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Extraction of Faloak Stem Bark (*Sterculia quadrifida* R. Br) Using Microwave-Assisted Extraction Method And LC-HRMS Profiling of the Extract

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Abstract

The extraction of bioactive plants is an essential step in isolating the targeted bioactive compounds. Microwave-assisted extraction (MAE) offers a green technology extraction that can minimize energy, time, and solvent and is a suitable method for extracting thermolabile plant bioactive compounds. The study aims to find out the optimal time and temperature for isolating the total phenolic content (TPC), total flavonoid (TF), and antioxidant activity (AO) of *faloak* stem bark (FSB) (*Sterculia quadrifida* R. Br) and to profile the phytochemicals in the FSB extract using sophisticated of LC-HRMS (Liquid Chromatography High-Resolution Mass Spectrometry). The research used the Randomized Block Design (RBD) method with two factors. The factors were the extraction time (5, 15, and 25 min) and temperature variation (50, 60, and 70°C). The data of observed parameters were calculated using Analysis of Variance (ANOVA) and followed by a further test with a 95% confidence interval. The results showed an interaction between temperature and time of extraction on TPC, TF, and AO activity. The best MAE condition for extracting FSB was achieved at 60°C for 25 min. The FSB extract had a TPC of 81.2 mg GAE/g, TF of 70.30 mg QE/g, and AO activity of 67.8%. LC-HRMS revealed the newly identified phenolic compounds such as methyl cinnamate, vanillin, apocynin, scopoletin, L(-)-pipecolinic acid, arecoline, δ-valerolactam, 3,4-dihydroxybenzaldehyde, 4-hydroxybenzaldehyde; flavonoids such as epicatechin and rutin and some fatty acids and its derivatives. Future research could focus on developing new therapies for promoting human health using extract FSB.

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Sterculia quadrifida R. Br.

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Introduction

The discoveries of crude drugs are sometimes based on the alternative medicine developed by indigenous people. *Faloak* is a stem bark from the *faloak* tree (*Sterculia quadrifida* R.Br) used by people in East Nusa Tenggara Indonesia, as traditional medicine (Figure 1). Locals people believe *faloak* stems bark (FSB) can cure liver dysfunction, cancer, gastroenteritis, anti-diabetic, and fatigue recovery.[1] Extract of *faloak* stems bark (FSB) contains bioactive compounds of alkaloids, flavonoids, phenols, and terpenoids.[1] Exploration of FSB is necessary to know the bioactive compounds and study the extract's biological activity.

Fig. 1: Faloak (*Sterculia quadrifida* R.Br) stem bark

Selecting a suitable extraction method is crucial in isolating bioactive compounds in plant materials. Conventional extractions were applied for years to obtain a plant bioactive compound extract. However, some conventional extractions are inefficient methods.[2] Nowadays, microwave-assisted extraction, a green technology extraction, offers many advantages, especially thermo-sensitive compound extraction.[3] Isolating of bioactive compounds from plant matrix using MAE is related to some parameters such as the chemical nature of the bioactive compounds and the plant matrix, time, ratio of ethanol and water, and temperature.[4] Ethanol, a green solvent with low toxicity compared to methanol, evaporates quickly and is commonly used in pharmaceutical industries. The ratio of water and ethanol needs to be optimized to obtain maximum bioactive compounds in the plant.[5] Water and ethanol are suitable for plant extraction using MAE, which has proved efficient for the phenolic compounds' extraction from plants.[6-10] In extraction involving a microwave, water is essential since entrapped water in the plant matrix can interact with the microwave, causing cell rupture and releasing targeted compounds into the solvent.[11] The temperature of extraction is necessary to be optimized. High temperature can reduce the viscosity and surface tension which solvent penetrates better into the plant matrix cell.[5] However, the degradation of bioactive compounds occurs at high temperatures. Extraction yields can be increased by extending the extraction time. However, a longer extraction time can lead to the degradation of heat-sensitive compounds.[12] The extraction time using MAE is generally less than 30 min.[13]

Phenolic compounds contain many hydroxyl groups, which can be conjugated with sugars, acids, or alkyl groups. Therefore, one plant can have very diverse phenolics. Developing one extraction condition to obtain all the phenolic compounds is difficult. In this study, the optimal temperature and time of MAE for isolating the bioactive compound present in the FSB should be determined as to how those factors affect the phenol and flavonoid content of the extract. Moreover, a powerful analytical technique, HRMS, was used to profile the phytochemicals of the FSB extract.

Materials and Methods

Materials

Stems bark of *faloak* (*Sterculia quadrifida* R. Br) was obtained from Kupang province of East Nusa Tenggara, Indonesia. All the chemical reagents were pro-analyze quality. Ethanol (Mallinkrodt), methanol (Merck), Gallic acid, Na_2CO_3, folin ciocalteau, quercetin, $NaNO_2$, $AlCl_3$, NaOH dan DPPH (2,2- diphenyl-1-picrylhydrazyl) (Sigma-Aldrich) were bought from local chemical reagent distributors.

Methods

Extraction of *Faloak* Stem Bark (FSB)

The steps of extraction using MAE are referred to Martati and Simamora.[14] The air-dried and powdered FSB (4 g) was added with 40 mL of ethanol. The mixture was extracted using MAE (Anton Paar) at a combination of different temperatures (50, 60, and 70 °C) and lengths of extraction (5, 15, and 25 min). The extract of FSB was brought to room temperature. Impurities were separated through fine filter paper. The extracts were pooled in a small dark glass bottle and kept at -20°C until further measurements.

Quantification of total phenol (TPC)

Quantification of the TPC of FSB extract was measured by the Folin Ciocalteu (FC) assay according to Martati *et al.*[14] Diluted FSB extract of 0.5 mL is reacted with 2.5 mL FC 10%, vortexed and then kept for 5 min. Then, the mixture was reacted with 2 mL of 7.5% Na_2CO_3. Keep the mixtures for 30 min at room temperature in a dark place. The absorbance of the FSB sample was read at 750 nm. Gallic acid (GA) was treated the same as the extract of FSB to obtain a calibration curve and used to quantify TPC as mg GAE/g.

Quantification of Total Flavonoid (TF)

Quantification of Total Flavonoid Content (TF) in the FSB extract was referred to Martati *et al.*[15] with modification. A sample of FSB extract 1 mL is mixed with 4 mL of distilled water and reacted with a volume of 0.3 mL of $NaNO_2$ 5%. After incubation for 5 min, 0.3 mL of $AlCl_3$ 10% was combined and kept for 6 min. After 6 min, NaOH 1 M of 2 mL was added, and the total volume was 10 mL with distilled water. The mixture was mixed thoroughly. For quantification, the absorbance of the sample was read at 510 nm. A standard compound of quercetin was treated in the same steps for the sample to make a calibration curve. TF was quantified as mg QE/g sample.

Radical Scavenging Activity (DPPH)

The antioxidant action of the extract FSB on free radicals was analyzed as in the method written by Martati *et al.*[15] with small changes. DPPH was diluted in methanol to make a concentration of 0.3 mM. A serial dilutions of the FSB extract in methanol were prepared. A diluted extract of 3 mL was added with 1 mL of DPPH 0.3 mM. The sample mixture was kept in a dark room for 30 min. The sample's absorbance value was measured at 517 nm. The radical scavenging activity was calculated using below equation

$$\text{Radical scavenging activity (\%)} = (Ab-Ae)/(Ab) \times 100$$

where A_b is the absorbance of the methanol and DPPH solution (a blank), and A_e is the absorbance of the diluted FSB extract and DPPH solution.

Analysis of LC-HRMS

Identification of the bioactive compounds in the extract of FSB was performed on Thermo Scientific Dionex Ultimate 3000 RSLCnano. The analytical column was Hypersil GOLD aQ 50 x 1 mm x 1.9 µm particle size. The column oven was 30° C. The mobile phase was formic acid 0.1% (phase A) in water and acetonitrile containing formic acid 0.1% (phase B). A linear gradient mobile phase with a 40 µL/min flow rate was applied. Mobile phase A was applied from 100% to 95% in 2 min. Then, it decreased to 40% in 13 min, then to 5% in 7 min and was held for 3 min. Finally, It was increased to 95% and kept for 5 min. The total running time until finished was 30 min. High-Resolution Mass Spectrometer (Thermo Scientific Q Exactive) was set as follows, full scan settings were 70,000, the orbitrap resolution was 17,500. The software for processing data was a Compound Discoverer with mzCloud MS/MS Library.

Design Experiment and Statistical Analysis

The research applied the Randomized Block Design (RBD) method consisting of two factors extraction time (5, 15, and 25 min) and temperature variation (50, 60, and 70°C). From the combination of these two factors with three replications of each treatment, 27 experimental units were obtained. The measured parameter data were assessed using Analysis of Variance (ANOVA). Followed by a test to explore the difference between means (95% confidence interval). The data obtained were written as mean and standard deviation. The data were statistically analyzed using SPSS.

Results

TPC

The TPC of FSB extract was obtained from the extraction using MAE at a combination of temperature and time range from 49.07-81.17 mg GAE/g. Figure 2 shows the trend of TPC of FSB extract at a different combination of temperature and extraction time. It indicates that the yield of TPC increased as the temperature rose from 50 °C to 60 °C. At 70 °C, the TPC decreased. The maximum amount of TPC was obtained at 60 °C for 25 min, amounting to 81.17 mgGAE/g. While the lowest TPC was extracted at 70 °C for 25 min, amounting to 49.07 GAE/g. Therefore, the yield of TPC was driven by the combination of temperature and extraction time.

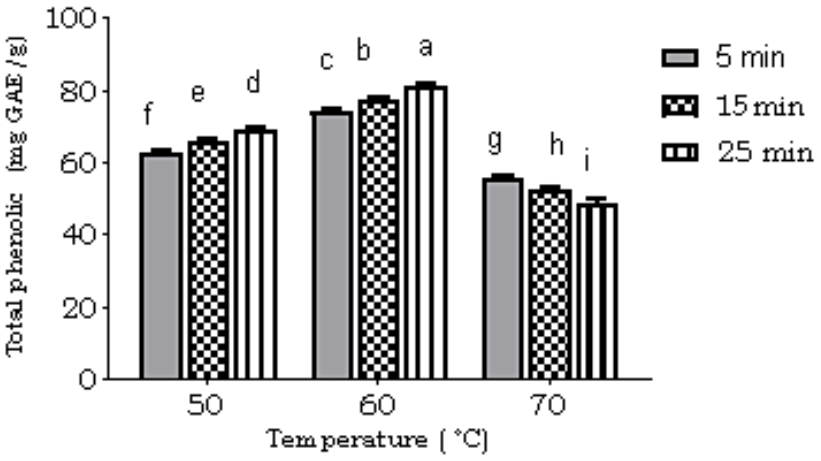


Fig. 2: TPC of FSB extract obtained at variation combination of temperature and time of extraction using MAE method. Means followed by different letters show significantly different at p<0.05

Total Flavonoid (TF)

The total flavonoid of FSB extract obtained from the extraction using MAE, at different temperatures and duration of extraction combinations ranged from 40.67 to 70.30 mg QE/g. The highest flavonoid was obtained by extraction at 60°C for 25 min.

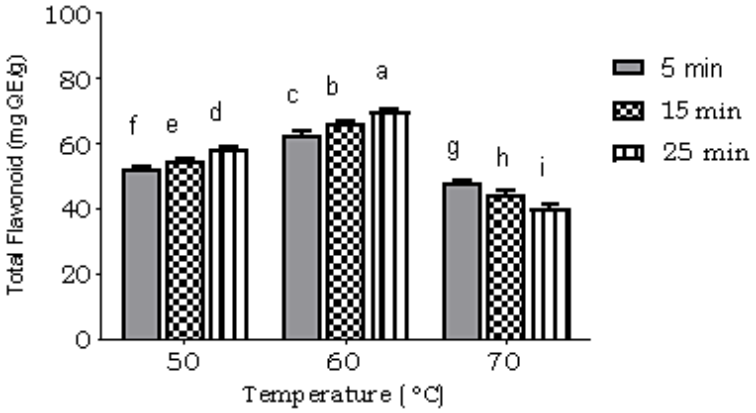


Fig. 3: TF of FSB extract obtained at various combinations of temperature and time of extraction using the MAE method. Means followed by different letters show significantly different at p<0.05

Figure 3 shows the highest TF obtained at a temperature of 60 °C for 25 min amounting to 70.30 mgQE/g. While the lowest TF value was obtained at a temperature treatment of 70°C with an extraction time of 25 min, amounting to 40.67 mgQE/g.

Radical Scavenging Activity (DPPH)

The radical scavenging activity of the FSB extract ranged from 47.96 to 73.40% (Figure 4). There is an increase in the radical scavenging activity of FSB extract obtained from extraction at 50 to 60 °C. Extraction of FSB at 70 °C resulted in a lower radical scavenging activity.

Identification of Bioactive Compound in FSB Extract

Figure 5 presents the chromatogram of the LC-HRMS analysis of FSB. The identified compounds are phenol, flavonoids, alkaloids, fatty acids, and their derivatives. Figure 6 presents

several fragmentation patterns of compounds extracted from FSB. Some of the identified compounds were methyl cinnamate, vanillin, apocynin, scopoletin, L(-)-pipecolinic acid, arecoline, δ-valerolactam, 3,4-dihydroxybenzaldehyde, 4-hydroxybenzaldehyde. A group of flavonoids was epicatechin and rutin. Fatty acids and their derivatives were eicosapentaenoic acid 9-oxo-10,12-octadecadienoic acid, 2,4-dihydroxy-heptadec-16-en-1-yl acetate, pinolenic acid, oleamide, α-eleostearic acid, 12-oxo phytodienoic acid, α-linolenoyl ethanolamide, palmitic acid, oleyl anilide dan 1-linoleoyl glycerol. The full list of compounds is attached in the supporting material (Table S1). There are some compounds identified as the same compounds, but they have different retention times, e.g. L(-)-Pipecolinic acid (1.01 and 0.87 min), (-)-Epicatechin (5.44 and 5.60 min) and Scopoletin (0.85 and 6.87 min). It might be that those compounds are isomers. Further analysis is needed to confirm this.

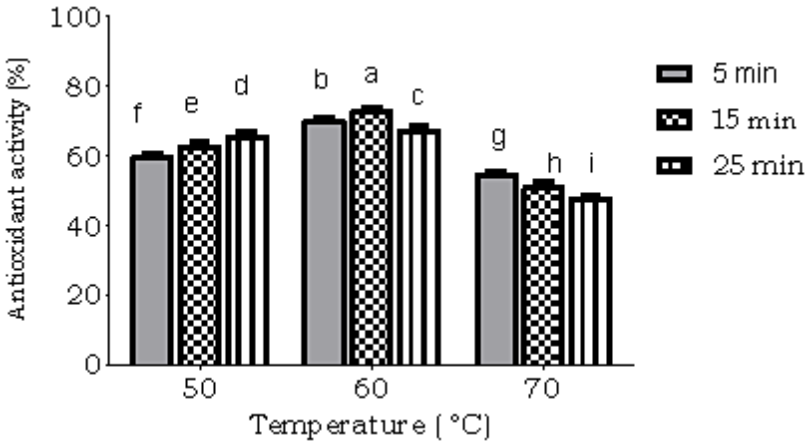
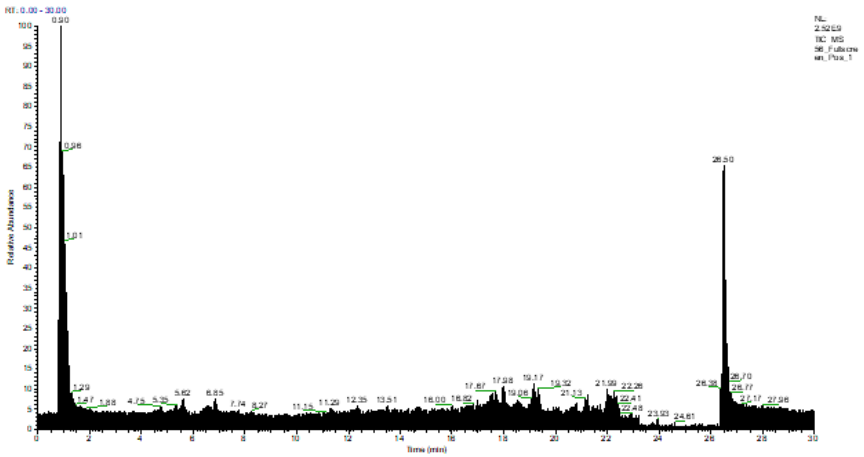


Fig.4: Radical scavenging activity of FSB extract obtained at variation combination of temperature and time of extraction using MAE method. Means followed by the different letters show significantly different at p<0.05



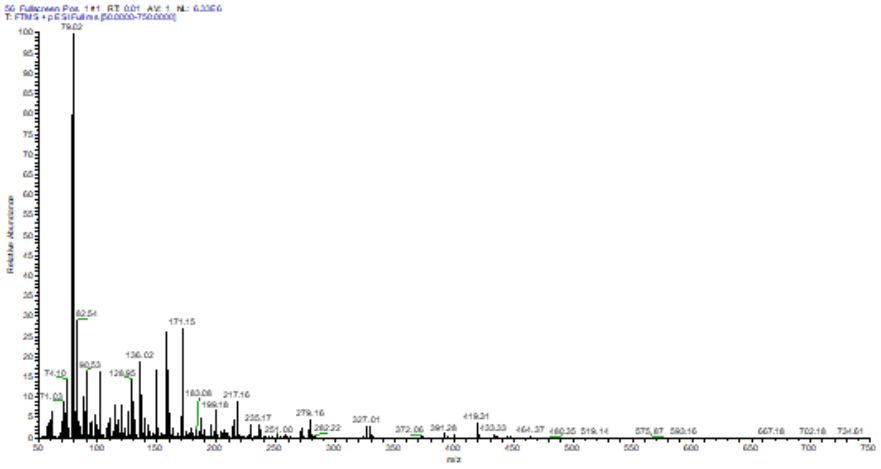
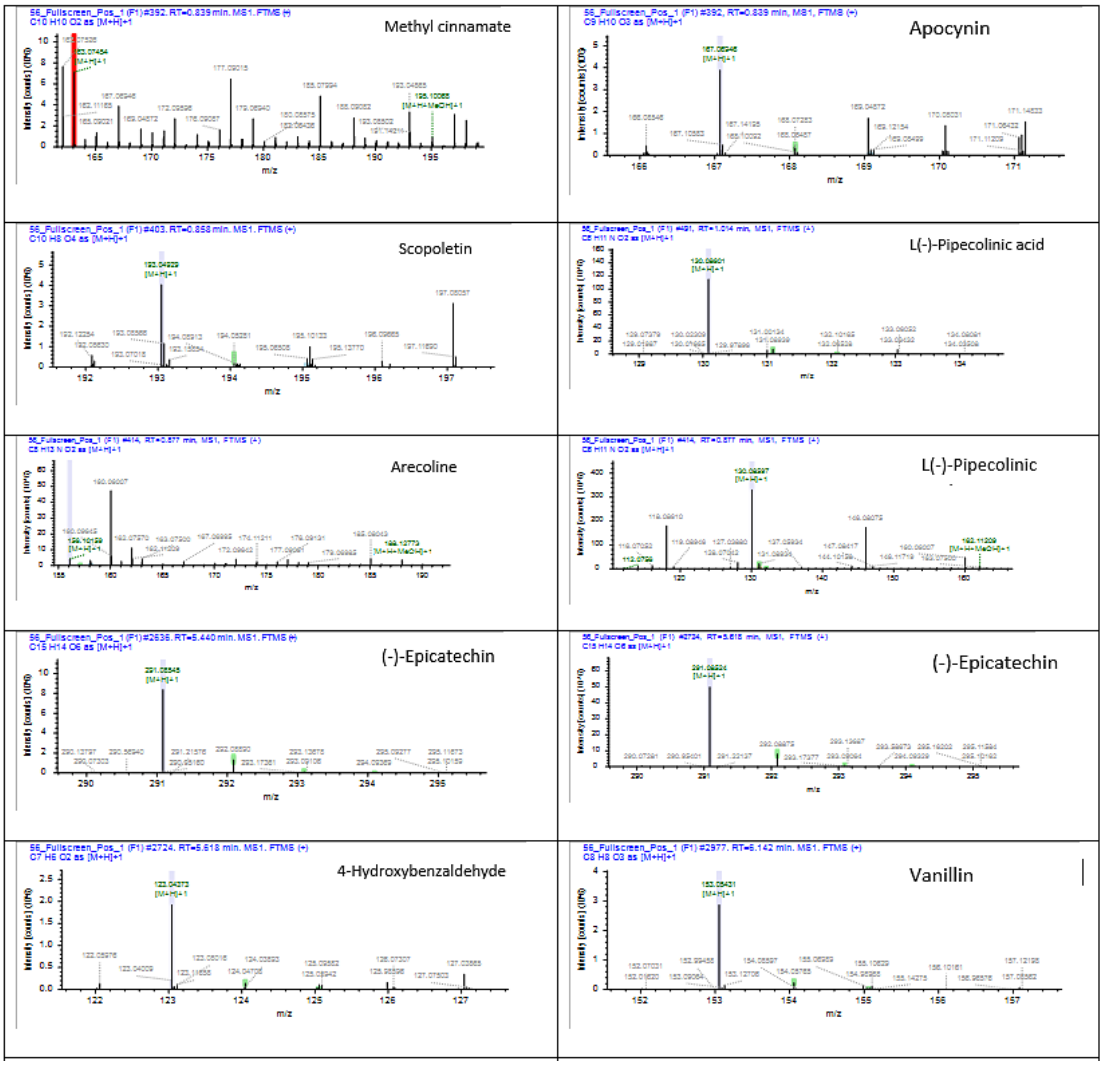


Figure 5: LC-HRMS chromatogram of FSB extract



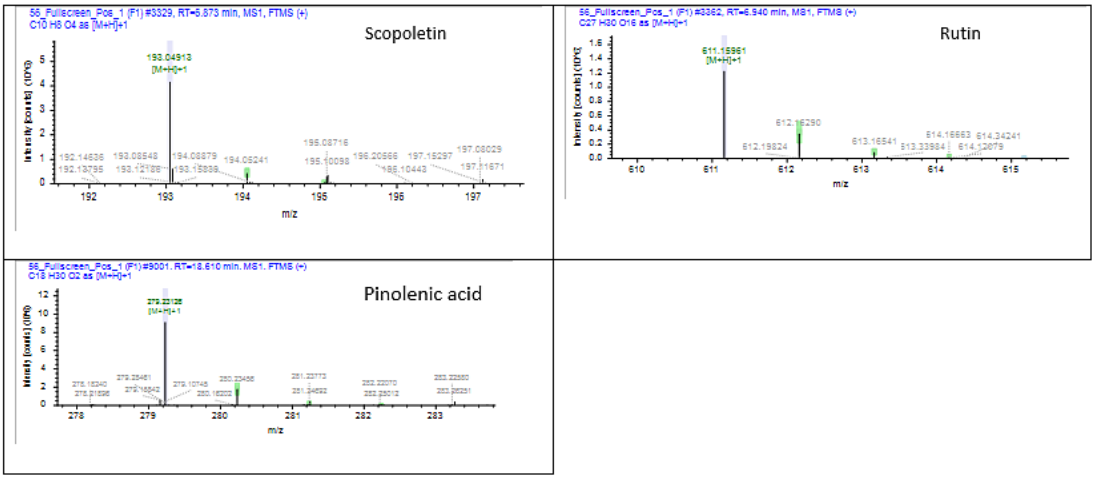


Fig. 6:LC-HRMS fragmentation patterns of some compounds extracted from FSB

Discussion

The yield of TPC and TF increased as the extraction temperature rose from 50 to 60 °C. Extraction at 70 °C resulted in a lower product of TPC and TF. At temperatures up to 60 °C, the heat from microwave energy can improve mass transfer, a better diffusion rate, and reduce viscosity and surface tension, resulting in higher yields of flavonoids.[16] Irradiation of microwave speeds up cell rupture by rapidly increasing temperature and internal pressure inside the cells as a booster for the destruction of the sample surface. It turns the release of the target compounds to the surrounding solvent.[17] Energy generated from the heat and microwave interact with polar solvent and allows the solvent to enter the matrix of plants resulting in more extracted bioactive compounds.[18] However, extraction time had a very low negative significant impact on the TF of citrus peel extraction, indicating that increasing extraction time could decrease the TF slightly.[19] Temperature gave a positive effect up to 60 °C meaning that increasing the extraction temperature resulted in a good impact on radical scavenging activity, which was in line with the increase of TF and TPC as the extraction temperature was higher. The longer the duration of extraction and temperature would increase the degradation of some heat-labile antioxidative compounds.

There is an increase in the antioxidant activity of FSB extract obtained from extraction at 50 to 60 °C. Extraction at 70 °C resulted in lower antioxidant activity. The microwave energy causes plant tissue degradation, cellulose dehydration, and weakening of the microstructure. Therefore, the solvent penetrates easily into the cellular channels to release the solute into the solvent.[12] At higher temperatures, the MAE will destroy the cell matrix's cell wall and the cells' solute can be released into the surrounding solvent.[20,21] In this study, the increase in the total phenol can be accredited to the heating effect. An increasing the solvent temperature was caused by the dipole rotation of the solvent in the microwave field, which was furthermore increasing the phenolic compounds' solubility. The combination of temperature and time could increase the solubility of phenolic compounds and lower the solvent's viscosity, therefore, accelerating the release and dissolution of these compounds. However, degradation of the phenolic compounds can occur at a higher temperature.[22] A lower extraction temperature may produce a more stable extract but may result in a lower extraction yield. The heat stability of a plant during extraction refers to its ability to retain its chemical and physical when subjected to high temperatures during extraction. The temperature significantly affected the extraction of flavonoids from citrus peel. Until 75 °C, the yield of flavonoids still increased, indicating that the extraction at 75 °C has not shown degradation of the flavonoids.[19]

Conclusion

This research showed an interaction between temperature and time of microwave-assisted extraction of FSB on TPC, TF, and radical scavenging

activity. The yield of TPC and TF has been higher as the rising temperature from 50 to 60 °C. Extraction at 70 °C decreased the yield TPC and TF. The newly identified specific phenolics and flavonoids were successfully profiled. Future research for testing the biological activity of the extract or the newly identified of phenol or flavonoid is necessary to study.

Authors' Contributions

Erryana Martati – Conceptualization and design of the study, laboratory supervision Interpretation of data, Writing the original draft, Visualization.
Vianney Evika Jemadu – Conceptualization and design of the study, Data curation, Interpretation of data, Investigation, Methodology
Ahmad Zaki Mubarok- Data analysis, Methodology, Analysis, and interpretation of data.

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Conflict of Interest

The authors have no conflicts of interest to declare.

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Supporting Material

Table S1 : Retention time (Rt), HRMS data, and proposed identification of detected features in Faloak Stem Bark (Sterculia quadrifida R. Br) by LC-HRMS

RT [min]	Calculated MW	Formula	Name
0.837	126.03121	C6 H6 O3	5-Hydroxymethyl-2-furaldehyde
0.845	162.06733	C10 H10 O2	Methyl cinnamate
0.845	166.06218	C9 H10 O3	Apocynin
0.854	192.04186	C10 H8 O4	Scopoletin
0.864	99.06847	C5 H9 N O	δ-Valerolactam
0.878	129.07869	C6 H11 N O2	L(-)-Pipecolinic acid
0.879	155.09429	C8 H13 N O2	Arecoline
0.88	115.06326	C5 H9 N O2	D-(+)-Proline
0.884	117.07885	C5 H11 N O2	Betaine
0.886	228.14691	C11 H20 N2 O3	Prolylleucine
0.894	197.12	C14 H15 N	Dibenzylamine
0.916	103.0997	C5 H13 N O	Choline

0.919	456.13893	C23 H19 F3 N4 O3	(1R,9S)-11-(2-Pyrazinylcarbonyl) -3-[4-(trifluoromethoxy)phenyl]-7, 11-diazatricyclo [7.3.1.02,7] trideca-2,4-dien-6-one
0.95	143.0943	C7 H13 N O2	1-Aminocyclohexanecarboxylic acid
1.01	129.07869	C6 H11 N O2	L(-)-Pipecolinic acid
1.021	135.05417	C5 H5 N5	Adenine
1.033	122.04785	C6 H6 N2 O	Nicotinamide
1.046	99.06847	C5 H9 N O	δ-Valerolactam
1.19	126.03121	C6 H6 O3	5-Hydroxymethyl-2-furaldehyde
4.766	410.12059	C19 H22 O10	6-(4-hydroxy-2-methyl-6-{[(2S,3R,4S,5S, 6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl]oxy}phenyl)-4-methoxy-2H-pyran-2-one
5.445	290.07796	C15 H14 O6	(-)-Epicatechin
5.607	290.07796	C15 H14 O6	(-)-Epicatechin
5.613	138.03121	C7 H6 O3	3,4-Dihydroxybenzaldehyde
5.613	122.03646	C7 H6 O2	4-Hydroxybenzaldehyde
6.142	152.04703	C8 H8 O3	Vanillin
6.581	226.15628	C13 H22 O3	NP-018660
6.872	192.04186	C10 H8 O4	Scopoletin
6.929	610.15233	C27 H30 O16	Rutin
7.439	197.12	C14 H15 N	Dibenzylamine
11.285	294.21866	C18 H30 O3	13(S)-HOTrE
11.759	191.13051	C12 H17 N O	DEET
12.377	157.14626	C9 H19 N O	2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)
12.858	246.12511	C15 H18 O3	2-[(4,5-dimethyl-2-furyl)methylidene]-5,5-dimethylcyclohexane-1,3-dione
13.693	292.20308	C18 H28 O3	12-Oxo phytodienoic acid
13.909	292.20308	C18 H28 O3	12-oxo Phytodienoic Acid
14.677	414.20333	C24 H30 O6	Bis(4-ethylbenzylidene)sorbitol
16.58	266.16405	C12 H27 O4 P	Triisobutyl phosphate
17.009	278.22365	C18 H30 O2	α-Eleostearic acid
17.017	234.16138	C15 H22 O2	3,5-di-tert-Butyl-4-hydroxybenzaldehyde
17.698	294.21867	C18 H30 O3	9-Oxo-10(E),12(E)-octadecadienoic acid
17.977	294.21867	C18 H30 O3	9-Oxo-10(E),12(E)-octadecadienoic acid
17.988	278.151	C16 H22 O4	Diisobutylphthalate
18.601	278.22365	C18 H30 O2	Pinolenic acid
19.018	323.2816	C20 H37 N O2	Linoleoyl Ethanolamide
20.005	354.27593	C21 H38 O4	1-Linoleoyl glycerol
20.028	292.23924	C19 H32 O2	9(Z),11(E),13(E)-Octadecatrienoic Acid methyl ester
20.101	321.26595	C20 H35 N O2	α-Linolenoyl ethanolamide
20.406	299.2816	C18 H37 N O2	Palmitoyl ethanolamide
20.471	325.2972	C20 H39 N O2	Oleoyl ethanolamide
20.615	120.05743	C8 H8 O	Acetophenone
21.073	282.25505	C18 H34 O2	Ethyl palmitoleate
21.181	281.27074	C18 H35 N O	Oleamide
21.291	356.29158	C21 H40 O4	Monoolein
21.661	281.27074	C18 H35 N O	Oleamide
22.006	283.28661	C18 H37 N O	Stearamide
22.014	282.25484	C18 H34 O2	Ethyl palmitoleate

22.02	255.25539	C16 H33 N O	Hexadecanamide
22.173	281.27074	C18 H35 N O	Oleamide
22.31	282.25485	C18 H34 O2	Ethyl palmitoleate
22.404	283.28661	C18 H37 N O	Stearamide
22.428	358.30724	C21 H42 O4	1-Stearoylglycerol
22.665	337.33296	C22 H43 N O	Erucamide
22.979	390.27562	C24 H38 O4	Bis(2-ethylhexyl) phthalate
23.169	390.27562	C24 H38 O4	Bis(2-ethylhexyl) phthalate
23.55	283.28661	C18 H37 N O	Stearamide
23.738	283.28661	C18 H37 N O	Stearamide
23.923	283.28661	C18 H37 N O	Stearamide
25.635	337.33296	C22 H43 N O	Erucamide
26.447	131.09449	C6 H13 N O2	6-Aminocaproic acid