Date : January 09, 2021

Certificate of Analysis – GC Profiling

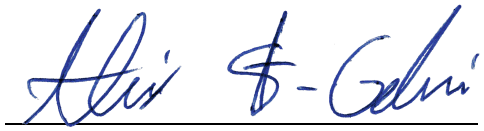
Sample identification

Internal code : 20L16-INT01
Customer identification : Mi Tesoro Agua de Violetas - Shane Carper
Type : Aqueous fragrance
Source : Fragrant 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 : January 09, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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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Conclusion

This sample features mostly ionone derivatives and synthetic musks, along with some fragrant alcohols and heliotropin. There is no indication whatsoever of the presence of essential oils, and in particular lavender (no linalool, linalyl acetate, lavandulol, lavandulyl acetate, beta-farnesene or caryophyllene) and tea tree (no terpinene-4-ol, no terpinenes, no viridiflorene, no aromadendrene).

Analysis summary

Identification	(mg/L)	% of total volatiles	Classe
Limonene	0.7	0.01	Monoterpene
Benzyl alcohol	209.0	4.22	Simple phenolic
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	24.6	0.50	Synthetic
Dipropylene glycol II	19.0	0.38	Synthetic
Dipropylene glycol III	21.7	0.44	Synthetic
Dipropylene glycol IV, stereoisomer I	6.5	0.13	Synthetic
Phenylethyl alcohol	236.9	4.79	Simple phenolic
Benzyl acetate	338.0	6.83	Phenolic ester
Dihydrocitronellol	2.9	0.06	Synthetic
cis-Florol	21.7	0.44	Synthetic
trans-Florol	47.9	0.97	Synthetic
Citronellol	227.9	4.61	Monoterpenic alcohol
Phenylethyl acetate	30.8	0.62	Phenolic ester
Geraniol	1.7	0.03	Monoterpenic alcohol
Ethyl 2-octynoate	1.7	0.03	Synthetic
Methyl 2-nonynoate	0.9	0.02	Synthetic
Heliotropin	167.4	3.38	Simple phenolic
Eugenol	6.1	0.12	Phenylpropanoid
Ethyl 2-nonynoate	11.5	0.23	Synthetic
Vanillin	0.5	0.01	Simple phenolic
Unknown	7.7	0.15	Unknown
Unknown	20.5	0.41	Unknown
(*E*)-α-Ionone	900.6	18.20	Ionone or analog
Unknown	58.0	1.17	Unknown
Unknown	25.2	0.51	Ionone or analog
Unknown	9.2	0.19	Unknown
Unknown	4.0	0.08	Unknown
(*E*)-α-Isomethyl-ionone	521.1	10.53	Ionone or analog
Unknown	9.1	0.18	Unknown
(*E*)-β-Ionone	448.3	9.06	Ionone or analog
Unknown	15.3	0.31	Unknown
β-Isomethylionone	34.0	0.69	Synthetic
Butylated hydroxytoluene (BHT)	9.4	0.19	Synthetic
α-Methyl-ionone	158.5	3.20	Ionone or analog
Unknown	16.9	0.34	Unknown
Nerolin bromelia	8.2	0.17	Synthetic
γ-Methyl-ionone?	5.2	0.11	Ionone or analog

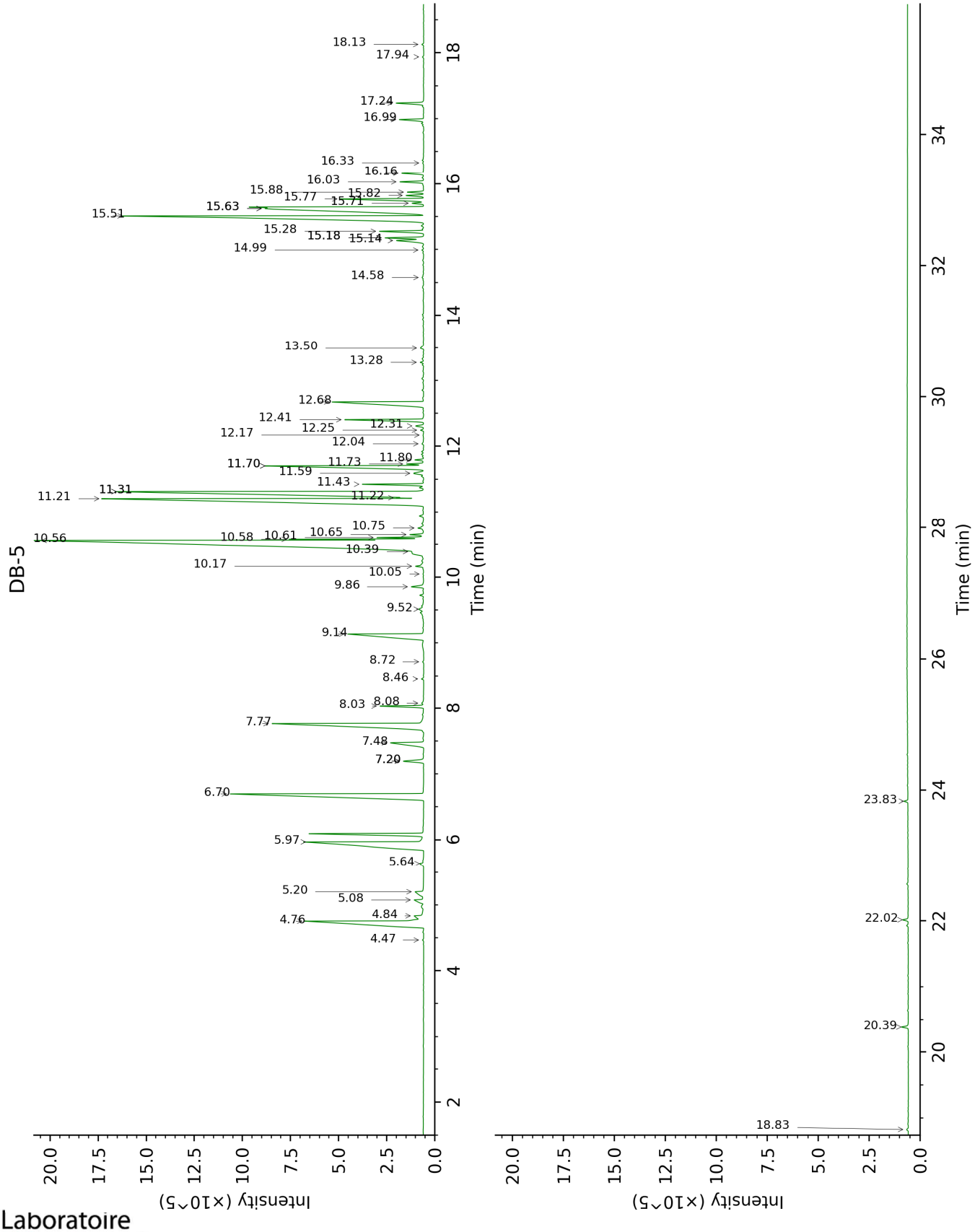
α-Elemol	1.4	0.03	Sesquiterpenic alcohol
Helional	0.6	0.01	Synthetic
Unknown	2.3	0.05	Unknown
Heliotropin diethyl acetal	8.1	0.16	Synthetic
β-Methyl-ionone	56.6	1.14	Ionone or analog
Diethyl phthalate	157.1	3.17	Synthetic
α-Eudesmol	2.1	0.04	Sesquiterpenic alcohol
3-Oxo-β-ionone?	2.3	0.05	Ionone or analog
Benzyl benzoate	1.2	0.02	Phenolic ester
Exaltone	1.0	0.02	Synthetic
Galaxolide analog 1	22.8	0.46	Synthetic
(13*E*)-Musk decenone	2.3	0.05	Synthetic
Galaxolide analog 2	20.6	0.42	Synthetic
Exaltolide	31.7	0.64	Aliphatic lactone
Isopropyl myristate	410.1	8.29	Synthetic
Galaxolide isomer I	161.3	3.26	Synthetic
Galaxolide isomer II	151.0	3.05	Synthetic
Galaxolide analog 3	6.5	0.13	Synthetic
Tonalide	58.3	1.18	Synthetic
Galaxolide isomer III	10.3	0.21	Synthetic
Galaxolide isomer IV	9.0	0.18	Synthetic
Galaxolide isomer V	13.4	0.27	Synthetic
Galaxolide isomer VI	12.2	0.25	Synthetic
Hexadecanolide	0.8	0.02	Aliphatic lactone
Musk ketone	25.4	0.51	Synthetic
Ethylene brassylate	24.6	0.50	Synthetic
Unknown	1.0	0.02	Unknown
Diethyl tridecanedioate?	1.4	0.03	Aliphatic ester
Unknown	1.7	0.03	Unknown
Unknown	5.7	0.12	Unknown
Unknown	4.7	0.10	Unknown
Dioctyl terephthalate	2.6	0.05	Synthetic
Consolidated total	**4838.4 mg/L**	**97.79%**	

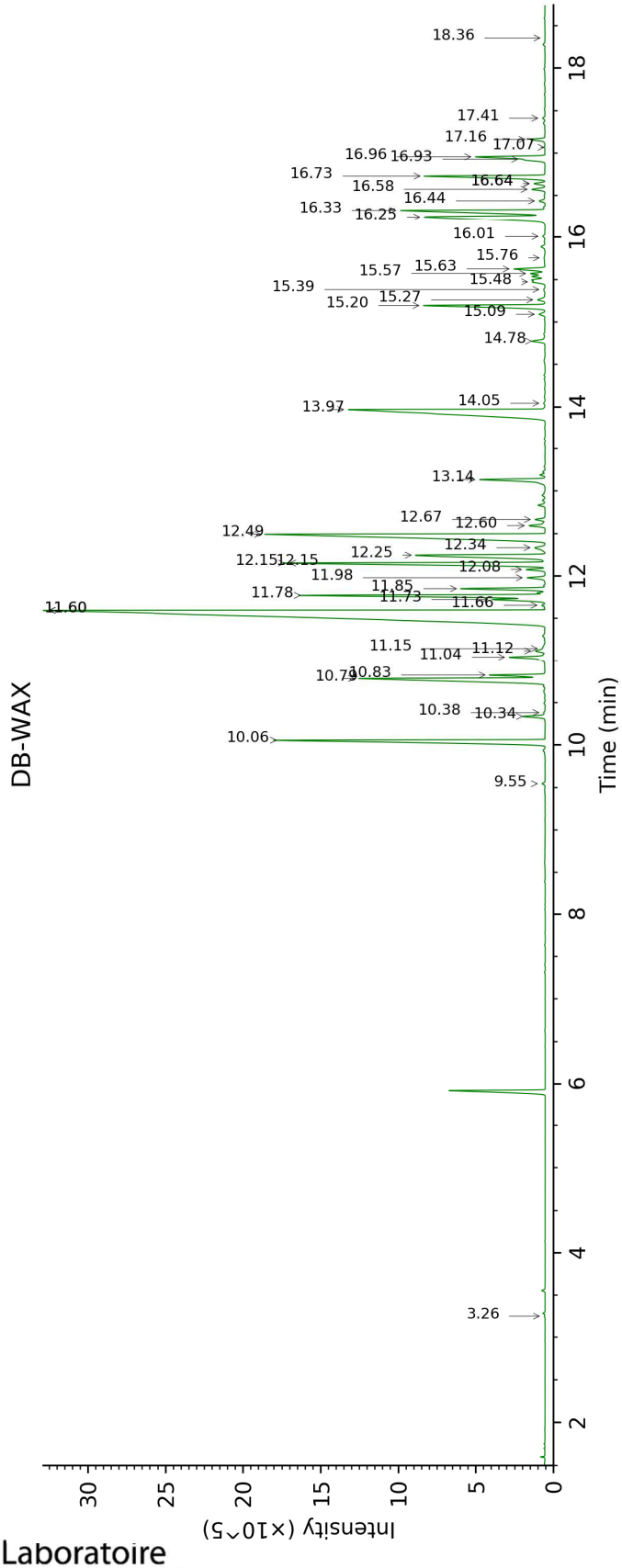
tr: < 0.05 mg/L

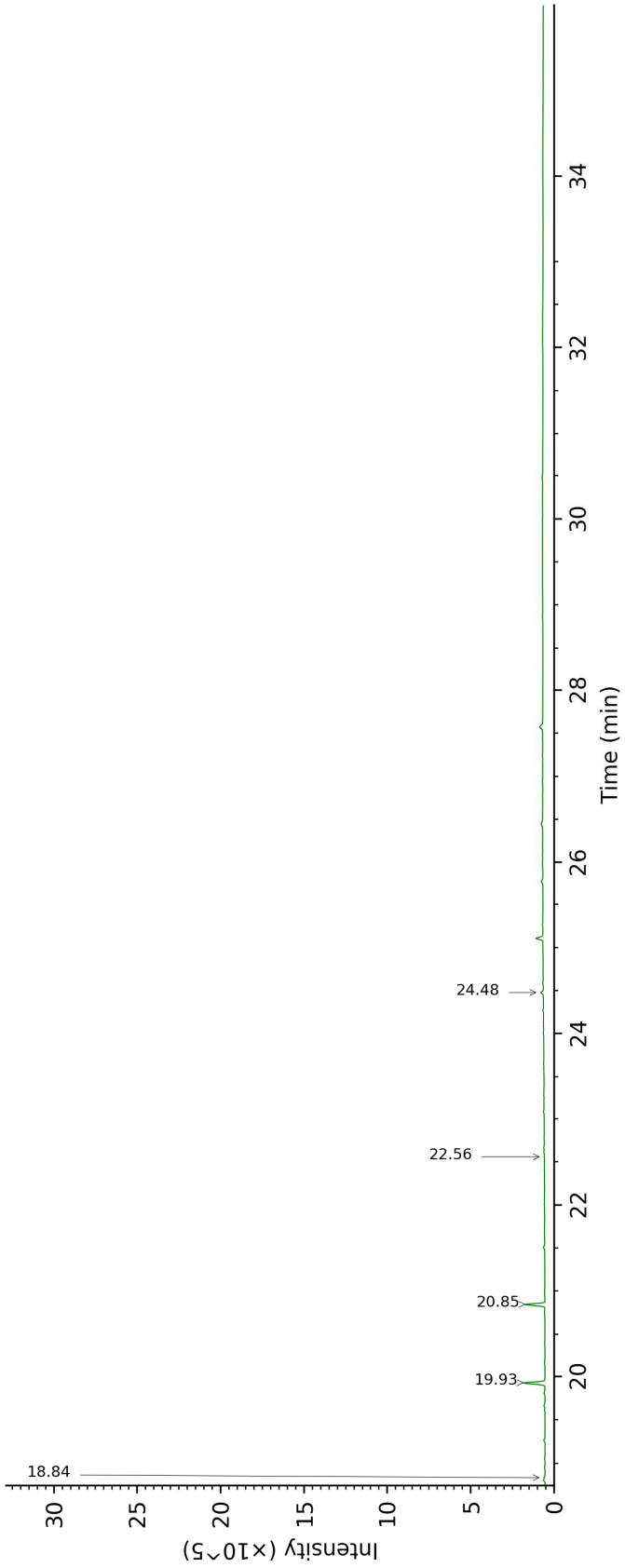
Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).
Unknown compounds are expressed in equivalents of internal standard without correction.

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)
18.13
17.94
17.24
16.99
16.33
16.16
16.03
15.88
15.82
15.77
15.71
15.63
15.51
15.28
15.18
15.14
14.99
14.58
13.50
13.28
12.68
12.41
12.25
12.31
12.17
12.04
11.70
11.73
11.80
11.59
11.43
11.31
11.21
11.22
10.75
10.65
10.61
10.58
10.56
10.39
10.17
10.05
9.86
9.52
9.14
8.72
8.46
8.08
8.03
7.77
7.48
7.20
6.70
5.97
5.64
5.20
5.08
4.84
4.76
4.47
23.83
22.02
20.39
18.83


DB-WAX
18.36
17.41
17.16
17.07
16.96
16.93
16.73
16.64
16.58
16.44
16.33
16.25
16.01
15.76
15.63
15.57
15.48
15.39
15.27
15.20
15.09
14.78
14.05
13.97
13.14
12.67
12.60
12.49
12.34
12.25
12.15
12.08
11.98
11.85
11.78
11.73
11.66
11.60
11.15
11.12
11.04
10.83
10.38
10.34
10.06
9.55
3.26
Time (min)
Intensity (×10^5)


24.48
22.56
20.85
19.93
18.84
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/L	R.T	R.I	mg/L
Limonene	4.47	1027	0.7	3.26	1164	0.6
Benzyl alcohol	4.76	1045	209.0	11.78	1820	212.0
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	4.84	1050	24.6			
Dipropylene glycol II	5.08	1066	19.0	11.98	1838	25.8
Dipropylene glycol III	5.20	1073	21.7	12.08	1847	24.1
Dipropylene glycol IV, stereoisomer I	5.64	1101	6.5	12.16*	1853	411.6
Phenylethyl alcohol	5.97	1122	236.9	12.16*	1853	[247.7]
Benzyl acetate	6.70	1169	338.0	10.06	1674	344.4
Dihydrocitronellol	7.20*	1201	18.7	9.55	1633	2.9
cis-Florol	7.20*	1201	[21.8]	10.34	1697	21.7
trans-Florol	7.48	1220	47.9	10.83	1738	48.1
Citronellol	7.77	1240	227.9	10.79	1735	238.6
Phenylethyl acetate	8.03	1258	30.8	11.04	1757	33.2
Geraniol	8.08	1261	1.7	11.66	1809	2.6
Ethyl 2-octynoate	8.46	1287	1.7			
Methyl 2-nonynoate	8.72	1300	0.9	10.38	1701	1.6
Heliotropin	9.14	1330	167.4	15.20	2140	174.6
Eugenol	9.52	1357	6.1	14.78	2098	14.9
Ethyl 2-nonynoate	9.86	1382	11.5	11.12	1763	12.4
Vanillin	10.05	1396	0.5	18.36	2475	0.3
Unknown [m/z 157, 142 (47), 172 (32), 141 (22), 158 (13), 115 (10)]	10.17	1404	7.7			
Unknown [m/z 43, 93 (41), 149 (34), 177 (29), 107 (28), 135 (27)...]	10.39	1421	20.5			
(*E*)-α-Ionone	10.56	1434	900.6	11.60*	1804	1448.4
Unknown [m/z 43, 82 (20), 107 (20), 93 (20), 81 (19), 106 (17)...]	10.58	1435	58.0	11.85	1827	76.0
Unknown [m/z 43, 149 (87), 121 (86), 109 (59), 81	10.60	1437	25.2			

(58), 41 (50)... 192 (12)]						
Unknown [m/z 108, 93 (77), 109 (55), 159 (50), 107 (45)...]	10.65	1440	9.2			
Unknown [m/z 95, 43 (53), 69 (48), 107 (41), 93 (30)...]	10.75	1448	4.0	11.15	1765	4.4
(*E*)-α-Isomethyl-ionone	11.21	1482	521.1	11.60*	1804	[1427.5]
Unknown [m/z 135, 43 (80), 163 (79), 123 (78), 177 (65), 107 (57)...]	11.22	1483	9.1			
(*E*)-β-Ionone	11.31*	1490	461.3	12.49	1883	448.3
Unknown [m/z 157, 172 (63), 142 (42), 141 (24), 156 (16), 158 (14)]	11.31*	1490	[541.2]			
β-Isomethylionone	11.43	1499	34.0	11.73	1815	44.8
Butylated hydroxytoluene (BHT)	11.59	1512	9.4	12.34	1869	12.6
α-Methyl-ionone	11.70*	1521	160.1	12.25	1861	158.5
Unknown [m/z 57, 107 (15), 134 (15), 106 (14), 93 (13)... 206 (3)]	11.70*	1521	[184.8]	12.60	1892	16.9
Nerolin bromelia	11.73	1523	8.2	15.09	2129	5.1
γ-Methyl-ionone?	11.80	1528	5.2	12.67	1899	8.7
α-Elemol	12.04	1547	1.4	14.05	2027	1.4
Helional	12.17	1558	0.6	17.07	2334	0.8
Unknown [m/z 109, 67 (49), 108 (43), 107 (36), 43 (30), 98 (26), 93 (24), 123 (19)... 206 (9)]	12.25	1564	2.3			
Heliotropin diethyl acetal	12.31	1569	8.1	15.26	2146	10.3
β-Methyl-ionone	12.41	1576	56.6	13.14	1942	61.5
Diethyl phthalate	12.68	1597	157.1	16.73	2297	156.5
α-Eudesmol	13.28	1647	2.1	15.39	2158	1.6
3-Oxo-β-ionone?	13.50	1665	2.3	17.41	2371	2.5
Benzyl benzoate	14.58	1757	1.2	18.84	2530	0.9
Exaltone	14.99	1793	1.0	15.76	2196	1.4
Galaxolide analog 1	15.14	1805	22.8	15.48	2167	19.7

(13*E*)-Musk decenone	15.18*	1809	25.5	16.01	2222	2.3
Galaxolide analog 2	15.18*	1809	[21.9]	15.57	2177	20.6
Exaltolide	15.28	1818	31.7	15.63	2183	29.8
Isopropyl myristate	15.51	1839	410.1	13.97	2020	407.0
Galaxolide isomer I	15.63*†	1849	314.8	16.25	2246	161.3
Galaxolide isomer II	15.63*†	1849	[314.8]	16.33	2255	151.0
Galaxolide analog 3	15.71	1857	6.5	16.44	2266	5.2
Tonalide	15.77	1862	58.3	16.96	2322	56.0
Galaxolide isomer III	15.82	1867	10.3	16.58	2281	10.7
Galaxolide isomer IV	15.88	1872	9.0	16.64*	2288	8.9
Galaxolide isomer V	16.03	1886	13.4	16.93	2318	14.7
Galaxolide isomer VI	16.16	1898	12.2	17.16	2344	12.7
Hexadecanolide	16.33	1913	0.8	16.64*	2288	[10.0]
Musk ketone	16.99	1975	25.4	20.85	2772	24.5
Ethylene brassylate	17.24	1999	24.6	19.93	2659	23.1
Unknown [m/z 291, 119 (40), 292 (23), 306 (17), 91 (16), 103 (7)...]	17.94	2067	1.0			
Diethyl tridecanedioate?	18.13	2086	1.4			
Unknown [m/z 257, 258 (19), 197 (10), 239 (8), 272 (8), 155 (6)...]	18.83	2157	1.7	22.56	2993	0.2
Unknown [m/z 98, 255 (85), 271 (83), 55 (55), 83 (45), 84 (41)...]	20.39	2320	5.7			
Unknown [m/z 176, 177 (14), 233 (7), 105 (3), 91 (3), 148 (2)...]	22.02	2502	4.7			
Dioctyl terephthalate	23.83	2718	2.6	24.48	3260	2.7

*: 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: < 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.

R.T.: Retention time (minutes)
R.I.: Retention index

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