

**Date :** September 29, 2020

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 20I21-PTH07

**Customer identification :** Grapefruit Pink - G50109207R

**Type :** Essential oil

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

**Customer :** Plant Therapy

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

**Analysis date :** September 23, 2020

Checked and approved by :

---

Alexis St-Gelais, M. Sc., 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*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.*

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright orange liquid

**Refractive index:** 1.4737 ± 0.0003 (20 °C; method PC-MAT-016)

*ISO 3053:2005 - OIL OF GRAPEFRUIT, OBTAINED BY EXPRESSION*

<b>Compound</b>	<b>Min. %</b>	<b>Max. %</b>	<b>Observed %</b>	<b>Complies?</b>
Nootkatone	0.01	0.80	0.10	Yes
β-Caryophyllene	0.2	0.5	0.3	Yes
Neral	0.02	0.04	0.12	No
Decanal	0.1	0.6	0.3	Yes
Nonanal	0.04	0.10	0.03	No
Octanal	0.2	0.8	0.3	Yes
Limonene	92	96	93	Yes
Myrcene	1.5	2.5	1.8	Yes
β-Pinene	0.05	0.20	0.05	Yes
Sabinene	0.1	0.6	0.4	Yes
α-Pinene	0.2	0.6	0.5	Yes
<b>Refractive index</b>	1.4740	1.4790	1.4737	No

*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
Heptane	tr	Alkane
Heptanal	0.01	Aliphatic aldehyde
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	0.52	Monoterpene
Camphene	0.01	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
$\beta$ -Pinene	0.05	Monoterpene
Sabinene	0.35	Monoterpene
Myrcene	1.84	Monoterpene
$\alpha$ -Phellandrene	0.03	Monoterpene
Pseudolimonene	tr	Monoterpene
Octanal	0.35	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	Monoterpene
Limonene	93.23	Monoterpene
$\beta$ -Phellandrene	0.26	Monoterpene
(Z)- $\beta$ -Ocimene	0.03	Monoterpene
(E)- $\beta$ -Ocimene	0.11	Monoterpene
$\gamma$ -Terpinene	0.02	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Octanol	0.03	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.05	Monoterpenic alcohol
Nonanal	0.03	Aliphatic aldehyde
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.01	Monoterpenic ether
<i>trans</i> -Limonene oxide	0.02	Monoterpenic ether
Citronellal	0.03	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	0.07	Monoterpenic alcohol
<i>trans</i> -Isopiperitenol	0.02	Monoterpenic alcohol
Decanal	0.29	Aliphatic aldehyde
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
<i>cis</i> -Carveol	0.02	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
Neral	0.12	Monoterpenic aldehyde
Geranial	0.11	Monoterpenic aldehyde
Undecanal	0.01	Aliphatic aldehyde
$\alpha$ -Terpinyl acetate	0.02	Monoterpenic ester
Limonene hydroperoxide IV	0.01	Monoterpenic peroxide
Neryl acetate	0.01	Monoterpenic ester
$\alpha$ -Copaene	0.07	Sesquiterpene
<i>cis</i> -para-Mentha-6,8-diene-2-hydroperoxide	0.01	Monoterpenic peroxide
Geranyl acetate	0.10	Monoterpenic ester
$\beta$ -Cubebene	0.04	Sesquiterpene

Dodecanal	0.02	Aliphatic aldehyde
β-Caryophyllene	0.26	Sesquiterpene
α-Humulene	0.03	Sesquiterpene
(E)-β-Farnesene	0.01	Sesquiterpene
Germacrene D	0.04	Sesquiterpene
Bicyclogermacrene	0.02	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
δ-Cadinene	0.07	Sesquiterpene
α-Elemol	0.02	Sesquiterpenic alcohol
Germacrene D-4-ol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
β-Sinensal	0.01	Sesquiterpenic aldehyde
Myristic acid	0.03	Aliphatic acid
Nootkatone	0.10	Sesquiterpenic ketone
Hexadecanal	0.01	Aliphatic aldehyde
Palmitic acid	0.05	Aliphatic acid
Bergapten	0.02	Furanocoumarin
Osthole	0.02	Coumarin
cis-Vaccenic acid?	0.01	Aliphatic acid
Stearic acid	0.17	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.01	Coumarin
Meranzin	0.02	Coumarin
Unknown	0.01	Coumarin
Auraptene	0.18	Coumarin
Tangeretin	0.02	Flavonoid
<b>Consolidated total</b>	<b>99.12%</b>	

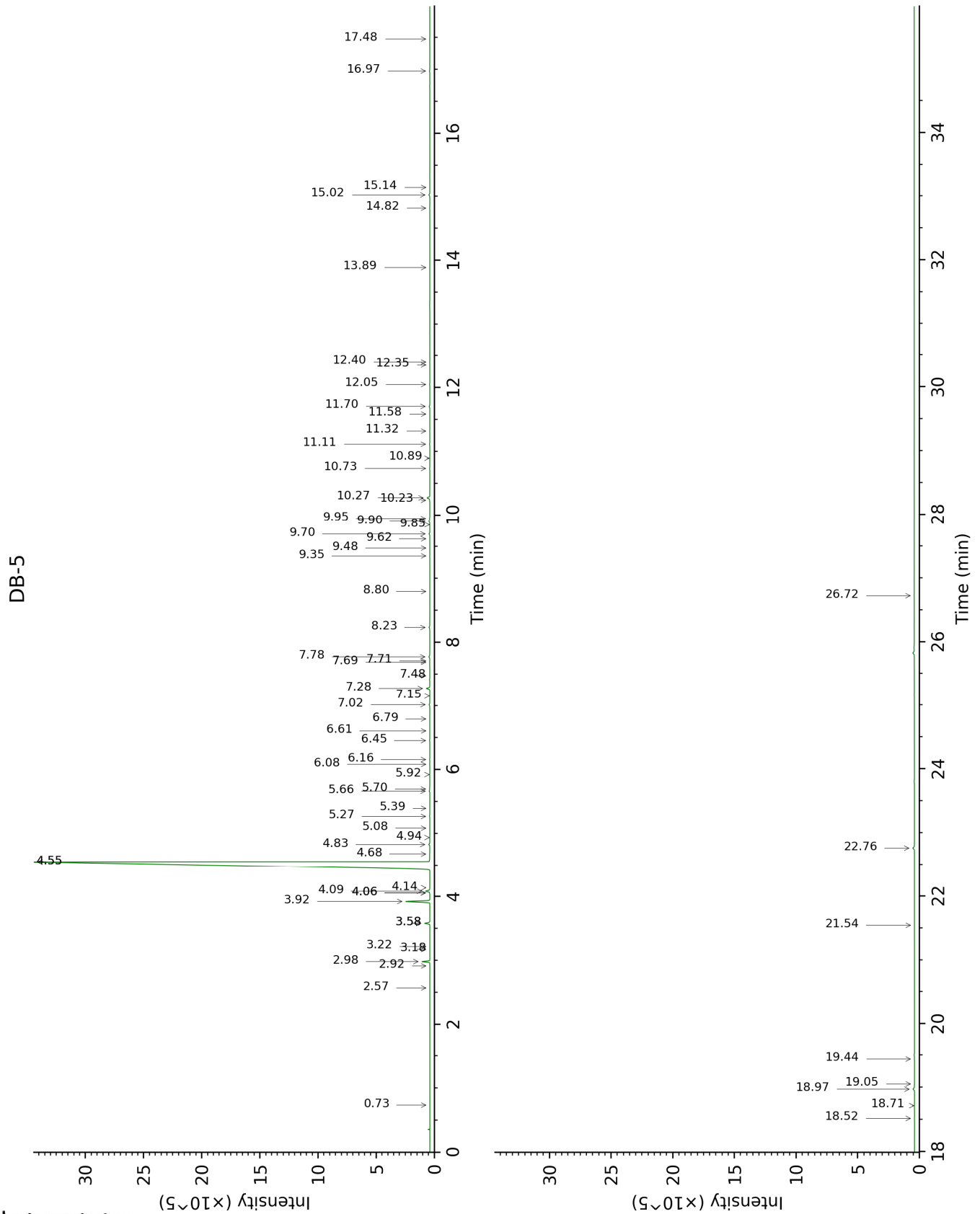
tr: The compound has been detected below 0.005% of total signal.

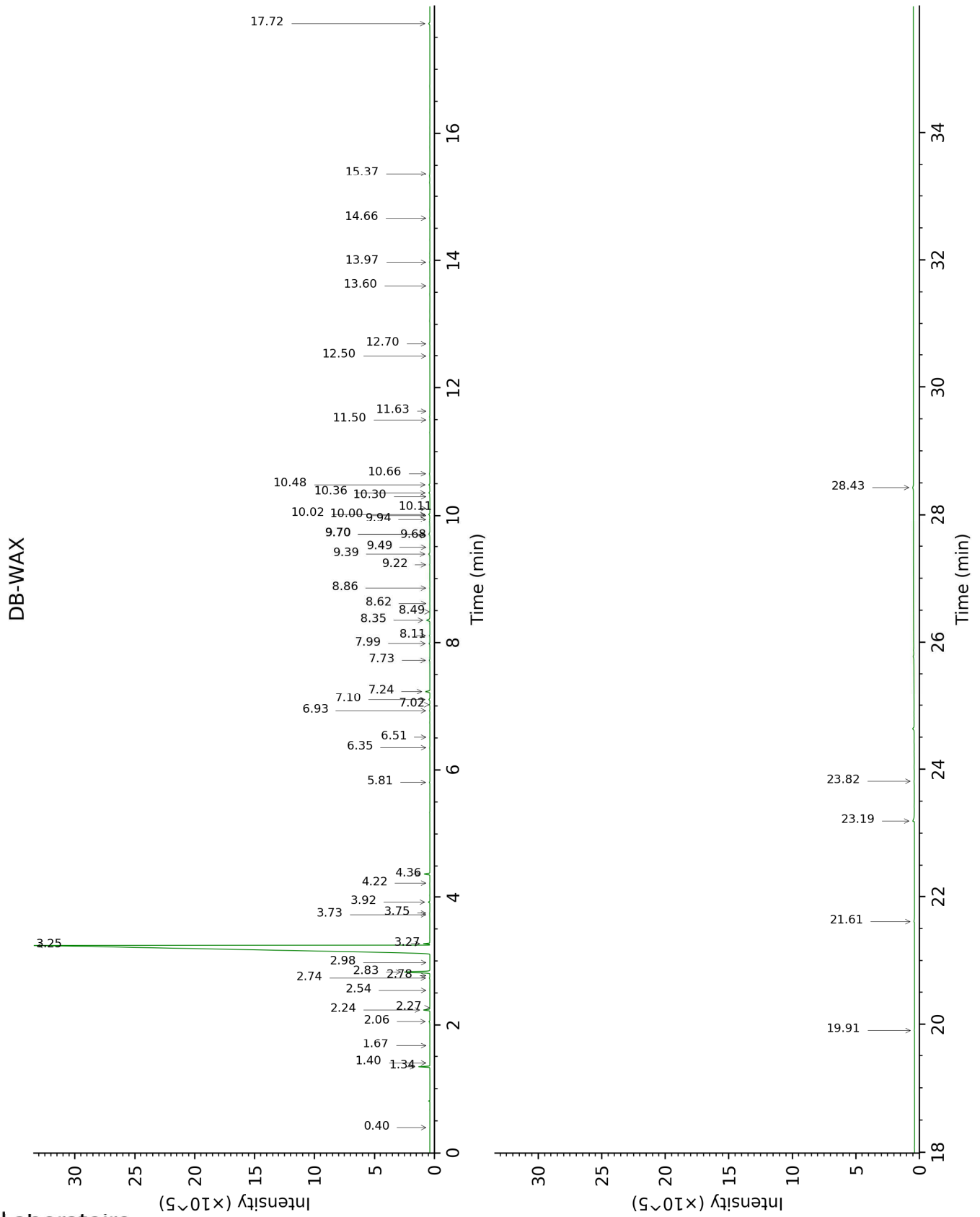
Note: no correction factor was applied

**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.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Heptane	0.73	700	tr	0.40	707	tr
Heptanal	2.57	902	0.01	2.98	1142	tr
$\alpha$ -Thujene	2.92	925	0.01	1.40	998	tr
$\alpha$ -Pinene	2.98	930	0.52	1.34	989	0.52
Camphene	3.18	942	0.01	1.67	1025	tr
Thuja-2,4(10)-diene	3.22	945	0.01	2.27	1085	0.01
$\beta$ -Pinene	3.58*	970	0.40	2.06	1064	0.05
Sabinene	3.58*	970	[0.40]	2.24	1081	0.35
Myrcene	3.92	992	1.84	2.83	1131	1.84
$\alpha$ -Phellandrene	4.06*	1001	0.03	2.74	1124	0.03
Pseudolimonene	4.06*	1001	[0.03]	2.78	1127	tr
Octanal	4.09	1003	0.35	4.36	1247	0.35
$\Delta^3$ -Carene	4.14	1006	0.01	2.54	1109	tr
Limonene	4.55*	1032	93.31	3.25	1163	93.23
$\beta$ -Phellandrene	4.55*	1032	[93.31]	3.27	1166	0.26
(Z)- $\beta$ -Ocimene	4.68	1040	0.03	3.75	1202	0.01
(E)- $\beta$ -Ocimene	4.83	1050	0.11	3.92	1215	0.09
$\gamma$ -Terpinene	4.94	1056	0.02	3.73	1200	0.01
cis-Sabinene hydrate	5.08	1066	0.01	6.93	1431	0.02
Octanol	5.27	1077	0.03	8.11	1520	0.04
Terpinolene	5.39	1085	0.01	4.22	1236	0.01
Linalool	5.66	1102	0.05	7.99	1510	0.05
Nonanal	5.70	1104	0.03	5.81	1348	0.03
trans-para-Mentha-2,8-dien-1-ol	5.92	1118	0.02	8.86	1578	0.01
cis-Limonene oxide	6.08	1129	0.01	6.35	1388	0.02
trans-Limonene oxide	6.16	1133	0.02	6.51	1400	0.01
Citronellal	6.45	1152	0.03	7.02	1438	0.03
Borneol	6.60	1162	0.01	9.70*	1646	0.10
Terpinen-4-ol	6.79	1174	0.01	8.49	1549	0.01
$\alpha$ -Terpineol	7.02	1188	0.07	9.70*	1646	[0.10]
trans-Isopiperitenol	7.15	1197	0.02	10.30	1694	0.01
Decanal	7.28	1205	0.29	7.24	1454	0.29
trans-Carveol	7.48	1218	0.02	11.50	1796	0.01
cis-Carveol	7.69	1232	0.02	11.63	1808	0.01
Citronellol	7.71	1234	0.02	10.66	1724	0.05
Neral	7.78	1238	0.12	9.39	1620	0.09
Geranial	8.23	1268	0.11	10.02	1671	0.08
Undecanal	8.80	1306	0.01	8.62	1559	0.01
$\alpha$ -Terpinyl acetate	9.35	1345	0.02	9.68	1644	0.01
Limonene hydroperoxide IV	9.48	1353	0.01			
Neryl acetate	9.62	1364	0.01	10.11	1679	0.01
$\alpha$ -Copaene	9.70	1369	0.07	7.10	1444	0.07
cis-para-Mentha-6,8-diene-2-hydroperoxide	9.84	1379	0.01			
Geranyl acetate	9.90	1383	0.10	10.48	1710	0.07
$\beta$ -Cubebene	9.95	1386	0.04	7.73	1490	0.04



Dodecanal	10.24	1407	0.02	9.94	1665	0.03
β-Caryophyllene	10.27	1410	0.26	8.35	1539	0.28
α-Humulene	10.73	1444	0.03	9.22	1607	0.02
(E)-β-Farnesene	10.89	1456	0.01	9.50	1629	0.01
Germacrene D	11.11	1472	0.04	9.70*	1646	[0.10]
Bicyclogermacrene	11.32	1488	0.02	10.00	1670	0.02
Cubebol	11.58	1508	0.01	12.50	1884	0.02
δ-Cadinene	11.70	1517	0.07	10.36	1699	0.07
α-Elemol	12.05	1544	0.02	13.97	2021	0.02
Germacrene D-4-ol	12.35	1568	0.01	13.60	1986	tr
Caryophyllene oxide	12.40	1572	0.01	12.70	1902	0.01
β-Sinensal	13.89	1694	0.01	15.36	2157	0.01
Myristic acid	14.82	1774	0.03	19.90	2654	0.03
Nootkatone	15.02	1792	0.10	17.72	2403	0.10
Hexadecanal	15.14	1802	0.01	14.66	2087	0.02
Palmitic acid	16.97	1973	0.05	21.61	2864	0.06
Bergapten	17.48	2022	0.02			
Osthole	18.52	2127	0.02			
cis-Vaccenic acid?	18.72	2148	0.01	23.82	3157	0.03
Stearic acid	18.97	2175	0.17	23.19	3072	0.25
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.05	2183	0.01			
Meranzin	19.44	2225	0.02			
Unknown [m/z 219, 247 (85), 217 (61), 161 (48), 189 (33), 232 (23)... 290 (18)]	21.54	2462	0.01			
Auraptene	22.76	2610	0.18	28.43	3752	0.12
Tangeretin	26.72	3140	0.02			
<b>Total identified</b>		<b>98.93%</b>			<b>98.94%</b>	
<b>Total reported</b>		<b>98.93%</b>			<b>98.94%</b>	

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

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

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