Date : April 28, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22D25-PTH03
Customer identification : Rose - R30111R
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 : Seydou Ka, Ph. D.
Analysis date : April 28, 2022

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 liquid
Refractive index: 1.4951 ± 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

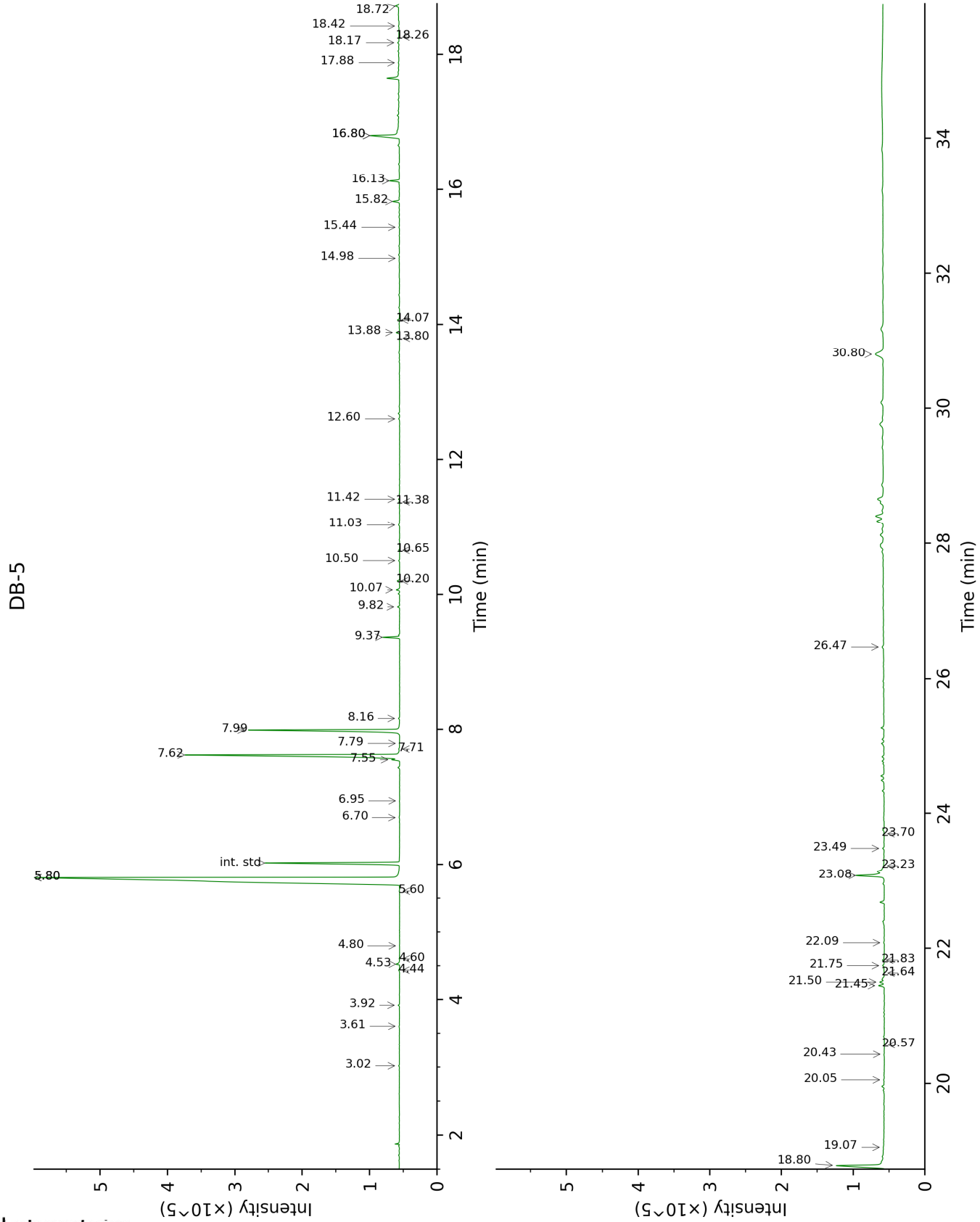
Identification	(mg/g)	% m/m	Classe
α-Pinene	0.14	0.01	Monoterpene
β-Pinene	0.11	0.01	Monoterpene
Myrcene	0.25	0.03	Monoterpene
Limonene	0.27	0.03	Monoterpene
Benzyl alcohol	1.03	0.10	Simple phenolic
(*Z*)-β-Ocimene	0.07	0.01	Monoterpene
(*E*)-β-Ocimene	0.03	0.00	Monoterpene
Linalool	0.12	0.01	Monoterpenic alcohol
cis-Rose oxide	0.08	0.01	Monoterpenic ether
Phenylethyl alcohol	306.76	30.68	Simple phenolic
Phenylethyl formate	0.18	0.02	Phenolic ester
α-Terpineol	0.06	0.01	Monoterpenic alcohol
Nerol	2.17	0.22	Monoterpenic alcohol
Citronellol	86.03	8.60	Monoterpenic alcohol
Neral	0.37	0.04	Monoterpenic aldehyde
(*Z*)-Isogeraniol	0.13	0.01	Monoterpenic alcohol
Geraniol	52.12	5.21	Monoterpenic alcohol
Geranial	0.28	0.03	Monoterpenic aldehyde
Eugenol	4.84	0.48	Phenylpropanoid
Geranyl acetate	0.62	0.06	Monoterpenic ester
Methyleugenol	1.09	0.11	Phenylpropanoid
β-Caryophyllene	0.65	0.07	Sesquiterpene
α-Guaiene	0.24	0.02	Sesquiterpene
α-Humulene	0.20	0.02	Sesquiterpene
Germacrene D	0.27	0.03	Sesquiterpene
Pentadecane	0.18	0.02	Alkane
γ-Cadinene	0.29	0.03	Sesquiterpene
Hexadecane	0.25	0.03	Alkane
(2*E*,6*Z*)-Farnesol	0.06	0.01	Sesquiterpenic alcohol
Heptadecane	0.82	0.08	Alkane
(2*E*,6*E*)-Farnesol	0.58	0.06	Sesquiterpenic alcohol
Octadecane	0.11	0.01	Alkane
Phenylethyl benzoate	0.17	0.02	Phenolic ester
(9*Z*)-Nonadecene	1.73	0.17	Alkene
Nonadecane	2.30	0.23	Alkane
(9*Z*)-Eicosene	0.17	0.02	Alkene
Palmitic acid	24.07	2.41	Aliphatic acid
(10*Z*)-Heneicosene	0.16	0.02	Alkene
Heneicosane	0.27	0.03	Alkane
Citronellyl caprate	0.07	0.01	Monoterpenic ester
Geranyl caprate	0.15	0.02	Monoterpenic ester
Ethyl oleate	0.91	0.09	Aliphatic ester
Docosene isomer	17.90	1.79	Alkene
Docosane	0.15	0.02	Alkane
Tricosane	0.18	0.02	Alkane
Geranyl laurate	0.13	0.01	Monoterpenic ester
Tetradecyl octanoate	0.08	0.01	Aliphatic ester
Tetradecyl nonanoate	1.87	0.19	Aliphatic ester

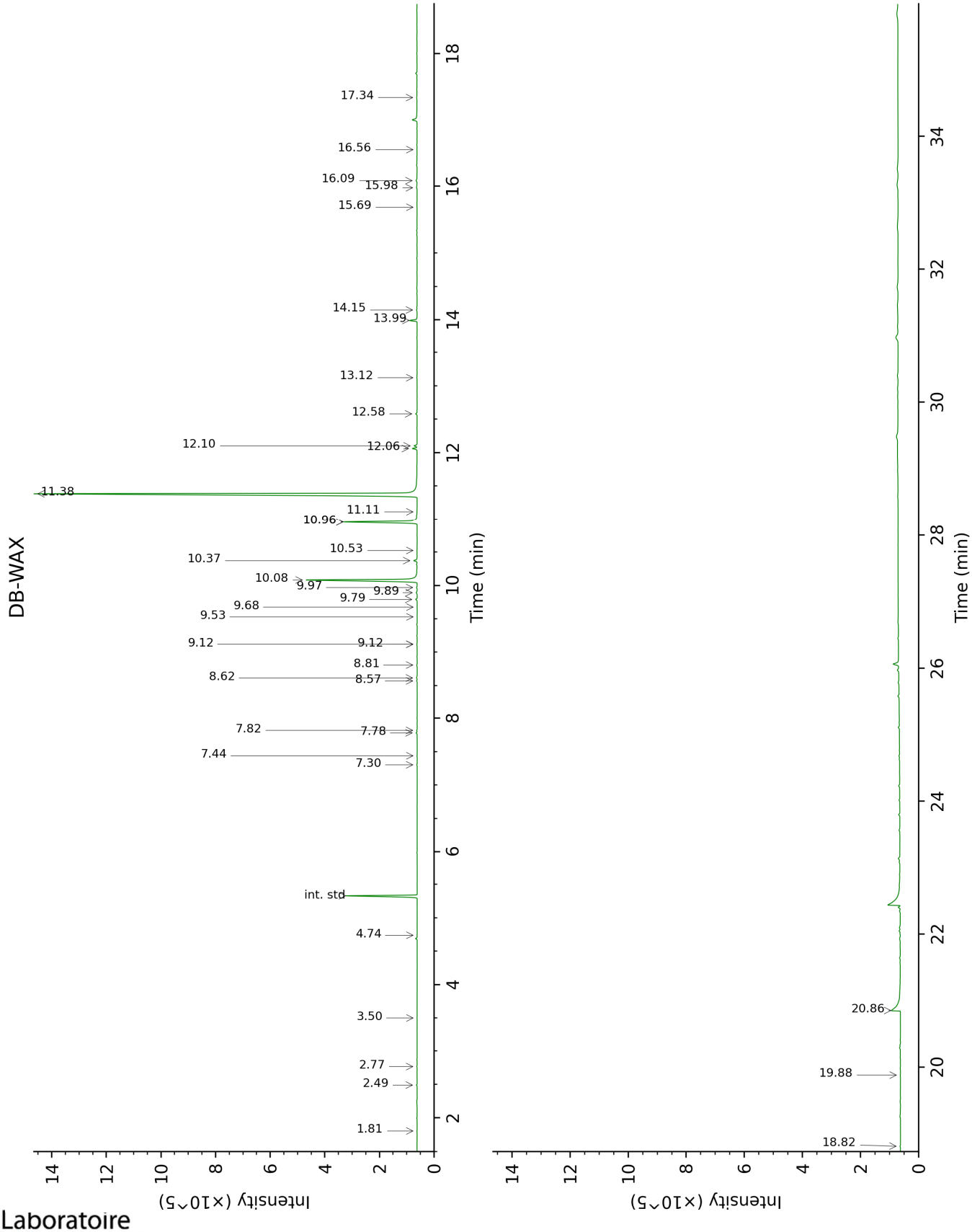
Pentadecyl octanoate	1.63	0.16	Aliphatic ester
Phenylethyl myristate	0.06	0.01	Phenolic ester
Pentacosane	0.39	0.04	Alkane
Citronellyl myristate	0.47	0.05	Monoterpenic ester
Geranyl myristate	0.18	0.02	Monoterpenic ester
Phenylethyl palmitoleate?	10.95	1.10	Phenolic ester
Phenylethyl palmitate	0.15	0.02	Phenolic ester
Citronellyl palmitate	0.51	0.05	Monoterpenic ester
Geranyl palmitate	0.15	0.02	Monoterpenic ester
α-Tocopherol	0.50	0.05	Tocopherol
Unknown	8.48	0.85	Oxygenated triterpene
Consolidated total	**534.16 mg/g**	**53.42%**	

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
18.72
18.42
18.17
18.26
17.88
16.80
16.13
15.82
15.44
14.98
14.07
13.88
13.80
12.60
11.42
11.38
11.03
10.65
10.50
10.20
10.07
9.82
9.37
8.16
7.99
7.79
7.71
7.62
7.55
6.95
6.70
int. std
5.80
5.60
4.80
4.60
4.53
4.44
3.92
3.61
3.02
Time (min)
Intensity (×10^5)
30.80
26.47
23.70
23.49
23.23
23.08
22.09
21.83
21.75
21.64
21.50
21.45
20.57
20.43
20.05
19.07
18.80
Time (min)
Intensity (×10^5)


DB-WAX
17.34
16.56
16.09
15.98
15.69
14.15
13.99
13.12
12.58
12.10
12.06
11.38
11.11
10.96
10.53
10.37
10.08
9.97
9.89
9.79
9.68
9.53
9.12
9.12
8.81
8.62
8.57
7.82
7.78
7.44
7.30
int. std
4.74
3.50
2.77
2.49
1.81
20.86
19.88
18.82
Intensity (×10^5)
Time (min)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
α-Pinene	3.02	932	0.14			
β-Pinene	3.61	973	0.11	1.81	1072	0.07
Myrcene	3.92	994	0.25	2.49	1136	0.27
Limonene	4.44	1027	0.27	2.77	1159	0.15
Benzyl alcohol	4.53	1033	1.03	11.11	1818	0.16
(*Z*)-β-Ocimene	4.60	1038	0.07			
(*E*)-β-Ocimene	4.80	1050	0.03	3.50	1218	0.04
Linalool	5.60	1102	0.12	7.44	1513	0.18
cis-Rose oxide	5.80*	1115	312.80	4.74	1310	0.08
Phenylethyl alcohol	5.80*	1115	[301.50]	11.38	1843	306.76
Phenylethyl formate	6.70	1174	0.18	9.97	1719	0.46
α-Terpineol	6.95	1190	0.06	9.12*	1648	0.42
Nerol	7.55	1232	2.17	10.37	1754	2.33
Citronellol	7.62	1236	86.03	10.08	1729	85.54
Neral	7.71	1242	0.37	8.81	1622	0.47
(*Z*)-Isogeraniol	7.79	1248	0.13	10.53	1767	0.13
Geraniol	7.99	1262	52.12	10.96*	1804	53.33
Geranial	8.16	1274	0.28	9.53	1682	0.08
Eugenol	9.37	1354	4.84	13.99	2088	5.34
Geranyl acetate	9.82	1386	0.62	9.89	1712	0.87
Methyleugenol	10.07	1404	1.09	12.58	1953	0.93
β-Caryophyllene	10.20	1414	0.65	7.78†	1540	0.98
α-Guaiene	10.50	1437	0.24	7.82†	1543	[0.98]
α-Humulene	10.65	1448	0.20	8.62	1606	0.56
Germacrene D	11.03	1476	0.27	9.12*	1648	[0.36]
Pentadecane	11.38	1502	0.18	7.30	1502	0.27
γ-Cadinene	11.42	1506	0.29	9.79	1704	0.80
Hexadecane	12.60	1600	0.25	8.57	1603	0.31
(2*E*,6*Z*)-Farnesol	13.80	1699	0.06	15.69	2263	0.11
Heptadecane	13.88	1706	0.82	9.68	1694	0.04
(2*E*,6*E*)-Farnesol	14.07	1722	0.58	16.09	2305	0.94
Octadecane	14.98	1802	0.11	10.96*	1804	[43.92]
Phenylethyl benzoate	15.44	1844	0.17	18.82	2616	0.34
(9*Z*)-Nonadecene	15.82	1879	1.73	12.10	1908	1.62
Nonadecane	16.13	1907	2.30	12.06	1904	2.35
(9*Z*)-Eicosene	16.80*	1972	13.82	13.12	2004	0.17
Palmitic acid	16.80*	1972	[16.59]	20.86	2871	24.07
(10*Z*)-Heneicosene	17.88	2078	0.16	14.15	2104	0.34
Heneicosane	18.17	2108	0.27			
Citronellyl caprate	18.26	2116	0.07	16.56	2357	0.15
Geranyl caprate	18.42	2133	0.15			

Ethyl oleate	18.72	2164	0.91	17.34	2444	0.45
Docosene isomer	18.80	2173	17.90			
Docosane	19.07	2201	0.15			
Tricosane	20.06	2308	0.18	15.98	2294	0.58
Geranyl laurate	20.43	2351	0.13			
Tetradecyl octanoate	20.57	2367	0.08			
Tetradecyl nonanoate	21.45	2468	1.87			
Pentadecyl octanoate	21.50	2474	1.63			
Phenylethyl myristate	21.64	2490	0.06			
Pentacosane	21.75	2503	0.39			
Citronellyl myristate	21.83	2512	0.47	19.88	2747	0.17
Geranyl myristate	22.08	2544	0.18			
Phenylethyl palmitoleate?	23.08	2667	10.95			
Phenylethyl palmitate	23.23	2685	0.15			
Citronellyl palmitate	23.49	2718	0.51			
Geranyl palmitate	23.70	2746	0.15			
α-Tocopherol	26.47	3121	0.50			
Unknown [m/z 109, 69 (43), 95 (41), 43 (27), 205 (25)... 424 (11)...]	30.80	3480	8.48			

*: 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