

**Date :** March 16, 2021

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 21B23-FEP14

**Customer identification :** Lemon - Argentina - 51307-19

**Type :** Essential oil

**Source :** *Citrus limonum*

**Customer :** Fern & Petal

*ANALYSIS*

**Method:** PC-MAT-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 :** Seydou Ka, M. Sc.

**Analysis date :** March 10, 2021

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4751 \pm 0.0003$  (20 °C; method PC-MAT-016)

*CONCLUSION*

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

## ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
2,6-Dimethyl-1,5-heptadiene	0.01	Normonoterpene
Heptanal	0.01	Aliphatic aldehyde
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.35	Monoterpene
$\alpha$ -Pinene	1.80	Monoterpene
Camphene	0.06*	Monoterpene
$\alpha$ -Fenchene	[0.06]*	Monoterpene
$\beta$ -Pinene	10.77	Monoterpene
Sabinene	1.94	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	1.46	Monoterpene
Pseudolimonene	0.01	Monoterpene
$\alpha$ -Phellandrene	0.02	Monoterpene
Octanal	0.05	Aliphatic aldehyde
$\Delta^3$ -Carene	0.02	Monoterpene
$\alpha$ -Terpinene	0.07	Monoterpene
para-Cymene	1.94	Monoterpene
$\beta$ -Phellandrene	0.32	Monoterpene
Limonene	68.07	Monoterpene
(Z)- $\beta$ -Ocimene	0.06	Monoterpene
(E)- $\beta$ -Ocimene	0.09	Monoterpene
$\gamma$ -Terpinene	5.61	Monoterpene
cis-Sabinene hydrate	0.06	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.26	Monoterpene
trans-Sabinene hydrate	0.06	Monoterpenic alcohol
Linalool	0.12	Monoterpenic alcohol
Nonanal	0.08	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
cis-Limonene oxide	0.18	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.04	Monoterpenic alcohol
trans-Limonene oxide	0.13	Monoterpenic ether
Epoxyterpinolene	0.04	Monoterpenic ether
Citronellal	0.06	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Unknown	0.04	Unknown
Terpinen-4-ol	0.04	Monoterpenic alcohol
Isogeranial	0.03	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.25	Monoterpenic alcohol
trans-Isopiperitenol	0.03	Monoterpenic alcohol
Decanal	0.03	Aliphatic aldehyde
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.09	Monoterpenic alcohol
2,3-Epoxygeranial?	0.04	Monoterpenic aldehyde
Neral	0.76	Monoterpenic aldehyde

Geraniol	0.02	Monoterpenic alcohol
Geranial	1.17	Monoterpenic aldehyde
Limonen-10-ol	0.01	Monoterpenic alcohol
Undecanal	0.02	Aliphatic aldehyde
Unknown	0.03	Unknown
Citronellyl acetate	0.04	Monoterpenic ester
Neryl acetate	0.39	Monoterpenic ester
$\alpha$ -Copaene	0.02	Sesquiterpene
$\beta$ -Bourbonene	0.01	Sesquiterpene
Geranyl acetate	0.15	Monoterpenic ester
Tetradecane	0.02	Alkane
$\beta$ -Caryophyllene	0.20	Sesquiterpene
<i>cis</i> - $\alpha$ -Bergamotene	0.01	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.40	Sesquiterpene
$\alpha$ -Humulene	0.02	Sesquiterpene
$\beta$ -Santalene	0.01	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.05	Sesquiterpene
<i>trans</i> - $\beta$ -Bergamotene	0.03	Sesquiterpene
Valencene	0.02	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.05	Sesquiterpene
$\beta$ -Bisabolene	0.59	Sesquiterpene
( <i>Z</i> )- $\gamma$ -Bisabolene	0.01	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.03	Sesquiterpene
Spathulenol	0.07	Sesquiterpenic alcohol
Caryophyllene oxide	0.05	Sesquiterpenic ether
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.04	Sesquiterpenic alcohol
Myristic acid	0.04	Aliphatic acid
Pentadecylic acid	0.04	Aliphatic acid
Citropten	0.11	Furanocoumarin
Palmitic acid	0.01	Aliphatic acid
Linoleic acid	0.10	Aliphatic acid
Oleic acid	0.03	Aliphatic acid
Stearic acid	0.21	Aliphatic acid
<b>Consolidated total</b>	<b>99.11%</b>	

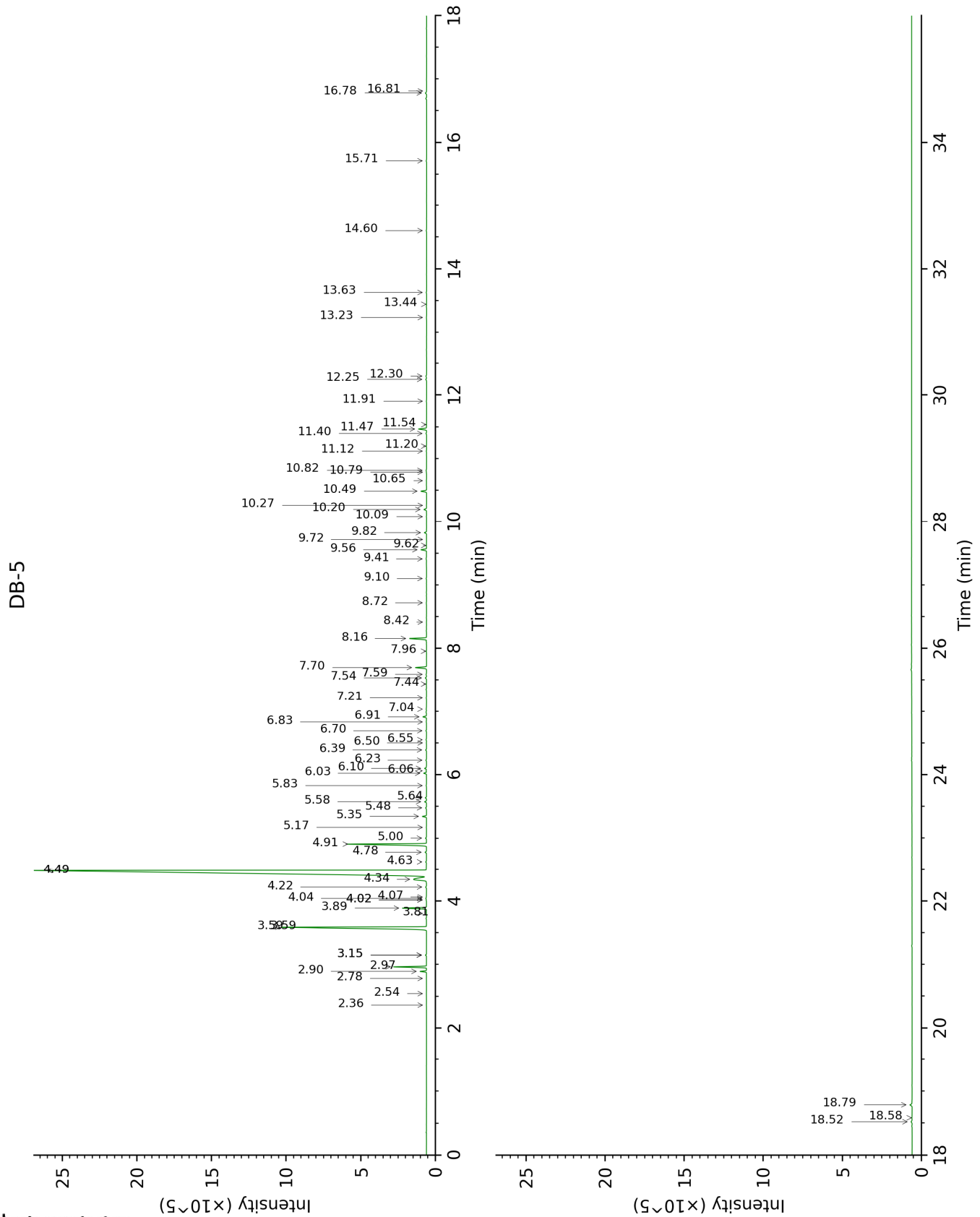
\*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered  
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

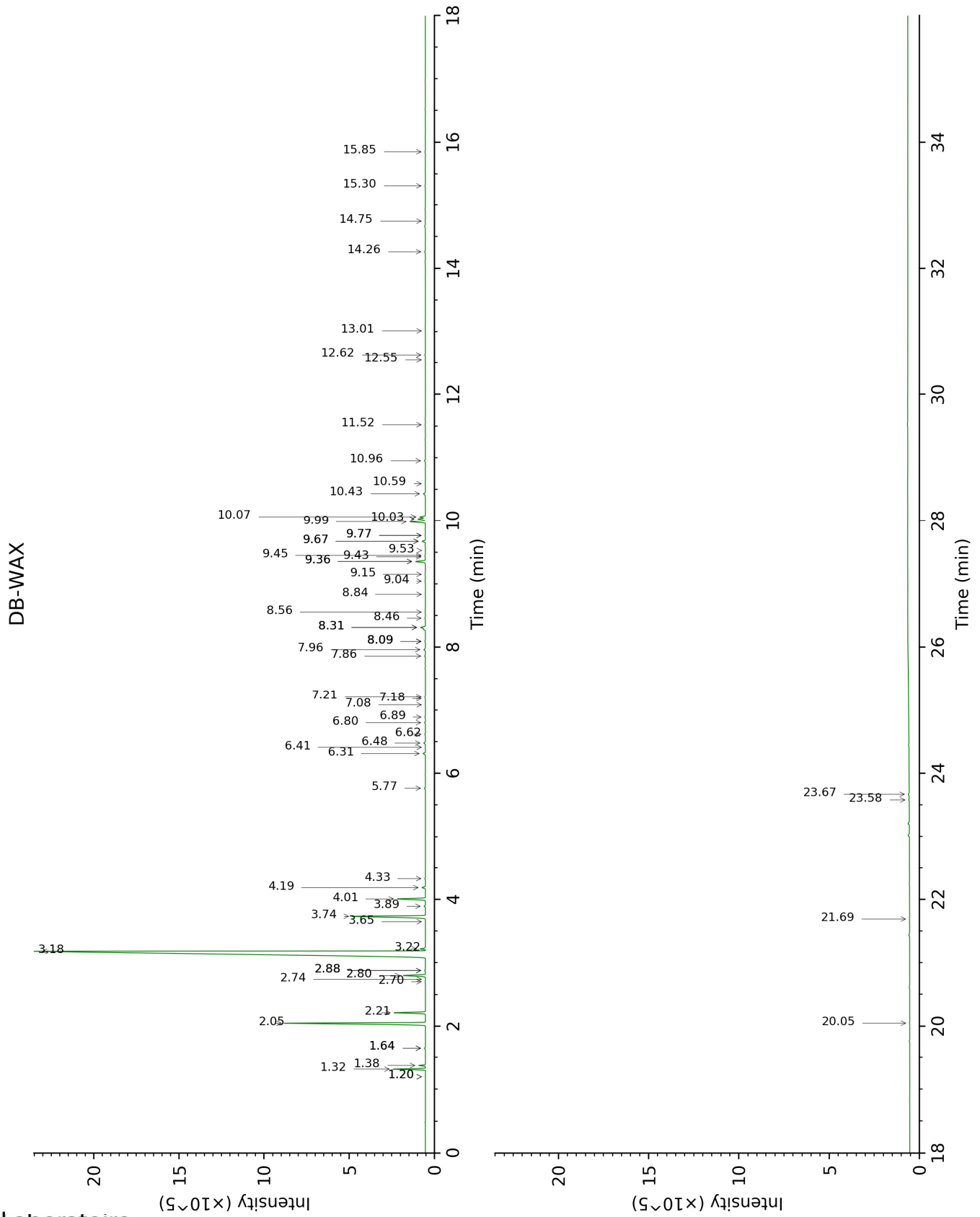
Note: no correction factor was applied

**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.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2,6-Dimethyl-1,5-heptadiene	2.36	885	0.01	1.20*	972	0.01
Heptanal	2.54	901	0.01	2.88*	1141	0.06
Tricyclene	2.78	917	0.01	1.20*	972	[0.01]
$\alpha$ -Thujene	2.90	925	0.35	1.38	1001	0.36
$\alpha$ -Pinene	2.97	930	1.80	1.32	992	1.79
Camphene	3.15*	942	0.06	1.64*	1028	0.06
$\alpha$ -Fenchene	3.15*	942	[0.06]	1.64*	1028	[0.06]
$\beta$ -Pinene	3.59*	972	12.67	2.05	1068	10.77
Sabinene	3.59*	972	[12.67]	2.22	1085	1.94
6-Methyl-5-hepten-2-one	3.81	986	0.01			
Myrcene	3.89	992	1.46	2.80	1134	1.50
Pseudolimonene	4.02*	1001	0.02	2.74	1130	0.01
$\alpha$ -Phellandrene	4.02*	1001	[0.02]	2.70	1127	0.02
Octanal	4.04	1002	0.05	4.33	1253	0.04
$\Delta$ 3-Carene	4.07	1004	0.02			
$\alpha$ -Terpinene	4.22	1014	0.07	2.88*	1141	[0.06]
para-Cymene	4.34	1022	1.94	4.01	1229	1.94
$\beta$ -Phellandrene	4.49*	1030	67.98	3.22	1168	0.32
Limonene	4.49*	1030	[67.98]	3.18	1165	68.07
(Z)- $\beta$ -Ocimene	4.63	1040	0.06	3.65	1202	0.01
(E)- $\beta$ -Ocimene	4.78	1049	0.09	3.89	1220	0.09
$\gamma$ -Terpinene	4.91	1058	5.61	3.74	1208	5.72
<i>cis</i> -Sabinene hydrate	5.00	1063	0.06	6.80	1430	0.06
Octanol	5.17	1074	0.01	8.09*	1528	0.05
Terpinolene	5.35	1085	0.26	4.19	1242	0.25
<i>trans</i> -Sabinene hydrate	5.48	1094	0.06	7.86	1510	0.06
Linalool	5.58	1100	0.12	7.96	1518	0.12
Nonanal	5.64	1104	0.08	5.77	1354	0.08
<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.83	1116	0.03	8.84	1586	0.02
<i>cis</i> -Limonene oxide	6.03	1129	0.18	6.31	1394	0.18
<i>cis</i> -para-Mentha-2,8-dien-1-ol	6.06	1132	0.04	9.43	1633	0.04
<i>trans</i> -Limonene oxide	6.10	1134	0.13	6.48	1406	0.13
Epoxyterpinolene	6.23	1142	0.04	6.62	1416	0.04
Citronellal	6.39	1153	0.06	6.89	1437	0.04
Borneol	6.50	1160	0.01	9.67*	1654	0.25
Unknown [m/z 43, 109 (68), 67 (62), 81 (36), 41	6.55	1163	0.04	7.21	1461	0.04



(31), 137 (29), 79 (26)...						
Terpinen-4-ol	6.70	1173	0.04	8.46	1556	0.06
Isogeranial	6.83	1182	0.03	8.09*	1528	[0.05]
$\alpha$ -Terpineol	6.91	1187	0.25	9.67*	1654	[0.25]
<i>trans</i> -Isopiperitenol	7.04	1195	0.03			
Decanal	7.21	1206	0.03	7.18	1459	0.03
2,3-Epoxyneral?	7.44	1222	0.02			
Nerol	7.54	1229	0.09	10.96	1761	0.08
2,3-Epoxygeranial?	7.59	1232	0.04			
Neral	7.70	1240	0.76	9.36*	1627	0.78
Geraniol	7.96	1257	0.02	11.52	1810	0.03
Geranial	8.16	1271	1.17	9.99	1679	1.22
Limonen-10-ol	8.42	1289	0.01	13.01	1944	0.01
Undecanal	8.72	1306	0.02	8.56	1564	0.03
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...	9.10	1333	0.03	12.55	1901	0.02
Citronellyl acetate	9.41	1355	0.04	9.36*	1627	[0.78]
Neryl acetate	9.56	1366	0.39	10.07	1686	0.43
$\alpha$ -Copaene	9.62	1370	0.02	7.08	1451	0.01
$\beta$ -Bourbonene	9.72	1377	0.01			
Geranyl acetate	9.82	1385	0.15	10.43	1716	0.16
Tetradecane	10.09	1403	0.02	6.41	1401	0.02
$\beta$ -Caryophyllene	10.20	1412	0.20	8.32*	1545	0.40
<i>cis</i> - $\alpha$ -Bergamotene	10.26	1416	0.01	8.09*	1528	[0.05]
<i>trans</i> - $\alpha$ -Bergamotene	10.49	1433	0.40	8.32*	1545	[0.40]
$\alpha$ -Humulene	10.65	1446	0.02	9.15	1611	0.04
$\beta$ -Santalene	10.79	1456	0.01	9.04	1602	0.04
( <i>E</i> )- $\beta$ -Farnesene	10.82	1458	0.05	9.45	1635	0.04
<i>trans</i> - $\beta$ -Bergamotene	11.12	1480	0.03	9.53	1642	0.01
Valencene	11.20	1486	0.02	9.77*	1661	0.03
( <i>Z</i> )- $\alpha$ -Bisabolene	11.40	1501	0.05			
$\beta$ -Bisabolene	11.47	1506	0.59	10.03	1683	0.59
( <i>Z</i> )- $\gamma$ -Bisabolene	11.54	1512	0.01	9.77*	1661	[0.03]
( <i>E</i> )- $\alpha$ -Bisabolene	11.91	1541	0.03	10.59	1730	0.02
Spathulenol	12.25	1568	0.07	14.26	2062	0.07
Caryophyllene oxide	12.30	1572	0.05	12.62	1908	0.06
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.24	1648	0.03	14.75	2110	0.03
Unknown [m/z 69, 95 (100), 41	13.44	1665	0.01	15.85	2222	0.05

(89), 109 (68), 67 (61)...222]						
α-Bisabolol	13.63	1681	0.04	15.30	2166	0.04
Myristic acid	14.60	1764	0.04	20.05	2693	0.01
Pentadecylic acid	15.71	1864	0.04			
Citropten	16.78	1964	0.11	23.67	3168	0.09
Palmitic acid	16.81	1967	0.01	21.69	2900	0.01
Linoleic acid	18.52	2137	0.10			
Oleic acid	18.58	2144	0.03	23.58	3155	0.04
Stearic acid	18.79	2165	0.21			
<b>Total identified</b>		<b>98.56%</b>			<b>98.34%</b>	
<b>Total reported</b>		<b>98.67%</b>			<b>98.47%</b>	

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

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

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index