

**Date :** June 25, 2020

## CERTIFICATE OF ANALYSIS – GC PROFILING

### SAMPLE IDENTIFICATION

**Internal code :** 20F15-PTH06

**Customer identification :** Rose Absolute - Morocco - R3010898R

**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<sup>1</sup>. Analysis with PC-PA-014 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Fanny Charlier, B. Sc., chimiste à l'entraînement

**Analysis date :** June 18, 2020

Checked and approved by :

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Alexis St-Gelais, M. Sc., chimiste 2013-174

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### REFERENCE

(1) Cachet, T.; Brevard, H.; Chaintreau, A.; Demyttenaere, J.; French, L.; Gassenmeier, K.; Joulain, D.; Koenig, T.; Leijts, 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.

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright orange viscous liquid

**Refractive index:**  $1.4948 \pm 0.0003$  (20 °C; method PC-MAT-016)

*CONCLUSION*

No adulterant, contaminant or diluent has been detected using this method.

## ANALYSIS SUMMARY

Identification	(mg/g) ††	%	Classe
α-Pinene	0.31	0.05	Monoterpene
β-Pinene	0.13	0.02	Monoterpene
Sabinene	0.13	0.02	Monoterpene
Myrcene	0.34	0.05	Monoterpene
Limonene	0.34	0.05	Monoterpene
Linalool	0.35	0.05	Monoterpenic alcohol
Phenylethyl alcohol	344.46	50.77	Simple phenolic
Phenylethyl formate	0.08	0.01	Phenolic ester
Terpinen-4-ol	0.28	0.04	Monoterpenic alcohol
Nerol	1.86	0.27	Monoterpenic alcohol
Citronellol	94.28	13.90	Monoterpenic alcohol
Neral	1.27	0.19	Monoterpenic aldehyde
Geraniol	54.35	8.01	Monoterpenic alcohol
Geranial	0.23	0.03	Monoterpenic aldehyde
Citronellyl formate	0.37	0.05	Monoterpenic ester
Citronellyl acetate	0.20	0.03	Monoterpenic ester
Eugenol	8.35	1.23	Phenylpropanoid
Geranic acid	1.98	0.29	Aliphatic acid
Geranyl acetate	0.90	0.13	Monoterpenic ester
Methyleugenol	1.40	0.21	Phenylpropanoid
β-Caryophyllene	2.51	0.37	Sesquiterpene
α-Guaiene	0.78	0.12	Sesquiterpene
α-Humulene	1.03	0.15	Sesquiterpene
Germacrene D	0.53	0.08	Sesquiterpene
Aciphyllene	0.10	0.01	Sesquiterpene
Pentadecane	0.17	0.02	Alkane
δ-Guaiene	0.14	0.02	Sesquiterpene
γ-Cadinene	0.29	0.04	Sesquiterpene
Hexadecane	0.44	0.07	Alkane
(8Z)-Heptadecene	0.22	0.03	Alkene
(2E,6Z)-Farnesol	0.16	0.02	Sesquiterpenic alcohol
Heptadecane	0.99	0.15	Alkane
(2E,6E)-Farnesol	0.82	0.12	Sesquiterpenic alcohol
Octadecane	0.53	0.08	Alkane
Phenylethyl benzoate	0.32	0.05	Phenolic ester
(9Z)-Nonadecene	2.18	0.32	Alkene
Nonadecane	3.21	0.47	Alkane
Palmitic acid	2.63	0.39	Aliphatic acid
(9Z)-Eicosene	0.24	0.04	Alkene
Eicosane	0.24	0.03	Alkane
(10Z)-Heneicosene	0.33	0.05	Alkene
Heneicosane	0.75	0.11	Alkane
Citronellyl caprate	0.20	0.03	Monoterpenic ester
Geranyl caprate	4.84	0.71	Monoterpenic ester
Phenylethyl undecanoate?	2.80	0.41	Phenolic ester
Ethyl oleate	1.58	0.23	Aliphatic ester
Ethyl linolenate	1.28	0.19	Aliphatic ester
Citronellyl laurate	0.72	0.11	Monoterpenic ester

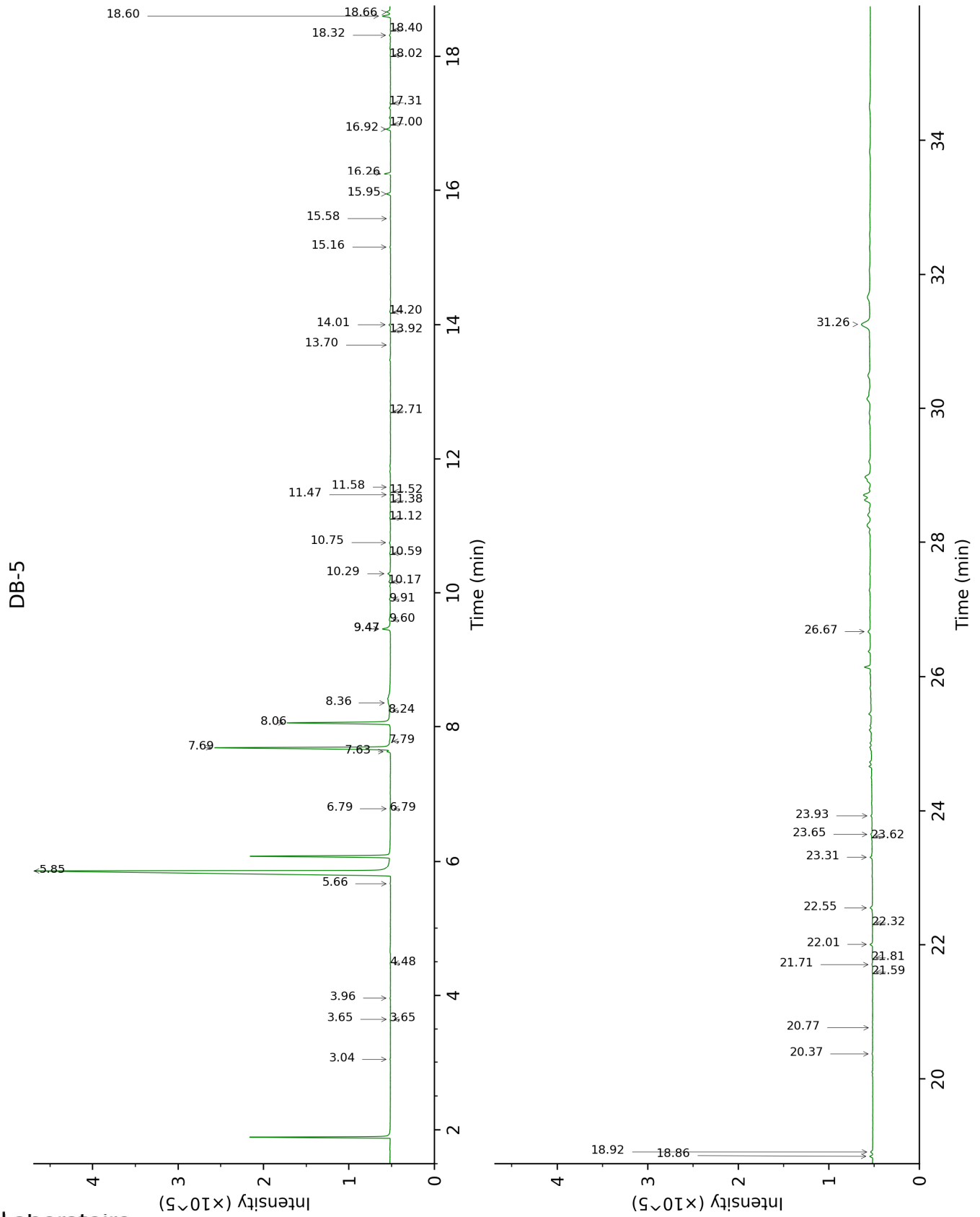
Tetradecyl octanoate	0.17	0.03	Aliphatic ester
Tetradecyl nonanoate	0.31	0.05	Aliphatic ester
Pentadecyl octanoate	0.50	0.07	Aliphatic ester
Phenylethyl myristate	0.50	0.07	Phenolic ester
Citronellyl myristate	1.42	0.21	Monoterpenic ester
Geranyl myristate	0.18	0.03	Monoterpenic ester
Unknown	1.49	0.22	Phenolic ester
Phenylethyl palmitoleate?	1.40	0.21	Phenolic ester
Geranyl palmitoleate?	0.54	0.08	Monoterpenic ester
Citronellyl palmitate	0.84	0.12	Monoterpenic ester
Geranyl palmitate	0.64	0.09	Monoterpenic ester
α-Tocopherol	2.43	0.36	Tocopherol
Unknown	16.01	2.36	Oxygenated triterpene
<b>Consolidated total</b>	<b>568.04 mg/g</b>	<b>83.72%</b>	

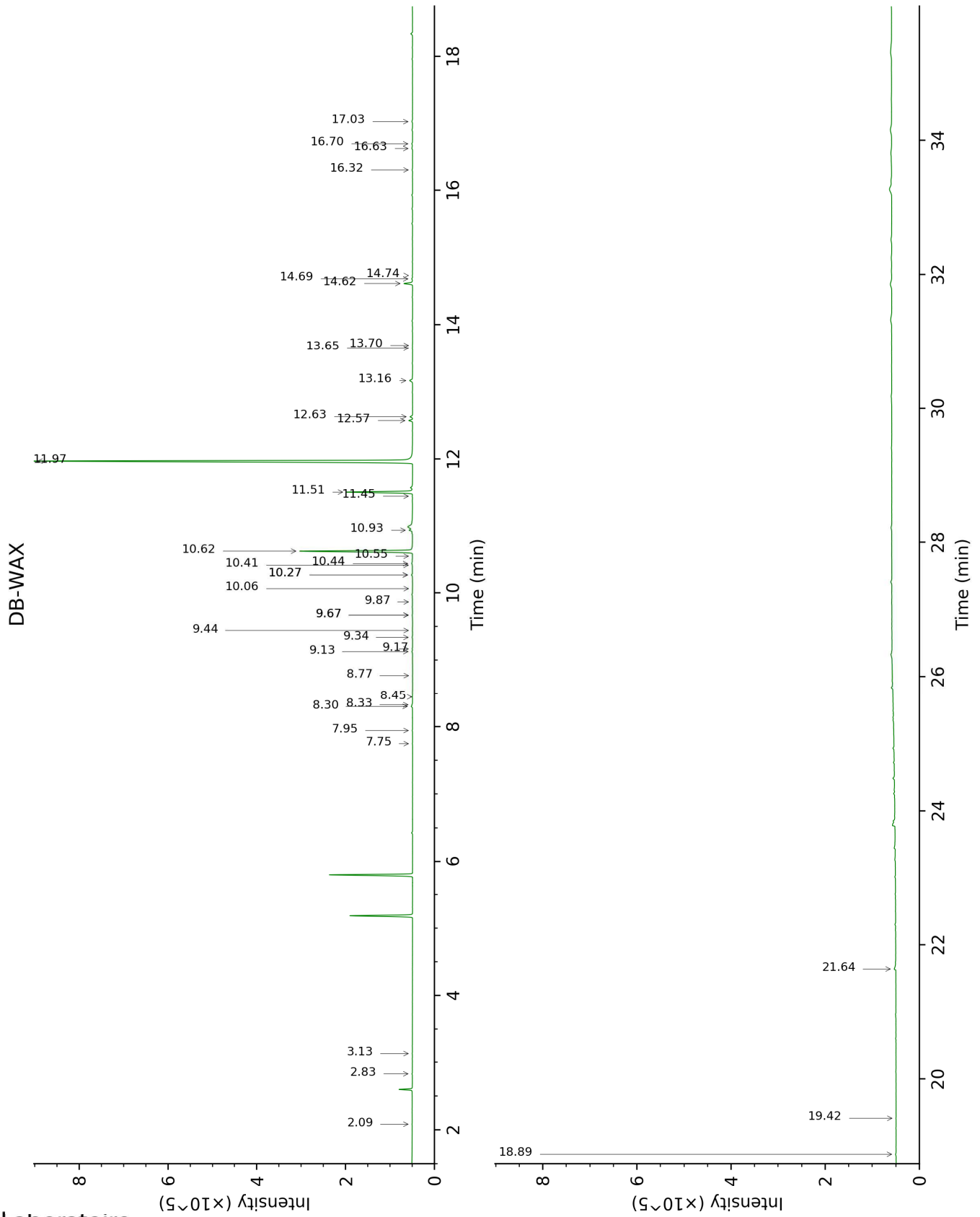
††: As Methyl octanoate equivalents

Note: no correction factor was applied

**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.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g ††	R.T	R.I	mg/g ††
α-Pinene	3.04	932	0.31	1.40	1002	0.17
β-Pinene	3.65*	972	0.26	2.09	1070	0.13
Sabinene	3.65*	972	[0.26]			
Myrcene	3.96	993	0.34	2.83	1135	0.34
Limonene	4.48	1026	0.34	3.13	1158	0.16
Linalool	5.66	1100	0.35	7.95	1512	0.48
Phenylethyl alcohol	5.85	1113	344.46	11.97	1844	357.55
Phenylethyl formate	6.78*	1173	0.38	10.55	1721	0.08
Terpinen-4-ol	6.78*	1173	[0.38]	8.45	1551	0.28
Nerol	7.63	1230	1.86	10.93	1753	3.31
Citronellol	7.69	1234	94.28	10.62	1727	96.88
Neral	7.79	1241	1.27	9.34	1622	0.70
Geraniol	8.06	1260	54.35	11.51	1802	55.78
Geranial	8.24	1272	0.23	10.06	1680	0.19
Citronellyl formate	8.36	1280	0.37	8.77	1576	0.12
Citronellyl acetate	9.47*	1354	6.79	9.44	1630	0.20
Eugenol	9.47*	1354	[6.79]	14.62	2090	8.35
Geranic acid	9.60	1363	1.98	16.63	2295	1.14
Geranyl acetate	9.91	1385	0.90	10.44	1711	0.97
Methyleugenol	10.17	1403	1.40	13.16	1952	3.70
β-Caryophyllene	10.29	1412	2.51	8.30	1540	1.32
α-Guaiene	10.59	1434	0.78	8.33	1542	0.70
α-Humulene	10.75	1446	1.03	9.17	1608	0.48
Germacrene D	11.12	1474	0.53	9.67*	1648	0.55
Aciphyllene	11.38	1493	0.10	9.67*	1648	[0.55]
Pentadecane	11.47	1500	0.17	7.75	1497	0.26
δ-Guaiene	11.52	1504	0.14	9.87	1664	0.31
γ-Cadinene	11.58	1509	0.29	10.27*	1697	1.05
Hexadecane	12.71	1597	0.44	9.13	1604	0.72
(8Z)-Heptadecene	13.70	1679	0.22	10.41	1709	0.19
(2E,6Z)-Farnesol	13.92	1697	0.16	16.32	2262	0.55
Heptadecane	14.01	1704	0.99	10.27*	1697	[1.05]
(2E,6E)-Farnesol	14.20	1720	0.82	16.70	2302	1.07
Octadecane	15.16	1804	0.53	11.45	1797	0.37
Phenylethyl benzoate	15.58	1843	0.32	19.42	2607	0.28
(9Z)-Nonadecene	15.95	1876	2.18	12.63	1902	2.48
Nonadecane	16.26	1904	3.21	12.57	1897	3.38
Palmitic acid	16.92	1968	2.63	21.64	2880	2.91
(9Z)-Eicosene	17.00	1975	0.24	13.70	2001	0.25
Eicosane	17.31	2005	0.24	13.65	1996	0.28

(10Z)- Heneicosene	18.02	2076	0.33	14.74	2101	0.42
Heneicosane	18.32	2105	0.75	14.69	2096	0.94
Citronellyl caprate	18.40	2114	0.20			
Geranyl caprate	18.60	2135	4.84			
Phenylethyl undecanoate?	18.66	2141	2.80			
Ethyl oleate	18.86	2162	1.58	17.03	2338	0.94
Ethyl linolenate	18.92	2169	1.28	18.89	2545	0.91
Citronellyl laurate	20.37	2325	0.72			
Tetradecyl octanoate	20.77	2370	0.17			
Tetradecyl nonanoate	21.59	2465	0.31			
Pentadecyl octanoate	21.71	2478	0.50			
Phenylethyl myristate	21.81	2490	0.50			
Citronellyl myristate	22.01	2514	1.42			
Geranyl myristate	22.32	2552	0.18			
Unknown [m/z 105, 79 (23), 104 (16), 67 (12), 95 (12), 106 (9)... 382 (1)]	22.55	2580	1.49			
Phenylethyl palmitoleate?	23.31	2675	1.40			
Geranyl palmitoleate?	23.62	2715	0.54			
Citronellyl palmitate	23.65	2718	0.84			
Geranyl palmitate	23.93	2755	0.64			
α-Tocopherol	26.67	3126	2.43			
Unknown [m/z 109, 69 (43), 95 (41), 43 (27), 205 (25)... 424 (11)...]	31.26	3488	16.01			

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

††: As Methyl octanoate equivalents

Note: no correction factor was applied  
R.T.: Retention time (minutes)  
R.I.: Retention index