Date : January 17, 2023

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 23A10-PTH01
Customer identification : Rose Absolute - Morocco - R30112R
Type : Absolute
Source : *Rosa centifolia*
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 : January 17, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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: Bright orange viscous liquid
Refractive index: 1.4953 ± 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
Hexanol	0.04	tr	Aliphatic alcohol
α-Pinene	0.20	0.02	Monoterpene
Benzaldehyde	0.11	0.01	Simple phenolic
β-Pinene	0.27	0.03	Monoterpene
Myrcene	0.41	0.04	Monoterpene
Limonene	0.24	0.02	Monoterpene
Benzyl alcohol	2.56	0.26	Simple phenolic
(*Z*)-β-Ocimene	0.25	0.03	Monoterpene
(*E*)-β-Ocimene	0.29	0.03	Monoterpene
cis-Sabinene hydrate	0.08	0.01	Monoterpenic alcohol
Linalool	0.32	0.03	Monoterpenic alcohol
cis-Rose oxide	1.59	0.16	Monoterpenic ether
Phenylethyl alcohol	555.99	55.60	Simple phenolic
Phenylethyl formate	0.29	0.03	Phenolic ester
Terpinen-4-ol	0.14	0.01	Monoterpenic alcohol
α-Terpineol	0.23	0.02	Monoterpenic alcohol
Nerol	1.66	0.17	Monoterpenic alcohol
Citronellol	137.31	13.73	Monoterpenic alcohol
Neral	1.39	0.14	Monoterpenic aldehyde
(*Z*)-Isogeraniol	0.69	0.07	Monoterpenic alcohol
Geraniol	75.48	7.55	Monoterpenic alcohol
Geranial	1.46	0.15	Monoterpenic aldehyde
Citronellyl formate	0.16	0.02	Monoterpenic ester
Eugenol	7.02	0.70	Phenylpropanoid
Geranic acid	1.16	0.12	Aliphatic acid
Geranyl acetate	0.38	0.04	Monoterpenic ester
Methyleugenol	1.73	0.17	Phenylpropanoid
β-Caryophyllene	1.90	0.19	Sesquiterpene
α-Guaiene	0.28	0.03	Sesquiterpene
α-Humulene	0.63	0.06	Sesquiterpene
Germacrene D	0.42	0.04	Sesquiterpene
Aciphyllene	0.15	0.02	Sesquiterpene
Pentadecane	0.20	0.02	Alkane
δ-Guaiene	0.17	0.02	Sesquiterpene
γ-Cadinene	0.19	0.02	Sesquiterpene
δ-Cadinene	0.03	tr	Sesquiterpene
α-Elemol	0.07	0.01	Sesquiterpenic alcohol
Hexadecane	0.09	0.01	Alkane
(8*Z*)-Heptadecene	0.10	0.01	Alkene
Heptadecane	0.87	0.09	Alkane
(2*E*,6*E*)-Farnesol	0.48	0.05	Sesquiterpenic alcohol
Benzyl benzoate	0.15	0.02	Phenolic ester
Octadecane	0.27	0.03	Alkane
Phenylethyl benzoate	0.36	0.04	Phenolic ester
(9*Z*)-Nonadecene	2.00	0.20	Alkene
Nonadecane	4.21	0.42	Alkane
Palmitic acid	4.03	0.40	Aliphatic acid
(9*Z*)-Eicosene	0.57	0.06	Alkene

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Eicosane	0.35	0.04	Alkane
(10*Z*)-Heneicosene	0.24	0.02	Alkene
Heneicosane	0.75	0.08	Alkane
Citronellyl caprate	0.18	0.02	Monoterpenic ester
Geranyl caprate	0.99	0.10	Monoterpenic ester
Phenylethyl undecanoate?	1.10	0.11	Phenolic ester
Stearic acid	16.94	1.69	Aliphatic acid
Docosane	0.13	0.01	Alkane
Tricosane	0.10	0.01	Alkane
Citronellyl laurate	0.21	0.02	Monoterpenic ester
Geranyl laurate	0.12	0.01	Monoterpenic ester
Tetradecyl octanoate	0.24	0.02	Aliphatic ester
Tetradecyl nonanoate	0.71	0.07	Aliphatic ester
Pentadecyl octanoate	0.21	0.02	Aliphatic ester
Phenylethyl myristate	0.46	0.05	Phenolic ester
Citronellyl myristate	0.17	0.02	Monoterpenic ester
Unknown	0.19	0.02	Phenolic ester
Unknown	0.36	0.04	Phenolic ester
Phenylethyl palmitoleate?	1.77	0.18	Phenolic ester
Heptacosane	0.23	0.02	Alkane
Citronellyl palmitate	0.69	0.07	Monoterpenic ester
Geranyl palmitate	0.29	0.03	Monoterpenic ester
Unknown	8.28	0.83	Oxygenated triterpene
(2*E*,6*Z*)-Farnesol	0.07	0.01	Sesquiterpenic alcohol
Consolidated total	**843.44 mg/g**	**84.34%**	

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.

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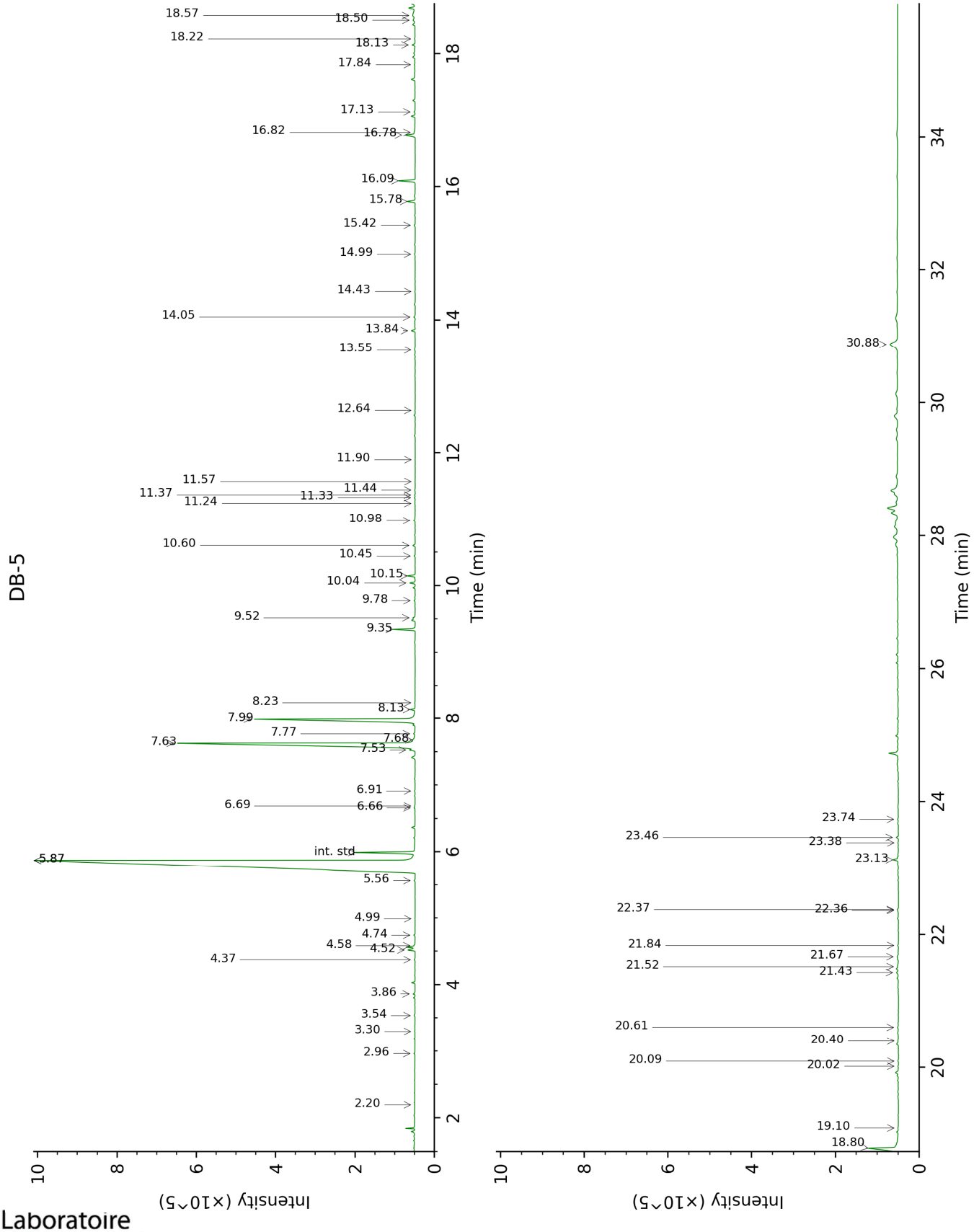
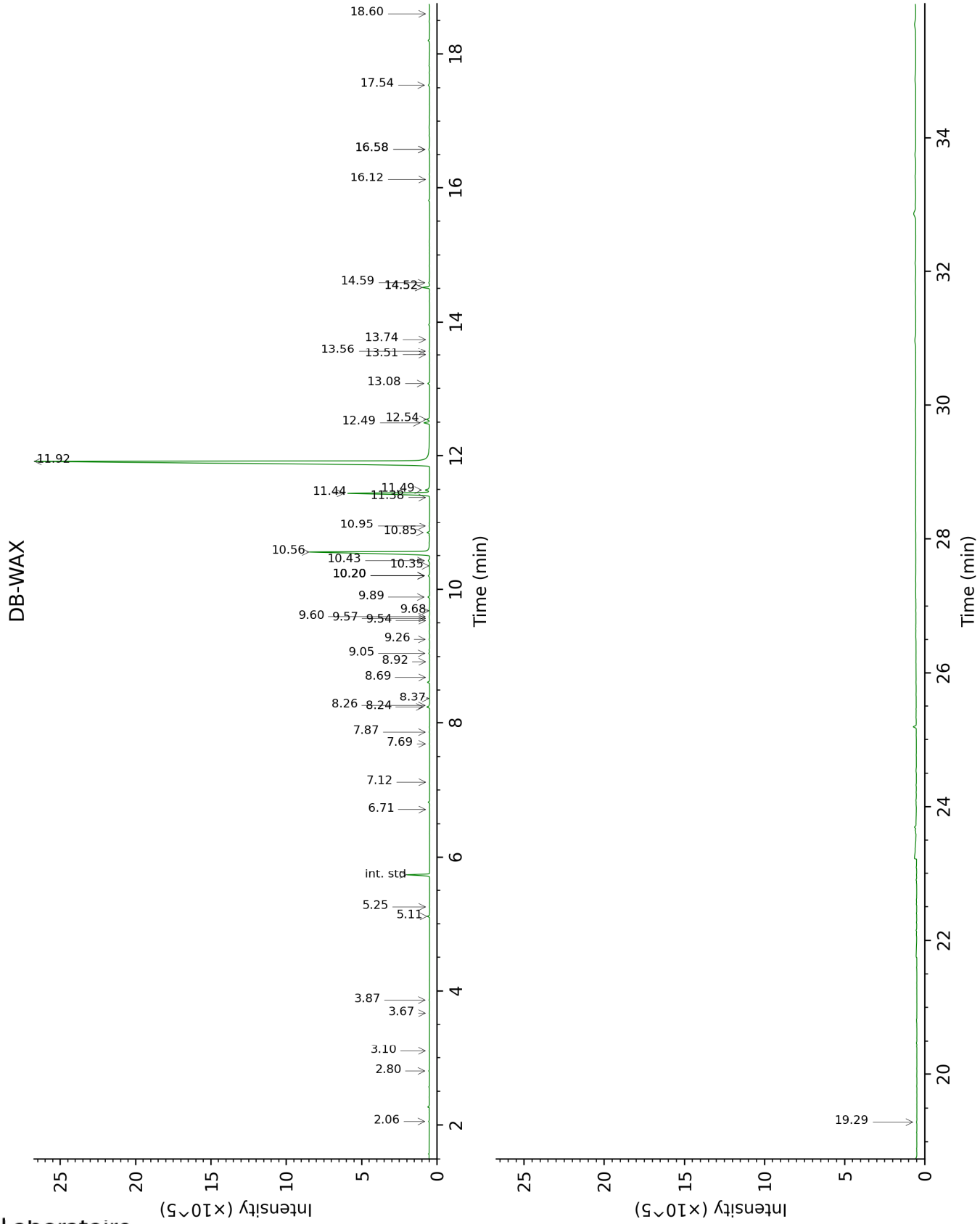

DB-5
18.57
18.50
18.22
18.13
17.84
17.13
16.82
16.78
16.09
15.78
15.42
14.99
14.43
14.05
13.84
13.55
12.64
11.90
11.57
11.44
11.37
11.33
11.24
10.98
10.60
10.45
10.15
10.04
9.78
9.52
9.35
8.23
8.13
7.99
7.77
7.68
7.63
7.53
6.91
6.69
6.66
int. std
5.87
5.56
4.99
4.74
4.58
4.52
4.37
3.86
3.54
3.30
2.96
2.20
30.88
23.74
23.46
23.38
23.13
22.37
22.36
21.84
21.67
21.52
21.43
20.61
20.40
20.09
20.02
19.10
18.80
Time (min)
Intensity (×10^5)


DB-WAX
Intensity (×10^5)
Time (min)
18.60
17.54
16.58
16.12
14.59
14.52
13.74
13.56
13.51
13.08
12.49
12.54
11.92
11.44
11.49
11.38
10.95
10.85
10.56
10.43
10.35
10.20
9.89
9.68
9.60
9.57
9.54
9.26
9.05
8.92
8.69
8.37
8.26
8.24
7.87
7.69
7.12
6.71
int. std
5.25
5.11
3.87
3.67
3.10
2.80
2.06
19.29

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Hexanol	2.20	874	0.04	5.25	1320	0.17
α-Pinene	2.96	933	0.20			
Benzaldehyde	3.30	956	0.11	7.12	1459	0.08
β-Pinene	3.54	972	0.27	2.06	1072	0.44
Myrcene	3.86	994	0.41	2.80	1138	0.43
Limonene	4.37	1027	0.24	3.10	1162	0.19
Benzyl alcohol	4.52	1036	2.56	11.49	1816	4.42
(*Z*)-β-Ocimene	4.58	1040	0.25	3.67	1208	0.18
(*E*)-β-Ocimene	4.74	1050	0.29	3.87	1223	0.35
cis-Sabinene hydrate	4.99	1066	0.08	6.71	1428	0.09
Linalool	5.56	1102	0.32	7.87	1516	0.35
cis-Rose oxide	5.87*	1122	539.51	5.11	1310	1.59
Phenylethyl alcohol	5.87*	1122	[520.03]	11.92	1854	555.99
Phenylethyl formate	6.66	1173	0.29	10.43	1724	1.77
Terpinen-4-ol	6.69	1175	0.14	8.37	1556	0.17
α-Terpineol	6.91	1189	0.23	9.57	1652	0.16
Nerol	7.53	1230	1.66	10.85	1760	2.26
Citronellol	7.63	1237	137.31	10.56	1735	141.99
Neral	7.68	1240	1.39	9.26	1627	0.54
(*Z*)-Isogeraniol	7.77	1246	0.69	10.95	1768	0.37
Geraniol	7.99	1261	75.48	11.44	1812	79.14
Geranial	8.13	1271	1.46	9.89	1679	1.47
Citronellyl formate	8.23	1278	0.16	8.69	1581	0.24
Eugenol	9.35	1355	7.02	14.52*	2098	6.41
Geranic acid	9.52	1367	1.16	16.58*	2310	1.17
Geranyl acetate	9.78	1385	0.38	10.35	1718	0.38
Methyleugenol	10.04	1404	1.73	13.08	1960	1.50
β-Caryophyllene	10.15	1412	1.90	8.24†	1546	2.34
α-Guaiene	10.44	1434	0.28	8.26†	1547	[2.34]
α-Humulene	10.60	1446	0.63	9.05	1610	0.60
Germacrene D	10.98	1474	0.42	9.60	1655	0.46
Aciphyllene	11.24	1494	0.15	9.54	1650	0.12
Pentadecane	11.33	1500	0.20	7.69	1502	0.17
δ-Guaiene	11.37	1503	0.17	9.68	1662	0.13
γ-Cadinene	11.44	1509	0.19	10.20*	1705	1.15
δ-Cadinene	11.57	1519	0.03	10.20*	1705	[1.15]
α-Elemol	11.90	1545	0.07	13.74	2023	0.08
Hexadecane	12.64	1603	0.09	8.92	1599	0.10
(8*Z*)-Heptadecene	13.55	1678	0.10	10.20*	1705	[1.11]
Heptadecane	13.84	1703	0.87	10.20*	1705	[1.10]
(2*E*,6*E*)-Farnesol	14.05	1721	0.48	16.58*	2310	[0.94]

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Benzyl benzoate	14.43	1754	0.15	18.60	2534	0.16
Octadecane	14.99	1803	0.27	11.38	1806	0.08
Phenylethyl benzoate	15.42	1842	0.36	19.29	2615	0.25
(9*Z*)-Nonadecene	15.78	1875	2.00	12.54	1910	2.21
Nonadecane	16.09	1903	4.21	12.49	1906	4.01
Palmitic acid	16.78	1969	4.03			
(9*Z*)-Eicosene	16.82	1973	0.57	13.56	2005	0.30
Eicosane	17.13	2002	0.35	13.51	2000	0.10
(10*Z*)-Heneicosene	17.84	2073	0.24	14.59	2105	0.68
Heneicosane	18.13	2102	0.75	14.52*	2098	[4.83]
Citronellyl caprate	18.22	2112	0.18			
Geranyl caprate	18.50	2141	0.99	17.54	2414	1.80
Phenylethyl undecanoate?	18.58	2148	1.10			
Stearic acid	18.80	2171	16.94			
Docosane	19.10	2202	0.13			
Tricosane	20.02	2302	0.10			
Citronellyl laurate	20.10	2310	0.21			
Geranyl laurate	20.40	2345	0.12			
Tetradecyl octanoate	20.61	2368	0.24			
Tetradecyl nonanoate	21.43	2463	0.71			
Pentadecyl octanoate	21.52	2473	0.21			
Phenylethyl myristate	21.67	2491	0.46			
Citronellyl myristate	21.84	2511	0.17			
Unknown [m/z 105, 79 (23), 104 (16), 67 (12), 95 (12), 106 (9)... 382 (1)]	22.36	2574	0.19			
Unknown [m/z 105, 104 (21), 67 (13), 81 (11), 106 (9)... 384 (1)]	22.37	2576	0.36			
Phenylethyl palmitoleate?	23.13	2670	1.77			
Heptacosane	23.38	2702	0.23			
Citronellyl palmitate	23.46	2712	0.69			

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Geranyl palmitate	23.74	2747	0.29			
Unknown [m/z 109, 69 (43), 95 (41), 43 (27), 205 (25)... 424 (11)...]	30.88	3477	8.28			
(2*E*,6*Z*)-Farnesol				16.12	2262	0.07

*: 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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