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RESEARCH ARTICLE

Identifying metabolite profiling in unripe fruits of Kayu Banana (Musa paradisiaca L. var.Kayu) by Using LCMS instruments in different extraction methods

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Abstract The unripe fruit of a wood banana (Moses paradisiaca L. Var. Wood) is used in traditional medicine as an antidiarrheal drug in Lumajang Regency, East Java which has antidiarrheal activity. Phenolic compounds in the unripe fruit of wood bananas have antidiarrheal activity in vivo and in vitro. This study aims to prove the influence of extraction methods on the acquisition of phenolic acid levels of unripe fruit of wood bananas (Musa paradisiaca L. Var. Wood) and its secondary metabolite profile. The research method used is an experimentally causative method The extraction method used in this study is 2, namely: cold extraction (remaseration and maceration) and heat extraction (reflux and soxhlet). The unripe fruit of a wood banana (Moses paradisiaca L. Var. Wood) is distracted using four methods namely remaseration, maceration, reflux and soxlet. The extract obtained was tested for the total phenolic content (TPC). Analysis of secondary metabolite profiles using the UPLC-Q-TOF/MS instrument. Total phenolic data obtained were followed by ANOVA analysis. The result obtained in the extraction method with the remaseration extraction method was 99.31 ± 1.11 mgGAE / gram. Based on the data from the interpretation of compound content analysis using UPLC-QToFMS, it can be seen that there are 92 compounds in the remaseration method, 133 compounds in the maceration method, 126 compounds in the reflux method, and 136 compounds in the soxlet method.

Keywords: metabolite profiling, unripe fruits of Kayu Banana, Musa paradisiaca L. var.Kayu, LCMS, extraction methods, Diarrhoeal diseases.

Introduction

Diarrheal Disease is an endemic disease that has the potential to cause Extraordinary Events (KLB) and is still a contributor to the mortality rate in Indonesia, especially in toddlers (KEMENKES RI, 2021). Based on WHO 2019 Diarrhea is one of the diseases with the highest incidence and mortality rate in the world. There are reportedly around 1.7 trillion cases annually (Shen et al., 2019). Diarrheal disease is the second leading cause of death in children under five years of age, and each year it can kill about 525,000 children. Diarrhea can last several days, and can leave the body without the water and salt necessary for survival(Putri et al., 2019).

The island of Java, especially the province of East Java, there is one city that has received the nickname "Banana City" which is none other than Lumajang City. One of them is the wooden banana, which has a special feature based on the empirical experience of the people of Senduro village, Lumajang, East Java, raw wood bananas can be used as an antidiarrheal medicine whose use is by burning, steaming, and boiling. research conducted by Ningsih, et al., in 2019 stated that ethanol extract of the raw fruit of wood banana has an antidiarrheal effect and has been tested on male mice of balb-C strains that make diarrhea(Ningsih, 2019).

Phenolics are a group of compounds consisting of aromatic rings containing one or more hydroxyl groups (Çoklar & Akbulut, 2017). All plants contain phenolic compounds in the form of glycosides and bind to proteins and then form a complex bond through hydrogen bonds (Rivai et al., 2010). Phenolic compounds in the unripe fruit of wood bananas have pharmacological activity as antidiarrheals in vitro and in vivo. The extraction method used may affect the concentration or loss of therapeutic effect of the extract due to the breakdown of the compounds and the decomposing contained during the extraction process(Hmidani et al., 2019).

The technique for obtaining phenolic compounds can use several extraction methods coldly and hotly. The cold extraction method uses remaseration and maceration extraction, while the hot extraction uses the soxhlet and reflux extraction method(Zhou Xu 1,†, Shiling Feng 1,†, Jipeng Qu 1, 2, Ming Yuan 1 & Ding, 2019). Several major industries have long applied continuous filtering so that they are efficient in terms of time, nutrient savings, and more extracted raw materials (Susanty & Bachmid, 2016). In general, various methods of extraction of bioactive compounds have their advantages and disadvantages therefore it is necessary to determine the most appropriate method of extraction of bioactive compounds taking into account factors such as temperature, extraction time, cost, yield and purity(Akyıl et al., 2020).

The choice of extraction method greatly affects the content of chemical compounds contained in a plant, especially compounds that are efficacious as antidiarrheals and affect the antidiarrheal activity produced. Based on the above background, a test will be carried out on the effect of the extraction method on phenolic levels and metabolite profiles in raw wood banana fruit (Musa paradisiaca L. Var. wood) with UPLC / Q-TOF MS analysis to characterize the differences in secondary metabolite profiles. This research is focused on profiling secondary metabolites of extracts with different extract methods and their phenolic content(Lee et al., 2014).

Material And Methods

Materials

The tools used in this study are oven, aluminum foil, scissors, blender, sieve No. 100, plastic jar, knife, glass jar, stirrer, filter paper, bunsen, hotplate, Buchner funnel, test tube, drip pipette, volume pipette, measuring pipette, measuring flask, porcelain cup, analytical balance, measuring cup, watch glass, glass beaker glass, erlenmeyer, glass funnel, macerator, rotary evaporator, drip plate, basin container, UV – vis spectrophotometry, UPLC-MS instrument, Ultrasonic Cleaner (Sonica) and cuvette.

The ingredients used in this study were raw wood bananas (Moses paradisiaca L. Var. Wood) which are characterized by banana peel that is still green and the fruit is still hard and is approximately 3 months old after the flower comes out, 96% ethanol, sterile aquadest, folin-ciocaltuae reagent, mayer reagent, dragendoorf, bouchardate, gelatin salt, HCl 2 N, magnesium, concentrated HCl, iron (III) chloride, CH3COOH, concentrated H2SO4, gallic acid, ethyl acetate, n-butanol, and methanol, methanol (hypergrade for UPLC), formic acid (ultrapure for UPLC), acetonitrile (hypergrade for UPLC), and water injection 0.05% for UPLC.

Plant Determination

The determination of the raw fruit of wood bananas was carried out at LIPI Purwodadi and the Food and Agricultural Security Service of Lumajang Regency.

Making Simplisia Unripe Fruit Banana Wood (Musa paradisiaca L.var. kayu)

A total of 12,959.9 g of unripe bananas were washed under running water until clean, drained, and weighed wet weight. Then the cutting is carried out, dried in a drying rack at a temperature of 50ºC, dry disortation, and weighed dry weight. The dry sample is then blended and then sifted and stored in a plastic container(Ningsih, 2019).

Extract Making

Remaseration: As much as 500 grams of simplicia powder of unripe fruit of wood banana (*Musa paradisiaca* L.var. Kayu) is macerated using 96% ethanol solvent at room temperature and stirring is carried out. The powder is soaked for 24 hours. Remaseration is carried out 2 times, filtering is carried out to separate residues and filtrates. The resulting maserat is then evaporated with a rotary evaporator at a temperature of 50ºC and evaporated until it becomes a viscous extract (Ningsih et al., 2020). Maceration: 500 grams of simplicia powder of raw fruit of banana wood is added with 96% ethanol solvent as much as 3,750 ml and maceration is carried out. After the whole powder is soaked, then stirring is done slowly and soaked for 5 days with stirring. The resulting maserat is then evaporated with a rotary evaporator at a temperature of 50ºC(Ningsih et al., 2020). Soxhlet :A total of 500 grams of simplicia powder is wrapped in filter paper and tied up and then put into the soxhlet extractor. A 96% ethanol solvent of 1.5 liters is put into a round base flask, then a soxhlet tool is assembled with a condenser. Extraction is carried out at a temperature of 60-80ºC until the liquid is colorless. The extract obtained was evaporated using a rotary evaporator at a temperature of 50ºC(Mokoginta et al., 2013). Reflux: A total of 500 grams of simplicia powder is put into the round base flask, then a 96% ethanol solvent is added. Assemble the reflux device, then the sample is extracted at a temperature of 50ºC for 2 hours. The solution obtained is filtered using filter paper and evaporated using a rotary evaporator at a temperature of 50ºC(Susanty & Bachmid, 2016).

Phytochemical Screening

Alkaloid Test: A total of 0.5 grams of wood banana fruit extract was added 1 ml of 2 N hydrochloric acid and 9 ml of distilled water, heated on a water bath for 2 minutes cooled and filtered. The filtrate is divided into 3 parts, each of which is added Mayer, Dragendorf, and Wagner reagents. Shows a positive result of alkaloids if with Mayer a white or yellow precipitate is formed, with Wagner a reddish-brown precipitate is formed and with Dragendorf a reddish-brown precipitate is formed(Endarini, 2016) (RI, 1980). Saponin Test: A total of 0.5 grams of powder is put into a test tube, 10 ml of hot water is added, cooled and then shaken for 10 seconds. If a stable foam of 1 to 10 cm high is formed for not less than 10 minutes and does not disappear with the addition of 1 drop of hydrochloric acid 2 N indicates the presence of saponins(Bonggol, 2018). Flavonoid Test: 0.5 grams of wood banana raw fruit extract is added to 20 ml of hot water, simmered for 10 minutes, and filtered hot. 5 ml of filtrate plus 0.1 g of Mg powder, 2 ml of amyl alcohol and 1 ml of concentrated hydrochloric acid, shaken and allowed to separate. The formation of a red, yellow, or orange color formed on the amyl alcohol layer indicates a positive presence of flavonoids (Ningsih et al., 2020). Tannin Test: 0.5 grams of raw fruit extract of banana wood is added with 10 ml of aquades. Then it is allowed to stand for 5 minutes and filtering is carried out. The filtrate is diluted with water until it is colorless. Next, the solution is taken as much as 2 ml added with 1 to 2 drops of 1 1% FeCl3%. Discoloration to green, blue or blackish indicates a positive result of tannins(Ningsih et al., 2020). Polyphenol Test: A total of 1 gram of raw fruit extract of banana wood was extracted with 15 ml of hot aquades then added 10% NaCl and filtered, the filtrate is divided into 3 parts (A, B, C). Filtrate A as a blank, filtrate B plus 3 drops of FeCl3 and filtrate C plus gelatin salt. Discoloration from green to blue-black indicates the presence of phenolic compounds(Hanani, 2015). Triterpenoid and Steroid Assay: A total of 0.1 gram of extract was added 3 drops of concentrated HCl and 1 drop of H2SO4. If red or purple color is formed then the positive contains terpenoids. If a green color is formed then positively contains steroids(Ergina et al., 2014). Anthraquinone Test: A total of 0.3 grams of the extract was extracted with 10 ml of aquades, then the filtrate was extracted with 3 ml of toluene and added ammonia. There is a change in color to red indicating positive anthraquinone(Muthia et al., 2019). Glycoside Test: 1 gram of viscous extract dissolved with ethanol, evaporated on a water bath, then dissolved in 5 ml of anhydrous acetic acid P. and added 10 drops of sulfuric acid P. blue or green color formed indicates the presence of glycosides(Program, 2014).

Determination of the total phenolic content of unripe wood banana fruit extract (Musa paradisiaca L. Var. Kayu)

The extract solution is picketed as much as 1 mL of raw wood banana fruit extract solution, then the sample is added with 0.4 mL of FolinCiocalteau reagent whipped and left for 4-8 minutes, add 4.0 mL of 7% Na2CO3 solution shake until homogeneous. Add aquades up to 10 mL and let stand for 2 hours at room temperature. Measure absorption at a maximum absorption wavelength of 750 nm. Do 3 repetitions so that the phenol levels obtained by the results are obtained as mg of gallic acid equivalent / g of extract(Campos et al., 2022).

$$TPC = \frac{x.v.fp}{g}$$

Information:
x = Phenolic concentration (ppm)

v = Extract volume used (mL)
fp = Dilution factor
g= Sample weight used (g)

Metabolite Profiling Using UPLC/Q-TOF MS

Thoroughly weighed 10.00 mg of extract then dissolved with methanol into a 10 ml measuring flask. The extract in methanol is taken with a microsyringe of 5 µl to be further injected into the sample site and entered into the UPLC column. Replication is carried out 4 times. The sample in the form of a liquid will be converted into droplets through the needle that has been given a positive ESI charge (+). The ions that have been generated by the detector will then be separated by a Q-ToF analyzer. The eluent used was a mixture of (A) water: formic acid (99.9:0.1) and (B) acetonitrile: formic acid (99.9:0.1) with a gradient elution system as listed in table 2 with an eluent flow velocity of 0.2 ml/min. A chromatogram with a polar compound will appear first then be followed by a compound whose polarity is lower. The separation results are then read by the QToF-MS detector resulting in a chromatogram peak. Peak chromatograms are then interpreted using the Masslynx application (Gong et al., 2020).

Results and Discussion

Plant determination

Sampling was carried out in Lumajang Regency, East Java. The selection of fruits taken is fresh and unripe fruit with a green color that has no yellow color, hard and aged 3 months after the flower tandan comes out. The determination of the raw fruit plant of wood bananas was carried out at LIPI Purwodadi and the raw fruit of wood bananas is indeed a wood variety by proving the determination of the raw fruit of wood bananas at the Food Security and Agriculture Office of Lumajang Regency.

Manufacture of simplisia

Table 1. Characteristic results of simplisia powdered unripe fruit banana wood

Simplisia	Temperature	Fresh Simplisia weight (gr)	Weight of dry Simplisia (gr)	% Shrinkage drying	Moisture content	Organoleptic
Unripe fruit of banana wood	Temperature 50^0C	12959,9 gram	4152,6 gram	32,04%	2,74%	Aromatic characteristic smell, ivory-white color, powder-shaped

The unripe fruit of wood bananas as much as 12,959.9 grams was washed thoroughly with running water to remove dirt and sap that was still attached to the wood banana fruit. The washed wooden banana fruit is then dried by aerating, then the wooden banana fruit is cut into thin strips to facilitate a drying process. Drying is carried out using a food dehydrator oven at a temperature of 50º and dry simplicia results are obtained. The dried simplisia is then mashed using a blender until it becomes a fine powder and the powder produced by 4152.6 grams.

Extract making

Simplisia extraction uses 2 extraction methods, namely cold and hot methods for cold extraction methods use remaseration and maceration while the hot extraction method uses reflux and Soxhlet uses 96% ethanol solvent with a temperature of 500 C according to table results 4.1% the highest amendment using the remaceration extraction method with results16.45%.

Table 2. % yield of amendments and phenolic total levels of wood banana raw fruit extract

No.	Extraction Methods	Powder Weight	Extract Weight	% Extract Amendments	KTFe±SD	Organoleptic Extract
1	Remaseration	750 gram	123,4 gram	16,45%	99.31±1.11	Color: brownish green Smell: slightly pungent Taste: slightly bitter and astringent

2	Maceration	750 gram	106,3 gram	14,17%	53.96±0.81	Color: brownish green Smell: slightly pungent Taste: slightly astringent and very bitter
3	Reflux	750 gram	85,7 gram	11,42%	54.65±0.80	Color: green-black Smell: slightly pungent Taste: slightly bitter and slightly astringent
4	Soxhlet	750 gram	76,8 gram	10,24%	54.47±0.65	Color: green-black Smell: very pungent Taste: bitter

Phytochemical screening examination

Table 3. Phytochemical screening results of unripe fruit of the wood banana

Organoleptic Examination	Extraction Method			
	Remaseration	**Maceration**	**Reflux**	**Soxhlet**
Alkaloid	+	+	+	+
Saponin	+	+	+	+
Flavonoid	+	+	+	+
Tanin	+	+	+	+
Polyphenol	+	+	+	+
Anthraquinone	+	+	+	+
Glikosida	-	-	-	-
Steroid	-	-	-	-
Triterpenoid	-	-	+	+

Phytochemical screening is carried out to determine the content of secondary metabolites contained in the extract of unripe fruit of banana wood. Phytochemical screening is carried out, namely tannins, alkaloids, saponins, flavonoids, polyphenols, glycosides, anthraquinones, terpenoids and steroids. Based on the results of phytochemical screening tests with the extraction method of remaseration and maceration, it produces a significant content of secondary metabolite compounds, namely containing alkaloids, saponins, flavonoids, tannins, polyphenols, and anthraquinones. Whereas in the reflux extraction method and Soxhlet produces compounds as secondary metabolites of alkaloids, saponins, flavonoids, tannins, polyphenols, anthraquinones, and triterpenoids. In this study, the results of phytochemical screening produced different secondary metabolite compounds because time and temperature greatly affect the number of compounds extracted so the extraction method by heating where the extraction method will provide an opportunity to obtain maximum secondary metabolite compounds.

DISCUSSION

The remaseration method is a modification method of the maceration method where the remaseration method is carried out by adding solvent repeatedly after the first extract filtering. In this study, the extract yield from the remaseration extraction method was 16.45% and for the results of obtaining phenolic compound levels produced 99.31±1.11 mgGAE / gram, it was suspected to produce the highest levels of amendments and phenolic compounds because at room temperature and protected from sunlight and heat, the withdrawal of active compounds for 2 days was carried out by soaking the simplicia powder with the appropriate solvent for 2 days and changing the solvent every time day. When it reaches the equilibrium phase, the plant cell will be entered by the solvent by passing through the cell wall. The equilibrium process occurs by exiting secondary metabolite compounds inside the cell because the concentration inside the cell is different from the concentration outside the cell. The equilibrium process occurs because there is a diffusion process caused by a difference in concentration where the concentration inside the cell is higher will cause secondary metabolite compounds to come out and be

replaced by solvent liquids outside the cell whose concentration is lower(Zhou Xu 1,†, Shiling Feng 1,†, Jipeng Qu 1, 2, Ming Yuan 1 & Ding, 2019). The event occurs repeatedly until there is a balance of concentration outside and inside the cell. During the remaseration process, a replacement of the igniting fluid is carried out every day for 2 days so that the effectiveness of the withdrawal will be maximized(Qiu et al., 2021).

The maceration method is a method of extraction of the cold way and the simplest method where the soldering liquid will penetrate the cell wall of the plant and will enter the cell cavity containing the active substance so that the active substance which is a sealed solution will be urged out of the cell because of the difference in concentration between the active substance solution inside the cell and the one outside the cell(Hasnaeni, Wisdawati, 2019). The resulting extract yield was 14.17% and the results of obtaining phenolic compound levels produced 53.96±0.81 mgGAE / gram. The yield is high because the time used is quite long and stirring is carried out many times, therefore the compounds contained in the unripe fruit of wood bananas are attracted quite a lot. The yield of the amendment is high enough that the level of phenolic compounds that should be produced must be high, but the principle of the maceration extraction method is not carried out by repeating the addition of solvents so that the active compounds contained in the raw fruit of wood bananas are not attracted to the maximum, therefore the levels of phenolic compounds produced are low.

The reflux method is a method of extraction with the help of heating. The thing that greatly affects extraction using reflux is the addition of heating and the solvent used will remain fresh due to the re-evaporation that is submerged in the material. Reflux extraction is used to extract materials that are heat-resistant and have a rough texture(Hasnaeni, Wisdawati, 2019). The resulting extract yield was 11.42% and the resulting phenolic content of 54.65±0.80 mgGAE / gram. High levels of phenolic compounds should produce high levels of amendments, but the time made for extraction is quite short, namely for 2 hours so that the withdrawal process of secondary metabolite compounds is not interested in the maximum, but the levels of phenolic compounds produced are quite high due to the heating process, causing the cell walls of banana wood fruit powder to open larger, in addition, the heating process also results in the viscosity of the solvent decreasing so that the ability of the solvent to penetrate the cell wall becomes easier and the amount of phenolic compounds extracted becomes high.

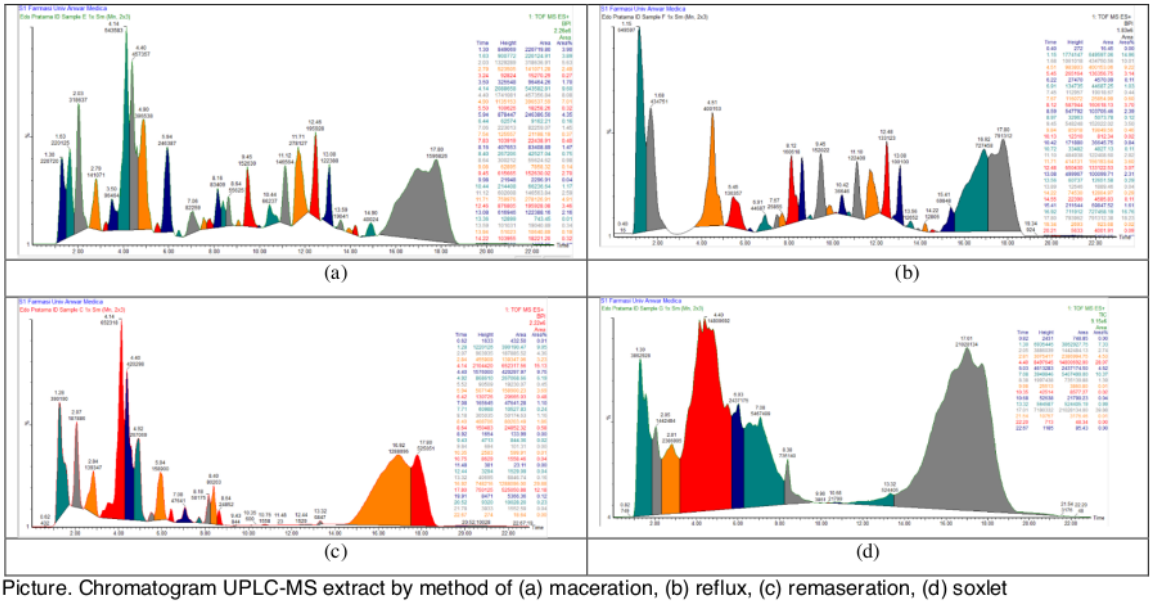
The soxhlet method is a heat extraction method. At this extraction, the solvent and the sample are placed separately. The principle of the soxhlet method is that it is carried out continuously using relatively few solvents. When the extraction is complete then the solvent can be evaporated so that an extract will be obtained. Usually, the solvent used is volatile or has a low boiling point(Susanty & Bachmid, 2016). The resulting extract yield was 10.24% and the resulting phenolic compound content was 54.47.47±.0.65 mgGAE / gram. The Soxhlet extraction method produces high yield levels but produces a fairly high level of phenolic compounds because the extraction process is quite long, which is 5 hours, and takes 3 days to be able to extract 750 grams of raw fruit powder of wood banana so that the time in the extraction process greatly affects the right extraction time will produce optimal compounds, but if the extraction time is too long it will damage the compound active and if the extraction time is too short it will result in low extract yield levels. The results of high phenolic compounds, it is suspected to be caused by the heating process so that the cell walls of banana powder can break and can secrete active compounds that can withstand heating.

Based on the results of phytochemical screening of extracts by extraction, the positive heat method contains triterpenoid compounds while in the cold way it does not contain triterpenoid compounds, where these triterpenoid compounds have antidiarrheal activity so that the extract with the soxhlet extraction method provides higher antidiarrheal activity than the maceration method. The reflux method has an average cross-marker length in the intestines of mice that is lower than the soxhlet method, the length of extraction will affect the attraction of chemical compounds. The soxhlet method takes quite a long time for extraction so the soxhlet method can attract more than the reflux method.

Based on the results of the one-way ANOVA test on phenolic level testing, it can be concluded that the results of hypothesis testing have significant differences in performance between types of extraction methods. This result is indicated by a Ftable value of 2.8951073 and a probability value (sig) of 0.000 H0 rejected, where the Fhitung ≥ Ftabel and its probability (sig) ≤ 0.05. The calculated F value from the ANOVA table is 3404,728 and the Ftabel value is 2.8951073 to 3404.728 ≥ 2.8951073 and the probability value (sig) in the ANOVA table is 0.000 while the signification level $\alpha = 0.05$ to 0.000≤0.05. It can be concluded that the test results have significant differences in the results of phenolic compound levels.

According to research by Hernanz, et all (2021) (Rebollo-Hernanz et al., 2021), The amendment of phenolic extraction from cocoa peels increases by modifying the extraction parameters including temperature, time, acidity, and S/L ratio. In the results of this study, the difference in extraction methods in a cold way produced the highest yield compared to the extraction method in a hot way because the temperature would affect the stability of the compound content. In the cold extraction method, namely, remaseration has the highest percentage of extract yield and the highest phenolic

content.



Picture. Chromatogram UPLC-MS extract by method of (a) maceration, (b) reflux, (c) remaseration, (d) soxlet

Analysis of the profile of the unripe fruit of the wood banana (Musa paradisiaca L.Var.Kayu) in this study using UPLC-MS. UPLC is one of the developmental techniques of liquid chromatography used for the segregation of different components in a mixture with a molecular level reaching two microns of analyte particles. The analysis method using UPLC can reduce the consumption of the phase of motion by up to 80% in a relatively shorter time of about 1.5 minutes than using HPLC. The UPLC-MS used in this study used an MS detector with an ESI ion source (+) and an MS analyst in the form of Q-ToF. Such instruments have several advantages, that is, selective and sensitive with high and fast resolution performance so that the analysis time is faster. The profile analysis of the metabolite of *Musa paradisiaca* L.Var.Kayu begins by injecting the sample, then the sample will enter the column so that a process of separation of metabolite components occurs. In this study, the silent phase used was column C18 or octimethyl silica. The advantage of octadecyl silica as a stationary phase is that this phase can separate compounds ranging from low, medium, to high polarity

Table 4. Results of interpretation of metabolite data profiling extract by remaseration method

No.	Rt (min)	m/z	Rumus Molekul	Nama Senyawa
1	0,051	327,2068	C12H2268	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
2	0,62	327,2077	C20H26N2O2	Dihydroquinidine
3	1,106	151,0358	C3H7N4OCl	Hydrochloride
4	1,169	212,8524	C3HS3Br	4-Bromo-1,3-dithiole-2-thione
5	1,232	381,0811	C9H20N2O12S	
6	1,282	381,0798	C9H20N2O12S	
7	1,457	381,0803	C9H16N8O5S2	
8	1,583	180,1018	C10H13NO2	Phenacetin
9	1,633	121,0648	C8H8O	Acetophenone
10	1,738	178,0865	C5H12N5Cl	2-Methyl-1-(1H-tetrazole-5yl)-1-propanamine hydrochloride (1:1)
11	1,809	178,0853	C10H11NO2	Acetoacetanilide
12	2,07	178,0839	C10H11NO2	Acetoacetanilide
13	2,357	178,0858	C6H7N7	
14	2,462	166,0841	C9H11NO2	DL-Phenylalanine
15	2,512	166,0872	C9H11NO2	DL-Phenylalanine
16	2,813	230,0943	C12H11N3O2	HC Red 1
17	2,84	230,0938	C12H11N3O2	HC Red 1

18	2,968	230,0917	C12H11N3O2	HC Red 1
19	3,039	230,0914	C7H11N5O4	Sanazole
20	3,1	208,1315	C6H10NO2Br	4-(bromoacetyl)morpholine
21	3,215	208,134	C8H13N7	{4,6-Bis(dimethylamino)-1,3,5-triazin-2-yl}cynamide
22	3,278	208,1341	C12H17NO2	Ciclopirox
23	3,341	180,0665	C6H13NO3S	Cyclamic acid
24	3,412	180,0664	C5H13N3S2	Piperazine Dithiocarbamate
25	3,454	180,0663	C6H13NO3S	Cyclamic acid
26	3,517	180,0663	C9H9NO3	Hippuric acid
27	3,567	180,0721	C3H13N3O4S	
28	3,671	188,0712	C11H9NO2	Benzylmaleimide
29	3,742	272,0928	C15H13NO4	4-Benzyloxy-3-nitroacethopenone
30	3,784	238,145	C13H19NO3	N-t-BOC-D-Phenylglycinol
31	3,868	257,1295	C15H16N2O2	Ancymidol
32	4,044	220,0973	C12H13NO3	Anirecetam
33	4,136	222,15	C13H19NO2	Ethyl-4-Butylamineobenzoate
34	4,395	256,1339	C16H17NO2	N,N-Dybenzylglycine
34	4,508	207,1384	C8H19N4Cl	8-Azido-1-octanamine hydrochloride (1:1)
35	4,56	207,1384	C11H7SCl	7-(3-Chloro-1-propyn-1-yl)-1-benzothiophene
36	4,571	308,1861	C17H25NO4	Buflomedil
37	4,663	365,1487	C21H20N2O4	1 [3-{(3-Propoxybenzoyl)amino}phenyl]-2-furamide
38	4,797	434,2039	C19H31NO10	21-(2,5-Dihydro-2,5-dioxo-1H-pyrrol-1-yl)-4,7,10,13,16,19-hexaoxaheneicosanoic acid
39	4,84	434,2016	C23H8N5Br	
40	4,92	236,164	C14H21NO2	Padimate A
41	4,952	236,1647	C14H21NO2	Padimate A
42	5,098	498,2608	C27H35N3O6	N-{3-(2,5-Dimethylphenyl)-1-oxo-1-[4-(3,4,5-trimethoxybenzoyl)-1-piperazinyl]-2-prpanyl)acetamide
43	5,148	490,2211	C24H31N3O8	Diethyl 1,1'-[(5-nitro-1,3-phenylene)dicarbonyl]dipiperidine-4-carboxylate
44	5,19	498,261	C27H35N3O6	N-(2-{[2-(Cyclohexylamino)-1-(3-methoxyphenyl)-2-oxoethyl](tetrahydro-2-furanylmethyl)amino}-2-oxoethyl)-2-furamide
45	5,232	352,2128	C19H29NO5	Dipivefrin
46	5,274	230,175	C12H23NO3	N-Boc-4-Piperidineethanol
47	5,324	330,1701	C5H15N17O	
48	5,408	482,2611	C21H39NO11	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
49	5,52	482,251	C21H39NO11	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
50	5,542	410,2553	C22H35NO6	Methyl 11-[(3,4,5-trimethoxybenzoyl)amino]undecanoate
51	5,605	245,1391	C12H20O5	Diisopropyl 3-hydroxy-1,1-cyclobutanedicarboxylate
52	5,676	445,2345	C29H32O4	2-(4-Biphenylyl)-2-oxoethyl 4-(octyloxy)benzoate
53	5,739	440,2296	C22H33NO8	4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenyl β-D-glucopyranosiduronic acid
54	5,801	197,1178	C11H16O3	1-carboxy-3-hydroxyadamantane
55	5,94	322,2019	C18H27NO4	Boc-4-tert-butyl-Phe-OH
56	5,956	336,2172	C19H29NO4	(3S)-3-({[(2-Methyl-2-propanyl)oxy]carbonyl}amino)-4-[4-(2-methyl-2-propanyl)phenyl]butanoic acid
57	6,027	333,1601	C21H20N2O2	1-Fmoc-4-Cyanopiperidine
58	6,153	333,1604	C21H20N2O2	1-Fmoc-4-Cyanopiperidine
59	6,203	333,1602	C26H20	Tetraphenylethylene
60	6,308	373,2226	C19H32O7	Byzantionoside B
61	6,421	280,1912	C16H25NO3	Moxisylyte
62	6,463	213,1488	C12H20O3	Ethyl 4-cyclohexyl-3-oxobutanoate
63	6,555	393,179	C23H24N2O4	(S)-Methyl 2-((4,6-dimethylpyrimidin-2-yl)oxy)-3-methoxy-3,3-diphenylpropanoate
64	6,638	373,2123	C21H28N2O4	3,5-Bis[(cyclohexylcarbonyl)amino]benzoic acid
65	6,68	373,213	C26H28O2	4'-Propyl-4-biphenylyl 4-butylbenzoate
66	6,73	207,1598	C10H22O4	Butoxytriglycol
67	6,772	294,2072	C17H27NO3	Nonivamide
68	6,835	336,2169	C19H29NO4	(3S)-3-({[(2-Methyl-2-propanyl)oxy]carbonyl}amino)-4-[4-(2-methyl-2-propanyl)phenyl]butanoic acid
69	6,906	442,2647	C17H27N15	
70	6,969	283,1544	C51H82O21	Pseudoprotodioscin
71	7,082	247,1329	C15H18O3	Loxoprofen
72	7,165	1175,584	C7H90O25	(3β,15α,16α,22α)-15,16,28-Trihydroxy-22-{[(2Z)-2-methyl-2-butenoyl]oxy}olean-12-en-3-yl β-D-galactopyranosyl-(1->2)-[β-D-

				xylopyranosyl-(1->2)-α-L-arabinopyranosyl-(1->3)]-β -D-glucopyranosiduronic acid
73	7,208	294,2074	C17H27NO3	Nonivamide
74	7,258	466,2671	C19H27N15	
75	7,32	291,0666	C18H10O4	2-(2-Furoyl)-3H-benzo[f]chromen-3-one
76	7,383	466,2671	C20H39NO10	α-D-Glucopyranosyl 6-deoxy-6-[(2-ethylhexyl)amino]-α-D-glucopyranoside
77	7,496	327,2113	C10H22N120	
78	7,559	378,2648	C22H35NO4	4-Nitrophenyl palmitate
79	7,609	432,2945	C23H37N5O3	1,3-Dicyclohexyl-5-({[2-(1-piperazinyl)ethyl]amino}methylene)-2,4,6(1H,3H,5H)-pyrimidinetrione
80	7,714	269,1718	C15H24O4	1,9-Nonanediol Diacrylate
81	7,806	441,2252	C18H32N8OS2	
82	7,85	372,2528	C23H33NO3	20-hydroxyiminopregna-5,16-dien-3-β-yl acetate
83	7,911	308,2208	C14H25N7O	4-[(4-Ethyl-1-piperazinyl)methyl]-6-(4-morpholinyl)-1,3,5-triazin-2-amine
84	7,961	416,3008	C23H37N5O2	(5-Isobutyl-1H-pyrazol-3-yl)[4-(1-pyrrolidinylcarbonyl)-1,4'-bipiperidin-1'-yl]methanone
85	7,982	275,2	C18H26O2	Nandrolone
86	8,003	278,2122	C17H27NO2	Venlafaxine
87	8,044	269,1756	C15H24O4	1,9-Nonanediol Diacrylate
88	8,086	346,2592	C18H35NO5	13-[(2R,3R,4R,5R)-3,4-Dihydroxy-5-(hydroxymethyl)-2-pyrrolidinyl]-1-hydroxy-4-tridecanone
89	8,18	269,1759	C15H24O4	1,9-Nonanediol Diacrylate
90	8,262	229,1443	C12H20O4	Dibutyl Fumarate
91	8,312	538,3234	C19H43N11O5S	
92	8,396	454,2294	C19H35NO11	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
93	8,488	488,2129	C30H25N5O2	N,N-Dimethyl-4-(4-{[4-(phenylcarbamoyl)phenyl]amino}-1-phthalazinyl)benzamide
94	8,614	295,2271	C18H30O3	Octoxynol-2
95	8,64	295,2268	C18H30O3	Octoxynol-2
96	8,839	327,2057	C20H26N2O2	Dihydroquinidine
97	8,902	468,2458	C21H33N5O7	N-[6-(2,5-Dioxo-2,5-dihydro-1H-pyrrol-1-yl)hexanoyl]-L-valyl-N5-carbamoyl-L-ornithine
98	8,92	468,2455	C21H33N5O7	N-[6-(2,5-Dioxo-2,5-dihydro-1H-pyrrol-1-yl)hexanoyl]-L-valyl-N5-carbamoyl-L-ornithine
99	9,078	181,1234	C8H20O2S	
100	9,409	324,2179	C18H29NO4	Guaiapate
101	9,43	324,2171	C19H25N5	4-benzyl-N-(4,6-dimethylpyrimidin-2-yl)piperidine-1-carboximidamide
102	9,47	279,0936	C20H10N2	Acridino[2,1,9,8-klmna]acridine
103	9,84	327,208	C20H26N2O2	dihydroquinidine
104	9,978	327,2061	C16H22N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
105	10,112	327,2062	C16H22N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
106	10,329	367,3326	C22H42N2O2	1,1'-(2,5-Dimethyl-1,4-piperazinediyl)di(1-octanone)
107	10,35	367,3323	C22H42N2O2	1,1'-(2,5-Dimethyl-1,4-piperazinediyl)di(1-octanone)
108	10,547	327,2066	C25H26	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
109	10,733	214,2531	C14H31N	Diheptylamine
110	10,75	214,2529	C14H31N	Diheptylamine
111	10,878	327,2076	C16H22N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
112	10,991	327,2069	C12H30N4O4S	Undecyl hydrogen sulfate - carbonohydrazonic diamide (1:1)
113	11,4	327,2066	C20H26N2O2	Dihydroquinidine
114	11,48	327,2067	C20H26N2O2	dihydroquinidine
115	12,44	327,2065	C20H26N2O2	Dihydroquinidine
116	13,317	279,1585	C16H22O4	Dibutyl phthalate
117	13,32	279,1585	C16H22O4	Dibutyl phthalate
118	14,878	960,8979	C62H113N5O2	
119	14,569	960,8963	C61H117NO6	
120	14,640	960,8960	C62H113N5O2	
121	14,765	960,8965	C61H117NO6	
122	15,033	960,8969	C55H113N11S	
123	16,523	960,9017	C56H113N9O3	
124	16,92	960,8978	C61H117NO6	
125	17,8	960,8975	C61H117NO6	
126	18,682	960,8943	C58H109N11	

127	19,645	327,2063	C20H26N2O2	Dihydroquinidine
128	19,91	327,2068	C20H26N2O2	dihydroquinidine
129	20,482	327,2070	C16H22N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
130	20,52	327,208	C20H26N2O2	dihydroquinidine
131	21,78	327,2068	C20H26N2O2	dihydroquinidine
132	22,106	327,2065	C25H26	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
133	22,67	327,2075	C20H26N2O2	dihydroquinidine
134	22,725	327,2066	C25H26	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
135	7,237	294,2075	C17H27NO3	Nonivamide
136	2,709	166,088	C9N3O	

Table 5. Results of interpretation of metabolite data profiling extracts by maceration method

No.	Rt (min)	m/z	Rumus Molekul	Nama Senyawa
1	0.156	327.2052	$C_{20\ 26}N_2O_2$	dihydroquinidine
2	0.311	327.2075	C16 H22 N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
3	1.169	212.8513	C4OCl2Br	unknown
4	1.232	381.0781	C5H12N14O3S2	unknown
5	1.303	381.0786	C9H20N2O12S	unknown
6	1.457	381.0791	C9H16N8O5S2	unknown
7	1.633	180.1019	C10H13NO2	phenacetin
8	1.759	121.0640	C8H8O	acetophenone
9	1.893	274.1076	C15H15NO4	thyronine
10	2.027	178.0868	C10H11NO2	AL9325000
11	2.160	178.0866	C5H12N5Cl	2-Methyl-1-(1H-tetrazol-5-yl)-1-propanamine hydrochloride (1:1)
12	2.244	178.0863	C3H11N7S	1-(1,2,3,4-Thiatriazolidin-5-yl)-1,2,4-triazolidin-3-amine
13	2.512	230.0924	C12H11N3O2	HC Red 1
14	2.533	166.0857	C9H11NO2	DL – Phenylalanine
15	2.638	120.0800	C8H9N	Indoline
16	2.989	230.0921	C7H11N5O4	Sanazole
17	3.039	164.0707	C9H9NO2	2,6 – Diacetylpyridine
18	3.060	220.1182	C13H17NS	1,3 – Diisopropyl– 2 – isothiocyanatobenzene
19	3.123	208.1334	C12H17NO2	Ciclopirox
20	3.215	208.1333	C8H13N7	[4,6 – Bis(dimethylamino) – 1,3,5 – triazin – 2 – yl]cyanamide
21	3.412	180.0654	C5H13N3S2	Piparazine Dithiocarbamate
22	3.516	180.0657	C9H9NO3	Hippuric Acid
23	3.587	188.0708	C11H9NO2	Benzylmaleimide
24	3.692	272.0904	C15H13NO4	4 – Benzyloxy – 3 – nitroacetophenone
25	3.868	238.1436	C13H19NO3	N – t – BOC – D – Phenylglycinol
26	3.960	257.1284	C15H16N2O2	Ancymidol
27	4.094	222.1499	C13H19NO2	Ethyl 4 – Butylaminobenzoate
28	4.220	240.1021	C15H13NO2	Fmoc – Amide
29	4.395	256.1331	C16H17NO2	N,N – Dibenzylglycine
30	4.571	308.1856	C17H25NO4	Buflomedil
31	4.663	365.1494	C18H24N2O4S	Dansyl – L – leucine
32	4.726	497.2366	C17H40N2O12S	unknown
33	4.797	434.2014	C19H31NO10	-(2,5-Dihydro-2,5-dioxo-1H-pyrrol-1-yl)-4,7,10,13,16,19-hexaoxaheneicosanoic acid
34	4.881	520.3289	C18H45N7O10	unknown
35	4.923	236.1647	C14H21NO2	Padimate A
36	5.036	564.3585	C24H53NO13	Tidak ada
37	5.098	498.2610	C27H35N3O6	N-{3-(2,5-Dimethylphenyl)-1-oxo-1-[4-(3,4,5-trimethoxybenzoyl)-1-piperazinyl]-2-propanyl}acetamide
38	5.211	608.3864	C25H57NO14	unknown
39	5.253	822.4492	C39H67NO17	unknown
40	5.324	293.1270	C18H16N2O2	BY8236000
41	5.387	652.4078	C25H53N11O9	unknown
42	5.408	482.2567	C21H39NO11	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
43	5.450	251.1738	C14H22N2O2	Rivastigmine
44	5.542	410.2532	C22H35NO6	Methyl 11-[(3,4,5-trimethoxybenzoyl)amino]undecanoate
45	5.626	245.1371	C12H20O5	Diisopropyl 3-hydroxy-1,1-cyclobutanedicarboxylate
46	5.676	445.2328	C24H32N2O6	Diethyl 1,1'-(1,3-phenylenedicarbonyl)dipiperidine-4-carboxylate
47	5.739	440.2281	C22H33NO8	249CZA0134

48	5.801	197.1172	C11H16O3	1 – carboxy – 3 – hydroxyadamantane
49	5.935	336.2160	C19H29NO4	(3S)-3-({[(2-Methyl-2-propanyl)oxy]carbonyl}amino)-4-[4-(2-methyl-2-propanyl)phenyl]butanoic acid
50	5.977	333.1607	C21H20N2O2	1 – Fmoc – 4 – Cyanopiperidine
51	8.044	269.1760	C21H20N2O2	1-Fmoc-4-Cyanopiperidine
52	8.157	275.2021	C15H30O2S	3-(Dodecylthio)propanoic acid
53	8.178	275.2003	C18H26O2	Nandrolone
54	8.312	538.3235	C25H47NO11	Octyl 4-O-(2-acetamido-2-deoxy-β-D-galactopyranosyl)-3-O-propyl-β-D-galactopyranoside
55	8.375	454.2287	C19H35NO11	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
56	8.396	454.2293	C19H35NO11	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
57	8.488	930.3048	C44H51NO21	unknown
58	8.614	277.2166	C18H28O2	MFCD00041917
59	8.789	293.2132	C14H30N3OCl	3-[2-(Cycloheptylamino)ethyl]-1,1-diethylurea hydrochloride (1:1)
60	8.839	211.0751	C14H10O2	Benzil
61	8.902	365.2328	C22H36S2	(8R,9S,10S,13S,14S)-10,13 Dimethylhexadecahydrospiro[cyclopenta[a]phenanthrene-17,2'-[1,3]dithiane]
62	8.965	293.2112	C14H32N2S2	2,2'-(1,2-Ethanediyldisulfanediyl)bis(N,N-diethylethanamine)
63	9.015	387.2732	C18H30N10	N,N,N',N',N'',N''-Hexaethyl-1,3,4,6,7,9,9b-heptaazaphenalene-2,5,8-triamine
64	9.036	387.2739	C21H38O6	MB2700000
65	9.120	275.2005	C13H27N4Cl	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
66	9.212	351.2516	C21H34O4	10-GINGEROL
67	9.254	269.1746	C15H24O4	1,9-NONANEDIOL DIACRYLATE
68	9.367	275.2003	C13H27N4Cl	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
69	9.451	291.1955	C18H26O3	octinoxate
70	9.584	289.0847	C19H12O3	7-Hydroxy-3-(2-naphthyl)-2H-chromen-2-one
71	9.668	303.1016	C20H14O3	Ĩ³-Oxo-1-pyrenebutyric acid
72	9.718	275.2001	C13H27N4Cl	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
73	9.781	369.2630	C21H36O5	Carboprost
74	9.844	277.2160	C18H28O2	MFCD00041917
75	9.894	275.0705	C18H10O3	Bindone
76	9.999	289.1797	C16H29SCl	2-[(4-Butylcyclohexyl)(chloro)methyl]-5-methyltetrahydrothiophene
77	10.020	289.1801	C13H25N4OCl	2-(Aminomethyl)-N-(1-isopropyl-1H-pyrazol-4-yl)-4-methylpentanamide hydrochloride (1:1)
78	10.070	351.2523	C21H35N2Cl	1-Methyl-4-[4-(2-methyl-2-propanyl)-1-phenylcyclohexyl]piperazine hydrochloride (1:1)
79	10.154	362.2883	C20H35N5O	(5-{[2-(Diethylamino)ethyl]amino}-1-methyl-4,5,6,7-tetrahydro-1H-indazol-3-yl)(1-piperidinyl)methanone
80	10.175	275.1996	C13H27N4Cl	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
81	10.246	848.3879	C47H53N5O10	Ethyl(5,13,31,37-tetraoxo-3,15,29,39-tetraoxa-6,9,12,32,36pentaazaheptacyclo [25.23.1.1^{17,41}.0^{2,47}.0^{16,21}.0^{23,28}.0^{40,45}] pentaconta-1,16,18,20,23,25,27,40,42,44,47,49-dodecaen-9-yl) acetate
82	10.329	317.0819	C20H12O4	6-Oxo-6H-benzo[c]chromen-3-yl benzoate
83	10.421	277.2174	C18H28O2	MFCD00041917
84	10.505	275.2017	C18H26O2	Nandrolone
85	10.526	275.2010	C13H27N4Cl	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
86	10.815	295.2272	C18H30O3	OCTOXYNOL-2
87	11.342	694.4023	C33H59NO14:	2-(aziridin-1-yl)ethanol; decanedioic acid; 2,2-dimethylpropane-1,3-diol; 2-ethyl-2-(hydroxymethyl)propane-1,3-diol; isophthalic acid
88	11.426	287.1070	C20H14O2	Binol
89	11.476	518.3249	C26H60N5S3Br	unknown
90	11.602	694.3992	C29H55N7O12	unknown
91	11.715	518.3247	C21H47N3O11	unknown
92	11.911	353.2688	C21H36O4	MONOLINOLENIN
93	12.024	494.3257	C26H43N3O6	N-[(4-{2-Hydroxy-3-[(2-methyl-2-propanyl)oxy]propyl}-2-morpholinyl)methyl]-3-methoxy-N-[2-(4-morpholinyl)ethyl]benzamide
94	12.066	351.2522	C17H38N2OS2	unknown

95	12.129	351.2535	C19H39OSCl	unknown
96	12.221	520.3435	C22H45N7O7	2-{(2R,3R,6S)-2-{[(1R,2S,3S,4R,6S)-4,6-Diamino-3-{[3-deoxy-4-C-methyl-3-(methylamino)-L-arabinopyranosyl]oxy}-2-hydroxycyclohexyl]oxy}-6-[(1R)-1-(methylamino)ethyl]tetrahydro-2H-pyran-3-yl}guanidine
97	12.355	696.4155	C33H61NO14	Hexadecyl 3-O-{(6R)-5-acetamido-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-β-L-threo-hex-2-ulopyranonosyl}-β-D-galactopyranoside
98	12.530	532.3519	C6H38N26OS	unknown
99	12.656	279.2324	C18H30O2	α-Linolenic acid
100	12.706	277.2170	C13H29N4Cl	N-[3-(3,4,5,6-Tetrahydro-2H-azepin-7-ylamino)propyl]-1,4-butanediamine hydrochloride (1:1)
101	13.079	496.3411	C20H45N7O7	Tidak ada
102	13.184	417.2387	C19H28N8O3	1-({(3R)-1-[(3-Amino-5,6-dimethyl-2-pyrazinyl)carbonyl]-3-piperidinyl}methyl)-N-(2-methoxyethyl)-1H-1,2,3-triazole-4-carboxamide
103	13.234	698.4329	C34H59N5O10	(1r,2r,3r,6r,7s,8s,9r,10r,12r,13s,17s)-3-Ethyl-2,10-Dihydroxy-2,6,8,10,12,15,15,17-Octamethyl-5-Oxo-9-(Prop-2-Yn-1-Yloxy)-4,14,16-Trioxabicyclo[11.3.1]heptadec-7-Yl {3-[n'-(Methylcarbamoyl) carbamimidamido]propyl}carbamate
104	13.359	534.3625	C27H51NO9	2-Methyl-2-propanyl-2,2-dimethyl-10-(2-{3-[(2-methyl-2-propanyl)oxy]-3-oxopropoxy}ethyl)-4-oxo-3,7,13-trioxa-10-azahexadecan-16-oate
105	13.409	424.3617	C23H45N5O2	N-[3-({4-[(3-Aminopropyl)amino]butyl}amino)propyl]-3-cyclohexyl-N^2-(cyclopropylcarbonyl)-L-alaninamide
106	13.472	468.3914	C24H53NO7	unknown
107	13.535	291.2328	C19H30O2	Androstanolone
108	13.690	644.4985	C33H65N5O7	2,2',2''-{10-[3-(Dioctylamino)-2-hydroxypropyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl}triacetic acid
109	13.761	393.2420	C21H32N2O5	Methyl N-(tert-butoxycarbonyl)-L-leucyl-L-phenylalaninate
110	13.937	590.4263	C30H59NO9	2-{[2-(Stearoyloxy)propanoyl]oxy}propanoic acid - 2,2',2''-nitrilotriethanol (1:1)
111	13.999	502.3742	C28H47N5O3	N-{3-[Cyclohexyl(methyl)amino]propyl}-1-{[(1R,2R)-6-oxo-7,11-diazatricyclo[7.3.1.0^{2,7}]tridec-11-yl]carbonyl}-4-piperidinecarboxamide
112	14.062	324.2896	C20H37NO2	MFCD00674434
113	14.112	305.2474	C20H32O2	Arachidonic acid
114	14.217	293.2477	C19H32O2	Methyl Linolenate
115	14.393	732.5536	C35H77N3O12	unknown
116	14.485	600.4708	C31H61N5O6	unknown
117	14.548	512.4185	C26H57NO8	unknown
118	14.640	394.3463	C28H43N	bis(4-Octylphenyl)amine
119	14.723	394.3446	C24H44N2O2	2,5-Bis[(dibutylamino)methyl]-1,4-benzenediol
120	15.188	960.9011	C62H113N5O2	unknown
121	15.364	960.8973	C61H117NO6	unknown
122	15.996	960.8954	C58H109N11	unknown
123	16.594	960.8855	C59H110N9O	unknown
124	16.699	960.8882	C63H113N3O3	unknown
125	17.929	960.9025	C60H117N3O5	unknown
126	18.331	960.8998	C62H113N5O2	unknown
127	18.506	960.8967	C57H113N7O4	unknown
128	18.984	327.2060	C20H26N2O2	dihydroquinidine
129	19.034	327.2070	C25H26	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
130	20.503	327.2064	C12H30N4O4S	Undecyl hydrogen sulfate - carbonohydrazonic diamide (1:1)
131	21.516	327.2076	C17H30N2O2S	N-[2-(Diethylamino)ethyl]-2,3,4,5,6-pentamethylbenzenesulfonamide
132	21.691	327.2097	C14H26N6O3	N-Isopropyl-2-{2-[1-(2-methoxyethyl)-1H-tetrazol-5-yl]-4-morpholinyl}-N-methylacetamide
133	21.846	327.2075	C15H26N4O4	(2-Methyl-1,4-piperazinediyl)bis(4-morpholinylmethanone)

Table 6. Results of Interpretation of metabolite data profiling extracts by the soxlet method

No.	Rt (min)	m/z	Rumus Molekul	Nama Senyawa
1	1,148	290,8486	C4O7S3Cl	unknown
2	1,232	381,0808	C9H20N2O12S	unknown
3	1,282	381,0808	C9H20N2O12S	unknown
4	1,562	180,1037	C10H13NO2	Phenacetin
5	1,633	121,0657	C8H8O	Acetophenone
6	1,809	178,0873	C10H11NO2	AL9325000
7	2,068	178,0875	C10H11NO2	AL9325000
8	2,336	178,0874	C3H11N7S	1-(1,2,3,4-Thiatriazolidin-5-yl)-1,2,4-triazolidin-3-amine
9	2,512	166,0878	C9H11NO2	DL-Phenylalanine

10	2,813	230,0938	C12H11N3O2	HC Red 1
11	2,843	230,0937	C12H11N3O2	HC Red 1
12	3,278	208,134	C12H17NO2	Ciclopirox
13	3,391	180,0665	C6H13NO3S	Cyclamic acid
14	3,496	180,0660	C9H9NO3	Hippuric acid
15	3,517	180,0656	C9H9NO3	Hippuric acid
16	3,671	188,0712	C11H9NO2	Benzylmaleimide
17	3,721	272,0927	C15H13NO4	4-Benzyloxy-3-nitroacetophenone
18	3,826	238,1445	C13H19NO3	N-t-BOC-D-Phenylglycinol
19	3,918	257,1290	C15H16N2O2	Ancymidol
20	4,136	222,1493	C13H19NO2	ETHYL 4-BUTYLAMINOBENZOATE
21	4,395	256,1349	C16H17NO2	N,N-Dibenzylglycine
22	4,529	207,1388	C8H19N4Cl	8-Azido-1-octanamine hydrochloride (1:1)
23	4,600	308,1872	C17H25NO4	Buflomedil
24	4,726	476,3053	C20H45NO11	unknown
25	4,797	434,2023	C19H31NO10	21-(2,5-Dihydro-2,5-dioxo-1H-pyrrol-1-yl)-4,7,10,13,16,19-hexaoxaheneicosanoic acid
26	4,818	434,2018	C19H31NO10	21-(2,5-Dihydro-2,5-dioxo-1H-pyrrol-1-yl)-4,7,10,13,16,19-hexaoxaheneicosanoic acid
27	4,881	520,3348	C22H49NO12	unknown
28	4,952	236,1669	C14H21NO2	Padimate A
29	5,036	564,3608	C24H53NO13	unknown
30	5,148	490,5148	C24H31N3O8	Diethyl 1,1'-[(5-nitro-1,3-phenylene)dicarbonyl]dipiperidine-4-carboxylate
31	5,190	608,3870	C27H53N5O10	unknown
32	5,408	503,1903	C18H34N2O12S	unknown
33	5,479	482,2613	C21H39NO11	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
34	5,500	482,2617	C21H39NO11	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
35	5,542	522,2933	C24H43NO11	Octyl 2-[(cyclopropylcarbonyl)amino]-2-deoxy-3-O-β-D-galactopyranosyl-β-D-glucopyranoside
36	5,605	245,1393	C12H20O5	Diisopropyl 3-hydroxy-1,1-cyclobutanedicarboxylate
37	5,739	461,1579	C23H28N2O4S2	1,1'-(9H-Fluorene-2,7-diyldisulfonyl)dipiperidine
38	5,831	197,1177	C11H16O3	1-carboxy-3-hydroxyadamantane
39	5,851	197,1179	C11H16O3	1-carboxy-3-hydroxyadamantane
40	5,914	322,2020	C16H27N5S	4-Ethyl-5-methyl-6-[4-(tetrahydro-2H-thiopyran-4-yl)-1-piperazinyl]-2-pyrimidinamine
41	5,956	336,2178	C19H29O4	(3S)-3-({[(2-Methyl-2-propanyl)oxy]carbonyl}amino)-4-[4-(2-methyl-2-propanyl)phenyl]butanoic acid
42	6,006	333,1606	C21H20N2O2	1-Fmoc-4-Cyanopiperidine
43	6,048	411,1784	C16H30N2O8S	(6R)-5-Acetamido-2-{3-[(2-aminoethyl)sulfanyl]propyl}-2,6-anhydro-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-L-xylo-hexonic acid
44	6,245	324,2167	C18H29NO4	guaiapate
45	6,308	373,2217	C19H32O7	O-dPEG6-OH
46	6,358	496,2752	C22H41NO11	Octyl 2-acetamido-2-deoxy-3-O-β-D-galactopyranosyl-β-D-glucopyranoside
47	6,421	280,1912	C16H25NO3	Moxisylyte
48	6,463	213,1496	C12H20O3	Ethyl 4-cyclohexyl-3-oxobutanoate
49	6,504	440,2489	C23H37NO5S	Leukotriene E4
50	6,596	383,1812	C19H30N2O2S2	2-[4-(1,4-Dithiepan-6-yl)-1-(3-methoxybenzyl)-2-piperazinyl]ethanol
51	6,659	373,2101	C21H28N2O4	3,5-Bis[(cyclohexylcarbonyl)amino]benzoic acid
52	6,751	207,1608	C10H22O4	toxytriglycol
53	6,835	496,2787	C21H41NO11	Octyl 2-acetamido-2-deoxy-3-O-β-D-galactopyranosyl-β-D-glucopyranoside
54	6,885	442,2675	C19H39NO10	MFCD11041146
55	7,082	247,1335	C15H18O3	Loxoprofen
56	7,166	517,2052	C23H36N2O7S2	(17β)-2-Methoxyestra-1(10),2,4-triene-3,17-diyl bis(dimethylsulfamate)
57	7,208	209,1536	C13H20O2	AC 45594
58	7,258	466,2652	C22H37N5O6	2-Methyl-2-propanyl N-[(5-{[5-({[(2-methyl-2-propanyl)oxy]carbonyl}amino)pentyl]carbamoyl}-1H-imidazol-4-yl)carbonyl]-L-alaninate
59	7,320	291,0653	C18H10O4	MFCD00192048
60	7,412	480,2445	C21H37NO11	6-O-(2-Acetamido-2-deoxyhexopyranosyl)-3-O-butyl-1,2-O-isopropylidenehexofuranose
61	7,475	605,2932	C28H48N2O8S2	Diethyl 2,2'-[(3,12-dioxo-4,11-dioxa-7,8-dithia-2,13-diazatetradecane-1,14-diyl)di-1,1-cyclohexanediyl]diacetate
62	7,588	211,1696	C13H22O2	4-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene-1-carbaldehyde
63	7,609	211,1694	C13H22O2	4-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene-1-carbaldehyde
64	7,714	441,2251	C22H36N2O3S2	N-[3-(Butylsulfanyl)propyl]-4-({[(4-methylphenyl)sulfonyl]amino}methyl)cyclohexanecarboxamide

65	7,869	549,2322	C25H28N10O5	4-{(Z)-[({1-(4-Amino-1,2,5-oxadiazol-3-yl)-5-[(diethylamino)methyl]-1H-1,2,3-triazol-4-yl}carbonyl)hydrazono]methyl}-2-methoxyphenyl phenylcarbamate
66	8,003	452,2141	C19H33NO11	6-O-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-3-O-ethyl-1,2-O-isopropylidene-β-L-idofuranose
67	8,044	452,2138	C19H33NO11	6-O-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-3-O-ethyl-1,2-O-isopropylidene-β-L-idofuranose
68	8,157	443,2410	C18H34N8OS2	unknown
69	8,375	454,2297	C19H35NO11	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
70	8,396	454,2294	C19H35NO11	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
71	8,902	489,1746	CH11N3O2	unknown
72	9,451	279,0951	C14H10N6O	3-[(2E)-2-(2-Furylmethylene)hydrazino]-5H-[1,2,4]triazino[5,6-b]indole
73	9,978	343,2936	C15H34N8O	2-(5-{[Isopropyl(methyl)amino]methyl}-1-tetrazolidinyl)-N-methyl-N-[2-(2-methyl-1-imidazolidinyl)ethyl]acetamide
74	9,999	327,2061	C16H22N8	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
75	10,196	327,2040	C20H26N2O2	dihydroquinidine
76	10,329	367,3330	C18H38N8	1,1'-(1,2-Ethanediyl)bis{3-[2-(1-imidazolidinyl)ethyl]imidazolidine}
77	10,618	288,2910	C17H37NO2	2,2'-(Tridecylimino)diethanol
78	10,639	288,2909	C17H37NO2	2,2'-(Tridecylimino)diethanol
79	10,752	214,7520	C14H31N	JR6600000
80	11,300	327,2067	C20H26N2O2	dihydroquinidine
81	12,003	316,3195	C19H41NO2	1-hexadecyl-2-amino-2-deoxy-sn-glycerol
82	12,066	327,2054	C20H26N2O2	dihydroquinidine
83	12,706	327,2080	C15H26N4O4	(2-Methyl-1,4-piperazinediyl)bis(4-morpholinylmethanone)
84	12,811	327,2076	C20H26N2O2	dihydroquinidine
85	13,317	279,1591	C16H22O4	Dibutyl phthalate
86	14,506	960,8987	C49H8N2O13S4	unknown
87	14,590	960,8883	C29H4N8O29S	unknown
88	14,765	960,8937	C35HN10O23S	unknown
89	14,836	960,8970	C47HN2O23	unknown
90	14,941	960,9005	C16H24N4O33S5	unknown
91	15,012	960,9003	C8H20N10O36S4	unknown
92	15,075	960,9001	C15H12N8O39S	unknown
93	15,209	960,8933	C17H9N12O32SCl	unknown
94	15,251	960,8942	C22H8N8O34S	unknown
95	15,343	960,8940	C16H16O47	unknown
96	15,385	960,8939	C50H113N13O2S	unknown
97	15,468	960,8890	C37HN6O27	unknown
98	15,539	960,8866	C49H4O19S2	unknown
99	15,715	960,9019	C38H8N8O16S4	unknown
100	15,757	960,9030	C12H24N4O38S4	unknown
101	15,820	960,9034	C27H12O39	unknown
102	15,870	960,9033	C39H4N12O12S4	unknown
103	15,975	960,9011	C37H4N8O21S2	unknown
104	16,067	960,8994	C22H12N2O41	unknown
105	16,109	960,8950	C38H8O29S	unknown
106	16,151	960,8983	C14H24O42S3	unknown
107	16,222	960,8966	C54H117N7O4S	unknown
108	16,284	960,8962	C31HN10O28	unknown
109	16,418	960,8958	C13H9N12O37Cl	unknown
110	16,523	960,8981	C41H12N4O15S5	unknown
111	16,573	960,8972	C40H8N4O20S3	unknown
112	16,678	960,8976	C19H12N8O34S2	unknown
113	16,749	960,8973	C62H113N5O2	unknown
114	16,833	960,9014	C16H8N12O35S	unknown
115	16,875	960,8997	C36H8N4O25S2	unknown
116	16,925	960,8989	C35H4N4O30	unknown
117	16,966	960,9007	C23H8N6O37	unknown
118	16,987	960,8997	C36H8N4O25S2	unknown
119	17,008	960,8990	C37H1N16O10S3Cl	unknown
120	17,100	960,8992	C34H4N14O14S4	unknown
121	17,184	960,8984	C33HN14O19S2	unknown
122	17,318	960,8952	C44HN8O16S2	unknown

123	17,381	960,8935	C29H8N2O36	unknown
124	17,473	960,8955	C23H4N12O30S	unknown
125	17,515	960,8943	C44H16O14S6	unknown
126	17,578	960,8963	C50H5O18SCl	unknown
127	17,649	960,8983	C14H24O42S3	unknown
128	17,691	960,8965	C41H1N16O5S4Cl	unknown
129	17,803	960,8969	C26H12N2O36S	unknown
130	17,979	960,8975	C34H8O34	unknown
131	18,155	960,8969	C26H13N2O36S	unknown
132	18,435	960,8932	C57H113N7O4	unknown
133	18,506	960,8938	C4H17N10O43SCl	unknown
134	19,16	327,2073	C20H26N2O2	dihydroquinidine
135	20,348	327,2070	C25H26	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
136	21,557	327,2062	C20H26N2O2	dihydroquinidine

Table 7. Results of Interpretation of metabolite data profiling extracts by reflux method

No	Rt (min)	m/z	Rumus Molekul	Nama Senyawa
1	0.156	327.2073	$C_{20}H_{26}N_2O_2$	dihydroquinidine
2	1.056	381.0796	$C_9H_{20}N_2O_{12}S$	unknown
3	1.499	222.1493	$C_{13}H_{19}NO_2$	ETHYL 4-BUTYLAMINOBENZOATE
4	1.633	256.1339	$C_6H_{13}N_{11}O$	unknown
5	1.675	256.1341	$C_{12}H_{13}N_7$	2-{[4-Amino-6-(dimethylamino)-1,3,5-triazin-2-yl]amino}benzonitrile
6	1.809	256.1333	$C_{16}H_{17}NO_2$	N,N-Dibenzylglycine
7	2.110	340.2601	$C_{18}H_{33}N_3O_3$	2-Methyl-2-propanyl 3-{[cyclopropyl(L-valyl)amino]methyl}-1-pyrrolidinecarboxylate
8	3.123	256.1313	$C_7H_{13}N_9O_2$	1,3,5,7-Tetraazatricyclo[3.3.1.1^{3,7}]decane - 5-nitro-1H-tetrazole (1:1)
9	3.215	256.1315	$C_9H_{17}N_7S$	4-(2-Aminoethyl)-N-(1H-1,2,4-triazol-3-yl)-1-piperazinecarbothioamide
10	3.567	256.1333	$C_5H_{17}N_7O_5$	unknown
11	3.868	256.1335	$C_6H_{13}N_{11}O$	unknown
12	4.044	434.2020	$C_{19}H_{31}NO_{10}$	21-(2,5-Dihydro-2,5-dioxo-1H-pyrrol-1-yl)-4,7,10,13,16,19-hexaoxaheneicosanoic acid
13	4.332	453.3423	$C_{24}H_{44}N_4O_4$	1,8,15,22-Tetraazacyclooctacosane-2,9,16,23-tetrone
14	4.445	236.1638	$C_{14}H_{21}NO_2$	Padimate A
15	4.684	136.0752	C_8H_9NO	Acetanilide
16	4.880	566.4326	$C_{30}H_{55}N_5O_5$	Cyclo(L-leucyl-L-valyl-N-methyl-L-leucyl-L-leucyl-L-leucyl)
17	5.015	359.1974	$C_{25}H_{26}O_2$	4-(5,5,8,8-Tetramethyl-5,6,7,8-tetrahydro-2-anthracenyl)benzoic acid
18	5.077	482.2609	$C_{21}H_{39}NO_{11}$	Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-β-D-mannopyranosyl)-β-D-glucopyranoside
19	5.274	197.1179	$C_{11}H_{16}O_3$	1-carboxy-3-hydroxyadamantane
20	5.542	322.2006	$C_{18}H_{28}ClN_3$	1-[1-(2-Chlorobenzyl)-4-piperidinyl]-4-ethylpiperazine
21	5.626	333.1602	$C_{21}H_{20}N_2O_2$	1-Fmoc-4-Cyanopiperidine
22	5.801	333.1634	$C_{26}H_{20}$	Tetraphenylethylene
23	5.914	324.2192	$C_{18}H_{29}NO_4$	guaiapate
24	5.977	324.2199	$C_{19}H_{25}N_5$	4-benzyl-N-(4,6-dimethylpyrimidin-2-yl)piperidine-1-carboximidamide
25	6.132	280.1909	$C_{16}H_{25}NO_3$	Moxisylyte
26	6.245	213.1486	$C_{12}H_{20}O_3$	Ethyl 4-cyclohexyl-3-oxobutanoate
27	6.329	324.2174	$C_{16}H_{29}N_5S$	2,4-Bis[(4-methyl-1-piperidinyl)methyl]-2,4-dihydro-3H-1,2,4-triazole-3-thione
28	6.379	309.2057	$C_{19}H_{24}N_4$	N-[4-(Dimethylamino)benzyl]-1-isopropyl-1H-benzimidazol-2-amine
29	6.504	373.2120	$C_{26}H_{28}O_2$	MFCD00056577
30	6.659	336.2160	$C_{15}H_{33}N_3OS_2$	unknown
31	6.793	247.1325	$C_{12}H_{22}O_3S$	3-(Octyloxy)-2,3-dihydrothiophene 1,1-dioxide
32	6.856	247.1321	$C_{15}H_{18}O_3$	Loxoprofen
33	7.032	570.3403	$C_{28}H_{47}N_3O_9$	2-Methyl-2-propanyl [(3S,6S,7R)-6-(cyclohexylmethyl)-7-hydroxy-10-(4-morpholinylmethyl)-4,8,14-trioxo-1,9-dioxa-5-azacyclotetradecan-3-yl]carbamate
34	7.103	1175.5892	$C_{49}H_{74}N_{24}O_9S$	unknown
35	7.187	466.2671	$C_{22}H_{35}N_5O_6$	5-[(3R)-4-(Cyclohexylcarbamoyl)-3-{[(3S)-2-oxo-3-piperidinyl]carbamoyl}-1-piperazinyl]-5-oxopentanoic acid
36	7.258	466.2650	$C_{21}H_{39}NO_{10}$	methyl 9-[(2S,3S,4S,5R)-5-[[(2S,3R,4R)-2-[(1R)-1,2-dihydroxyethyl]-3,4-dihydroxy-pyrrolidin-1-yl]methyl]-3,4-dihydroxy-tetrahydrofuran-2-yl]oxynonanoate
37	7.299	294.2064	$C_{17}H_{27}NO_3$	Nonivamide
38	7.341	167.0857	$C_{13}H_{10}$	Fluorene

39	7.475	308.2214	$C_{18}H_{29}NO_3$	Betaxolol
40	7.559	432.2954	$C_{23}H_{37}N_5O_3$	1,3-Dicyclohexyl-5-({[2-(1-piperazinyl)ethyl]amino}methylene)-2,4,6(1H,3H,5H)-pyrimidinetrione
41	7.609	269.1747	$C_{15}H_{24}O_4$	1,9-NONANEDIOL DIACRYLATE
42	7.735	372.2514	$C_{23}H_{33}NO_3$	20-hydroxyiminopregna-5,16-dien-3-β-yl acetate
43	7.785	372.2528	$C_{23}H_{34}O_4$	Digitoxigenin
44	7.869	275.2001	$C_{18}H_{26}O_2$	Nandrolone
45	7.911	278.2109	$C_{17}H_{27}NO_2$	Venlafaxine
46	8.003	269.1757	$C_{13}H_{24}N_4S$	4-Cyclohexyl-5-(1-(dimethylamino)propyl)-4H-1,2,4-triazole-3-thiol
47	8.086	275.2008	$C_{15}H_{30}O_2S$	3-(Dodecylthio)propanoic acid
48	8.312	454.2273	$C_{19}H_{35}NO_{11}$	5-Aminopentyl 3-O-(2-O-acetyl-6-deoxy-α-L-talopyranosyl)-β-D-glucopyranoside
49	8.438	930.3079	$C_{44}H_{51}NO_{21}$	unknown
50	8.488	467.2429	$C_{25}H_{26}N_{10}$	6-[(1E,3E)-3-(4,5-Dihydro-1H-imidazol-2-ylhydrazono)-1-propen-1-yl]-2-{4-[(1E,3E)-3-(4,5-dihydro-1H-imidazol-2-ylhydrazono)-1-propen-1-yl]phenyl}imidazo[1,2-a]pyridine
51	8.551	295.2283	$C_{18}H_{30}O_3$	OCTOXYNOL-2
52	8.593	277.2168	$C_{18}H_{28}O_2$	MFCD00041917
53	8.768	554.3457	$C_{28}H_{47}N_3O_8$	2-Methyl-2-propanyl [1-(bicyclo[6.1.0]non-4-yn-9-yl)-3,19-dioxo-2,8,11,14-tetraoxa-4,18-diazaicosan-20-yl]carbamate
54	8.860	365.2314	$C_{22}H_{36}S_2$	(8R,9S,10S,13S,14S)-10,13-Dimethylhexadecahydrospiro[cyclopenta[a]phenanthrene-17,2'-[1,3]dithiane]
55	8.965	181.1216	$C_{11}H_{16}O_2$	5-Pentylresorcinol
56	9.015	387.2738	$C_{21}H_{38}O_6$	MB2700000
57	9.191	351.2522	$C_{21}H_{34}O_4$	10-GINGEROL
58	9.367	291.1953	$C_{16}H_{31}ClS$	4-Butyl-1-(chloromethyl)-1-[3-(ethylsulfanyl)propyl]cyclohexane
59	9.430	291.1957	$C_{15}H_{30}O_3S$	3-(Dodecylsulfinyl)propanoic acid
60	9.492	313.2376	$C_{18}H_{32}O_4$	(9E)-9-Octadecenedioic acid
61	9.584	289.0860	$C_{19}H_{12}O_3$	7-Hydroxy-3-(2-naphthyl)-2H-chromen-2-one
62	9.718	275.200	$C_{13}H_{27}ClN_4$	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
63	9.760	369.2636	$C_{21}H_{36}O_5$	Carboprost
64	9.823	362.2890	$C_{19}H_{39}NO_5$	Ethyl decyl{2-[2-(2-hydroxyethoxy)ethoxy]ethyl}carbamate
65	10.020	227.1634	$C_{13}H_{22}O_3$	Hedione
66	10.196	293.2106	$C_{16}H_{32}SCl$	unknown
67	10.246	309.2421	$C_{19}H_{32}O_3$	4-Nonylphenol diethoxylate
68	10.371	371.2788	$C_{21}H_{38}O_5$	(5Z)-5-Heptenoic acid - (1S,3R,4R,5R)-4-[(1E,3S)-3-hydroxy-1-octen-1-yl]-5-methyl-1,3-cyclopentanediol (1:1)
69	10.505	275.2018	$C_{13}H_{27}ClN_4$	(2E)-2-(4-Cyclohexyl-4-methyl-2-pentanylidene)-1-(diaminomethylene)hydrazinium chloride
70	10.949	295.2262	$C_{14}H_{34}N_2S_2$	N,N'-(Disulfanediyldi-2,1-ethanediyl)bis(N,N-dimethyl-2-propanaminium)
71	11.074	295.2268	$C_{15}H_{34}O_3S$	unknown
72	11.250	295.2272	$C_{13}H_{31}ClN_4O$	N,N-Bis[3-(dimethylamino)propyl]alaninamide hydrochloride (1:1)
73	11.476	518.3246	$C_{28}H_{43}N_3O_6$	N-[(trans-4-{[(N-{[(2-Methyl-2-propanyl)oxy]carbonyl}-L-leucyl)amino]methyl}cyclohexyl)carbonyl]-L-phenylalanine
74	11.581	694.4052	$C_{33}H_{59}NO_{14}$	2-(aziridin-1-yl)ethanol; decanedioic acid; 2,2-dimethylpropane-1,3-diol; 2-ethyl-2-(hydroxymethyl)propane-1,3-diol; isophthalic acid
75	11.715	518.3239	$C_{23}H_{43}N_5O_8$	Bis(2-methyl-2-propanyl) [(Z)-({5-[methoxy(methyl)amino]-4-({[(2-methyl-2-propanyl)oxy]carbonyl}amino)-5-oxopentyl}amino)methylylidene]biscarbamate
76	11.777	353.2675	$C_{21}H_{36}O_4$	MONOLINOLENIN
77	12.0003	494.3242	$C_{26}H_{43}N_3O_6$	N-[(4-{2-Hydroxy-3-[(2-methyl-2-propanyl)oxy]propyl}-2-morpholinyl)methyl]-3-methoxy-N-[2-(4-morpholinyl)ethyl]benzamide
78	12.066	351.2528	$C_{17}H_{38}N_2OS_2$	unknown
79	12.129	351.2542	$C_{21}H_{35}ClN_2$	1-Methyl-4-[4-(2-methyl-2-propanyl)-1-phenylcyclohexyl]piperazine hydrochloride (1:1)
80	12.200	520.3421	$C_{28}H_{45}N_3O_6$	3-c-3-(Z-amino)-L-alanine (dicyclohexylammonium) salt
81	12.221	520.3423	$C_{22}H_{45}N_7O_7$	2-{(2R,3R,6S)-2-{[(1R,2S,3S,4R,6S)-4,6-Diamino-3-{[3-deoxy-4-C-methyl-3-(methylamino)-L-arabinopyranosyl]oxy}-2-hydroxycyclohexyl]oxy}-6-[(1R)-1-(methylamino)ethyl]tetrahydro-2H-pyran-3-yl}guanidine
82	12.305	351.2527	$C_{17}H_{38}N_2OS_2$	unknown
83	12.355	696.4171	$C_{33}H_{61}NO_{14}$	Hexadecyl 3-O-{(6R)-5-acetamido-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-β-L-threo-hex-2-ulopyranonosyl}-β-D-galactopyranoside
84	12.530	279.2326	$C_{18}H_{30}O_2$	α-Linolenic acid
85	12.706	277.2168	$C_{13}H_{29}ClN_4$	N-[3-(3,4,5,6-Tetrahydro-2H-azepin-7-ylamino)propyl]-1,4-butanediamine hydrochloride (1:1)

86	13.058	496.3408	$C_{26}H_{45}N_3O_6$	1-(β-D-Arabinofuranosyl)-4-(heptadecanoylamino)-2(1H)-pyrimidinone
87	13.079	496.3407	$C_{22}H_{41}N_9O_4$	N^5-(Diaminomethylene)-L-ornithyl-L-prolyl-L-lysyl-L-prolinamide
88	13.184	417.2404	$C_{23}H_{32}N_2O_5$	Tritace
89	13.234	698.4322	$C_{33}H_{63}NO_{14}$	unknown
90	13.359	522.3527	$C_{24}H_{43}N_9O_4$	unknown
91	13.409	522.3538	$C_{28}H_{47}N_3O_6$	1-(2,3-Dideoxy-3-{hydroxy[(9E)-9-octadecenoyl]amino}pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione
92	13.472	468.3870	$C_{24}H_{53}NO_7$	unknown
93	13.535	291.2302	$C_{19}H_{30}O_2$	Androstanolone
94	13.669	600.4661	$C_{30}H_{65}NO_{10}$	unknown
95	13.711	644.4918	$C_{30}H_{57}N_{15}O$	unknown
96	13.761	228.2317	$C_{14}H_{29}NO$	Myristamide
97	13.845	393.2397	$C_{16}H_{32}N_4O_7$	unknown
98	13.887	393.2410	$C_{21}H_{32}N_2O_5$	Methyl N-(tert-butoxycarbonyl)-L-leucyl-L-phenylalaninate
99	13.958	546.4022	$C_{30}H_{51}N_5O_4$	N-{[4-(5-Aminopentyl)phenyl]acetyl}-L-seryl-N-(2-cyclohexylethyl)-L-lysinamide
100	13.979	502.3760	$C_{27}H_{51}NO_7$	1-(Dodecylamino)-3-{[(3aR,5aS,8aS,8bR)-2,2,7,7-tetramethyltetrahydro-3aH-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-5-yl]methoxy}-2-propanol
101	14.062	324.2890	$C_{20}H_{37}NO_2$	MFCD00674434
102	14.112	305.2479	$C_{20}H_{32}O_2$	Arachidonic acid
103	14.196	293.2475	$C_{19}H_{32}O_2$	Methyl Linolenate
104	14.361	368.3518	$C_{23}H_{45}NO_2$	N-(Tetrahydro-2-furanylmethyl)octadecanamide
105	14.393	732.5457	$C_{34}H_{65}B_{15}O_3$	unknown
106	14.414	688.5164	$C_{34}H_{73}NO_{12}$	unknown
107	14.464	644.4927	$C_{32}H_{69}NO_{11}$	unknown
108	14.506	556.4396	$C_{28}H_{61}NO_9$	unknown
109	14.640	309.2417	$C_{16}H_{36}O_3S$	unknown
110	14.723	300.2889	$C_{18}H_{37}NO_2$	Palmitylethanolamide
111	14.815	307.2630	$C_{20}H_{34}O_2$	Ethyl linolenate
112	14.857	960.8978	$C_{61}H_{117}NO_6$	unknown
113	14.991	960.8975	$C_{62}H_{113}N_5O_2$	unknown
114	15.054	609.2717	$C_{34}H_{40}O_{10}$	Scortechinone C
115	15.385	378.2213	$C_{28}H_{27}N$	4,4'-BIS(1-PHENYLETHYL)DIPHENYLAMINE
116	15.736	960.8998	$C_{55}H_{113}N_{11}S$	unknown
117	16.523	960.8996	$C_{61}H_{117}NO_6$	unknown
118	16.749	960.9011	$C_{56}H_{113}N_9O_3$	unknown
119	18.331	960.9026	$C_{60}H_{117}N_3O_5$	unknown
120	18.435	960.8989	$C_{58}H_{109}N_{11}$	unknown
121	18.745	960.8931	$C_{53}H_{109}N_{13}O_2$	unknown
122	18.808	327.2052	$C_{16}H_{22}N_8$	N-[3-(1H-Imidazol-1-yl)propyl]-1-methyl-4-(1-pyrrolidinyl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine
123	19.385	327.2045	$C_{15}H_{26}N_4O_4$	(2-Methyl-1,4-piperazinediyl)bis(4-morpholinylmethanone)
124	19.561	327.2076	$C_{25}H_{26}$	1,5-Diphenyl-3-(2-phenylethyl)-2-pentene
125	19.779	327.2078	$C_{10}H_{22}N_{12}O$	unknown
126	21.093	327.2046	$C_{12}H_{30}N_4O_4S$	Undecyl hydrogen sulfate - carbonohydrazonic diamide (1:1)

The eluent used is a mixture of water: formic acid (99.9:0,1) (v:v) and acetonitrile: formic acid (99.9:0.1) (v:v) with a gradient elution system, which is an elution system in which the eluent used changes its composition every time. The mixture of water and formic acid with acetonitrile and formic acid is an eluene mixture that facilitates the separation process in the column in a fast period, which is less than 10-15 minutes. A chromatogram with a polar compound will appear first then be followed by a compound whose polarity is lower. Next, the eluation results in the column go to the MS detector so that the results can be read easily. The sample in the form of a liquid will be converted into droplets and then pass through a needle that has been assigned an ESI (+) charge to produce ions that will be read by the MS detector. The result of the separation will appear as a chromatogram which is then processed using the Masslynx 4.1 application so that the spectra of each chromatogram peak can be known. Figure 1 is a chromatogram of the results of the analysis of the metabolite profile of Moses paradisiaca L.var.wood. The chromatogram is then processed using the Masslynx 4.1 application so that it can be known and

predictable the molecular formula of each compound. Each peak of a chromatogram indicates one compound. Based on the measured mass and calculated mass values on the spectra, it can be known the prediction of the molecular formula of the spectra. The value of measured mass and calculated mass must also be reduced by the mass of 1 H atom, which is 1.0078 because at the time of separation using the column there is an addition of H atoms derived from the firing of ESI ions (+). The prediction of the molecular formula that appears in the data is then selected as whose difference between measured mass and calculated mass ± 0.0005. Predictions of the molecular formula that have been selected are then searched with the help of the chemspider.com website. The molecular formula written on this website must be reduced by 1 H atom first because in the separation process there is an addition of 1 H atom derived from firing ESI ions (+). After the search is completed, the compound ID number is selected based on the number of publications, then the name ADC / IUPAC is selected to be further converted using the Chemdraw Ultra 12.0 application so that the structure of the desired compound can be known. Based on the data from the interpretation of compound content analysis using UPLC-QToFMS, it can be seen that there are 136 compounds in the remaseration method, 133 compounds in the maceration method, 126 compounds in the reflux method, and 136 compounds in the soxhlet method (table 1-table 4). Based on these data, it is known that there are differences in metabolite profiles in different extraction methods characterized by differences and the number of types of compounds contained in each extract. Based on the results of the interpretation of the data that has been obtained, it can be known several major compounds, namely compounds that have a higher percentage area compared to other compounds. The major compounds in the remaseration method are 15.13% ethyl-4-butylaminobenzoate, 29.88% unknown compounds, and 12.18% unknown compounds. The major compounds in the maceration method are 9.6% ethyl-4-butylaminobenzoate, 8.08% N compounds, N-dibenzyl glycine, and 7.01% bisphenol A dicyamate compounds. The major compounds in the soxhlet method are 11.79% ethyl-4-butylaminobenzoate, 29.92% N,N-dibenzyl glycine compounds, and 13.35% unknown compounds. The major compounds in the reflux method are 14.96% unknown compounds, 16.76%% unknown compounds and 18.23% unknown compounds.

Conclusions

Based on the results of the research that has been carried out, it can be concluded that differences in extraction methods affect phenolic levels and metabolite profiles in the unripe fruit of wood bananas (Musa paradisiaca L.Var.Kayu). In the remaseration extraction method, the highest phenolic content is 55.82%. In the remaseration method, it was found that there were 136 compounds, the maceration method of 133 compounds, the reflux method of 126 compounds, and the soxhlet method of 136 compounds.

Conflicts of Interest

The authors state there is no conflict of interest.

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