	0.07	Diterpene
Phytone	1.08	0.11	Terpenic ketone
Phytadiene isomer I	1.10	0.11	Diterpene
Benzyl salicylate	0.54	0.05	Phenolic ester
Phytadiene isomer II	0.49	0.05	Diterpene
Methyl palmitate	4.16	0.42	Aliphatic ester
Isophytol	75.77	7.58	Diterpenic alcohol
Palmitic acid	4.45	0.45	Aliphatic acid

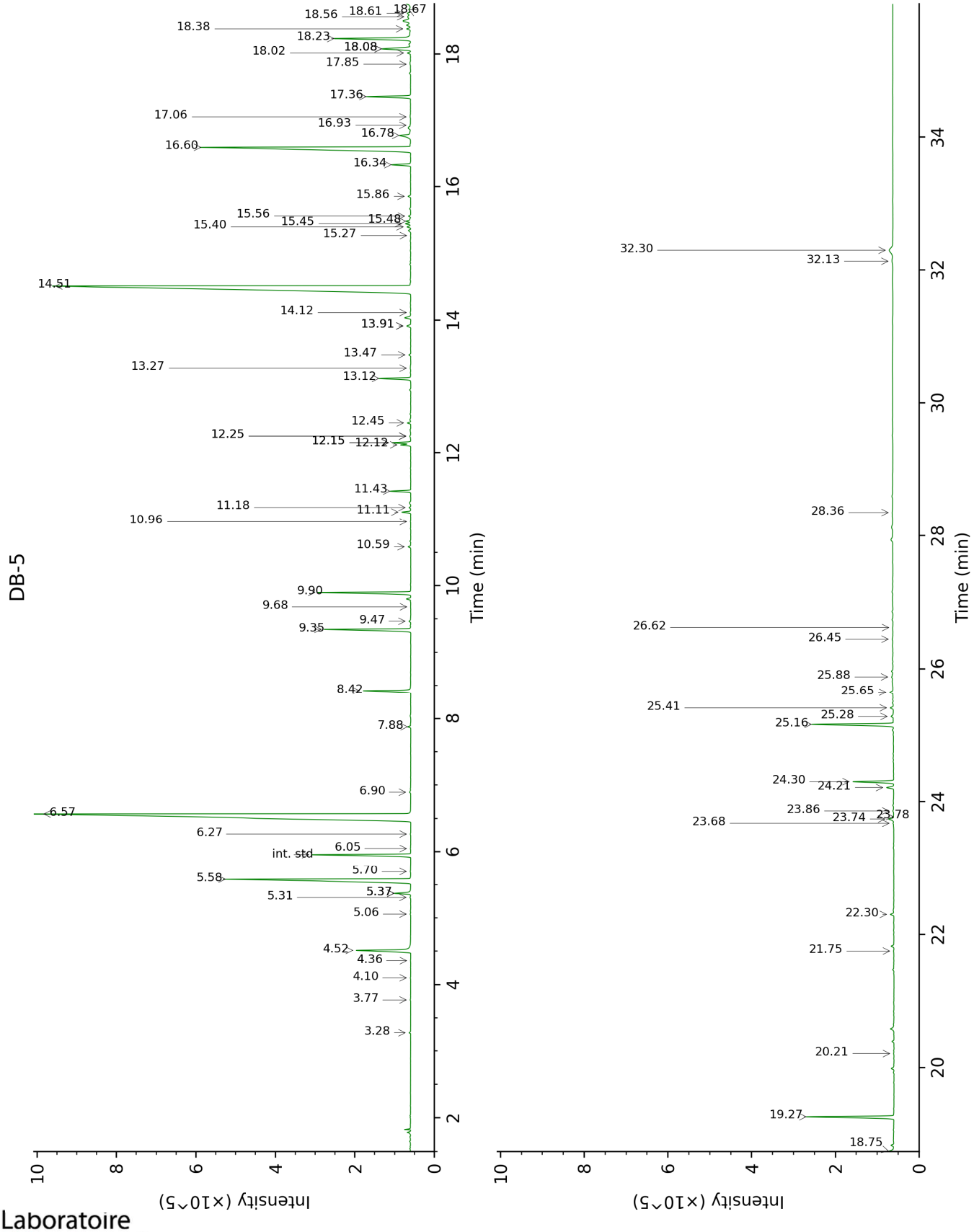
(3*E*,6*E*,10*E*)-α-Springene	0.16	0.02	Diterpene
Ethyl palmitate	0.16	0.02	Aliphatic ester
(*E*,*E*)-Geranyllinalool	9.27	0.93	Diterpenic alcohol
Unknown	0.12	0.01	Phenolic ester
Methyl linoleate	0.72	0.07	Aliphatic ester
Methyl α-linolenate	6.51	0.65	Aliphatic ester
Methyl oleate	2.07	0.21	Aliphatic ester
Phytol	17.37	1.74	Diterpenic alcohol
Methyl stearate	0.96	0.10	Aliphatic ester
α-Linolenic acid	1.25	0.13	Aliphatic acid
Ethyl linoleate	1.10	0.11	Aliphatic ester
Ethyl α-linolenate	0.59	0.06	Aliphatic ester
Methyl (*E*)-phytenate	1.98	0.20	Diterpenic ester
(*E*)-Phytyl acetate	19.29	1.93	Diterpenic ester
4,8,12,16-Tetramethylheptadecan-4-olide?	0.14	0.01	Terpenic lactone
2-Monopalmitin	0.21	0.02	Glyceride
Benzyl palmitate	0.82	0.08	Phenolic ester
Benzyl oleate	0.19	0.02	Phenolic ester
Benzyl α-linolenate	1.33	0.13	Phenolic ester
Squalene isomer I	0.09	0.01	Diterpene
Benzyl stearate	0.32	0.03	Phenolic ester
(*E*)-Phytyl benzoate?	1.56	0.16	Phenolic ester
Squalene	8.00	0.80	Triterpene
2,3-Oxidosqualene	18.16	1.82	Triterpenic ether
2,3-Dihydro-3-oxosqualene?	0.65	0.07	Triterpenic ketone
Benzyl arachidate	0.71	0.07	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	0.97	0.10	Triterpenic alcohol
Unknown	0.59	0.06	Triterpenic alcohol
α-Tocopherol	0.34	0.03	Tocopherol
Unknown	0.14	0.01	Unknown
β-Amyrin	0.40	0.04	Triterpenic alcohol
(*E*)-Phytyl palmitate	0.53	0.05	Diterpenic ester
Jasminum grandiflorum marker I	1.85	0.19	Unknown
Consolidated total	**799.51 mg/g**	**79.95%**	

tr: The compound has been detected below 0.005% of total signal.

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)
18.56
18.61
18.67
18.38
18.23
18.02
18.08
17.85
17.36
17.06
16.93
16.78
16.60
16.34
15.86
15.56
15.45
15.48
15.40
15.27
14.51
14.12
13.91
13.47
13.27
13.12
12.45
12.25
12.15
12.12
11.43
11.18
11.11
10.96
10.59
9.90
9.68
9.47
9.35
8.42
7.88
6.90
6.57
6.27
6.05
int. std
5.70
5.58
5.37
5.31
5.06
4.52
4.36
4.10
3.77
3.28
32.30
32.13
28.36
26.62
26.45
25.88
25.65
25.41
25.28
25.16
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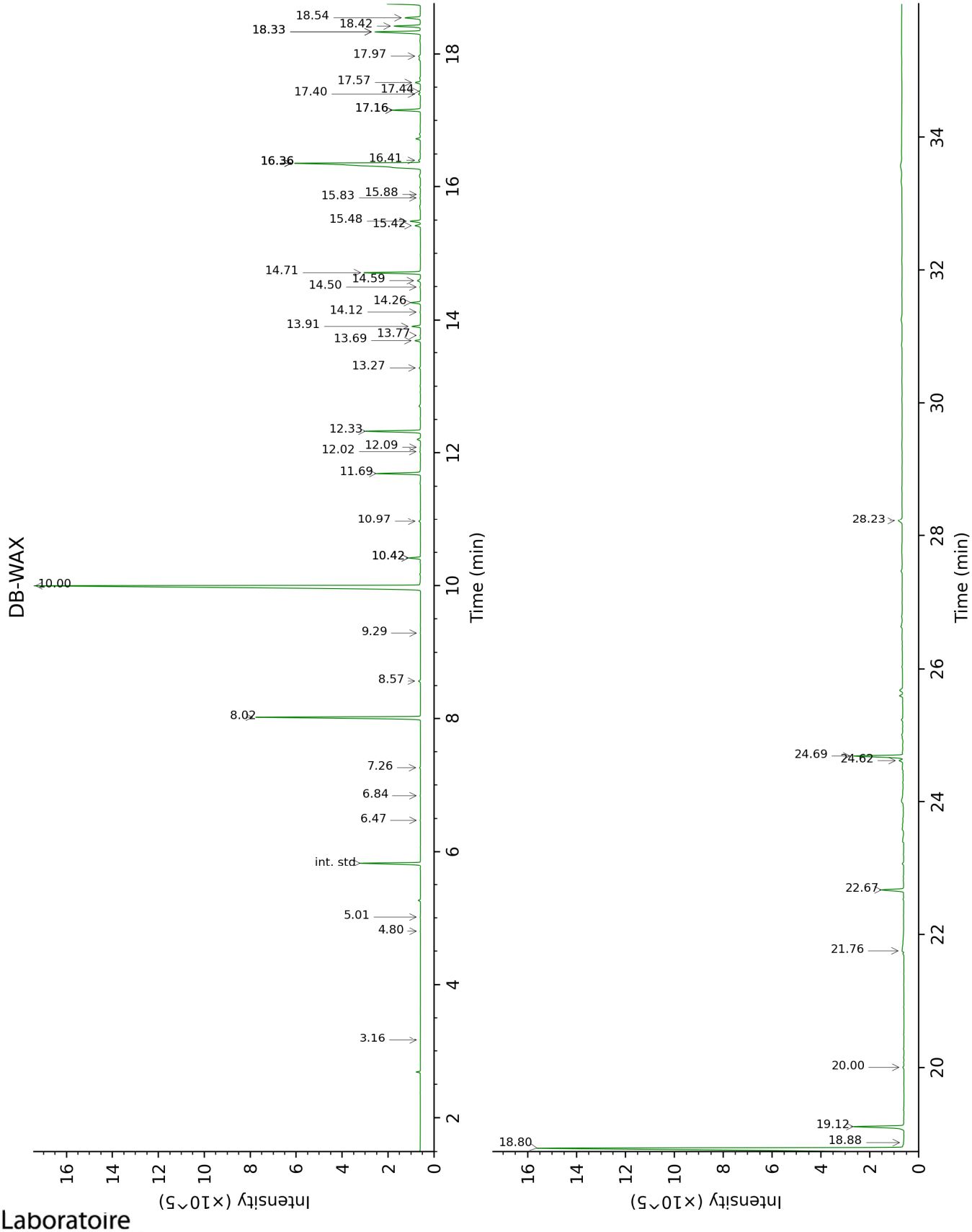
23.68
22.30
21.75
20.21
19.27
18.75


DB-WAX
Intensity (×10^5)
Time (min)
18.54
18.42
18.33
17.97
17.57
17.40
17.44
17.16
16.36
16.41
15.83
15.88
15.48
15.42
14.71
14.59
14.50
14.26
14.12
13.91
13.69
13.77
13.27
12.33
12.02
12.09
11.69
10.97
10.42
10.00
9.29
8.57
8.02
7.26
6.84
6.47
int. std
5.01
4.80
3.16
28.23
24.69
24.62
22.67
21.76
20.00
19.12
18.88
18.80

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Benzaldehyde	3.28	956	0.30	7.26	1461	0.33
6-Methyl-5-hepten-2-one	3.77	990	0.11	5.02	1297	0.12
(3*Z*)-Hexenyl acetate	4.10	1012	0.12	4.80	1281	0.11
Limonene	4.36	1028	0.07	3.16	1159	0.03
Benzyl alcohol	4.52	1038	14.92	11.69	1820	15.82
cis-Linalool oxide (fur.)	5.06	1072	0.15	6.47	1402	0.15
trans-Linalool oxide (fur.)	5.31	1088	0.24	6.84	1430	0.20
para-Cresol	5.37*	1092	3.79	13.91	2021	3.13
Methyl benzoate	5.37*	1092	[4.50]	8.57	1562	0.90
Linalool	5.58	1106	63.68	8.02	1519	65.29
Phenylethyl alcohol	5.70	1113	0.19	12.02	1849	0.26
Benzeneacetonitrile	6.05	1136	0.12	12.09	1854	0.11
para-Vinylanisole	6.27	1150	0.12	9.29	1618	0.10
Benzyl acetate	6.57	1169	244.13	10.00	1676	250.83
Methyl salicylate	6.90	1190	0.47	10.42*	1710	5.79
Phenylethyl acetate	7.88	1256	0.64	10.97	1758	0.70
Indole	8.42	1292	10.14	17.16*	2349	10.41
Eugenol	9.35	1357	22.79	14.71	2098	22.90
8-Hydroxylinalool isomer	9.47	1366	0.56	16.36*	2265	108.81
Unknown [m/z 95, 67 (82), 41 (50), 166 (33), 66 (31), 94 (30)]	9.68	1381	0.06			
(*Z*)-Jasmone	9.90	1396	21.81	12.33	1876	21.96
(*E*)-Isoeugenol	10.58	1447	0.65	16.41	2269	1.02
Unknown [m/z 43, 67 (65), 71 (56), 68 (34), 55 (33), 82 (30)...]	10.96	1475	0.13			
(*Z*)-Jasmin lactone	11.11	1487	2.27	15.42	2168	2.66
Benzyl tiglate	11.18	1492	0.40	14.12	2041	0.24
(3*E*,6*E*)-α-Farnesene	11.43	1510	3.54	10.42*	1710	[3.63]
(*E*)-Nerolidol	12.12	1565	1.92	13.69	2000	1.93
Unknown [m/z 99, 71 (39), 145 (22), 55 (21), 41 (18)...]	12.15*	1568	4.37	15.83	2210	0.28
(3*Z*)-Hexenyl benzoate	12.15*	1568	[3.92]	14.26	2055	3.76
Hexyl benzoate	12.25*	1575	0.43	13.77	2008	0.18
(2*E*)-Hexenyl benzoate	12.25*	1575	[0.43]	14.50	2077	0.21
Methyl N-acetylanthranilate	12.45	1591	0.98	17.40	2375	1.04
Methyl *cis*-jasmonate	13.12	1646	8.46	16.36*	2265	[115.34]
Unknown [m/z 150, 135 (67), 91 (32), 79 (23), 105 (21), 133 (18)]	13.27	1658	0.22			
Methyl *trans*-jasmonate	13.47	1675	0.56	17.16*	2349	[13.55]
Jasmine ketolactone	13.91*	1712	1.46			
Pentadecanal	13.91*	1712	[1.05]	13.27	1962	0.55

(*E*)-Coniferyl alcohol	14.12	1729	0.26			
Benzyl benzoate	14.51	1764	202.85	18.80	2532	209.58
Phytadiene analog?	15.27	1831	0.06			
Neophytadiene	15.40	1843	0.72			
Phytone	15.45	1847	1.08	14.59	2086	1.32
Phytadiene isomer I	15.48	1851	1.10			
Benzyl salicylate	15.56	1858	0.54	20.00	2673	0.64
Phytadiene isomer II	15.86	1885	0.49			
Methyl palmitate	16.34	1930	4.16	15.48	2175	4.03
Isophytol	16.60	1955	75.77	16.36*	2265	[84.59]
Palmitic acid	16.78	1972	4.45	21.76	2892	4.29
(3*E*,6*E*,10*E*)-α-Springene	16.93	1986	0.16			
Ethyl palmitate	17.06	1998	0.16	15.88	2216	0.15
(*E*,*E*)-Geranyllinalool	17.36	2028	9.27	18.42	2488	9.57
Unknown [m/z 91, 57 (27), 71 (20), 43 (17), 109 (17)...]	17.85	2077	0.12			
Methyl linoleate	18.02	2094	0.72	17.97	2438	1.07
Methyl α-linolenate	18.08*	2100	8.34	18.54	2502	6.51
Methyl oleate	18.08*	2100	[8.17]	17.57	2394	2.07
Phytol	18.23	2116	17.37	19.12	2569	19.34
Methyl stearate	18.38	2131	0.96	17.44	2379	0.44
α-Linolenic acid	18.56	2149	1.25			
Ethyl linoleate	18.61	2155	1.10	18.33*	2478	20.17
Ethyl α-linolenate	18.67	2161	0.59	18.88	2541	0.62
Methyl (*E*)-phytenate	18.76	2170	1.98			
(*E*)-Phytyl acetate	19.27	2224	19.29	18.33*	2478	[19.67]
4,8,12,16-Tetramethylheptadecan-4-olide?	20.21	2327	0.14			
2-Monopalmitin	21.75	2504	0.21			
Benzyl palmitate	22.30	2571	0.82			
Benzyl oleate	23.68	2744	0.19			
Benzyl α-linolenate	23.74	2752	1.33			
Squalene isomer I	23.78	2757	0.09			
Benzyl stearate	23.86	2768	0.32			
(*E*)-Phytyl benzoate?	24.21	2814	1.56	24.62	3283	1.89
Squalene	24.30	2825	8.00	22.67	3012	8.06
2,3-Oxidosqualene	25.16	2942	18.16	24.69	3294	19.85
2,3-Dihydro-3-oxosqualene?	25.28	2958	0.65			
Benzyl arachidate	25.41	2976	0.71			
2,6,10,15,19,23-Hexamethyl-(6*E*,10*E*,14*E*,18*E*)-1,6,10,14,18,22-tetracosahexaen-3-ol	25.65	3009	0.97			
Unknown [m/z 41, 119 (14), 147 (13), 40 912), 94 (12), 133 (12)...]	25.88	3042	0.59			
α-Tocopherol	26.45	3118	0.34			

Unknown [m/z 109, 95 (52), 69 (51), 57 (47), 97 (45)... 278 (9)...]	26.62	3139	0.14			
β-Amyrin	28.36	3312	0.40			
(*E*)-Phytyl palmitate	32.13	3544	0.53			
Jasminum grandiflorum marker I	32.30	3552	1.85	28.23	3748	1.83

*: Two or more compounds are coeluting on this column
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

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