

**Date :** March 24, 2020

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 20C11-PSC06

**Customer identification :** Nerolina - Australia - JF20698

**Type :** Essential oil

**Source :** *Melaleuca quinquenervia* ct. Nerolina (linalool/nerolidol)

**Customer :** Pacha Soap Co.

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

**Analysis date :** March 23, 2020

Checked and approved by :

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

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### PHYSICOCHEMICAL DATA

**Physical aspect:** Clear liquid

**Refractive index:**  $1.4714 \pm 0.0003$  (20 °C)

### CONCLUSION

The sample contains plinol isomers, which are considered by some authors as being indicative of addition of foreign linalool. We recommend this observation is considered when evaluating this batch. Furthermore, the important presence of (*Z*)-nerolidol is not, to the best of our knowledge, expected in the species<sup>1,2</sup>, and could indicate addition of foreign nerolidol.

### REFERENCES

- (1) Ramanoelina, P. A. R.; Bianchini, J. P.; Gaydou, E. M. Main Industrial Niaouli (*Melaleuca Quinquenervia*) Oil Chemotype Productions from Madagascar. *J. Essent. Oil Res.* **2008**, *20* (3), 261–266. <https://doi.org/10.1080/10412905.2008.9700007>.
- (2) Ramanoelina, P. A. R.; Viano, J.; Bianchini, J. P.; Gaydou, E. M. Occurrence of Various Chemotypes in Niaouli (*Melaleuca Quinquenervia*) Essential Oils from Madagascar Using Multivariate Statistical Analysis. *J. Agric. Food Chem.* **1994**, *42* (5), 1177–1182. <https://doi.org/10.1021/jf00041a024>.

## ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Classe
Isobutyral	tr	Aliphatic aldehyde
$\alpha$ -Thujene	0.02	Monoterpene
$\alpha$ -Pinene	0.22	Monoterpene
Sabinene	tr	Monoterpene
$\beta$ -Pinene	0.05	Monoterpene
Myrcene	0.07	Monoterpene
$\alpha$ -Phellandrene	0.08	Monoterpene
$\alpha$ -Terpinene	0.12	Monoterpene
para-Cymene	0.48	Monoterpene
Limonene	0.51	Monoterpene
1,8-Cineole	5.77	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.01	Monoterpene
$\gamma$ -Terpinene	0.36	Monoterpene
cis-Linalool oxide (fur.)	0.04	Monoterpenic alcohol
Terpinolene	0.06	Monoterpene
trans-Linalool oxide (fur.)	0.04	Monoterpenic alcohol
Plinol (A?)	0.02	Monoterpenic alcohol
Linalool	35.29	Monoterpenic alcohol
endo-Fenchol	0.02	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.02	Monoterpenic alcohol
Plinol (C?)	0.07	Monoterpenic alcohol
trans-para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.77	Monoterpenic alcohol
trans-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	0.09	Monoterpenic alcohol
Hodiendiol	0.02	Monoterpenic alcohol
trans-Piperitol	0.01	Monoterpenic alcohol
Citronellol	2.23	Monoterpenic alcohol
Piperitone	1.10	Monoterpenic ketone
Eugenol	0.03	Phenylpropanoid
Longifolene	0.02	Sesquiterpene
$\beta$ -Caryophyllene	0.05	Sesquiterpene
Aromadendrene	0.02	Sesquiterpene
Nerylacetone	0.02	Terpenic ketone
Geranylacetone	0.13	Monoterpenic ketone
allo-Aromadendrene	tr	Sesquiterpene
Viridiflorene	0.05	Sesquiterpene
(Z)-Nerolidol	20.68	Sesquiterpenic alcohol
Unknown	0.02	Unknown
(E)-Nerolidol	29.71	Sesquiterpenic alcohol
Unknown	0.05	Unknown
Unknown	0.17	Unknown
<b>Consolidated total</b>	<b>98.47%</b>	

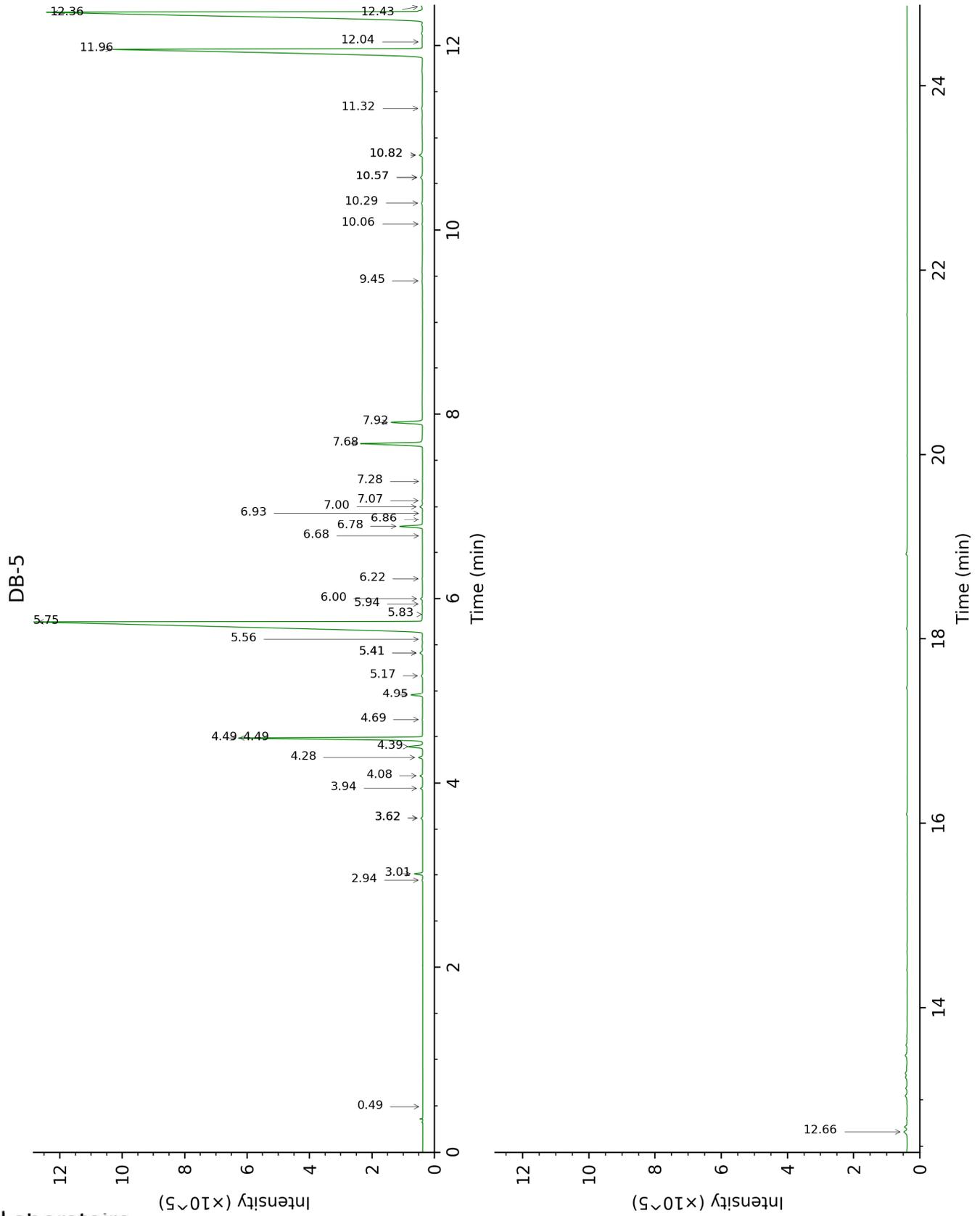
tr: The compound has been detected below 0.005% of total signal.

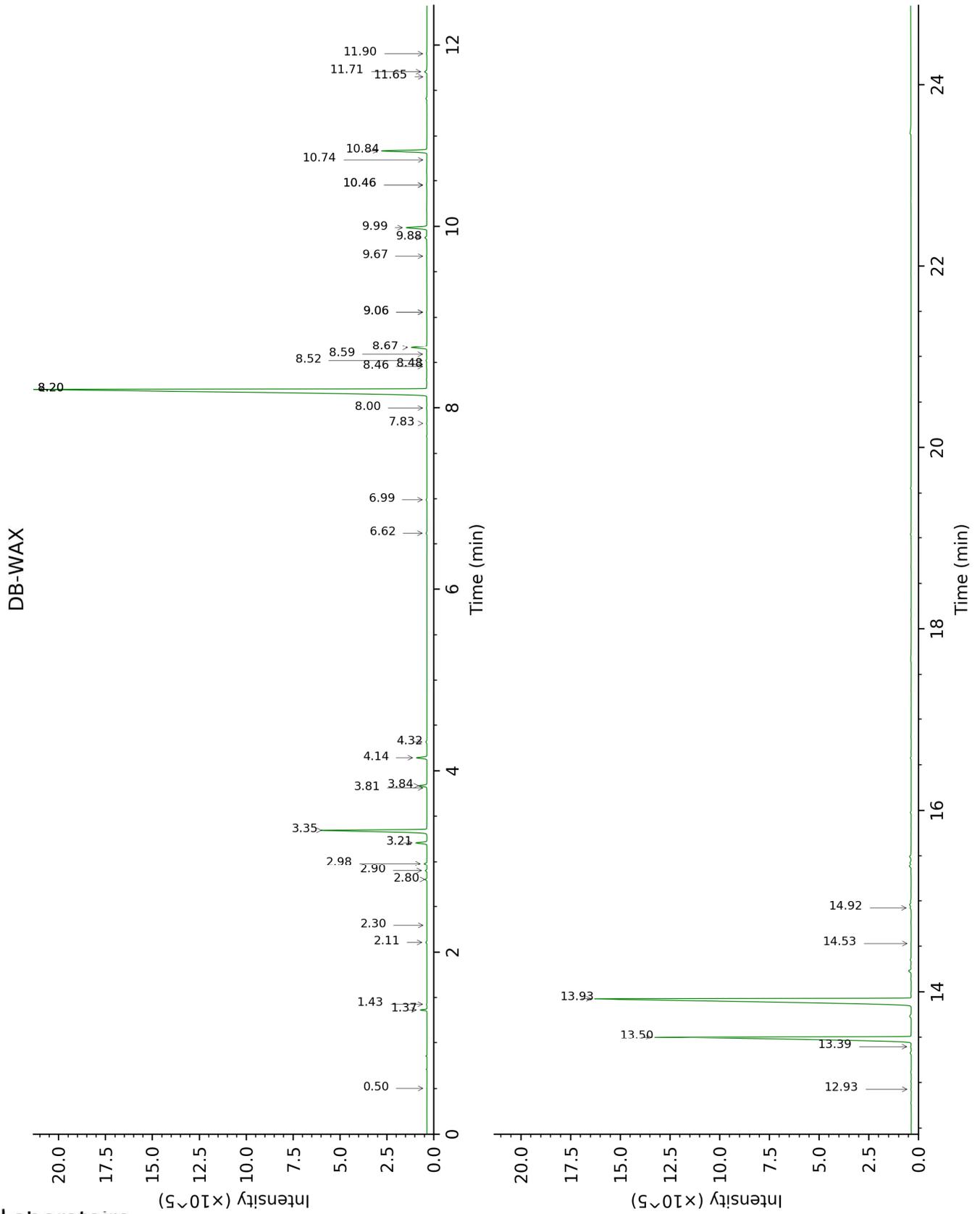
Note: no correction factor was applied

**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.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutyral	0.49	587	tr	0.50	780	tr
α-Thujene	2.94	925	0.02	1.43	996	0.01
α-Pinene	3.01	930	0.22	1.37	988	0.22
Sabinene	3.62*	970	0.05	2.30	1082	tr
β-Pinene	3.62*	970	[0.05]	2.11	1064	0.05
Myrcene	3.94	991	0.07	2.90	1131	0.07
α-Phellandrene	4.08	1000	0.08	2.80	1124	0.08
α-Terpinene	4.28	1013	0.12	2.98	1138	0.13
para-Cymene	4.39	1020	0.48	4.14	1225	0.49
Limonene	4.49*	1026	6.28	3.21	1156	0.51
1,8-Cineole	4.49*	1026	[6.28]	3.35	1166	5.77
(Z)-β-Ocimene	4.69	1038	0.01	3.81†	1201	0.38
γ-Terpinene	4.95	1055	0.36	3.84†	1203	[0.38]
cis-Linalool oxide (fur.)	5.17	1069	0.04	6.62	1403	0.04
Terpinolene	5.41*	1084	0.10	4.32	1237	0.06
trans-Linalool oxide (fur.)	5.41*	1084	[0.10]	6.99	1430	0.04
Plinol (A?)	5.56	1094	0.02	7.83	1492	0.02
Linalool	5.75	1106	35.29	8.20*	1521	35.15
endo-Fenchol	5.83	1111	0.02	8.46	1540	0.02
cis-para-Menth- 2-en-1-ol	5.94	1118	0.02	8.20*	1521	[35.15]
Plinol (C?)	6.00	1122	0.07	8.48	1542	0.02
trans-para- Menth-2-en-1-ol	6.22	1136	0.01	9.06*	1587	0.02
cis-Linalool oxide (pyr.)	6.68	1166	0.01	10.46*	1699	0.02
Terpinen-4-ol	6.78	1173	0.77	8.67	1556	0.77
trans-Linalool oxide (pyr.)	6.86	1178	0.01	10.74	1723	tr
para-Cymen-8- ol	6.93	1183	0.01	11.65	1800	0.01
α-Terpineol	7.00	1187	0.09	9.88	1652	0.10
Hodiendiol	7.07	1192	0.02	12.93	1912	0.02
trans-Piperitol	7.28	1205	0.01	10.46*	1699	[0.02]
Citronellol	7.68	1234	2.23	10.84	1731	2.27
Piperitone	7.92	1250	1.10	9.99	1661	1.11
Eugenol	9.45	1352	0.03	14.92	2099	0.07
Longifolene	10.06	1395	0.02	8.00	1505	0.02
β- Caryophyllene	10.29	1412	0.05	8.52	1545	0.04
Aromadendrene	10.57*	1432	0.10	8.59	1551	0.02
Nerylacetone	10.57*	1432	[0.10]	11.90	1822	0.02
Geranylacetone	10.82*	1451	0.13	11.71	1805	0.13
allo- Aromadendrene	10.82*	1451	[0.13]	9.06*	1587	[0.02]
Viridiflorene	11.32	1488	0.05	9.67	1636	0.02

(Z)-Nerolidol	11.96	1538	20.68	13.50	1964	20.58
Unknown [m/z 123, 131 (67), 91 (60), 105 (58), 109 (56), 93 (48), 124 (47)...]	12.04	1544	0.02	14.53	2061	0.02
(E)-Nerolidol	12.36	1570	29.71	13.92	2004	29.33
Unknown [m/z 109, 69 (60), 43 (40), 93 (28), 41 (25), 111 (22)...]	12.43	1575	0.05	13.39	1955	0.03
Unknown [m/z 69, 81 (86), 95 (69), 137 (51), 41 (44)...]	12.66	1593	0.17			
<b>Total identified</b>		<b>98.30%</b>			<b>97.61%</b>	
<b>Total reported</b>		<b>98.53%</b>			<b>97.65%</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

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