

**Date :** February 23, 2018

**CERTIFICATE OF ANALYSIS - GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 18B20-PLG11-1-CC

**Customer identification :** Pink Grapefruit

**Type :** Essential oil

**Source :** *Citrus x paradisi* cv. Pink

**Customer :** Plant Guru

*ANALYSIS*

**Method:** PC-PA-014-17J19 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste

**Analysis date :** February 23, 2018

Checked and approved by :

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

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#### *PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright orange liquid

**Refractive index:**  $1.4723 \pm 0.0003$  (20 °C)

#### *CONCLUSION*

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

## ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
Ethanol	0.01	0.01	Aliphatic alcohol
Heptanal	tr	tr	Aliphatic aldehyde
$\alpha$ -Thujene	0.01	0.01	Monoterpene
$\alpha$ -Pinene	0.50	0.51	Monoterpene
Camphene	tr	tr	Monoterpene
Sabinene	0.40*	0.36	Monoterpene
$\beta$ -Pinene	[0.40]*	0.06	Monoterpene
Heptanol	tr	tr	Aliphatic alcohol
Myrcene	1.75	1.76	Monoterpene
$\alpha$ -Phellandrene	0.02	0.03	Monoterpene
Octanal	0.34	0.33	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	0.01	Monoterpene
$\alpha$ -Terpinene	tr	0.01	Monoterpene
Limonene	93.95*	93.96	Monoterpene
para-Cymene	[93.95]*	0.05	Monoterpene
1,8-Cineole	[93.95]*	0.25	Monoterpenic ether
(Z)- $\beta$ -Ocimene	tr	0.01	Monoterpene
(E)- $\beta$ -Ocimene	0.10	0.10	Monoterpene
$\gamma$ -Terpinene	0.02	0.03	Monoterpene
cis-Sabinene hydrate	tr	0.01	Monoterpenic alcohol
Octanol	0.03	0.04	Aliphatic alcohol
Terpinolene	0.01	0.01	Monoterpene
Linalool	0.03	0.03	Monoterpenic alcohol
Nonanal	0.02	0.02	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.01	0.01	Monoterpenic alcohol
cis-Limonene oxide	0.01	0.01	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.01	0.09*	Monoterpenic alcohol
Citronellal	0.01	0.01	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.07	0.12*	Monoterpenic alcohol
trans-Isopiperitenol	0.01	0.01	Monoterpenic alcohol
Decanal	0.29	0.27	Aliphatic aldehyde
Octyl acetate	0.02	0.02	Aliphatic ester
trans-Carveol	0.01	0.01	Monoterpenic alcohol
cis-Carveol	0.01	tr	Monoterpenic alcohol
Neral	0.10	[0.09]*	Monoterpenic aldehyde
(E)-Isogeraniol?	0.01	tr	Monoterpenic alcohol
Geranial	0.12	0.10	Monoterpenic aldehyde
cis-para-Mentha-2,8-diene-1-hydroperoxide	0.01*		Monoterpenic peroxide
Undecanal	[0.01]*	tr	Aliphatic aldehyde
$\alpha$ -Terpinyl acetate	0.01	0.02	Monoterpenic ester
Limonene hydroperoxide IV	0.02		Monoterpenic peroxide
Neryl acetate	0.01	0.01	Monoterpenic ester
$\alpha$ -Copaene	0.06	0.06	Sesquiterpene
Geranyl acetate	0.11*	0.06	Monoterpenic ester
cis-para-Mentha-6,8-diene-2-hydroperoxide	[0.11]*		Monoterpenic peroxide
$\beta$ -Cubebene	[0.11]*	0.04	Sesquiterpene

$\beta$ -Elemene	[0.11]*	0.24*	Sesquiterpene
Dodecanal	0.04*	0.02	Aliphatic aldehyde
Limonen-10-yl acetate	[0.04]*	0.01	Monoterpnic ester
$\beta$ -Caryophyllene	0.25	[0.24]*	Sesquiterpene
$\alpha$ -Humulene	0.05	0.05	Sesquiterpene
(E)- $\beta$ -Farnesene	0.02	0.02	Sesquiterpene
Germacrene D	0.05	[0.12]*	Sesquiterpene
Bicyclogermacrene	0.02	0.02	Sesquiterpene
$\alpha$ -Muurolene	0.01	tr	Sesquiterpene
Cubebol	0.01	0.01	Sesquiterpenic alcohol
$\delta$ -Cadinene	0.07	0.07	Sesquiterpene
$\alpha$ -Elemol	0.02	0.02	Sesquiterpenic alcohol
(E)-Nerolidol	0.01	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	0.01	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	0.01	Sesquiterpenic ether
$\beta$ -Sinensal	0.01	0.01	Sesquiterpenic aldehyde
Myristic acid	0.02	0.01	Aliphatic acid
Nootkatone	0.10	0.09	Sesquiterpenic ketone
Palmitic acid	0.05	0.06	Aliphatic acid
Bergapten	0.01		Furanocoumarin
Osthole	0.02		Coumarin
Linoleic acid	0.02	0.03	Aliphatic acid
Oleic acid	0.03		Aliphatic acid
cis-Vaccenic acid?	0.04	0.08*	Aliphatic acid
Stearic acid	0.07	[0.08]*	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.01		Coumarin
Isoauraptene	0.04		Coumarin
Meranzin	0.07		Coumarin
Auraptenol	0.01		Coumarin
Unknown	tr		Coumarin
Auraptene	0.21		Coumarin
Epoxyaurapten	0.08		Coumarin
Tangeretin	0.01		Flavonoid
<b>Total identified</b>	<b>99.44%</b>	<b>99.16%</b>	

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

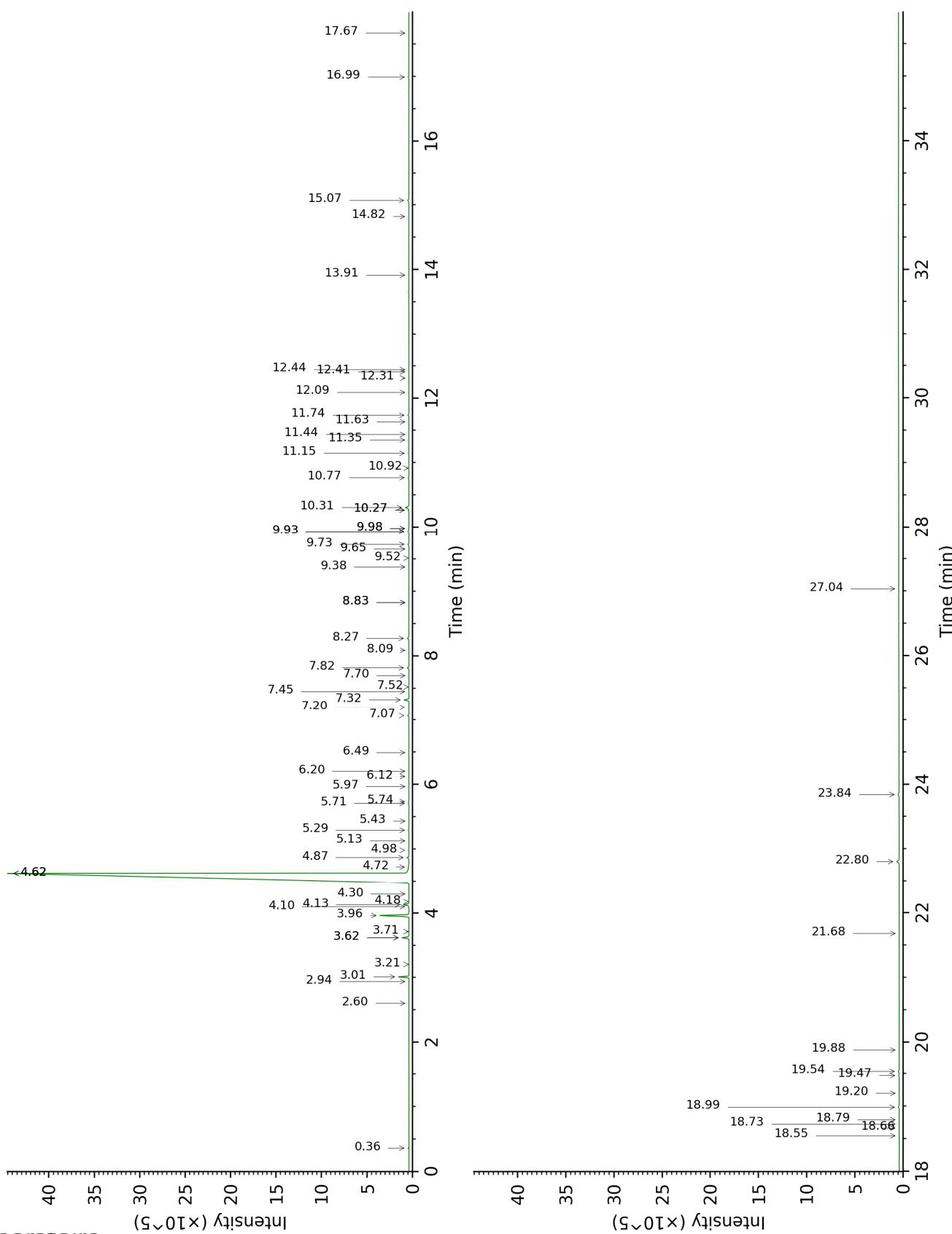
[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

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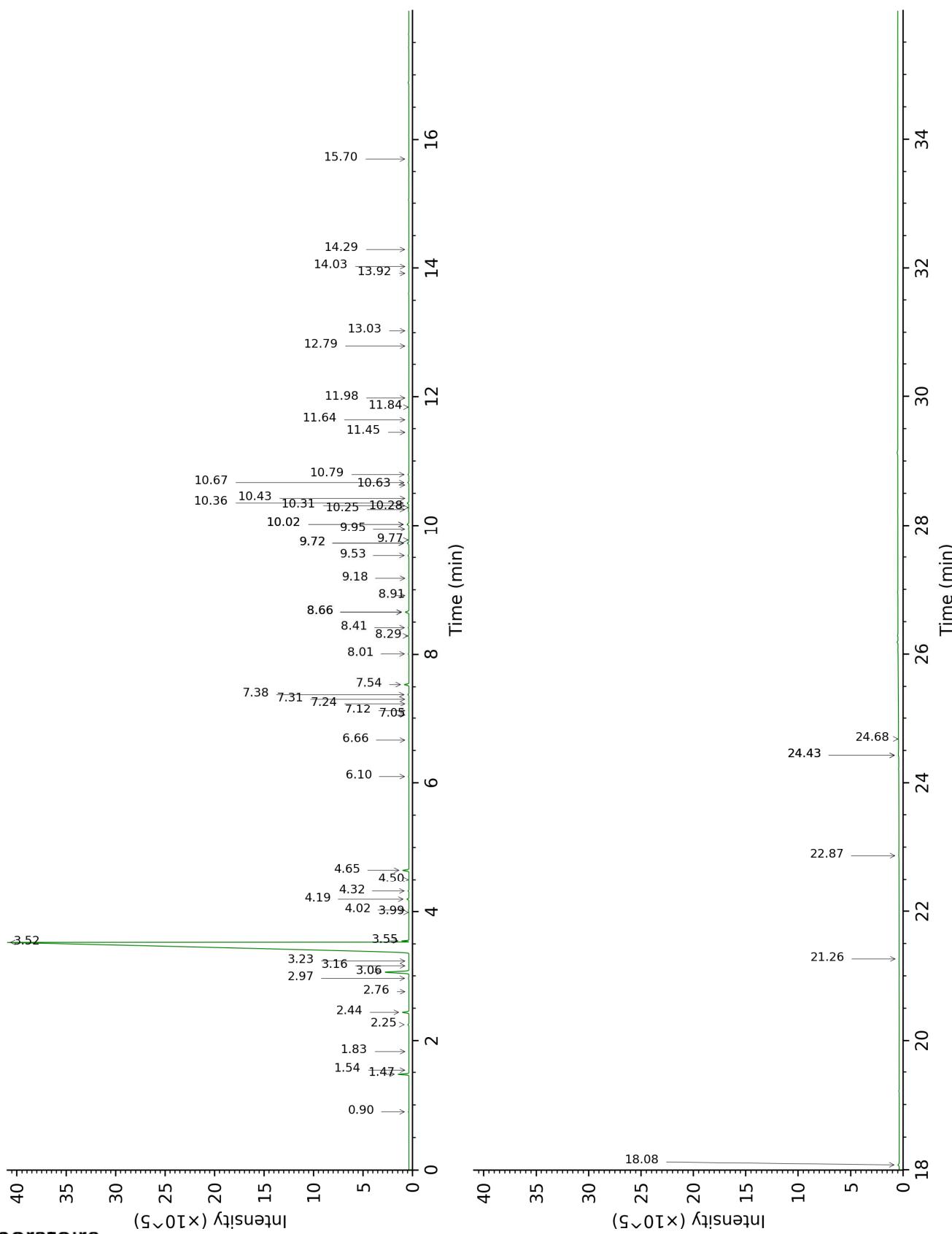
DB-5



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Plus que des analyses... des conseils

DB-WAX



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**PhytoChemia**

Plus que des analyses... des conseils

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.36	495	0.01	0.90	902	0.01
Heptanal	2.60	897	tr	3.24	1148	tr
$\alpha$ -Thujene	2.94	920	0.01	1.54	1002	0.01
$\alpha$ -Pinene	3.01	925	0.50	1.47	995	0.51
Camphene	3.21	938	tr	1.83	1030	tr
Sabinene	3.62*	966	0.40	2.44	1087	0.36
$\beta$ -Pinene	3.62*	966	[0.40]	2.25	1069	0.06
Heptanol	3.71	972	tr	7.05	1424	tr
Myrcene	3.96	988	1.75	3.06	1135	1.76
$\alpha$ -Phellandrene	4.10	998	0.02	2.97	1128	0.03
Octanal	4.13	1000	0.34	4.65	1252	0.33
$\Delta^3$ -Carene	4.18	1002	0.01	2.76	1112	0.01
$\alpha$ -Terpinene	4.30	1010	tr	3.16	1143	0.01
Limonene	4.62*	1031	93.95	3.52	1170	93.96
para-Cymene	4.62*	1031	[93.95]	4.32	1228	0.05
1,8-Cineole	4.62*	1031	[93.95]	3.55	1172	0.25
(Z)- $\beta$ -Ocimene	4.72	1037	tr	3.99	1205	0.01
(E)- $\beta$ -Ocimene	4.87	1046	0.10	4.19	1219	0.10
$\gamma$ -Terpinene	4.98	1053	0.02	4.02	1207	0.03
cis-Sabinene hydrate	5.13	1062	tr	7.12	1429	0.01
Octanol	5.29	1072	0.03	8.42	1526	0.04
Terpinolene	5.43	1081	0.01	4.50	1241	0.01
Linalool	5.71	1098	0.03	8.29	1516	0.03
Nonanal	5.74	1100	0.02	6.10	1355	0.02
trans-para-Mentha-2,8-dien-1-ol	5.97	1115	0.01	9.18	1584	0.01
cis-Limonene oxide	6.12	1125	0.01	6.66	1395	0.01
cis-para-Mentha-2,8-dien-1-ol	6.20	1130	0.01	9.72*	1628	0.09
Citronellal	6.49	1149	0.01	7.24	1437	0.01
$\alpha$ -Terpineol	7.07	1185	0.07	10.02*	1652	0.12
trans-Isopiperitenol	7.20	1194	0.01	10.63	1702	0.01
Decanal	7.32	1201	0.29	7.54	1459	0.27
Octyl acetate	7.45	1210	0.02	7.31	1442	0.02
trans-Carveol	7.52	1215	0.01	11.64	1786	0.01
cis-Carveol	7.70	1226	0.01	11.98	1816	tr
Neral	7.82	1235	0.10	9.72*	1628	[0.09]
(E)-Isogeraniol?	8.09	1253	0.01	11.45	1770	tr
Geranial	8.27	1265	0.12	10.36	1678	0.10
cis-para-Mentha-2,8-diene-1-hydroperoxide	8.83*	1302	0.01			
Undecanal	8.83*	1302	[0.01]	8.91	1564	tr
$\alpha$ -Terpinyl acetate	9.38	1341	0.01	9.95	1646	0.02
Limonene hydroperoxide IV	9.52	1350	0.02			
Neryl acetate	9.65	1360	0.01	10.43	1684	0.01
$\alpha$ -Copaene	9.73	1366	0.06	7.38	1448	0.06
Geranyl acetate	9.93*†	1380	0.11	10.80	1715	0.06

<i>cis</i> -para-Menta-6,8-diene-2-hydroperoxide	9.93*†	1380	[0.11]			
β-Cubebene	9.98*†	1383	[0.11]	8.01	1494	0.04
β-Elemene	9.98*†	1383	[0.11]	8.66*	1544	0.24
Dodecanal	10.27*	1404	0.04	10.25	1670	0.02
Limonen-10-yl acetate	10.27*	1404	[0.04]	11.84	1804	0.01
β-Caryophyllene	10.31	1407	0.25	8.66*	1544	[0.24]
α-Humulene	10.77	1441	0.05	9.53	1612	0.05
(E)-β-Farnesene	10.92	1452	0.02	9.77	1632	0.02
Germacrene D	11.15	1469	0.05	10.02*	1652	[0.12]
Bicyclogermacrene	11.35	1484	0.02	10.31	1675	0.02
α-Muurolene	11.44	1491	0.01	10.28	1673	tr
Cubebol	11.63	1505	0.01	12.79	1888	0.01
δ-Cadinene	11.74	1513	0.07	10.67	1705	0.07
α-Elemol	12.09	1541	0.02	14.29	2026	0.02
(E)-Nerolidol	12.31	1558	0.01	14.02	2001	0.01
Germacrene D-4-ol	12.41	1566	0.01	13.92	1991	0.01
Caryophyllene oxide	12.44	1569	0.01	13.03	1909	0.01
β-Sinensal	13.92	1688	0.01	15.70	2164	0.01
Myristic acid	14.82	1766	0.02	21.26	2792	0.01
Nootkatone	15.07	1788	0.10	18.08	2416	0.09
Palmitic acid	16.99	1963	0.05	22.87	3001	0.06
Bergapten	17.67	2029	0.01			
Osthole	18.55	2117	0.02			
Linoleic acid	18.66	2129	0.02	24.68	3253	0.03
Oleic acid	18.73	2135	0.03			
<i>cis</i> -Vaccenic acid?	18.79	2142	0.04	24.42*	3216	0.08
Stearic acid	18.99	2162	0.07	24.42*	3216	[0.08]
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.20	2184	0.01			
Isoauraptene	19.47	2213	0.04			
Meranzin	19.54	2220	0.07			
Auraptenol	19.88	2256	0.01			
Unknown [m/z 219, 247 (85), 217 (61), 161 (48), 189 (33), 232 (23)... 290 (18)]	21.68	2458	tr			
Auraptene	22.80	2592	0.21			
Epoxyaurapten	23.84	2721	0.08			
Tangeretin	27.04	3135	0.01			
<b>Total identified</b>		<b>99.44%</b>			<b>99.16%</b>	
<b>Total reported</b>		<b>99.44%</b>			<b>99.16%</b>	

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

[xx]: Duplicate percentage due to coelutions, not taken account in the identified 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.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index