

## Characteristics and Identification of the Metabolite Profile of Arabica Coffee Oil by Using the Gas Chromatography-Mass Spectrometry (GC-MS)

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### ABSTRACT

Indonesia is a tropical country that is suitable for coffee cultivation, and each coffee producing region has its own unique and distinct taste characteristics. This study aimed to determine the characteristics and identification of the metabolite profile of arabica coffee oil. The material used is coffee beans obtained from several coffee Micro, Small, and Medium Enterprises (MSMEs) in Bukanagara Hamlet, Cupunagara Village, Cislak, Subang-West Java. Coffee beans were roasted until medium to dark roast level. Coffee oil was extracted from the ground coffee using n-hexane. Parameters to be observed included oil yield, specific gravity, acid number, peroxide number and identification of metabolite profiles by using Gas Chromatography-Mass Spectrometry (GC-MS). The results of the study showed that Bukanagara arabica coffee had an oil yield of 9.43% with specific gravity of 0.94, acid number of 0.78 mg NaOH/g, and a peroxide number of 8.23 meq/kg. There was total of 20 metabolite compounds identified in arabica coffee oil and based on the area of their distribution there were 11 compounds exist in high proportion.

## 1. INTRODUCTION

Coffee is one of the most popular drinks in the world. For some adult peoples, drinking coffee is a lifestyle and daily habit, including Indonesians (Wolska *et al.*, 2017). Indonesia is a tropical country that is suitable for coffee cultivation, so that Indonesia has a major contribution in providing coffee in the world. Each coffee-producing region in Indonesia has a unique and distinct taste strength that is called local coffee. Apart from climatic factors, soil factors, namely nutrient in the soil, cultivation techniques, and post-harvest handling also determine the taste of coffee (Narulita *et al.*, 2014). Some of the local coffees that are already famous for their taste to foreign countries are Javanese, Mandailing, Gayo, Flores, Lintong, Kintamani, Toraja coffee, and so on (Wahyudi & Jati, 2012).

Bukanagara coffee is a type of local arabica coffee originating from Subang Regency, West Java. Like other local coffees, the named of this coffee was taken from the name of the area where the coffee was grown, namely Bukanagara Hamlet, Cupunagara Village, Cisolak, Subang-West Java. Bukanagara coffee is one of the potentials possessed by Subang Regency, but not many studies have been carried out in an effort to develop its potential. The identification of metabolite profiles is an effort to develop the potential of local coffee in Indonesia so that it becomes basic information regarding the chemical components of the coffee. The metabolite profile is related to the chemical components contained in coffee, however, information related to this is still limited ([Happyana et al., 2020](#)).

Gas Chromatography-Mass Spectrometry (GC-MS) is a spectroscopic technique using the principle of mixture separation based on variations in the velocity of the component constituents. The use of the GC-MS method can be carried out to identify the coffee profile metabolites [not only the main location](#) of chemical content, this is because the GC-MS method can identify compounds found in the volatile coffee gas mixture and can also determine the concentration of these compounds ([Kenyanu et al., 2014](#)). Based on the stated background, this study aimed to determine the characteristics and identification of the metabolite profile of arabica coffee oil.

## 2. MATERIALS AND METHODS

This research was conducted from Mei to Desember 2019 at the Extraction Laboratory Griin.id, Tugu village, Cisarua, West Bandung, West Java. Parameters of specific gravity, acid number, peroxide number were analyzed at Testing Laboratory of Food and Feed, Indonesian Institute of Science (LIPI). Analysis of metabolite profile was conducted at Universitas Pendidikan Indonesia (UPI), West Java.

### 2.1. Materials

The material used in this research is Arabica coffee beans obtained from several coffee Micro, Small, and Medium Enterprises (MSMEs) in Bukanagara Hamlet, Cupunagara Village, Cisolak, Subang, West Java. The coffee beans were roasted at a level of medium to dark with a temperature of 180 °C for 10 min. Before roasting, the coffee fruit is sorted, peeled the skin of the curry bean coffee, fermentation, drying, stripping the parchment (husk), and final sorting. The other materials are filter paper, Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>, n-hexane, NaOH, PP Indicator, chloroform, gracial acetate, potassium iodide, aquadest. The tools used in this research are roaster, thermometer, stopwatch, pycnometer, stative, clamps, burette, dropper, Erlenmeyer, grinder, analytical scale, soxhlet extractor, evaporator, oven, measuring cup, glass bottle, and GC-MS Shimadzu-QP 5050.

### 2.2. Methods

The methods of the research were described in Figure 1. Green beans are roasted at 180 °C for approximately 10 minutes until level medium to dark and further grinding (60 mesh) to reduce size and expand the surface ([Sacchetti et al., 2009](#)). Green beans that have been ground are called ground coffee. The ground coffee was then extracted with a modified method ([Lamona & Nurman, 2018](#)): the ground coffee was weighed as much as 100 g and put in a thimble using filter paper in the extractor tube for further extraction. The solvent used in the extraction was 500 ml of n-hexane which was put into the soxhlet. The extraction process was carried out for 8 h at a temperature of 69° C. The extracted samples then evaporated to the solvent for one hour at a temperature

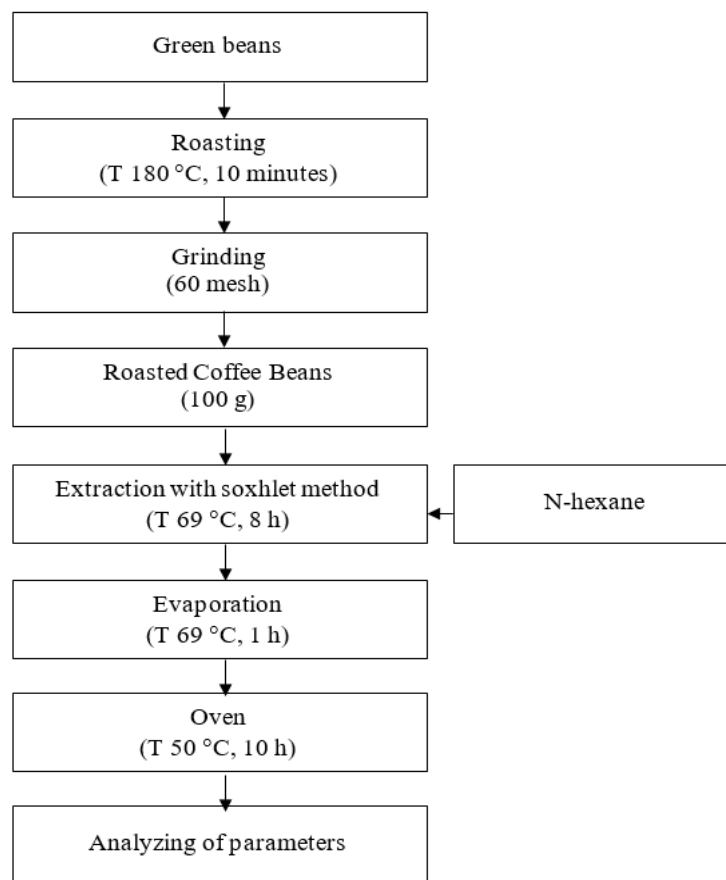
of 69°C. The evaporated sample was then subjected to an oven for 10 h at temperature 50 °C, and then observed the parameters.

### 2.3. Analysis and Measurements

#### 2.3.1. Oil yield

Oil yield is defined as the ratio of the final weight of coffee oil produced to the initial weight of coffee beans and multiplied by 100%. Oil yield off coffee oil was calculated with Equation (1) (Aziz *et al.*, 2009):

$$\text{Oil yield (\%)} = \frac{\text{Final weight}}{\text{Initial weight}} \times 100\% \quad (1)$$



**Figure 1.** The flow chart of coffee oil extraction and analysis

#### 2.3.2. Specific gravity

Specific gravity (SG) was analyzed using a pycnometer and was calculated according to the following formula (Maradesa *et al.*, 2014):

$$SG \text{ (g/mL)} = \frac{\text{(weigh pycno + the sample)} - \text{weigh empty pycno}}{\text{Sample mass}} \quad (2)$$

### 2.3.3. Acid number

Acid number (AN) was analyzed by weighing 10 g of sample, and adding 50 mL of 95% alcohol. The solution was heated in a water bath for 10 minutes while stirring until temperature of 50 °C. The solution was titrated with 0.05 N NaOH and add 3-5 drops of 1% PP indicator until appeared a pink color (Hutapea *et al.*, 2021).

$$AN \text{ (mg NaOH/g)} = \frac{\text{amount of titran NaOH (mL)} \times N \text{ NaOH} \times 39,997}{\text{Sample mass}} \quad (3)$$

### 2.3.4. Peroxide number

Peroxide number (PN) was analyzed by mixing in a closed Erlenmeyer flask 5 g oil and 12 mL of chloroform and 18 mL of glacial acetate. The sample was shaken until homogeneous, 0.5 mL of a potassium iodide saturated solution was then added. The solution was left in a dark room for 30 minutes, and then added 30 mL aquadest. Then into the solution mixture, 0.5 mL of 1% starch was added and immediately titrated with Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> 0.1 N until the blue color disappeared. In the same way, a blank titration was performed (Hutapea *et al.*, 2021).

$$PN \text{ (mg NaOH/g)} = \frac{(V_0 - V_1) \times N \text{ Na}_2\text{S}_2\text{O}_3 \times 1000}{\text{Sample mass (g)}} \quad (4)$$

where V<sub>0</sub> = Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> titration volume in the sample, V<sub>1</sub> = Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> titration volume in the blank, N = Normality Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>.

### 2.3.5. Metabolite Profile

Identification of the metabolite profile contained in the coffee oil was performed by GC-MS (Shimadzu-QP 5050) immediately after the derivatization reaction. The derivatized samples (1 µL) were injected in split mode at temperature of 230 °C and were analyzed. Helium was used as carrier gas, and the column temperature was held at 80 °C for 2 min until temperature increased. Mass spectra were recorded at 20 scans per second. A standard alkane mixture was injected as a solution at the beginning of the GC-MS run of the analysis to calculate retention indices (RIs) used for tentative identification (Putri *et al.*, 2019).

## 3. RESULTS AND DISCUSSION

### 3.1. Characteristics of Bukanagara Arabica Coffee Oil

Bukanagara arabica coffee oil was obtained from the extraction process and had an average oil yield of 9.43%. The yield is an important value in the manufacture of the product because oil yield is related to the amount of bioactive content in the samples (Yuniarifin *et al.*, 2006; Sani *et al.*, 2014; Dewatisari *et al.*, 2018). The average yield of coffee oil with a roasting temperature of 180 °C ranged from 8.54% to 12.87%. The factor that affects the yield is the roasting temperature, at a higher roasting temperature the coffee texture will be more fragile. The more fragile the beans, the easier solvent to penetrate the coffee beans so that they can extract higher coffee oil (Yuwanti *et al.*, 2016). Other factors that affect the yield are extraction time, type, and volume of solvent. Research conducted by (Aziz *et al.*, 2009) proved that the extraction time, type and volume solvent are effect in the yield of coffee oil produced, the many solvent and the longer the extraction, the greater the yield. The result of specific gravity is 0.94, and coffee oil already meets existing standards where the quality

requirement of specific gravity for coffee oil is from 0.94 to 0.98 (Schuette *et al.*, 1934). An acid number of 0.78 mg NaOH/g is considerably lower than the standard 2.1-7.9 mg NaOH/g, whereas a peroxide number of 8.23 meq/kg is significantly higher than the standard 0.69-1.07 meq/kg (Schuette *et al.*, 1934). The higher the roasting temperature, the higher the acid number of coffee oil obtained as well as the peroxide number, the higher the roasting temperature will accelerate the oxidation process of coffee oil so that the resulting peroxide number is higher (Yuwanti *et al.*, 2016).

### 3.2. Identification of The Bukanagara Arabica Coffee Oil Metabolite Profiles

Based on the research conducted, the total metabolite compounds identified in Bukanagara Arabica coffee oil were 23 compounds. Another research stated that roasted Arabica coffee contained 35 compounds, dominated by volatile compounds, organic acids, sugars, alcohols, and long chains (Casas *et al.*, 2017). There are several things that affect this, one of which is the extraction process. The extraction process will produce a large enough pressure on the coffee, so that the temperature inside also increases, as a result, long-chain compounds with high boiling points can evaporate (Lutfiah, 2021). The following is the result of the GC-MS chromatogram at Figure 2. Based on the area of distribution, there are 11 compounds that have a larger distribution area than other metabolite compounds. The results of metabolite compounds in Bukanagara arabica coffee oil are listed in Table 1.

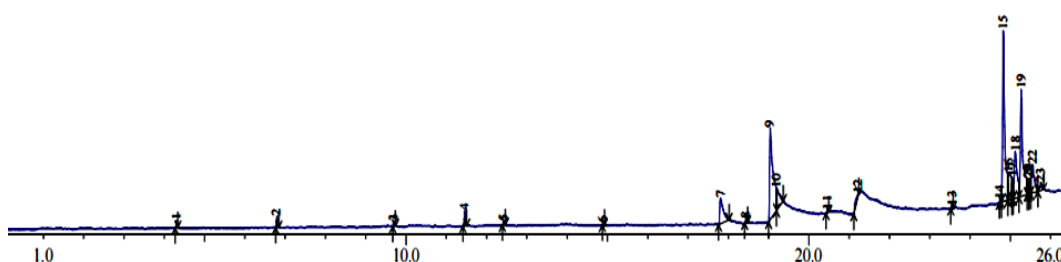


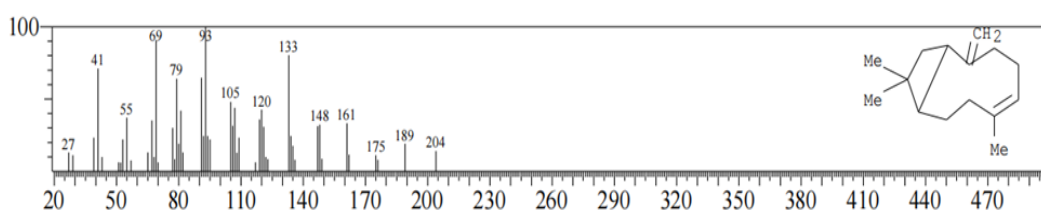
Figure 1. Chromatogram from GC of Bukanagara arabica coffee oil

Table 1. Metabolite compounds in Bukanagara arabica coffee oil

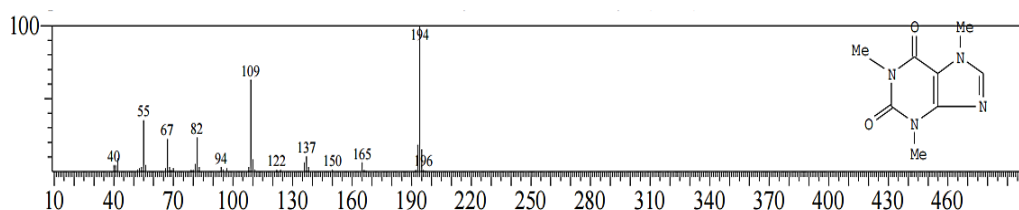
Peak	R.Time	Area	Area%	Height	A/H	Name
4	11.457	107708	1.02	57595	1.87	Caryophyllene
7	17.810	602358	5.70	99640	6.05	Caffeine
9	19.044	2104370	19.91	361677	5.82	Pentadecanoic acid (CAS) Pentadecylic acid
10	19.210	391695	3.71	83159	4.71	Hexadecanoic acid (CAS) Palmitic acid
12	21.225	128005	1.21	8831	14.49	9,12-Octadecadienoic acid- (CAS) Linoleic acid
16	24.963	523890	4.96	103799	5.05	2,3-Dimethylbenzofuran
17	25.050	203874	1.93	84195	2.42	5-N-Pentadecyl-1,2,3,4-Tetrahydronaphthalene
18	25.125	920437	8.71	183857	5.01	Benzene, (2-methyl-1-butenyl)- (CAS) 1-Butene, 2-methyl
19	25.272	1839148	17.40	421340	4.36	Pregnenolone acetate
21	25.489	167602	1.59	59384	2.82	9-Dehydro-1-Methyl Estrone Methyl Ether
23	25.764	121459	1.15	30184	4.02	Tetracosane (CAS) n-Tetracosane

Note : CAS = Chemical Abstracts Service

The metabolite compounds of caryophyllene have a content fragmentation pattern as in Figure 3. The results of the GC chromatogram that have been carried out show that Bukanagara arabica coffee oil contains caryophyllene obtained at peak 4 with a retention time 11.457 and an area of 1.02%. According to Nugraha *et al.* (2020), who conducted research on the volatile components of the ari skin of coffee beans (*coffea robusta*), was found caryophyllene at a retention time of 10.509, and an area of 4.56%. Caryophyllene was also found in robusta coffee flowers at a retention time of 24.175 but at 0.00% (Hafsah *et al.*, 2020). Caryophyllene is a naturally occurring bicyclic sesquiterpene which is an important constituent of plants (Freire *et al.*, 2012; Gertsch *et al.*, 2008). Caryophyllene enters into an active *sesquiterpene bi-cyclic*, produced by plants in response to threats from herbivores (Araniti *et al.*, 2017). In addition, caryophyllene have activities antimicrobials and analgesics (Nugraha *et al.*, 2020). These compounds can be used as additives for food or cosmetics (Sköld *et al.*, 2006).



**Figure 3.** Fragmentation patterns caryophyllene

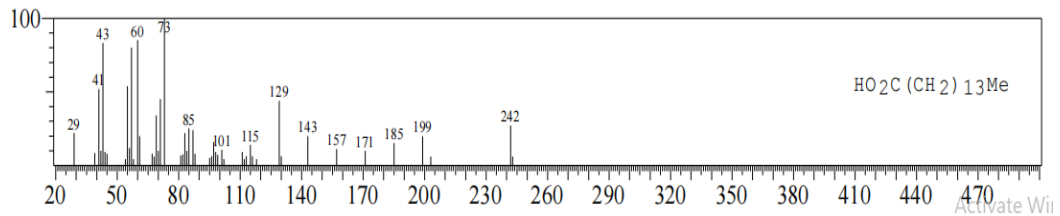


**Figure 4.** Fragmentation patterns caffeine

Bukanagara Arabica coffee oil contains caffeine compounds with retention time 17.810 and an area of 5.70% at Figure 4. According to Hafsah *et al.* (2020), who conducted research on the volatile compounds from flowers and secondary metabolites from the skin pulp, green beans, and peaberry green beans of robusta coffee, was founded caffeine caffeine is in every part of the coffee studied. Skin pulp have retention time 15.891- 15.805 and relative peak area 16.02-4.51%; pea berry skin-pulp have retention time 15.883-15.801 and relative peak area 10.26-5.52%; green bean retention time 16.160-16.117 and relative peak area 79-51.15%; and pea berry green bean have retention time 16.280 -6.607 and relative peak area 52.46-74.88%. Caffeine is one of the main compounds contained in coffee, caffeine is also an indicator of good or bad coffee (Happyana *et al.*, 2020). Caffeine (1,3,7-trimethylxanthine) is the main active ingredient in coffee, belongs to the group of alkaloids methylxanthine which acts as antagonists of adenosine receptors A1, A2A, and A2B, it also too contributes to the taste of coffee (Nugraha *et al.*, 2020).

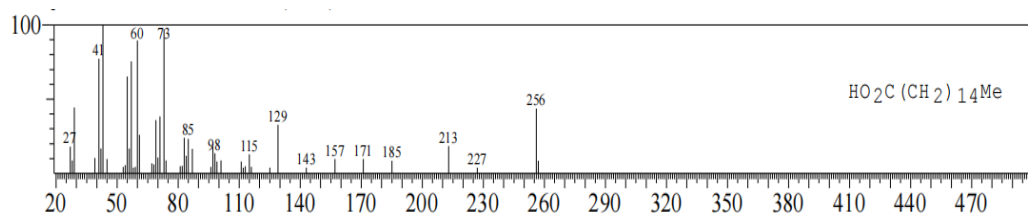
Pentadecanoic acid (CAS) Pentadecylic acid appeared at peak 9 have retention time 19.044 and an area of 19.91% at Figure 5. Research conducted by Chuaca *et al.* (2022) also found the same components in coffee oil compositions from RTD coffee, with the

retention time of 17.525 and area of 2.72%. Pentadecanoic acid was also found in Arabica coffee bean oil at a retention time of 19,151 and an area of 4.08%. Pentadecanoic acid is the active compound contained in coffee oil which is a saturated fatty acid (Lamona & Nurman, 2018).

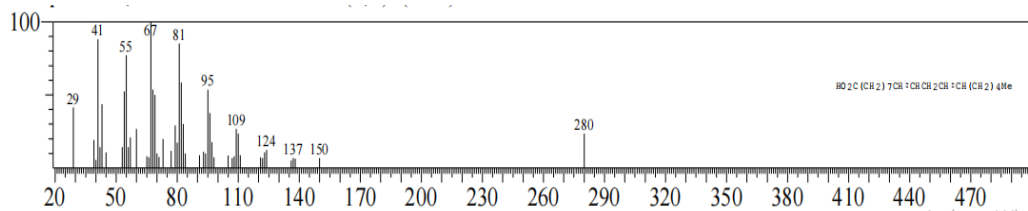


**Figure 5.** Fragmentation patterns Pentadecanoic acid (CAS) Pentadecylic acid

The compound hexadecanoic acid (CAS) Palmitic acid also appeared in Bukanagara arabica coffee oil at peak 10 with retention time 19.044 and an area of 3.71% at Figure 6. Nugraha *et al.* (2020) stated that on ari's coffee beans also contained hexadecanoic acid at a retention time of 16,196 and an area of 11.48%. Chuaca *et al.* (2022) also stated in coffee oil compositions from freshly brewed coffee there was also a retention time of 11,396 and an area of 0.02% and retention time of 11,277 and an area of 1.05% at coffee oil compositions from RTD coffee. This compound was a fatty acid found in both arabica and robusta coffee oil extracts, besides palmitic acid is found in green beans coffee and roasted beans coffee. The main fatty acids contained in Colombian roasted bean coffee were palmitic (46.1%), linoleic (32.9%), oleic (8.0%), stearic (6.6%) and arachidic (1.9%) (Yu *et al.*, 2016). These compounds are volatile compounds from coffee oil which can be used for the food and cosmetic industries.



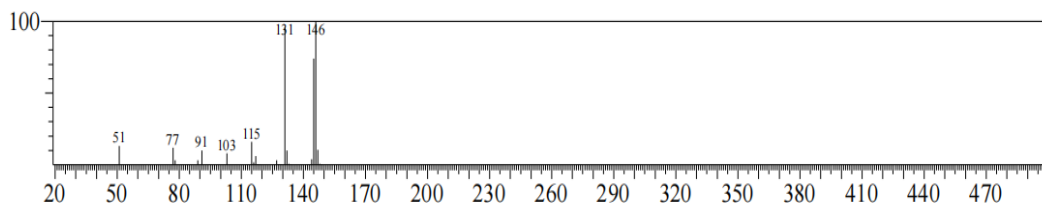
**Figure 6.** Fragmentation patterns Hexadecanoic acid (CAS) Palmitic acid



**Figure 7.** Fragmentation patterns 9,12-Octadecadienoic acid- (CAS) Linoleic acid

Bukanagara arabica coffee also contains 9,12-Octadecadienoic acid - (CAS) Linoleic acid at peak 12 with retention time 21.225 and area 1.21% Figure 7. Coffee oil compositions from RTD coffee has linoleic acid with retention time 16.935 and area 0.74%, while coffee oil compositions from freshly brewed coffee has linoleic acid with

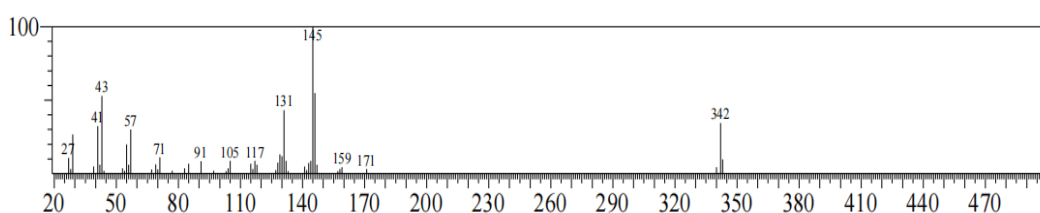
retention time 19.501 and area 2.89%. Linoleic acid is one of the fatty acids that can be used for biodiesel (Chuaca *et al.*, 2022). This compound is an antioxidant compound and in the study Lamona & Nurman (2018) it was concluded that arabica ground coffee has an oil component, one of which is linoleic acid, which retention time 21.198 and area 2.61%. The linoleic acid content in coffee is related to the roasting process, the longer the roasting process will reduce the linoleic acid content.



**Figure 8.** Fragmentation patterns 2,3-Dimethyl benzofuran

2,3-Dimethylbenzofuran was found in the peaks of 16 areas with retention time 24.963 and area 4.96% at Figure 8. Aziz *et al.* (2009) through his research stated that there are several compounds contained in coffee oil, one of which is 2,3-Dimethylbenzofuran. Coffee beans contain 10-15% coffee oil or coffee bean oil. Coffee oil is a compound that mostly contains triacylglycerol with number of aromatic compound constituents, one of the compounds and total fatty acids in coffee oil is 2,3-Dimethylbenzofuran.

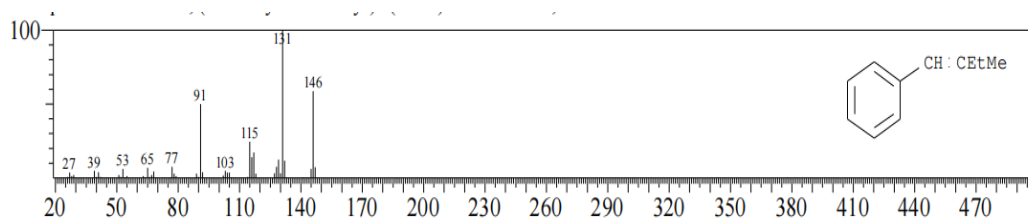
5-N-Pentadecyl-1,2,3,4- Tetrahydronaphthalene appeared in Bukanagara arabica coffee oil at peak 17 with retention time 25.050 and an area of 1,93% at Figure 9. This compound is an indication of the ink given from the packaging used. Lago & Ackerman (2016) through the research there are other compounds that can be identified when examining a sample, these compounds can come from packaging ink that is in direct contact with the sample. GC-MS is a method that can be identified from the printing ink that is on the packaging (Peters *et al.*, 2019). Another study conducted by Asensio *et al.* (2019) can also exclude compounds from various types of packaging used by coffee sellers.



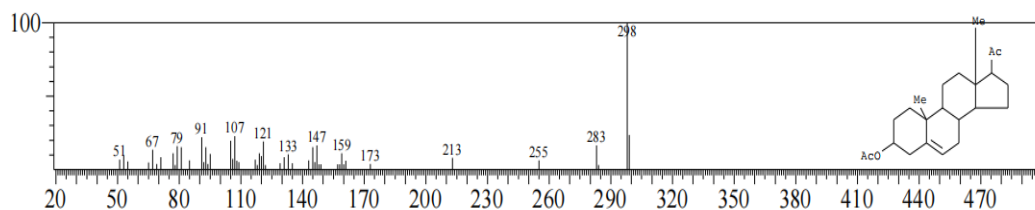
**Figure 9.** Fragmentation patterns 5-N-Pentadecyl-1,2,3,4-Tetrahydronaphthalene

Benzene, (2-methyl-1-butenyl) - (CAS) 1-Butene, 2-methyl was also found in the samples studied. Benzene, (2-methyl-1-butenyl) - (CAS) 1-Butene, 2-methyl was found on peak 19 with retention time 25.125 and an area of 8,71% at Figure 10, this compound is one of the volatile compounds in coffee that plays a role in providing flavor coffee. These compounds were also found in green beans through the Total Ion Chromatogram (TIC) method (Kim *et al.*, 2019). In addition, these compounds also appear in roasting coffee at 13.54 minutes (Agresti *et al.*, 2008).

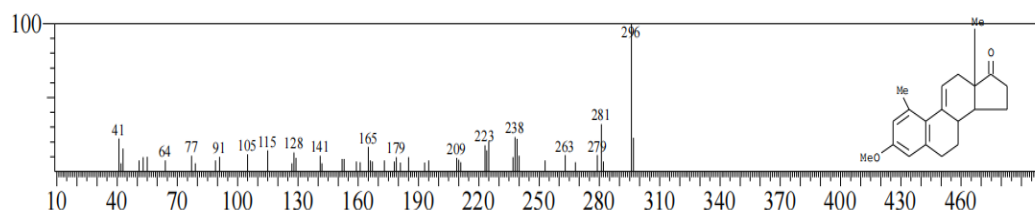




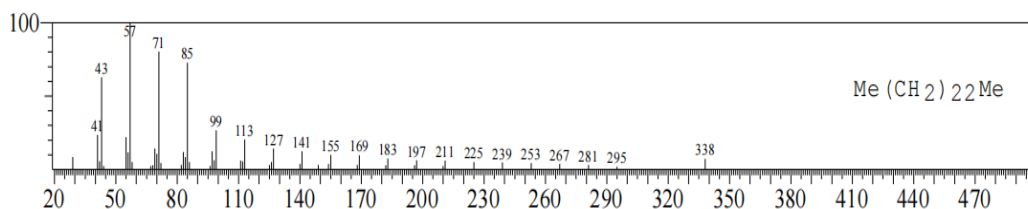
**Figure 10.** Fragmentation patterns Benzene, (2-methyl-1-butenyl)- (CAS) 1-Butene, 2-methyl



**Figure 11.** Fragmentation patterns Pregnenolone acetate



**Figure 12.** Fragmentation patterns 9-Dehydro-1-Methyl Estrone Methyl Ether



**Figure 13.** Fragmentation patterns Tetracosane (CAS) n-Tetracosane

In addition, the compound Pregnenolone acetate was also found. Pregnenolone acetate was found at retention time 25.272 and an area of 17,40% at Figure 11, Pregnenolone acetate is a steroid compound that has been isolated recently in various studies (Abdel-Lateff *et al.*, 2019). In coffee, the aroma itself varies depending on the lipid composition contained. Pregnenolone acetate is one of the volatile compounds that is responsible for the aroma of coffee (Wang *et al.*, 2012).

9-Dehydro-1-Methyl Estrone Methyl Ether at peak 21 at the retention time 25.489 and an area of 2,82% Figure 12 is a type of unsaturated estrone derivative and is classified as an aromatic compound (Djerassi *et al.*, 1962). The final metabolite compound that has a large surface area in non-tarred coffee is Tetracosane (CAS) n-Tetracosane. Tetracosane (CAS) n-Tetracosane is a volatile compound which was identified in 5% green bean arabica coffee using HS-SPME-GC-MS (Poyraz *et al.*, 2016) which was found in retention time 25.764 and an area of 4.02% at Figure 13.

#### 4. CONCLUSIONS

The result showed that characteristic parameters of Bukanagara coffee oil there are parameters that not up to standards, which are caused by temperature, extraction time, type, and volume of solvent. Bukanagara arabica coffee oil has a yield of 9.43%, a specific gravity of 0.94, an acid number of 0.78 mg NaOH/g and a peroxide number of 8.23 meq/kg. While in identification metabolite profiles, there are differences in content, retention time, and percent area caused by extraction process and temperature. There are 23 metabolite compounds identified in Bukanagara arabica coffee oil, from this number and based on the area there are 11 compounds that have a larger distribution area than other metabolite compounds.

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