Date : November 18, 2020

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 20J23-INT02
Customer identification : Violetas Francesas
Type : Aqueous fragrance
Source : Fragrant extract(s) and isolate(s)
Customer : Interne

Analysis

Method: Addition of salt and extraction with dichloromethane 3 times. Addition of an internal standard to estimate concentrations of individual compounds[1]. Concentration of the organic phase. Analysis with PC-MAT-009 - Analysis of the composition of an hydrosol by GC-FID.
Analyst : Alexis St-Gelais, M. Sc., chimiste
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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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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Conclusion

This sample features mostly isolates and/or synthetic single ingredients, ionone derivatives in particular. Despite the presence of linalool and terpinen-4-ol, the absence of sesquiterpenes and some other key monoterpenols, like lavandulol, do not suggest that either lavender or tea tree oils are present, or in no more than negligible amounts.

Analysis summary

Identification	(mg/L)	% of total volatiles	Classe
para-Methylanisole	22.6	0.13	Simple phenolic
Benzyl alcohol	158.0	0.92	Simple phenolic
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer II	850.5	4.96	Synthetic
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	500.2	2.91	Synthetic
Dipropylene glycol II	968.0	5.64	Synthetic
Dipropylene glycol III	778.9	4.54	Synthetic
Linalool	39.4	0.23	Monoterpenic alcohol
Dipropylene glycol IV, stereoisomer II	372.3	2.17	Synthetic
Phenylethyl alcohol	1087.5	6.34	Simple phenolic
Benzyl acetate	1377.5	8.03	Phenolic ester
Dihydrocitronellol	73.2	0.43	Synthetic
Methyl 2-octynoate	87.1	0.51	Synthetic
Citronellol	629.0	3.66	Monoterpenic alcohol
para-Anisaldehyde	745.8	4.35	Simple phenolic
Phenylethyl acetate	148.1	0.86	Phenolic ester
Ethyl salicylate	5.8	0.03	Phenolic ester
Ethyl 2-octynoate	36.6	0.21	Synthetic
Hydroxycitronellal	301.6	1.76	Synthetic
Heliotropin	387.4	2.26	Simple phenolic
Geranyl acetate	7.9	0.05	Monoterpenic ester
α-Gurjunene	4.0	0.02	Sesquiterpene
Ethylvanillin	115.2	0.67	Synthetic
(*E*)-α-Isomethyl-ionone	4608.1	26.85	Ionone or analog
β-Isomethylionone	283.9	1.65	Synthetic
Unknown	50.8	0.30	Unknown
α-Methyl-ionone	1335.5	7.78	Ionone or analog
Unknown	70.2	0.41	Unknown
γ-Methyl-ionone?	46.6	0.27	Ionone or analog
Hydroxycitronellal diethyl acetal	11.6	0.07	Aliphatic acetal
Unknown	20.2	0.12	Unknown
Heliotropin diethyl acetal	10.4	0.06	Synthetic
β-Methyl-ionone	483.6	2.82	Ionone or analog
Diethyl phthalate	94.2	0.55	Synthetic
Galaxolide impurity I	1.6	0.01	Synthetic
Benzyl benzoate	130.8	0.76	Phenolic ester
Galaxolide analog 1	11.9	0.07	Synthetic

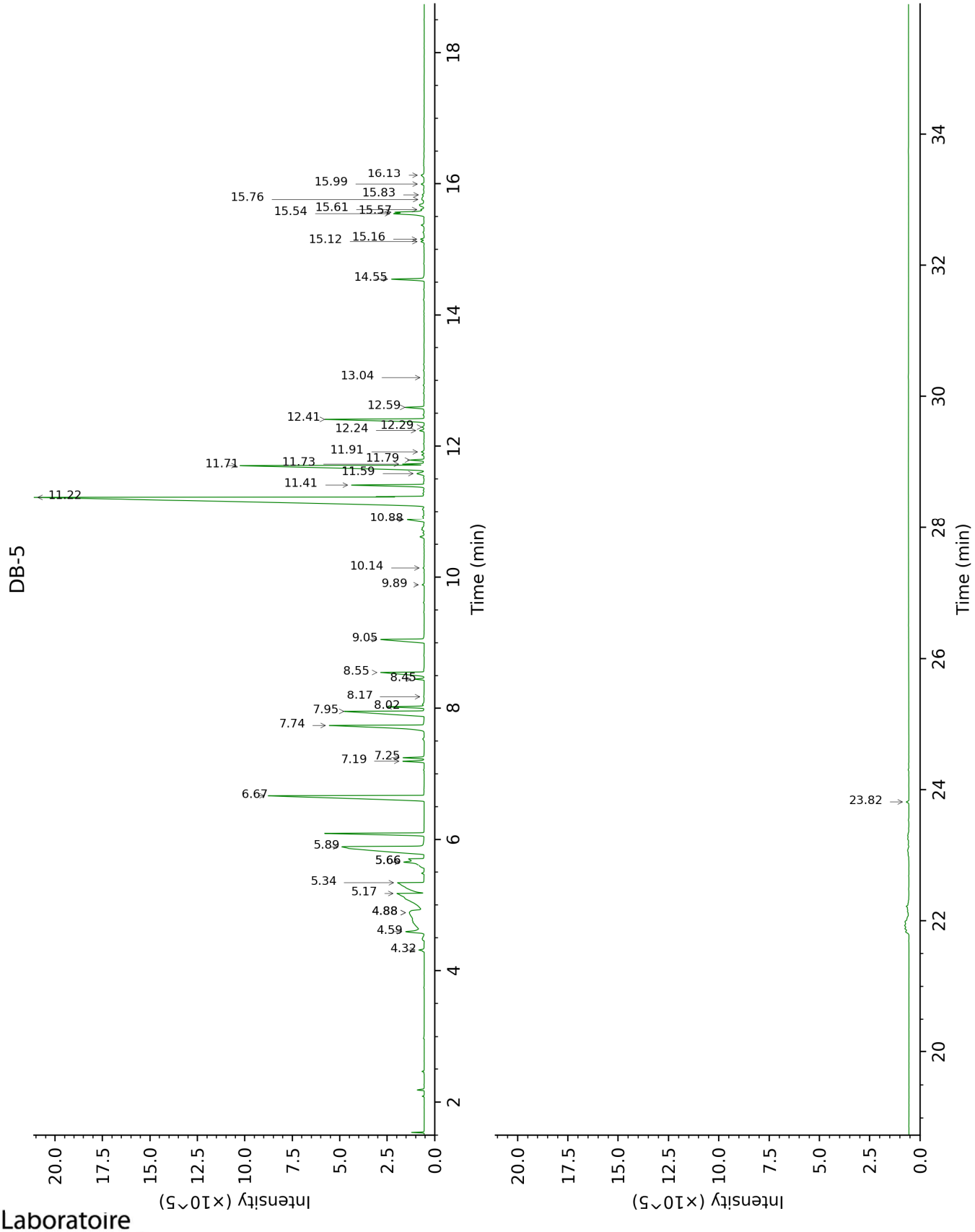
Galaxolide analog 2	11.8	0.07	Synthetic
Galaxolide isomer I	92.3	0.54	Synthetic
Galaxolide isomer II	84.3	0.49	Synthetic
Galaxolide analog 3	11.5	0.07	Synthetic
Galaxolide isomer III	8.0	0.05	Synthetic
Galaxolide isomer IV	6.9	0.04	Synthetic
Galaxolide isomer V	10.4	0.06	Synthetic
Galaxolide isomer VI	14.5	0.08	Synthetic
Dioctyl terephthalate	11.5	0.07	Synthetic
Dipropylene glycol IV, stereoisomer I	299.3	1.74	Synthetic
Consolidated total	**16406.2 mg/L**	**95.59%**	

tr: < 0.05 mg/L

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)
16.13
15.99
15.83
15.76
15.61
15.57
15.54
15.16
15.12
14.55
13.04
12.59
12.41
12.29
12.24
11.91
11.79
11.73
11.71
11.59
11.41
11.22
10.88
10.14
9.89
9.05
8.55
8.45
8.17
8.02
7.95
7.74
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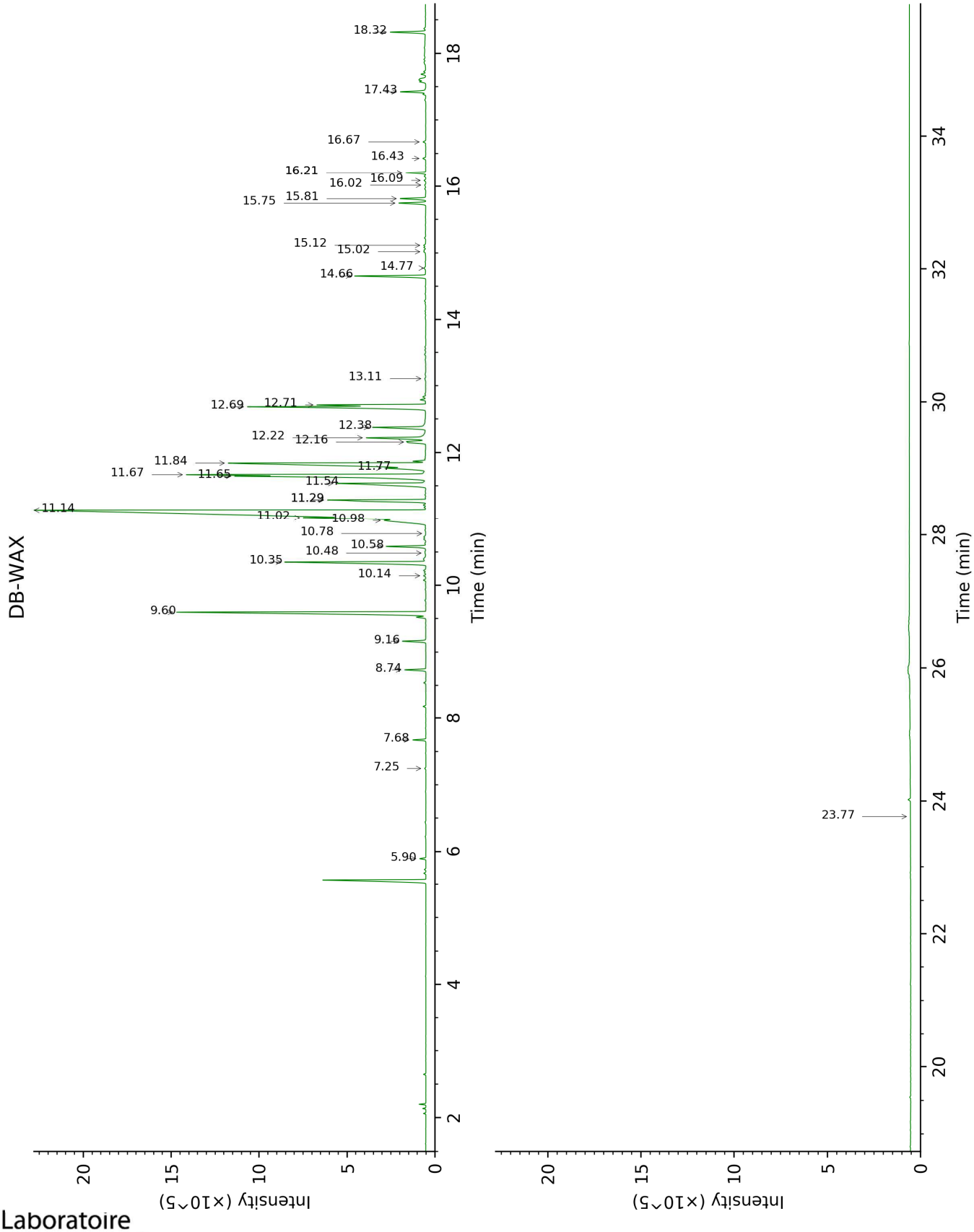
5.34
5.17
4.88
4.59
4.32
23.82



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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/L	R.T	R.I	mg/L
para-Methylanisole	4.32	1018	22.6	5.90	1383	17.8
Benzyl alcohol	4.60†	1035	710.9	11.29*	1814	448.3
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer II	4.88*†	1054	[1151.6]	11.02	1790	850.5
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	4.88*†	1054	[1151.6]	10.98	1786	500.2
Dipropylene glycol II	5.18	1072	968.0	11.54	1836	780.6
Dipropylene glycol III	5.34	1082	778.9	11.65†	1846	2591.2
Linalool	5.66*†	1103	270.3	7.68	1516	39.4
Dipropylene glycol IV, stereoisomer II	5.66*†	1103	[432.9]	12.38	1912	372.3
Phenylethyl alcohol	5.89	1118	1087.5	11.67†	1848	[1559.6]
Benzyl acetate	6.67	1168	1377.5	9.60	1670	1380.7
Dihydrocitronellol	7.19	1202	73.2	9.16	1634	76.5
Methyl 2-octynoate	7.25	1206	87.1	8.74	1599	85.1
Citronellol	7.74	1239	629.0	10.35	1733	623.4
para-Anisaldehyde	7.95	1254	745.8	12.69†	1941	1332.0
Phenylethyl acetate	8.02	1259	148.1	10.58	1753	155.7
Ethyl salicylate	8.17	1269	5.8	10.48	1744	4.1
Ethyl 2-octynoate	8.45	1288	36.6			
Hydroxycitronellal	8.55	1295	301.6	12.22	1898	297.7
Heliotropin	9.06	1327	387.4	14.66	2134	397.4
Geranyl acetate	9.89	1386	7.9	10.14	1715	8.9
α-Gurjunene	10.14	1404	4.0	7.25	1484	3.7
Ethylvanillin	10.88	1459	115.2	17.42	2432	121.8
(*E*)-α-Isomethyl-ionone	11.22	1484	4608.1	11.14	1800	4274.7
β-Isomethylionone	11.41	1498	283.9	11.29*	1814	[438.5]
Unknown [m/z 57, 149 (36), 93 (30), 107 (24), 135 (22), 191 (21), 109 (18), 91 (18)... 206? (4)]	11.59	1512	50.8			

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α-Methyl-ionone	11.71	1522	1335.5	11.84	1864	1310.5
Unknown [m/z 57, 107 (15), 134 (15), 106 (14), 93 (13)... 206 (3)]	11.73	1523	70.2			
γ-Methyl-ionone?	11.79	1528	46.6	12.16	1892	58.8
Hydroxycitronellal diethyl acetal	11.92	1538	11.6	13.11	1981	5.4
Unknown [m/z 109, 67 (49), 108 (43), 107 (36), 43 (30), 98 (26), 93 (24), 123 (19)... 206 (9)]	12.24	1563	20.2			
Heliotropin diethyl acetal	12.29	1568	10.4	14.77	2146	12.8
β-Methyl-ionone	12.41	1577	483.6	12.71†	1944	[1096.5]
Diethyl phthalate	12.59	1591	94.2	16.21*	2296	93.8
Galaxolide impurity I	13.04	1628	1.6	10.78	1769	0.7
Benzyl benzoate	14.55	1755	130.8	18.32	2536	124.7
Galaxolide analog 1	15.12	1805	11.9	15.02	2171	8.5
Galaxolide analog 2	15.16	1808	11.8	15.12	2181	7.1
Galaxolide isomer I	15.54†	1844	225.1	15.75	2247	92.3
Galaxolide isomer II	15.57†	1846	[225.1]	15.82	2254	84.3
Galaxolide analog 3	15.61	1849	11.5	16.02	2276	4.5
Galaxolide isomer III	15.76	1863	8.0	16.09	2284	5.4
Galaxolide isomer IV	15.83	1870	6.9	16.21*	2296	[63.5]
Galaxolide isomer V	15.99	1885	10.4	16.43	2320	10.2
Galaxolide isomer VI	16.13	1897	14.5	16.67	2348	9.6
Dioctyl terephthalate	23.82	2743	11.5	23.77	3266	0.5
Dipropylene glycol IV, stereoisomer I				11.77	1857	299.3

*: 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
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

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