

**Date :** March 16, 2021

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 21B23-FEP16


**Customer identification :** Lime - Mexico - 51247-13

**Type :** Essential oil

**Source :** *Citrus aurantifolia*

**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 :** Alexis St-Gelais, M. Sc., chimiste

**Analysis date :** March 15, 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:** Yellow liquid

**Refractive index:**  $1.4801 \pm 0.0003$  (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
Heptanal	0.01	Aliphatic aldehyde
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.55	Monoterpene
$\alpha$ -Pinene	2.16	Monoterpene
Thuja-2,4(10)-diene	0.16	Monoterpene
$\beta$ -Pinene	12.31	Monoterpene
Sabinene	1.71	Monoterpene
Geranic oxide	0.02	Monoterpenic ether
Myrcene	1.23	Monoterpene
Pseudolimonene	0.01	Monoterpene
$\alpha$ -Phellandrene	0.04	Monoterpene
Octanal	0.01	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.23	Monoterpene
para-Cymene	1.13	Monoterpene
$\beta$ -Phellandrene	0.31*	Monoterpene
1,8-Cineole	[0.31]*	Monoterpenic ether
Limonene	51.66	Monoterpene
(Z)- $\beta$ -Ocimene	0.05	Monoterpene
(E)- $\beta$ -Ocimene	0.10	Monoterpene
$\gamma$ -Terpinene	11.11	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
Terpinolene	0.54	Monoterpene
trans-Sabinene hydrate	0.03	Monoterpenic alcohol
Linalool	0.16	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
cis-Limonene oxide	0.04	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
trans-Limonene oxide	0.03	Monoterpenic ether
cis- $\beta$ -Terpineol	0.04	Monoterpenic alcohol
Citronellal	0.42	Monoterpenic aldehyde
trans- $\beta$ -Terpineol	0.01	Monoterpenic alcohol
Borneol	0.03	Monoterpenic alcohol
$\alpha$ -Phellandren-8-ol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.07	Monoterpenic alcohol
para-Cymen-8-ol	0.03	Monoterpenic alcohol
$\alpha$ -Terpineol	0.23	Monoterpenic alcohol
$\gamma$ -Terpineol	0.04	Monoterpenic alcohol
Decanal	0.04	Aliphatic aldehyde
trans-Carveol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.07	Monoterpenic alcohol
cis-Carveol	0.01	Monoterpenic alcohol
2,3-Epoxygeranial?	0.05	Monoterpenic aldehyde

Neral	1.62	Monoterpenic aldehyde
Geraniol	0.06	Monoterpenic alcohol
Geranial	2.67	Monoterpenic aldehyde
Unknown	0.03	Oxygenated monoterpene
<i>cis</i> -Ascaridole glycol	0.02	Monoterpenic alcohol
Undecanal	0.01	Aliphatic aldehyde
$\delta$ -Elemene	0.06	Sesquiterpene
Citronellyl acetate	0.02	Monoterpenic ester
Neryl acetate	1.01	Monoterpenic ester
Geranyl acetate	0.21	Monoterpenic ester
$\beta$ -Elemene	0.15	Sesquiterpene
Dodecanal	0.02	Aliphatic aldehyde
<i>cis</i> - $\alpha$ -Bergamotene	0.07	Sesquiterpene
$\beta$ -Caryophyllene	0.64	Sesquiterpene
$\alpha$ -Santalene	0.02	Sesquiterpene
$\gamma$ -Elemene	0.02	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	1.12	Sesquiterpene
$\alpha$ -Humulene	0.10	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.04	Sesquiterpene
$\beta$ -Santalene	0.07	Sesquiterpene
Selina-4,11-diene	0.02	Sesquiterpene
Germacrene D	0.04	Sesquiterpene
<i>trans</i> - $\beta$ -Bergamotene	0.09	Sesquiterpene
$\alpha$ -Selinene	0.05	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.16	Sesquiterpene
$\beta$ -Bisabolene	1.63	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	0.17	Sesquiterpene
$\gamma$ -Cadinene	0.01	Sesquiterpene
$\delta$ -Cadinene	0.02	Sesquiterpene
Selina-4(15),7(11)-diene	0.01	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.05	Sesquiterpene
Germacrene B	0.15	Sesquiterpene
Caryophyllene oxide	0.06	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Tetradecanal	0.02	Aliphatic aldehyde
10-epi- $\gamma$ -Eudesmol	0.01	Sesquiterpenic alcohol
Alismol	0.08	Sesquiterpenic alcohol
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.05	Sesquiterpenic alcohol
Herniarin	0.31	Coumarin
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	0.01	Sesquiterpenic aldehyde
Myristic acid	0.03	Aliphatic acid
meta-Camphorene	0.01	Diterpene
Citropten	0.11	Furanocoumarin
Palmitic acid	0.10	Aliphatic acid
Bergapten	0.05	Furanocoumarin
Heneicosane	0.02	Alkane
Linoleic acid	0.05	Aliphatic acid
Stearic acid	0.37	Aliphatic acid
Isopimpinellin	0.05	Furanocoumarin
Tricosane	0.06	Alkane

Heraclenin	0.01	Furanocoumarin
Pentacosane	0.02	Alkane
Hexacosane	0.01	Alkane
Heptacosane	0.02	Alkane
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
<b>Consolidated total</b>	<b>96.65%</b>	

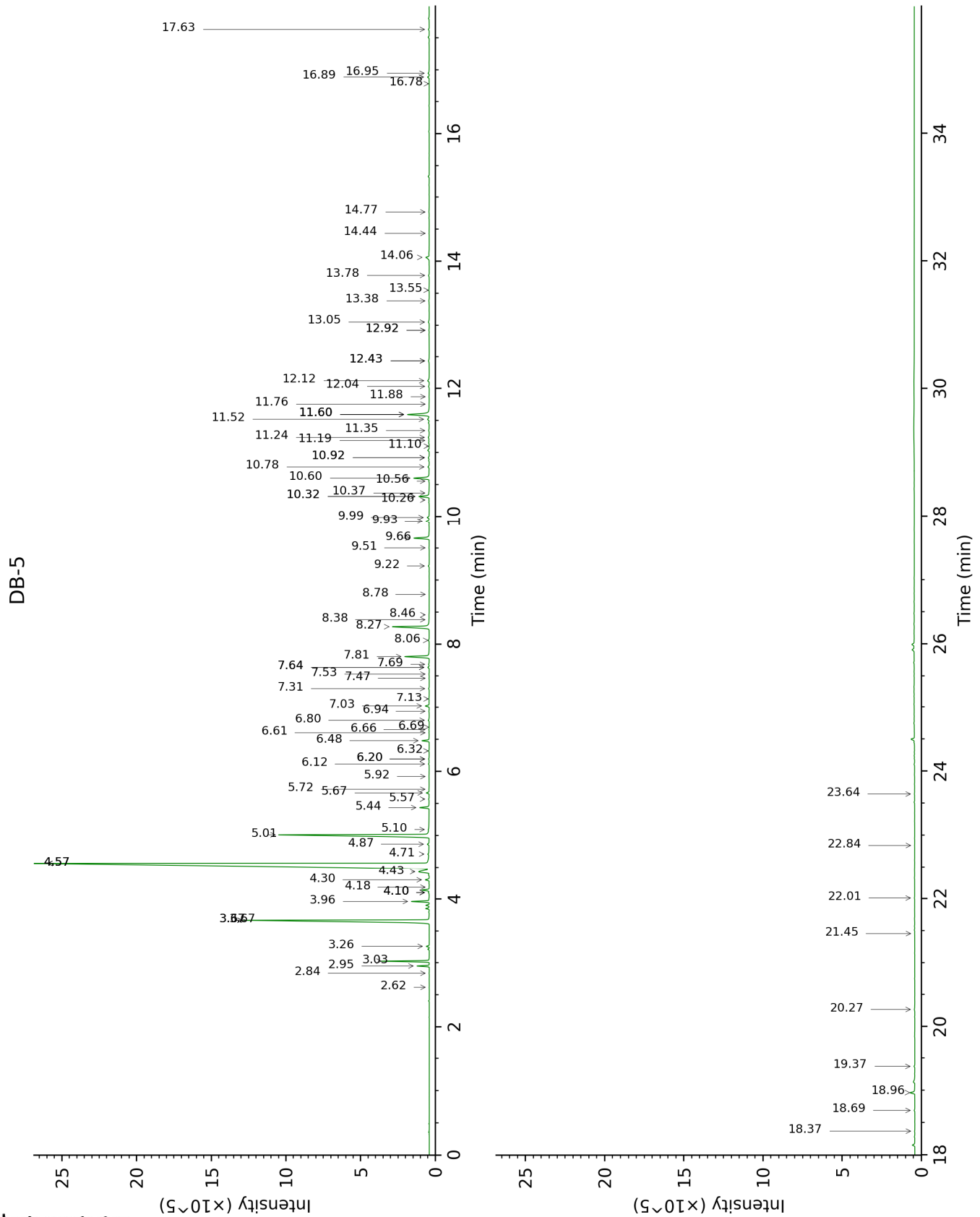
\*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered [xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

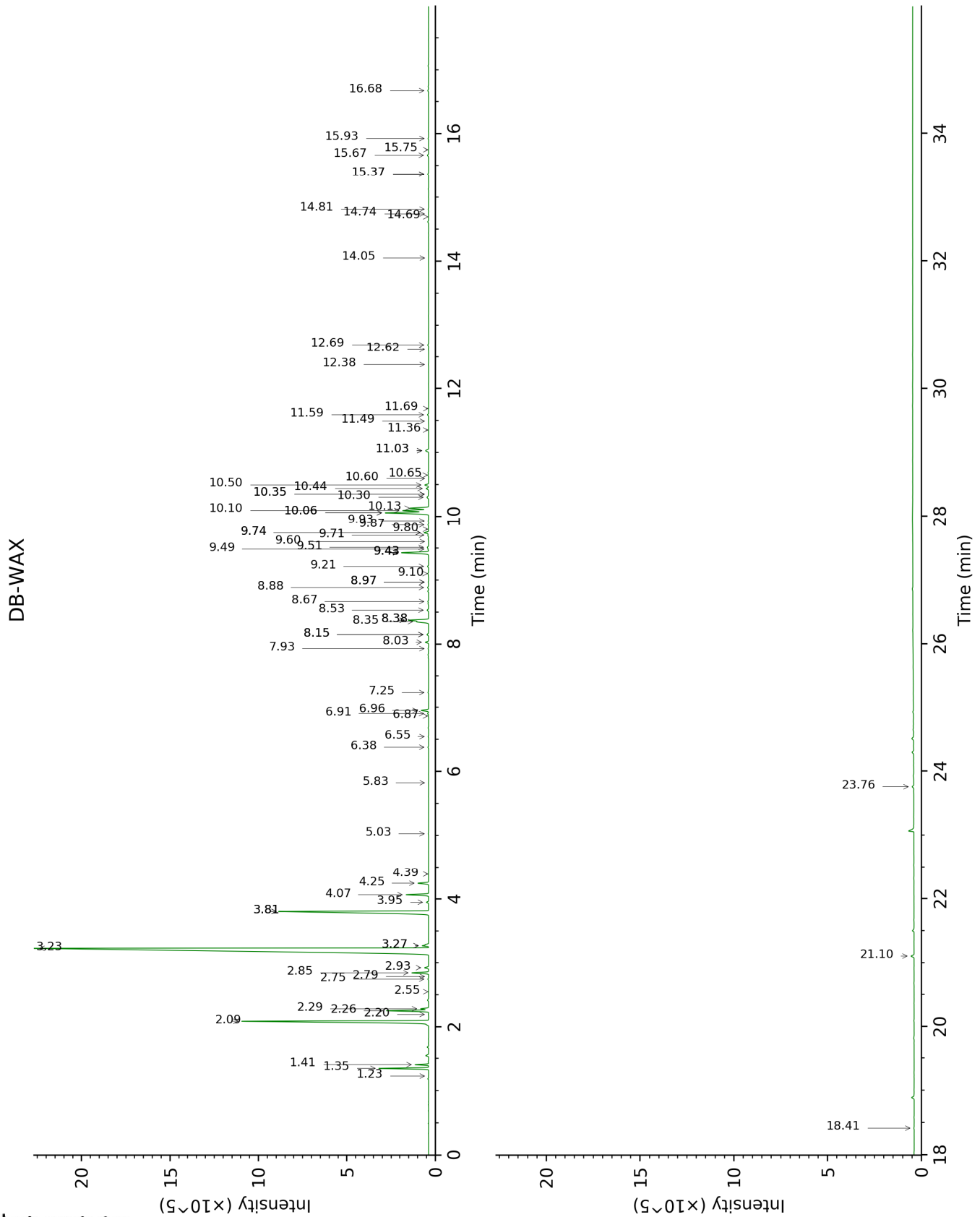
Note: no correction factor was applied

**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	%
Heptanal	2.62	903	0.01			
Tricyclene	2.84	917	0.01	1.23	972	0.01
$\alpha$ -Thujene	2.95	925	0.55	1.41	1000	0.54
$\alpha$ -Pinene	3.03	930	2.16	1.35	992	2.15
Thuja-2,4(10)-diene	3.26	945	0.16	2.29†	1087	[2.44]
$\beta$ -Pinene	3.67*	972	14.04	2.09	1068	12.31
Sabinene	3.67*	972	[14.04]	2.26†	1084	2.44
Geranic oxide	3.67*	972	[14.04]	2.20	1078	0.02
Myrcene	3.96	992	1.23	2.85	1134	0.88
Pseudolimonene	4.10*	1001	0.05	2.79	1129	0.01
$\alpha$ -Phellandrene	4.10*	1001	[0.05]	2.75	1126	0.04
Octanal	4.10*	1001	[0.05]	4.39	1250	0.01
$\Delta$ 3-Carene	4.18	1007	0.01	2.55	1111	0.01
$\alpha$ -Terpinene	4.30	1014	0.23	2.93	1140	0.24
para-Cymene	4.43	1022	1.13	4.07	1226	1.19
$\beta$ -Phellandrene	4.57*	1031	51.97	3.27*	1166	0.42
1,8-Cineole	4.57*	1031	[51.97]	3.27*	1166	[0.42]
Limonene	4.57*	1031	[51.97]	3.23	1163	51.66
(Z)- $\beta$ -Ocimene	4.71	1040	0.05	3.81*	1208	11.36
(E)- $\beta$ -Ocimene	4.87	1050	0.10	3.95	1218	0.11
$\gamma$ -Terpinene	5.01	1059	11.11	3.81*	1208	[11.36]
cis-Sabinene hydrate	5.10	1064	0.01	6.87	1430	0.03
Terpinolene	5.44	1086	0.54	4.25	1239	0.57
trans-Sabinene hydrate	5.57	1094	0.03	7.93	1510	0.04
Linalool	5.67	1100	0.16	8.03	1517	0.18
Nonanal	5.72	1104	0.02	5.82	1353	0.01
trans-para-Mentha-2,8-dien-1-ol	5.92	1117	0.01	8.88	1584	0.08
cis-Limonene oxide	6.12	1129	0.04	6.38	1394	0.04
cis-para-Mentha-2,8-dien-1-ol	6.20*	1134	0.04	9.43*	1627	1.66
trans-Limonene oxide	6.20*	1134	[0.04]	6.55	1406	0.03
cis- $\beta$ -Terpineol	6.32	1142	0.04	8.97*	1590	0.03
Citronellal	6.48	1153	0.42	6.96	1436	0.42
trans- $\beta$ -Terpineol	6.61	1161	0.01	9.60	1642	0.01
Borneol	6.66	1164	0.03	9.74*†	1653	[0.34]
$\alpha$ -Phellandren-8-ol	6.69	1166	0.01	10.06*†	1679	4.31
Terpinen-4-ol	6.80	1173	0.07	8.53	1556	0.10
para-Cymen-8-ol	6.94	1182	0.03	11.49	1800	0.02
$\alpha$ -Terpineol	7.02	1188	0.23	9.74*†	1653	[0.34]

$\gamma$ -Terpineol	7.14	1195	0.04	9.80	1657	0.03
Decanal	7.31	1206	0.04	7.25	1458	0.04
<i>trans</i> -Carveol	7.47	1217	0.01	11.36	1788	0.01
2,3-Epoxyneral?	7.53	1221	0.02			
Nerol	7.64*	1229	0.08	11.03*	1760	0.24
<i>cis</i> -Carveol	7.64*	1229	[0.08]	11.69	1817	0.01
2,3-Epoxygeranial?	7.69	1232	0.05			
Neral	7.81	1240	1.62	9.43*	1627	[1.66]
Geraniol	8.06	1257	0.06	11.59	1808	0.07
Geranial	8.27	1272	2.67	10.06*†	1679	[4.31]
Unknown [m/z 95, 67 (45), 41 (42), 110 (42), 43 (41), 59 (36)]	8.38	1279	0.03	12.38	1878	0.02
<i>cis</i> -Ascaridole glycol	8.46	1284	0.02	14.74	2100	0.03
Undecanal	8.78	1306	0.01	8.67	1567	0.05
$\delta$ -Elemene	9.22	1334	0.06	6.91	1433	0.06
Citronellyl acetate	9.50	1353	0.02	9.43*	1627	[1.66]
Neryl acetate	9.66	1364	1.01	10.13	1685	1.13
Geranyl acetate	9.93	1383	0.21	10.50	1715	0.24
$\beta$ -Elemene	9.99	1388	0.15	8.38*	1544	1.25
Dodecanal	10.26	1407	0.02	9.93	1668	0.03
<i>cis</i> - $\alpha$ -Bergamotene	10.32*	1411	0.70	8.15*	1527	0.11
$\beta$ -Caryophyllene	10.32*	1411	[0.70]	8.35	1542	0.64
$\alpha$ -Santalene	10.37	1415	0.02	8.15*	1527	[0.11]
$\gamma$ -Elemene	10.56	1429	0.02	8.97*	1590	[0.03]
<i>trans</i> - $\alpha$ -Bergamotene	10.60	1432	1.12	8.38*	1544	[1.25]
$\alpha$ -Humulene	10.78	1446	0.10	9.22	1610	0.07
( <i>E</i> )- $\beta$ -Farnesene	10.92*	1456	0.08	9.49	1632	0.04
$\beta$ -Santalene	10.92*	1456	[0.08]	9.10	1601	0.07
Selina-4,11-diene	11.10	1470	0.02	9.43*	1627	[1.66]
Germacrene D	11.19	1476	0.04	9.70†	1650	0.34
<i>trans</i> - $\beta$ -Bergamotene	11.24	1480	0.09	9.51	1634	0.10
$\alpha$ -Selinene	11.35	1488	0.05	9.87	1663	0.05
( <i>Z</i> )- $\alpha$ -Bisabolene	11.52	1501	0.16	10.30	1699	0.13
$\beta$ -Bisabolene	11.60*	1506	1.82	10.10†	1682	[4.31]
(3 <i>E</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	11.60*	1506	[1.82]	10.44	1710	0.17
$\gamma$ -Cadinene	11.60*	1506	[1.82]	10.35*	1703	0.03
$\delta$ -Cadinene	11.76	1519	0.02	10.35*	1703	[0.03]
Selina-4(15),7(11)-diene	11.88	1528	0.01	10.60	1724	0.01
( <i>E</i> )- $\alpha$ -Bisabolene	12.04	1541	0.05	10.65	1728	0.05
Germacrene B	12.12	1548	0.15	11.03*	1760	[0.24]

Caryophyllene oxide	12.43*	1572	0.09	12.69	1909	0.06
Caryophyllene oxide isomer	12.43*	1572	[0.09]	12.62	1899	0.02
Tetradecanal	12.92*	1611	0.03			
10-epi-γ-Eudesmol	12.92*	1611	[0.03]	14.05	2034	0.01
Alismol	13.05	1621	0.08	15.67	2192	0.09
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.38	1649	0.04	14.81	2108	0.03
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.55	1662	0.03	15.93	2219	0.03
α-Bisabolol	13.78	1681	0.05	15.37*	2163	0.06
Herniarin	14.06	1705	0.31	21.10	2811	0.21
(2E,6E)-Farnesal	14.44	1737	0.01	15.75	2201	0.02
Myristic acid	14.77	1766	0.03			
meta-Camphorene	16.78	1949	0.01	15.37*	2163	[0.06]
Citropten	16.89	1958	0.11	23.76	3168	0.11
Palmitic acid	16.95	1964	0.10			
Bergapten	17.63	2030	0.05			
Heneicosane	18.37	2103	0.02	14.69	2096	0.02
Linoleic acid	18.69	2136	0.05			
Stearic acid	18.96	2165	0.37			
Isopimpinellin	19.37	2207	0.05			
Tricosane	20.27	2303	0.06	16.68	2297	0.06
Heraclenin	21.45	2437	0.01			
Pentacosane	22.01	2501	0.02	18.42	2488	0.02
Hexacosane	22.84	2601	0.01			
Heptacosane	23.64	2701	0.02			
6-Methyl-5-hepten-2-one				5.03	1296	0.02
<b>Total identified</b>		<b>96.51%</b>			<b>96.61%</b>	
<b>Total reported</b>		<b>96.60%</b>			<b>96.70%</b>	

\*: 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

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index