

Date : September 17, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 20A20-PTH07

**Customer identification :** Grapefruit, Pink - USA - G5010893R

**Type :** Essential oil

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

**Customer :** Plant Therapy

ANALYSIS

**Method:** PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sarah-Eve Tremblay, M. Sc. A., Chimiste

**Analysis date :** January 23, 2020

Checked and approved by :

Sylvain Mercier, M. Sc., chimiste 2014-005

*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.*

*This report is an update of the version first issued on February 3, 2020 to indicatively present comparison to a standard.*

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright orange liquid

**Refractive index:** 1.4763 ± 0.0003 (20 °C)

*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	0.13	Yes
β-Caryophyllene	0.2	0.5	0.3	Yes
Neral	0.02	0.04	0.05	No
Decanal	0.1	0.6	0.2	Yes
Nonanal	0.04	0.10	0.05	Yes
Octanal	0.2	0.8	0.3	Yes
Limonene	92	96	92	Yes
Myrcene	1.5	2.5	2.0	Yes
β-Pinene	0.05	0.20	0.18	Yes
Sabinene	0.1	0.6	0.4	Yes
α-Pinene	0.2	0.6	0.6	Yes
<b>Refractive index</b>	1.4740	1.4790	1.4763	Yes

*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	%	Classe
Heptane	tr	Alkane
Heptanal	tr	Aliphatic aldehyde
$\alpha$ -Thujene	tr	Monoterpene
$\alpha$ -Pinene	0.57	Monoterpene
Camphene	tr	Monoterpene
meta-Cymene	tr	Monoterpene
Sabinene	0.38	Monoterpene
$\beta$ -Pinene	0.18	Monoterpene
Myrcene	1.96	Monoterpene
Pseudolimonene	tr	Monoterpene
$\alpha$ -Phellandrene	0.02	Monoterpene
Octanal	0.32	Aliphatic aldehyde
$\Delta^3$ -Carene	tr	Monoterpene
Limonene	92.01	Monoterpene
1,8-Cineole	0.31	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.01	Monoterpene
(E)- $\beta$ -Ocimene	0.08	Monoterpene
$\gamma$ -Terpinene	tr	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.08	Monoterpenic alcohol
Nonanal	0.05	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
cis-Limonene oxide	0.01	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	tr	Monoterpenic alcohol
trans-Limonene oxide	0.01	Monoterpenic ether
Citronellal	0.05	Monoterpenic aldehyde
Terpinen-4-ol	tr	Monoterpenic alcohol
$\alpha$ -Terpineol	0.04	Monoterpenic alcohol
trans-Isopiperitenol	0.03	Monoterpenic alcohol
Decanal	0.24	Aliphatic aldehyde
Octyl acetate	0.03	Aliphatic ester
trans-Carveol	0.01	Monoterpenic alcohol
cis-Carveol	0.01	Monoterpenic alcohol
Citronellol	0.01	Monoterpenic alcohol
Neral	0.05	Monoterpenic aldehyde
Geraniol	0.01	Monoterpenic alcohol
Isopiperitenone	tr	Monoterpenic ketone
Geranial	0.02	Monoterpenic aldehyde
Unknown	0.07	Oxygenated monoterpene
Undecanal	0.01	Aliphatic aldehyde
$\alpha$ -Terpinyl acetate	0.01	Monoterpenic ester
Limonene hydroperoxide IV	0.02	Monoterpenic peroxide
Neryl acetate	0.01	Monoterpenic ester
$\alpha$ -Copaene	0.10	Sesquiterpene
Geranyl acetate	0.04	Monoterpenic ester

β-Cubebene	0.09	Sesquiterpene
β-Elemene	0.02	Sesquiterpene
Dodecanal	0.03	Aliphatic aldehyde
β-Caryophyllene	0.28	Sesquiterpene
α-Humulene	0.04	Sesquiterpene
(E)-β-Farnesene	tr	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
Bicyclogermacrene	0.03	Sesquiterpene
α-Murolene	0.03	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
δ-Cadinene	0.10	Sesquiterpene
α-Elemol	0.02	Sesquiterpenic alcohol
(E)-Nerolidol	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
β-Sinensal	0.03	Sesquiterpenic aldehyde
(2E,6E)-Farnesal	tr	Sesquiterpenic aldehyde
Myristic acid	0.03	Aliphatic acid
Nootkatone	0.13	Sesquiterpenic ketone
Hexadecanal	tr	Aliphatic aldehyde
Palmitic acid	0.08	Aliphatic acid
Bergapten	0.02	Furanocoumarin
Osthole	0.06	Coumarin
Linoleic acid	0.05	Aliphatic acid
Oleic acid	0.05	Aliphatic acid
cis-Vaccenic acid?	0.01	Aliphatic acid
Stearic acid	0.07	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.03	Coumarin
Isoauraptene	0.11	Coumarin
Meranzin	0.24	Coumarin
Meranzin hydrate	0.01	Coumarin
Unknown	tr	Coumarin
Auraptene	0.81	Coumarin
Epoxyaurapten	0.24	Coumarin
Tangeretin	0.12	Flavonoid
3,5,6,7,8,3',4'-Heptamethoxyflavone?	0.04	Flavonoid
3,3',4',5,6,7,8-Heptamethoxyflavone	0.04	Flavonoid
<b>Consolidated total</b>	<b>99.79%</b>	

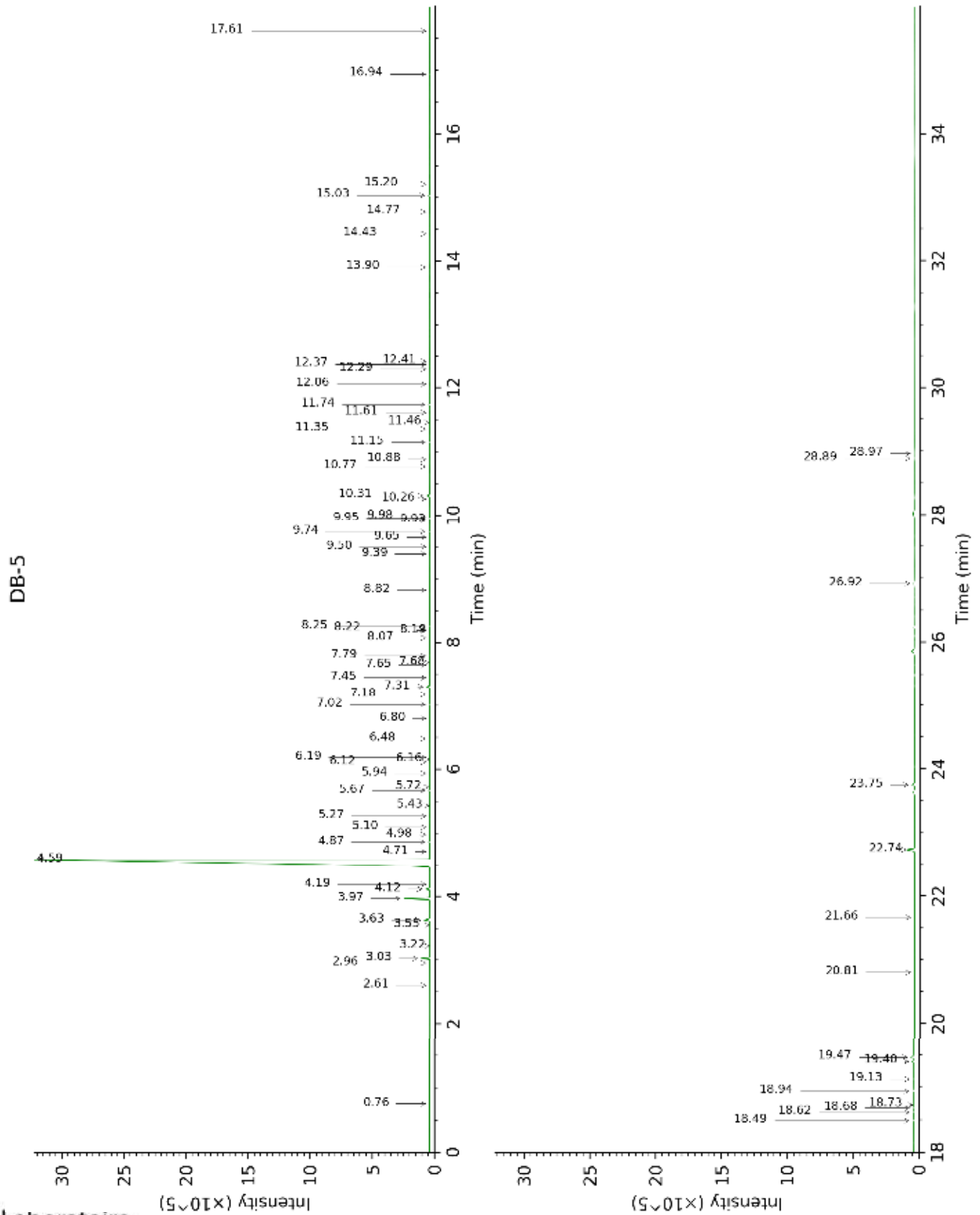
tr: The compound has been detected below 0.005% of total signal.

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	0.76	705	tr	0.42	708	tr
Heptanal	2.61	901	tr	3.07	1148	tr
$\alpha$ -Thujene	2.96	925	tr	1.43	1000	tr
$\alpha$ -Pinene	3.03	930	0.57	1.37	992	0.57
Camphene	3.22	942	tr	1.71	1028	tr
meta-Cymene	3.55	964	tr	2.90*	1135	1.98
Sabinene	3.63*	969	0.56	2.29	1085	0.38
$\beta$ -Pinene	3.63*	969	[0.56]	2.11	1067	0.18
Myrcene	3.97	992	1.96	2.90*	1135	[1.98]
Pseudolimonene	4.12*	1002	0.34	2.84	1130	tr
$\alpha$ -Phellandrene	4.12*	1002	[0.34]	2.80	1127	0.02
Octanal	4.12*	1002	[0.34]	4.46	1252	0.32
$\Delta$ 3-Carene	4.19	1006	tr	2.59	1111	tr
Limonene	4.59*	1032	91.82	3.31	1167	92.01
1,8-Cineole	4.59*	1032	[91.82]	3.34	1169	0.31
(Z)- $\beta$ -Ocimene	4.71	1040	0.01	3.82	1206	tr
(E)- $\beta$ -Ocimene	4.87	1049	0.08	4.00	1219	0.09
$\gamma$ -Terpinene	4.98	1056	tr	3.85	1208	tr
cis-Sabinene hydrate	5.10	1064	0.01	6.88	1427	0.01
Octanol	5.27	1075	0.02	8.24	1528	0.02
Terpinolene	5.43	1085	0.01	4.30	1240	0.01
Linalool	5.67	1100	0.08	8.11	1519	0.09
Nonanal	5.72	1104	0.05	5.90	1355	0.06
trans-para-Mentha-2,8-dien-1-ol	5.94	1118	0.01	8.99	1587	0.01
cis-Limonene oxide	6.12	1129	0.01	6.46	1395	0.01
cis-para-Mentha-2,8-dien-1-ol	6.16	1132	tr	9.48	1626	0.02
trans-Limonene oxide	6.19	1134	0.01	6.62	1408	0.01
Citronellal	6.48	1153	0.05	7.04	1438	0.05
Terpinen-4-ol	6.80	1174	tr	8.61	1557	0.04
$\alpha$ -Terpineol	7.02	1188	0.04	9.80	1651	0.08
trans-Isopiperitenol	7.18	1199	0.03	10.40	1700	0.03
Decanal	7.31	1207	0.24	7.33	1460	0.24
Octyl acetate	7.45*	1217	0.03	7.11	1444	0.03
trans-Carveol	7.45*	1217	[0.03]	11.45	1789	0.01
cis-Carveol	7.65	1231	0.01	11.79	1819	tr
Citronellol	7.68	1234	0.01	10.71	1727	0.01
Neral	7.79	1241	0.05	9.52	1629	0.07
Geraniol	8.07	1260	0.01	11.69	1810	0.01
Isopiperitenone	8.19	1268	tr	11.23	1771	0.01
Geranial	8.22	1271	0.02	10.15	1680	0.13
Unknown [m/z 41, 43 (84), 72 (81), 97 (90), 95 (60)... 150 (4)]	8.25	1273	0.07	12.80	1908	0.01
Undecanal	8.82	1307	0.01	8.70	1565	0.02
$\alpha$ -Terpinyl acetate	9.39	1347	0.01	9.74	1647	0.02
Limonene	9.50	1355	0.02			



hydroperoxide IV						
Neryl acetate	9.65	1366	0.01	10.23	1686	0.01
$\alpha$ -Copaene	9.74	1372	0.10	7.15	1447	0.10
Geranyl acetate	9.93	1385	0.04	10.59	1717	0.06
$\beta$ -Cubebene	9.95	1387	0.09	7.79	1494	0.09
$\beta$ -Elemene	9.98	1389	0.02	8.54	1552	0.01
Dodecanal	10.26	1409	0.03	10.02	1670	0.05
$\beta$ -Caryophyllene	10.31	1413	0.28	8.42	1543	0.27
$\alpha$ -Humulene	10.77	1447	0.04	9.37	1617	0.12
( <i>E</i> )- $\beta$ -Farnesene	10.88	1455	tr	9.60	1636	0.01
Germacrene D	11.15	1475	0.08	9.83	1654	0.05
Bicyclogermacrene	11.35	1490	0.03	10.08*	1674	0.06
$\alpha$ -Muurolene	11.46	1498	0.03	10.08*	1674	[0.06]
Cubebol	11.61	1510	0.01	12.59	1890	0.01
$\delta$ -Cadinene	11.74	1520	0.10	10.44	1704	0.11
$\alpha$ -Elemol	12.06	1545	0.02	14.09	2029	0.03
( <i>E</i> )-Nerolidol	12.29	1564	0.01	13.83	2004	0.01
Germacrene D-4-ol	12.37	1569	0.02	13.71	1992	0.02
Caryophyllene oxide	12.42	1573	0.02	12.72	1902	tr
$\beta$ -Sinensal	13.90	1694	0.03	15.49	2165	0.03
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	14.43	1739	tr	15.88	2205	0.02
Myristic acid	14.77	1769	0.03			
Nootkatone	15.02	1791	0.13	17.85	2414	0.13
Hexadecanal	15.20	1806	tr	14.73	2090	0.01
Palmitic acid	16.94	1966	0.08	21.72	2873	0.12
Bergapten	17.61	2032	0.02			
Osthole	18.49	2118	0.06			
Linoleic acid	18.62	2132	0.05	23.88	3162	0.09
Oleic acid	18.68	2139	0.05	23.51	3111	0.07
<i>cis</i> -Vaccenic acid?	18.73	2143	0.01			
Stearic acid	18.94	2165	0.07	23.30	3083	0.17
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.13	2184	0.03			
Isoauraptene	19.40	2213	0.11			
Meranzin	19.47	2220	0.24			
Meranzin hydrate	20.81	2366	0.01			
Unknown [m/z 219, 247 (85), 217 (61), 161 (48), 189 (33), 232 (23)... 290 (18)]	21.66	2464	tr			
Auraptene	22.74	2590	0.81			
Epoxyaurapten	23.75	2716	0.24			
Tangeretin	26.92	3126	0.12			
3,5,6,7,8,3',4'-Heptamethoxyflavone?	28.89	3305	0.04			
3,3',4',5,6,7,8-Heptamethoxyflavone	28.97	3310	0.04			
<b>Total identified</b>		<b>99.20%</b>			<b>98.52%</b>	
<b>Total reported</b>		<b>99.27%</b>			<b>98.53%</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