

Date : March 20, 2016

SAMPLE IDENTIFICATION

Internal code : 16C09-CRH1-1-HM

Customer identification : Young Living - Cinnamon Bark - Lot #15B10032 - Untampered seal

Type : Essential oil

Source : *Cinnamomum verum*

Customer : Crystal Heck

ANALYSIS

Method : PC-PA-001-15E06, "Analysis of the composition of a liquid essential oil by GC-FID" (in French).

Identifications double-checked by GC-MS.

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

Analysis date : 2016-03-19

Checked and approved by :

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

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IDENTIFIED COMPOUNDS

Identification	Column: BP5			Column: WAX			Molecular Class
	R.T.	R.I.	%	%	R.I.	R.T.	
Tricyclene	2.99	915	0.01	tr	930	0.82	Monoterpene
α -Thujene	3.07	920	0.03	0.05	958	0.94	Monoterpene
α -Pinene	3.17	926	0.85	0.82	950	0.90	Monoterpene
Camphene	3.44*	943	0.37	0.30	1005	1.13	Monoterpene
α -Fenchene	3.44*	943	[0.37]	0.07	995	1.09	Monoterpene
Sabinene	3.86	969	0.05	0.05	1060	1.57	Monoterpene
Benzaldehyde	3.88	970	0.34	0.35	1442	6.59	Simple phenolic
β -Pinene	3.92	972	0.52	0.40	1042	1.43	Monoterpene
Myrcene	4.20	989	0.06	0.06	1118	2.07	Monoterpene
α -Phellandrene	4.46*	1005	1.01	0.84	1111	2.00	Monoterpene
Δ 3-Carene	4.46*	1005	[1.01]	0.16	1093	1.83	Monoterpene
Octanal	4.61	1013	tr	0.01	1241	3.58	Aliphatic aldehyde
α -Terpinene	4.65	1015	0.02	0.02	1124	2.14	Monoterpene
meta-Cymene	4.74	1020	0.03				Monoterpene
para-Cymene	4.83	1026	2.99	3.07	1214	3.20	Monoterpene
Limonene	4.87*	1028	0.68	0.66	1142	2.35	Monoterpene
β -Phellandrene	4.87*	1028	[0.68]	0.49	1148	2.43*	Monoterpene
1,8-Cineole	4.94	1032	0.47	[0.49]	1148	2.43*	Monoterp. ether
<i>trans</i> - β -Ocimene	5.23	1048	tr	tr	1207	3.10	Monoterpene
Benzyl alcohol	5.28	1051	0.03	0.11	1792	19.98*	Simple phenolic
γ -Terpinene	5.41	1058	0.24	0.24	1191	2.92	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	5.70	1074	0.01	0.01	1389	5.68	Monoterp. alcohol
Terpinolene	5.88*	1084	0.18	0.16	1226	3.38	Monoterpene
Octanol	5.88*	1084	[0.18]	0.02	1516	8.05	Aliphatic alcohol
<i>trans</i> -Linalool oxide (fur.)	6.00	1091	0.01	0.02	1415	6.09	Monoterp. alcohol
α -Linalool	6.05	1094	0.33	6.56	1509	7.87*	Monoterp. alcohol
Linalool	6.31	1107	5.87	[6.56]	1509	7.87*	Monoterp. alcohol
Nonanal	6.42	1111	0.06	0.05	1343	5.01	Aliphatic aldehyde
Unknown (m/z = 70, 43 (93), 81 (74), 55 (68), 41 (62)... 136 (7)?)	6.63	1119	0.01				
endo-Fenchol	6.67	1121	0.01	6.37	1527	8.35*	Monoterp. alcohol
Linalyl methyl ether	6.78	1125	tr	tr	1290	4.27	Monoterp. ether
Ipsdienol	6.84	1127	0.05	0.04	1569	9.61	Monoterp. alcohol
Plinol isomer II	6.90	1130	0.01	0.01	1538	8.68	Monoterp. alcohol
1-Terpineol	7.04	1136	0.02	[6.37]	1527	8.35*	Monoterp. alcohol
Camphor	7.26	1144	0.09	0.09	1430	6.35	Monoterp. ketone
<i>cis</i> - β -Terpineol	7.39	1149	0.02	0.01	1570	9.66	Monoterp. alcohol
Isomenthone	7.67	1160	0.01	tr	1419	6.16	Monoterp. ketone
Isoborneol	7.87	1168	0.01	tr	1593	10.37	Monoterp. alcohol
Borneol	7.93*	1171	0.04	0.01	1622	11.30	Monoterp. alcohol

<i>trans</i> - β -Terpineol	7.93*	1171	[0.04]	0.02	1628	11.57	Monoterp. alcohol
Terpinen-4-ol	8.14	1179	0.02	0.05	1537	8.65*	Monoterp. alcohol
para-Cymen-8-ol	8.55	1195	0.01	0.01	1777	19.11	Monoterp. alcohol
α -Terpineol	8.69	1200	0.86	0.89	1634	11.84	Monoterp. alcohol
α -Phellandrene epoxide	8.78*	1203	0.02	0.01	1731	16.41	Monoterpene
Methylchavicol	8.78*	1203	[0.02]	0.01	1589	10.25	Phenylpropanoid
γ -Terpineol	8.83	1205	0.15	0.15	1637	11.99	Monoterp. alcohol
(<i>Z</i>)-Cinnamaldehyde	9.66	1224	0.27	0.22	1780	19.30	Phenylpropanoid
Unknown (m/z = 137, 43 (35), 152 (31), 91 (27), 109 (24), 119 (22), 41 (20))	9.80	1227	0.01				Oxygenated monoterpene
Cuminal	10.41	1242	0.09	0.08	1678	13.83	Monoterp. aldehyde
Geraniol	10.94	1254	0.08	[0.11]	1792	19.98*	Monoterp. alcohol
2-(1-propenyl)-phenol	11.10	1258	0.01				Phenylpropanoid
(<i>E</i>)-Cinnamaldehyde	12.63	1294	66.53	66.32	1927	29.08	Phenylpropanoid
α -Methylcinnamaldehyde	14.57	1328	0.02				Phenylpropanoid
(2 <i>Z</i> ,4 <i>Z</i>)-5-Phenylpentadienal	15.22	1339	0.01				Synthetic
Eugenol	16.23*	1355	5.19	5.26	2073	36.72*	Phenylpropanoid
α -Copaene	16.23*	1355	[5.19]	tr	1433	6.41	Sesquiterpene
Isocaryophyllene	18.22	1387	0.07	[6.56]	1509	7.87*	Sesquiterpene
β -Ylangene	18.79	1396	0.02				Sesquiterpene
β -Caryophyllene	19.29	1404	6.24	[6.37]	1527	8.35*	Sesquiterpene
(2 <i>Z</i> ,4 <i>E</i>)-5-Phenylpentadienal	19.84*	1410	0.04	0.02	2008	34.01	Synthetic
α -Guaiene	19.84*	1410	[0.04]	[0.05]	1537	8.65*	Sesquiterpene
Aromadendrene	19.96*	1412	0.11	0.06	1530	8.44	Sesquiterpene
Methyleugenol	19.96*	1412	[0.11]	0.08	1942	30.05	Phenylpropanoid
(2 <i>E</i> ,4 <i>Z</i>)-5-Phenylpentadienal	21.50	1431	0.04	[5.26]	2073	36.72*	Synthetic
α -Humulene	21.80*	1434	1.02	1.03	1584	10.07	Sesquiterpene
allo-Aromadendrene	21.80*	1434	[1.02]	0.01	1560	9.38	Sesquiterpene
(<i>E</i>)-Cinnamyl acetate	23.23	1452	3.56	3.44	2049	35.89	Phenylpropanoid ester
Butylated hydroxytoluene	26.86	1496	0.01	0.02	1846	23.46	Synthetic
δ -Cadinene	27.76	1508	0.01	0.01	1672	13.54	Sesquiterpene
<i>trans</i> -Calamenene	28.35	1515	0.01	0.01	1729	16.29	Sesquiterpene
Caryophyllene oxide	32.18*	1565	0.05	0.04	1851	23.80	Sesquiterp. ether
(2 <i>E</i> ,4 <i>E</i>)-5-Phenylpentadienal	32.18*	1565	[0.05]	0.01	2151	39.25	Synthetic
Benzyl benzoate	41.26	1763	0.94	0.88	2489	47.04	Phenolic ester
Total identified			99.8%	99.68%			

*: Two or more compounds are coeluting on this column

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

Note: no correction factor was applied

OTHER DATA

Physical aspect : Slightly yellow liquid

Refractive index : 1.5775 ± 0.0003 (20 °C)

CONCLUSION

This sample is adulterated with synthetic cinnamaldehyde and possibly synthetic linalool. The adulteration is determined from the presence of 5-phenylpentadienal isomers, which are known markers of addition of synthetic cinnamaldehyde¹⁻³. These molecules can be found from their peculiar mass spectra, with peaks $m/z = 129, 158$ being diagnostic^{4,5}. Figure 1 shows a portion of the total ion chromatogram (from *E*-cinnamaldehyde to benzyl benzoate) with extracted peaks in blue (129) and red (158). The four isomers are marked by their configuration in positions 2 and 4. Figure 2 shows the extracted spectrum of (2Z,4Z)-5-phenylpentadienal obtained from this sample.



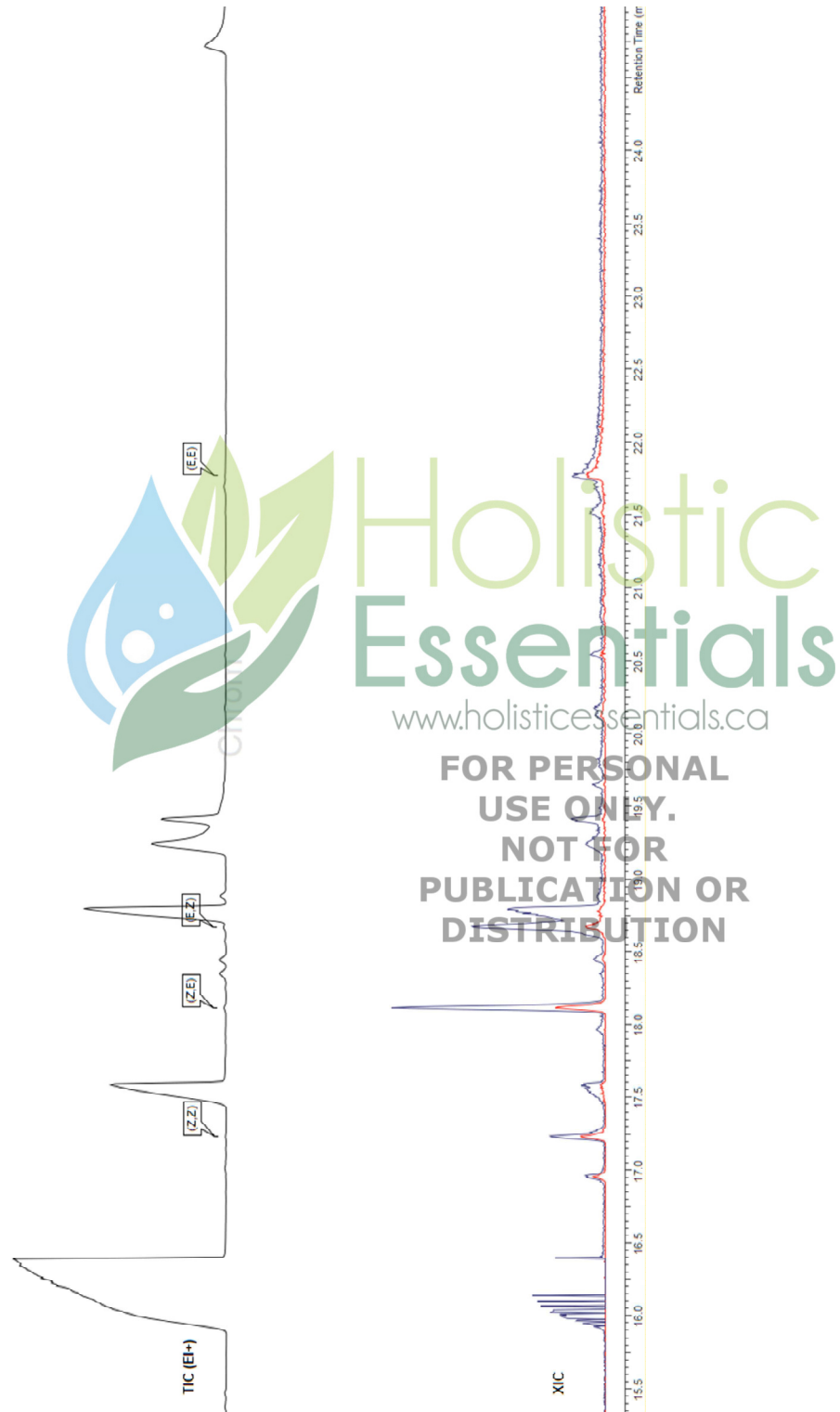


Figure 1. Zoomed section of the total ion chromatogram of the studied sample, with extracted traces for $m/z = 129$ (in blue) and $m/z = 158$ (in red). Matching peaks correspond to the four isomers of the synthetic marker.

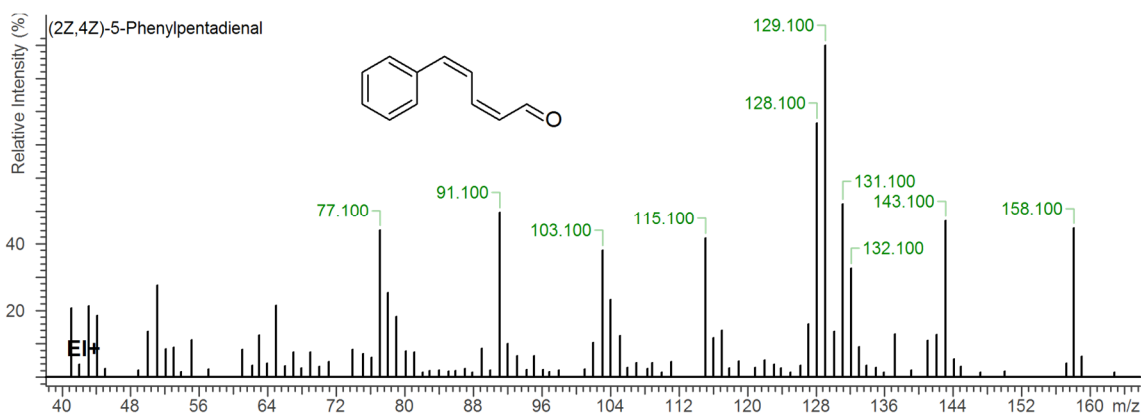
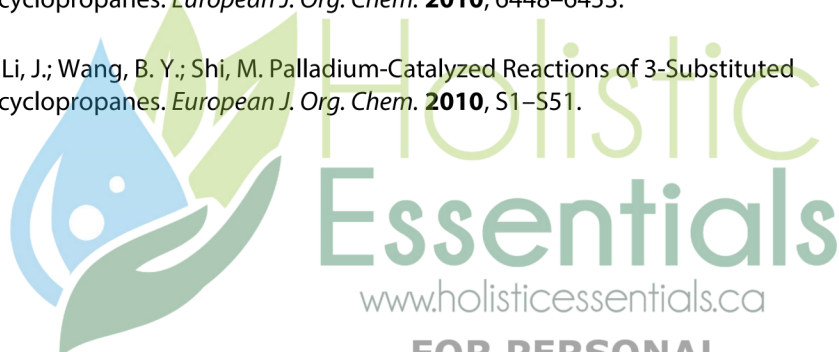


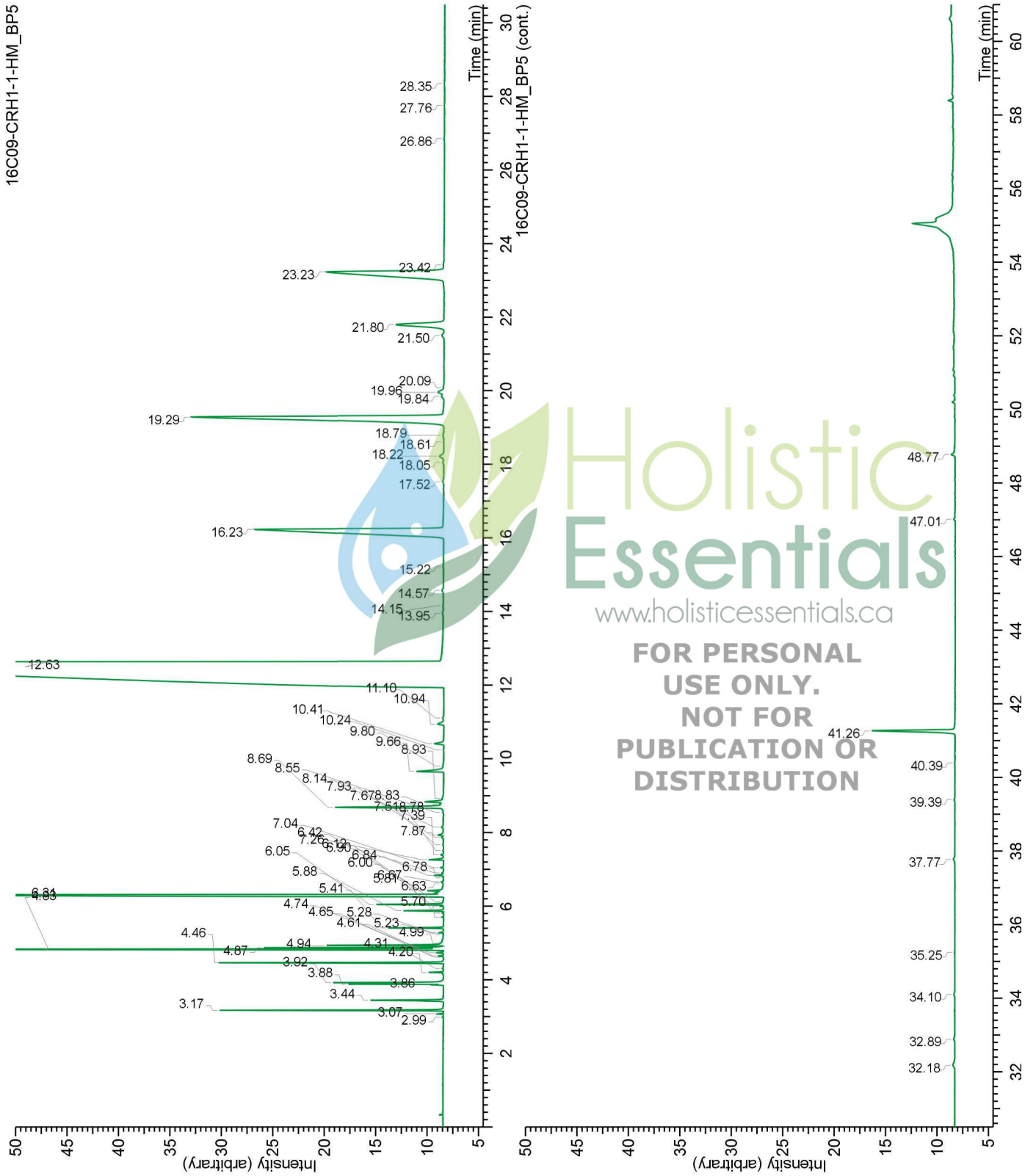
Figure 2. Mass spectrum of the first isomer of phenylpenta-2,4-dienal from the studied sample.

REFERENCES

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- (3) Zhu, M.; Liu, S.; Luo, R.; Bu, Y. GC/MS Detection of Synthetic Cinnamic Aldehyde Added to Cassia Oil. *Yaoxue Xuebao* **1996**, *31*, 461–465.
- (4) Shao, L. X.; Li, J.; Wang, B. Y.; Shi, M. Palladium-Catalyzed Reactions of 3-Substituted Methylene cyclopropanes. *European J. Org. Chem.* **2010**, 6448–6453.
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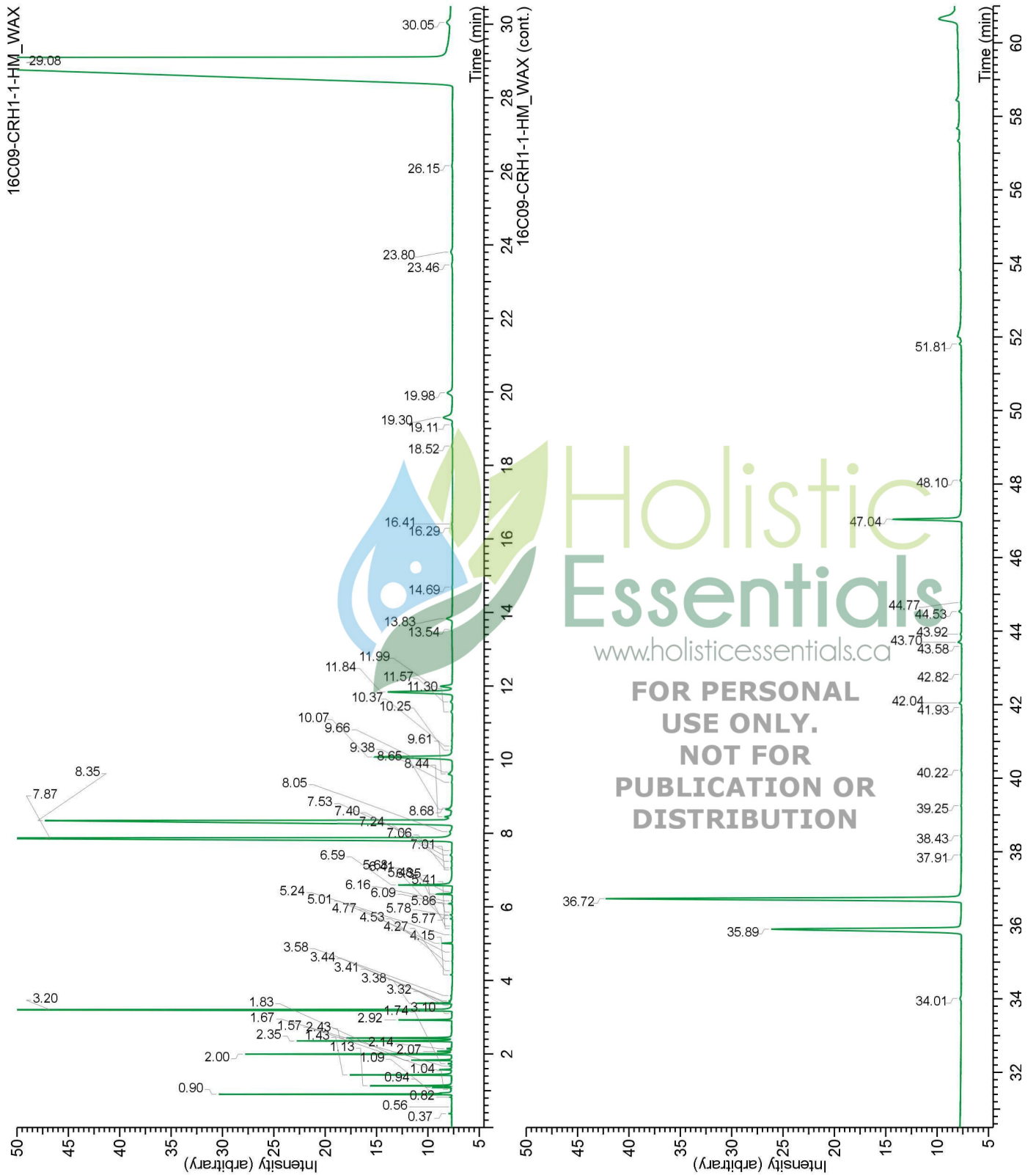
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