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## Isolation and characterization of methyl caprylate from virgin coconut oil (VCO)

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# Isolation and characterization of methyl caprylate from virgin coconut oil (VCO)

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**Abstract.** Caprylic acid is a medium length fatty acid with many potential applications, from bioherbicides to dietary supplements. It was found as a minor constituent of coconut oil and palm kernel oil fatty acids. This study prepared isolated methyl caprylate from virgin coconut oil (VCO) using low pressured fractionated distillation and review its potency as a by-product of Lauric acids production. Neutralized VCO was esterified using basic catalyzed transesterification reaction producing methyl esters of mixed fatty acids. Low pressured fractionated distillation of methyl esters was performed using temperature of 80-120°C, 120-130°C, and 130-150°C. This process produced three fractions of distillates with a volume ratio of 21:19:1, respectively. Gas chromatography analysis using a flame ionization detector confirmed the first fraction of distillates as methyl caprylate.

## 1. Introduction

One of an 8-carbon medium length fatty acid is Caprylic acid, present in coconut oil, bovine milk, and breast milk [11]. It has low solubility in water and oily liquid, smell and taste rancid-like [1]. The major uses of caprylic acid are for the food additive and dietary supplements due to its characteristic as a medium length fatty acid. Some studies described that medium length triglycerides can be used in the weight loss process and burning calorie [12].

Besides food additive and dietary supplements, caprylic acid is also known as a natural herbicide. It disrupts the integrity of the plasmalemma of plant cells, causing desiccation [9]. Some studies reported that Caprylic acid and its monoglyceride can inactive common mastitis pathogens, including *Streptococcus agalctiae*, *Streptococcus dysgalactiae*, *Streptococcus uberis*, *Staphylococcus aureus*, and *Escherichia coli* [6]. Liu et al also reported that caprylic acid suppresses mycelial growth and inhibit spore germination of four phytopathogenic fungi: *Alternaria solani*, *Colletotrichum lagenarium*, *Fusarium oxysporum* f. sp. *cucumerinum* and *Fusarium oxysporum* f. sp. *Lycopersici*.

Virgin coconut oil (VCO) which is extracted by a wet process directly from coconut milk under controlled temperature may have more beneficial effects than refined, bleached, and deodorized (RBD) coconut oil since it retains most of the beneficial components [5]. Compared to RBD coconut oil, VCO contains less unsaturated bond, less peroxide value, and higher phenolic content. A study reported that the production of lauric acid from CCO could be more effective than from RBD due to its chemical properties [8]. Nitbani et al. have studied to isolated lauric acid using low pressured fractionated distillation method with the promising result from crude coconut oil (CCO). This study aims to isolated methyl caprylate from VCO using low pressured distillation and review its potency as a by-product of lauric acids production.



## 2. Materials

VCO used in this study were purchased from the local market. Hydrochloric Acid, Hexane, Methanol,  $\text{Na}_2\text{SO}_4$  anhydrous,  $\text{K}_2\text{CO}_3$ , NaOH,  $\text{Na}_2\text{SO}_4$ , and distilled water. All reagent were purchased from Merck.

## 3. Methods

In order to achieve the research objectives, the step of the research method was adopted by Nitbani et al., 2016. VCO neutralization, VCO neutral transesterification, and isolation of methyl caprylate. Furthermore, methyl ester characterization was conducted using gas chromatography employing an FID detector.

### 3.1. Neutralization of VCO

In separating funnel, dissolved fifty grams of VCO with 50 mL of hexane. Added 30 mL  $\text{Na}_2\text{CO}_3$  30% (w/w) to the funnel and slowly shaken. To make a neutral pH of the upper layer, Added distilled water to it. The yellow liquid dried with anhydrous  $\text{Na}_2\text{SO}_4$ .

### 3.2. Transesterification of neutral VCO

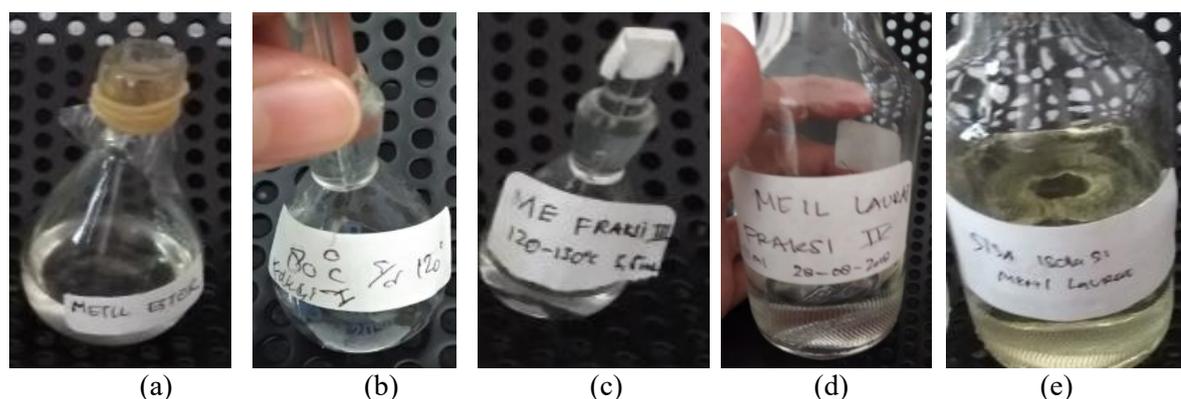
Dissolved  $\text{K}_2\text{CO}_3$  0.25% (w/w) from the total weight of yellow liquid oil with 0.21 mol of methanol. This process was conducted in three neck flask. 0.1 mol of neutral oil was added into the mixture and heated at  $55^\circ\text{C}$  for 3 hours. Dissolved the product in hexane and washed with hot distilled water until a neutral pH reached.

### 3.3. Isolation of methyl caprylate

The isolation process was done by using the low-pressure fractional distillation technique. The fraction from distillation was taken a variety of range of temperature including 80-120, 120-130, and 130- $150^\circ\text{C}$  under 20 cm Hg pressure. Each fraction was further analyzed using GC.

## 4. Results and discussion

Transesterification product from the previous process contained methyl ester from various fatty acids contained in VCO



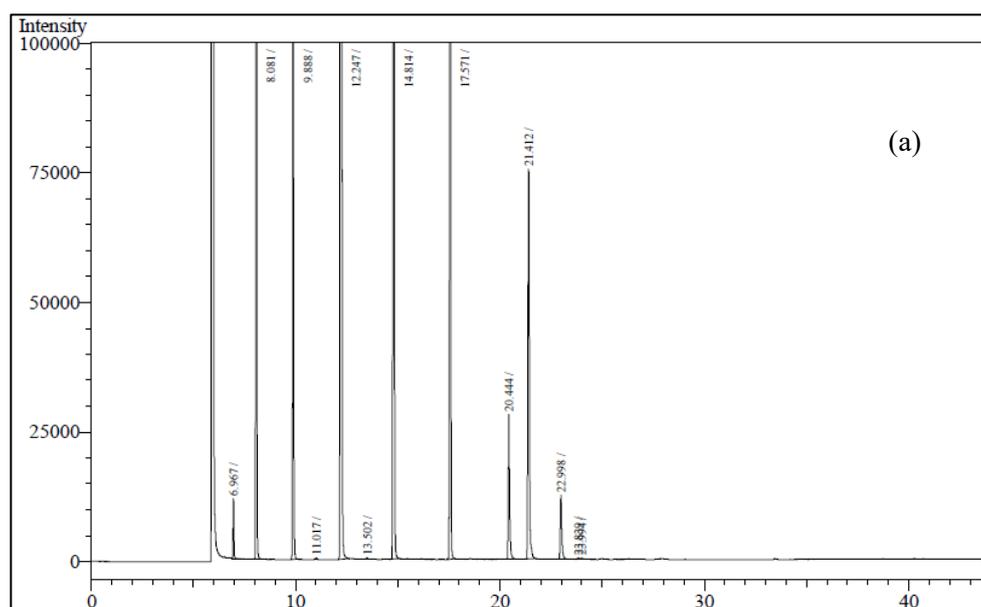
**Figure 1.** (a) Fatty acids product contain a mixture of Methyl ester (b) Distillate of fraction I ( $80-120^\circ\text{C}$ ); (c) Distillate of fraction II ( $120-130^\circ\text{C}$ ); (d) Distillate of fraction III ( $130-150^\circ\text{C}$ ); (e) Distillate of fraction IV ( $>150^\circ\text{C}$ ).

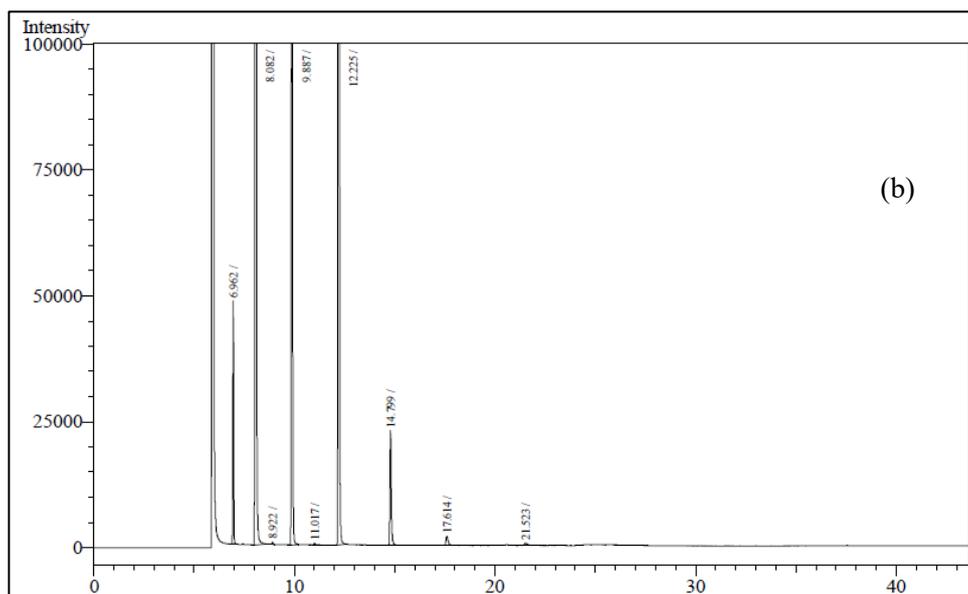
Theoretically, this mixture can be separated using a distillation method based on the difference of the boiling point of each compound. Since the boiling point of these compound at 76 cm, Hg ranged from  $192$  to  $443^\circ\text{C}$ , the distillation using atmospheric pressure is difficult. Low-pressure fractional

distillation was used to decrease the boiling point of each compound to the process can be separated at low temperature. The distillation was conducted under the fractional temperature range of 80-120, 120-130, and 130-150 °C produced three fractions with volume ratio 21:19:1, respectively. The transparent viscous liquid in Fig 1 a, b, c, and d is the product from transesterification reaction. Fig 1e shows fatty acids product contain methyl esters which are yellow viscous liquid.

Furthermore, by using the GC technique to analyze the product of transesterification reaction present in Figure 2. Figure 2a shows the chromatogram of twelve peaks with retention times ranging from 6.96 to 23.99 minute. The greatest peak is shown by the highest peak with 12.24 minutes a retention time and having a relative percentage of 50.38%, indicates that this peak is methyl laurate. Chromatogram of other peaks in figure 2a shows good evidence that the final product of transesterification is purely contained a mixture of fatty acid methyl ester. Figure 2b shows the chromatogram of nine peaks with retention time ranging from 6.96 to 21.52 minute. The greatest peak is shown by the highest peak with 8.08 minute as retention time and having a relative percentage of 62.90%, indicate that this peak is methyl caprylate and can be isolated with low-pressure fractional distillation with high abundance as a by-product of lauric acids production.

The GC analysis of each fraction showed the relative composition methyl ester (Figure 3). Methyl caprylate were highly abundance on fraction 80-120 OC and 120-130 OC with relative composition more than 60%. However, a single distillation process was not effectively separated methyl ester into fractions. Re-distillation can be performed to increase the effectiveness of this process.

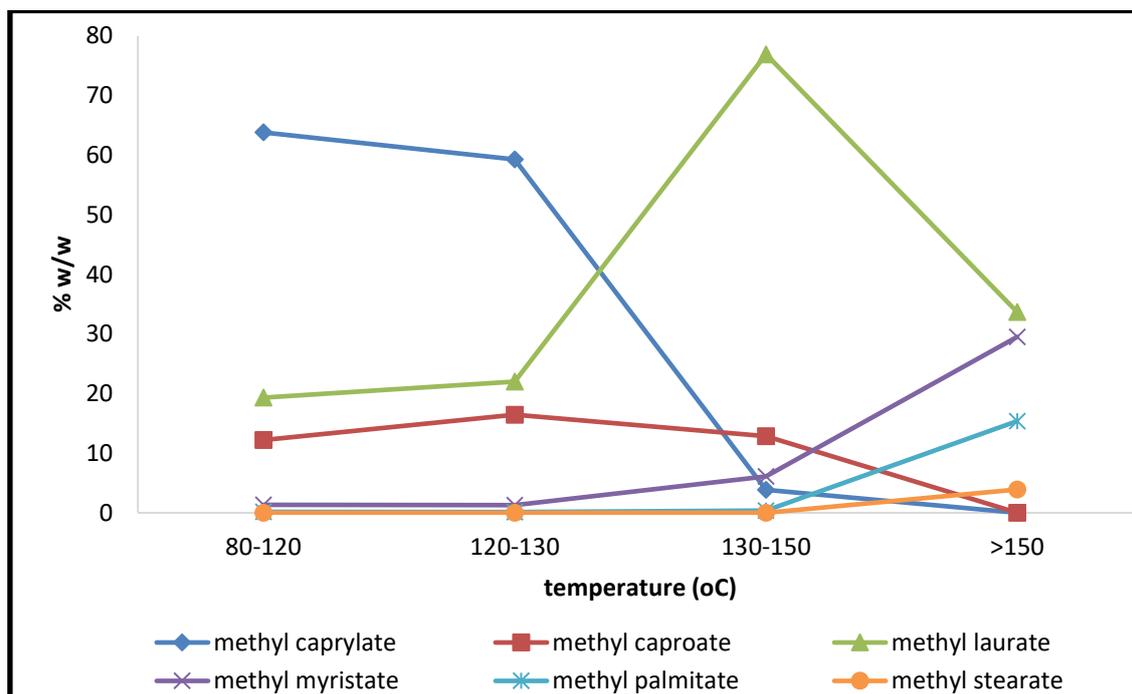




**Figure 2.** Gas chromatogram of (a) Fatty acids product contains a mixture of methyl ester and (b) Product distillate of fraction I (80-120 °C)

**Table 1.** Result (% w/w) composition of methyl ester from each fraction

Parameter	Result (% w/w)				
	Methyl ester	80-120 °C	120-130 °C	130-150 °C	>150 °C
Fatty Acid					
Caproic (C6:0)	0.61	2.04	0.36	-	-
Caprylic (C8:0)	8.25	63.82	59.30	3.85	-
Capryc (C10:0)	6.00	12.21	16.46	12.86	0.02
Undecanoic (C11:0)	0.02	0.02	0.02	0.04	-
Lauric (C12:0)	48.63	19.32	21.99	76.94	33.71
Tridecanoic (C13:0)	0.02	-	-	0.02	0.03
Myristic (C14:0)	17.34	1.32	1.29	6.08	29.51
Palmitic (C16:0)	7.70	0.16	0.13	0.40	15.38
Palmitoleic (C16:1)	-	-	-	-	0.02
Stearic (C18:0)	1.92	-	-	0.01	3.91
Oleic (C18:1n9c)	5.08	0.04	0.02	0.06	9.43
Linoleic (C18:2n6c)	1.11	-	-	-	1.08
Arachidic (C20:0)	0.02	-	-	-	0.09
Linolenic (C18:3n3)	-	-	-	-	0.05
Lignoceric (C24:0)	-	-	-	-	0.03
Fatty acid total	96.70	98.93	99.58	100.27	93.26



**Figure 3.** Relative composition of methyl ester.

## 5. Conclusions

Neutralized VCO was esterified using basic catalyzed transesterification reaction producing methyl ester of mixed fatty acids. Low pressured fractionated distillation of methyl ester was performed using temperature of 80-120 °C, 120-130 °C, and 130-150 °C. This process produced three fractions of distillates with a volume ratio of 21:19:1, respectively. Gas chromatography analysis using a flame ionization detector confirmed the first fraction of distillates as a methyl caprylate.

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