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Original Article

Metabolite Profiling of Different Parts of *Syzygium cumini* var. album and Physicochemical Testing of its Identical Compounds

Yanu Andhiarto[1,2], Faisal Akhmal Muslikh[2], Suciati[3], Sukardiman[3]*

ABSTRACT

Indonesia is the second most biodiverse country in the world and is classified as a megadiverse country. *Syzygium cumini* is known to have various pharmacological activities, such as anti-inflammatory, antioxidant, antibacterial, antifungal, antidiarrheal, and others. This study aims to explore the metabolite profile of 70% ethanolic extract from the leaves and bark of *Syzygium cumini* var. *album* and analyze the physicochemical properties of its identical compounds. Phytochemical screening was conducted using commonly used methods, and metabolite profiling was carried out using UPLC-QToF-MS/MS. Pharmacological bioactivity and physicochemical properties of the identified compounds were analyzed using web tools such as Way2Drug, SwissADME, and ProTox II. The results showed that the ethanolic extract of *Syzygium cumini* var. *album* leaves contain 33 compounds, while the bark extract contains 26 compounds. Morin and alnusiin were identified in both samples. Based on PASS activity testing, morin exhibited Chlordecone reductase inhibitor activity and has potential for further development due to its favorable physicochemical properties and safety profile based on toxicity tests. This study demonstrates that the leaf and bark extracts of *Syzygium cumini* var. *album* contain morin and alnusiin, with morin showing potential as an effective and safe therapeutic agent as a Chlordecone reductase inhibitor.

Keywords: *Syzygium cumini* var. album; Chlordecone reductase inhibitor; biological activity; physicochemistry; toxicity analysis.

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INTRODUCTION

Indonesia is one of the most biodiverse countries and it is classified as a megadiverse country and of the approximately 40,000 types of medicinal plants recognized globally, it is estimated that 30,000 species are located in Indonesia. This accounts for 90% of the medicinal plants found across Asia.[1,2] Medicinal plants are widely recognized by the community for their medicinal properties and are used as raw materials in traditional medicine.[3] The transmission of knowledge about medicinal plants and the development of modern medicine is currently advancing rapidly due to their effectiveness and the minimal or non-existent side effects compared to synthetic and chemical (modern) medicines.[4,5]

Syzygium cumini var. *album* (L.) is a large tree reaching up to 30 meters in height and with a trunk circumference of 3-6 meters. It can be found in South Asia, Indonesia, India, Bangladesh, Nepal, and Sri Lanka.[6] Traditionally, various parts of the plant (bark, leaves, fruit, and seeds) have been used in the treatment of various diseases.[7] Various parts of *Syzygium cumini* have also been reported to exhibit anti-inflammatory, antioxidant, antibacterial, antifungal, antidiarrheal, antifertility, anorexigenic, gastroprotective, and radioprotective activities.[8] In addition, it has therapeutic activities such as analgesic, antidiabetic, anticancer, and antimalarial effects.[7]

Studies in medicinal plants is continually advancing to harness their medicinal potential for health benefits. Method to determine the variation in metabolite profiles is the metabolomic approach.[9] Metabolomics is the study of metabolite profiles in biological samples, tissues, and cells. The goal is to identify all analytes, their concentrations, and their metabolite profiles in plants.[10] Metabolite profiling can be conducted using several techniques, such as a combination of chromatography and spectrophotometry.[11]

In this study, UPLC-QToF-MS/MS was used to characterize the metabolite profiles. UPLC-QToF-MS/MS is a chemical analysis method that combines the physical separation capabilities of liquid chromatography with mass spectrometry. This tool has several advantages, such as enhancing the efficiency of compound separation, speeding up analysis time, requiring smaller sample volumes, offering more accurate monoisotopic mass measurements, providing high-resolution spectra for compound confirmation, and providing better.[12] This study aims to investigate the metabolite profile of 70% ethanolic extract from the leaves and bark of *Syzygium cumini* var. *album* using UPLC-QToF-MS/MS and to analyze the physicochemical properties of its identical compounds.

MATERIALS AND METHODS

Plant Material

Syzygium cumini var. *album* was collected from Surabaya, the capital of East Java. It was identified and characterized at Materia Medika, Batu, East Java, with specimen letter number 074/636/102.20-A/2022. The leaves and bark were then prepared by cutting, drying, and grinding to obtain simplicia powder.

Chemical Substances

70% ethanol, water, acetonitrile, and formic acid were used as solvents and mobile phases in UPLC-QToF-MS/MS. They were purchased from Merck (Darmstadt, Germany).

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Extraction

The simplicia powder of the leaves and bark of *Syzygium cumini* var. *album* was extracted using the maceration method for 3 x 24 hours with 70% ethanol as the solvent. The solution was then filtered, and the filtrate was evaporated at 50°C and 70 rotations per minute using a Heidolph G3 rotary evaporator. The extract was then concentrated until a thick extract was obtained in an oven at 50°C.

Phytochemical Screening

Alkaloid Group Test: A total of 2 mL of the extract solution was mixed with 2 mL of 2% hydrochloric acid, followed by the addition of Mayer's reagent (a positive result is indicated by the formation of a yellowish-white precipitate), Dragendorff's reagent (a positive result is indicated by turbidity or the formation of an orange precipitate), and Wagner's reagent (a positive result is indicated by the formation of a brown precipitate).

Flavonoid Group Test: Magnesium powder and 4 drops of concentrated hydrochloric acid were added to 2 mL of the extract solution. A positive reaction is indicated by the development of a red, orange, or dark-colored solution. Additionally, the flavonoid group was tested using TLC with an eluent mixture of ethyl acetate: formic acid: distilled water (100:15:17) and quercetin as a standard compound. After elution, the TLC plate was sprayed with borate citrate reagent and observed for spot formation under UV light at 366 and 254 nm.

Phenolic Group Test: Three drops of 1% ferric chloride reagent were added to 2 mL of the extract solution. The presence of phenolic compounds is indicated by a blue or black coloration.

Saponin Group Test: A volume of 2-3 mL of the extract solution was placed in a test tube, followed by the addition of 10 mL of hot water. The solution was cooled, shaken vigorously for 10 seconds, and 1 drop of 2 N hydrochloric acid was added. The presence of saponins is indicated by the formation of stable foam, 1-10 cm in height, persisting for at least 10 minutes.

Steroid/Triterpenoid Group Test: Ten drops of acetic anhydride and 2 drops of concentrated sulfuric acid were added to 2 mL of the extract solution. Steroids are indicated by a blue or green color, while triterpenoids are indicated by a red or purple color. The steroid group was also tested using TLC with an eluent mixture of n-hexane: ethyl acetate (4:1) and stigmasterol as a standard compound. After elution, the TLC plate was sprayed with anisaldehyde-sulfuric acid reagent, heated, and the spots were observed.

Polyphenol Group Test: A total of 2 mL of the extract solution was added to 3 drops of 1% ferric chloride reagent. A blue or black color indicates the presence of phenolic compounds.

Metabolite Profiling

The profiling of metabolites was carried out using UPLC-QToF-MS/MS equipment at the Forensic Laboratory Center of the Indonesian National Police Criminal Investigation Agency. Extracts and fractions were acquired through the Solid Phase Extraction (SPE) method. Each sample, in a volume of 5 µl (100 ppm), was injected into an ACQUITY UPLC® H-Class System with an MS Xevo G2-S QToF detector (Waters, USA). The samples were then separated on an ACQUITY BEH C18 column (1.7 µm; 2.1 x 50 mm) at a flow rate of 0.2 ml/min, using acetonitrile + 0.1% formic acid (A) and water + 0.1% formic acid (B) as the mobile phases (gradient). Chromatogram data and m/z (0-1200 m/z) spectra were obtained from the UPLC-QToF-MS/MS analysis results for each peak using the MassLynx 4.1 software. Newly identified compounds were validated using ChemSpider and MassBank.

PASS Activity Online

Identical compounds found in *Syzygium cumini* var. *album* were obtained from the PubChem library portal (https://pubchem.ncbi.nlm.nih.gov/). PubChem provides complete information on various chemical compounds, including data from the Simplified Molecular Input Line Entry System (SMILES). The SMILES codes found in PubChem were then copied and entered into the Way2Drug webtool (https://www.way2drug.com/passonline/predict.php) to evaluate the potential pharmacological effects of a compound.[13,14]

Physicochemical Analysis

The SMILES format was also used to evaluate the molecules based on their physical properties using the SwissADME webtool (http://www.swissadme.ch). It was used to determine the pharmacokinetics and pharmacodynamics of the compounds, including their topological polar surface area (TPSA), molecular weight, log P, hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), and whether they meet the five parameters of Lipinski's rule of five. The SwissADME webtool is freely accessible.[15]

Toxicity Testing

The online tool ProTox II (http://tox.charite.de/protox II/) was used to estimate the LD50 value using the SMILES format. Both of these web tools are freely accessible.[5]

RESULTS

The results of the phytochemical screening of the ethanolic extract from the leaves and bark of *Syzygium cumini* var. *album* are shown in Table 1. They indicate that the leaves and bark of *Syzygium cumini* var. *album* contain alkaloid, flavonoid, saponin, steroid, terpenoid, and polyphenol compounds.

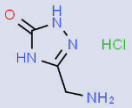
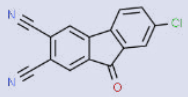
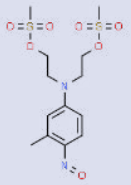
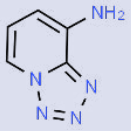
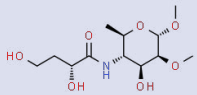
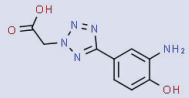
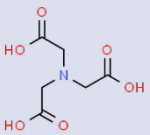
The metabolite profiling of the ethanolic extract from *Syzygium cumini* var. *album* leaves using the UPLC-QToF-MS/MS instrument as a total ion chromatogram (TIC), as shown in Figure 1. The retention time (RT), % area, m/z, molecular formula, and compound name, as shown in Table 2. Thirty-three compounds were identified with Myricetin was the dominant compound in the ethanolic extract from the leaves of *Syzygium cumini* var. *album*, as it had the largest % area, indicating a high concentration.

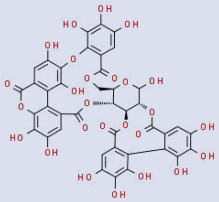
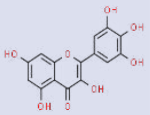
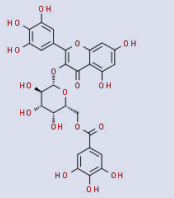
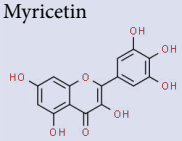
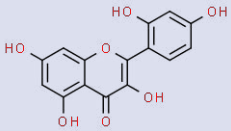
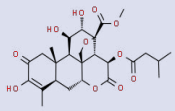
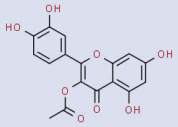
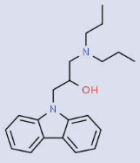
The results of the metabolite profiling of the ethanolic extract from the bark of *Syzygium cumini* var. *album* using the UPLC-QToF-MS/MS instrument, in the form of a total ion chromatogram (TIC), can be seen in Figure 2. The retention time (RT), % area, m/z, molecular formula, and compound name can be seen in Table 3. The results demonstrated that 26 compounds were identified, with N-[(9Z)-9-Octadecen-1-yl]-2-oxohexadecanamide is the dominant compound in the ethanolic extract from the bark of *Syzygium cumini* var. *album*.

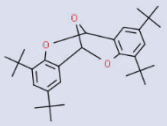
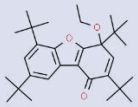
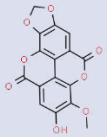
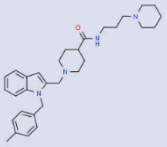
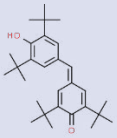
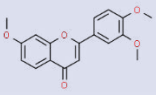
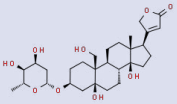
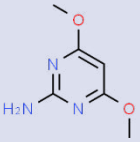
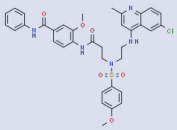
The metabolite profiling indicated that morin and alnusiin are the active marker compounds of *Syzygium cumini* var. *album*, either the leaves or bark. PASS activity prediction was conducted on the

Table 1. Phytochemical Screening Results of the Ethanolic Extract from the Leaves and Bark of *Syzygium cumini* var. album.

Secondary Metabolite Group	Leaves	Bark
Alkaloid	+	+
Flavonoid	+	+
Saponin	+	+
Steroid dan terpenoid	+	+
Polyphenol	+	+

No	Rt (min)	% area	Meazured (m/z)	Calculated (m/z)	Formula	IUPAC Name and Chemical Structure
1	0.95	4.52	151.0363	151.0387	$C_3H_7ClN_4O$	5-(aminomethyl)-2,4-dihydro-3H-1,2,4-triazol-3-one hydrochloride 
2	0.97	0.31	265.0168	265.0196	$C_{15}H_5N_2OCl$	7-Chloro-9-oxo-9H-fluorene-2,3-dicarbonitrile 
3	1,21	1,3	381,0804	381,0790	$C_{13}H_{20}N_2O_7S_2$	[(3-Methyl-4-nitrosophenyl)imino]di-2,1-ethanediyl dimethanesulfonate 
4	1,83	0,19	136,0630	136,0623	$C_5H_5N_5$	Tetrazolo[1,5-a]pyridin-8-amine 
5	2,09	0,31	294,1556	294,1553	$C_{12}H_{23}NO_7$	1,2-di-O-methyl-4-[(2R)-2,4-dihydrobutyramido]-4,6-dideoxy-α-D-mannopyranoside 
6	2,44	0,47	236,0772	236,0784	$C_9H_9N_5O_3$	5-(3-Amino-4-hydroxyphenyl)-2H-tetrazole-2-acetic acid 
7	2,77	0,05	192,0511	192,0508	$C_6H_9NO_6$	nitrilotriacetic acid 
8	3,28	0,59	120,0823	120,0813	C_8H_9N	Indoline 

9	3.69	5.39	935.0799	935.0791	$C_{41}H_{26}O_{26}$	Alnusiin 
10	4.42	0.1	291.0872	291.0869	$C_{15}H_{14}O_6$	D-(+)-Catechin 
11	4.80	0.1	633.1086	633.1092	$C_{28}H_{24}O_{17}$	5,7-Dihydroxy-4-oxo-2-(3,4,5-trihydroxyphenyl)-4H-chromen-3-yl 6-O-(3,4,5-trihydroxybenzoyl)-β-D-galactopyranoside 
12	5.37	15.88	319.0454	319.0454	$C_{15}H_{10}O_8$	Myricetin 
13	6.13	0.47	303.0501	303.0505	$C_{15}H_{10}O_7$	Morin 
14	6.36	1.03	523.2210	523.2179	$C_{26}H_{34}O_{11}$	Brucein A 
15	7.06	7,80	345.0603	345.0610	$C_{17}H_{12}O_8$	Quercetin acetate 
16	7.43	0.11	325.2282	325.2280	$C_{21}H_{28}N_2O$	1-(9H-Carbazol-9-yl)-3-(dipropylamino)-2-propanol 

17	7.98	0.74	451.3213	451.3212	$C_{30}H_{42}O_3$	4,6,12,14-Tetrakis(2-methyl-2-propanyl)-8,16,17-trioxatetracyclo[7.7.1.0^{2,7}.0^{10,15}]heptadeca-2,4,6,10,12,14-hexaene 
18	8.51	0.69	453.3371	453.3369	$C_{30}H_{44}O_3$	2,4,6,8-tetra-tert-butyl-4-ethoxydibenzo[b,d]furan-1(4H)-one 
19	9.21	0.1	329.0296	329.0297	$C_{16}H_8O_8$	2-Hydroxy-3-methoxychromeno[5,4,3-cde][1,3]dioxolo[4,5-h]chromene-5,11-dione 
20	10.07	1.57	487.3431	487.3437	$C_{31}H_{42}N_4O$	1-{[1-(4-Methylbenzyl)-1H-indol-2-yl]methyl}-N-[3-(1-piperidinyl)propyl]-4-piperidinecarboxamide 
21	11.34	2.29	423.3263	423.3263	$C_{29}H_{42}O_2$	Galvinol 
22	11.95	6.84	313.1096	313.1076	$C_{18}H_{16}O_5$	Fasciculiferin 
23	12.79	2.64	537.3038	537.3064	$C_{29}H_{44}O_9$	(3Î²,5Î²)-3-[(2,6-Dideoxy-Î²-D-ribo-hexopyranosyl)oxy]-5,14,19-trihydroxycard-20(22)-enolide 
24	13.36	3.18	496.3416	496.3387	$C_6H_9N_3O_2$	4,6-Dimethoxy-2-pyrimidinamine 
25	14.18	0.68	702.2156	702.219	$C_{36}H_{36}ClN_5O_6S$	4-[(N-{2-[(6-Chloro-2-methyl-4-quinolinyl)amino]ethyl}-N-[(4-methoxyphenyl)sulfonyl]-β-alanyl)amino]-3-methoxy-N-phenylbenzamide 

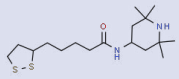
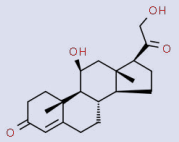
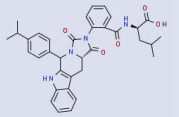
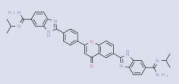
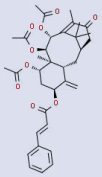
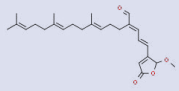
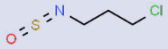
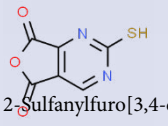
26	14,92	5.17	345.2064	345.2034	$C_{17}H_{32}N_2OS_2$	5-(1,2-Dithiolan-3-yl)-N-(2,2,6,6-tetramethyl-4-piperidinyl)pentanamide 
27	15.64	7.18	347.2219	347.2222	$C_{21}H_{30}O_4$	Corticosterone 
28	16.50	0.10	593.2774	593.2764	$C_{35}H_{36}N_4O_5$	N-{2-[(11aS)-5-(4-Isopropylphenyl)-1,3-dioxo-5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]pyrido[3,4-b]indol-2(3H)-yl]benzoyl}-D-leucine 
29	17.14	1.25	623.2904	623.2883	$C_{37}H_{34}N_8O_2$	N'-Isopropyl-2-(4-{6-[6-(N'-isopropylcarbamimidoyl)-1H-benzimidazol-2-yl]-4-oxo-4H-chromen-2-yl}phenyl)-1H-benzimidazole-6-carboximidamide 
30	17.54	6.06	607.2891	607.2907	$C_{35}H_{42}O_9$	2-Deacetoxytaxinin B 
31	17.85	1.44	413.2672	413.2692	$C_{26}H_{36}O_4$	(2E,5E,9E)-2-[(2E)-3-(2-Methoxy-5-oxo-2,5-dihydro-3-furanyl)-2-propen-1-ylidene]-6,10,14-trimethyl-5,9,13-pentadecatrienal 
32	18.79	3.92	139.9898	139.9937	C_3H_6ClNOS	1-Chloro-3-(sulfinylamino)propane 
33	20.48	0.21	182.9865	182.9864	$C_6H_2N_2O_3S$	2-Sulfanylfuro[3,4-d]pyrimidine-5,7-dione 

Table 4. Biological activity of Morin.

Pa	Pi	Activity
0.979	0.001	Chlordecone reductase inhibitor
0.974	0.002	Membrane integrity agonist
0.971	0.002	HIF1A expression inhibitor
0.961	0.001	Aryl-alcohol dehydrogenase (NADP+) inhibitor
0.959	0.001	P-benzoquinone reductase (NADPH) inhibitor
0.959	0,001	Kinase inhibitor
0.956	0.002	Membrane permeability inhibitor
0.956	0.001	2-Dehydropantoate 2-reductase inhibitor
0.947	0.001	Antimutagenic
0.941	0.002	CYP1A inducer
0.941	0.002	HMOX1 expression enhancer

Table 5. Biological activity of Alnusiin.

Pa	Pi	Activity
0.953	0.002	Antioxidant
0.917	0.005	HIF1A expression inhibitor
0.910	0.002	Hepatoprotectant
0.902	0.005	Antineoplastic
0.897	0.002	Protein kinase A inhibitor
0.882	0.005	Antiinflammatory
0.877	0.005	Apoptosis agonist
0.858	0.002	Free radical scavenger
0.850	0.003	Chemopreventive
0.807	0.010	TP53 expression enhancer
0.953	0.002	Antioxidant

Table 6. Physicochemical and Toxicity Analysis of Morin and Alnusiin.

Parameter	Morin	Alnusiin
BM ≤500 g/mol	302.24	934.63
Log P ≤ 5	1.20	0.01
HBA ≤ 5	7	26
HBD ≤ 5	5	14
Lipinski's Rule of Five	Yes	No
TPSA (Å2)	131.36 Å²	437.09 Å²
Toxicity class (Prediction of LD50)	5 (3919 mg/kg)	4 (1000mg/kg)

dominant compounds present in *Syzygium cumini* var. *album* to assess the potential pharmacological effects. Table 4 shows that morin has the highest Pa value of 0.979, with activity as a Chlordecone reductase inhibitor. Meanwhile, Table 5 shows that alnusiin has the highest Pa value of 0.953, with antioxidant activity.

The physicochemical and toxicity analysis results of morin and alnusiin can be seen in Table 6. The results indicate that morin meets Lipinski's parameters with a molecular weight of 302.24 g/mol, a log P value of 1.20, HBA (Hydrogen Bond Acceptors) of 7, HBD (Hydrogen Bond Donors) of 5, "yes" for Lipinski's rule compliance, and a TPSA (Topological Polar Surface Area) value of 131.36 Å². On the other hand, the toxicity class of morin is better compared to alnusiin, as it classified into toxicity class 5 with a predicted LD_{50} of 3919 mg/kg.

DISCUSSION

The pharmacological activities of *Syzygium cumini* var. *album*, such as anti-inflammatory, antioxidant, analgesic, antibacterial, antidiabetic, and antifungal,[7,8] are likely due to the presence of phytochemical compounds. We found that the leaf and bark extracts of *Syzygium cumini* var. *album* contain alkaloids, flavonoids, saponins, steroids, terpenoids, and polyphenols (see Table 1).

Based on the metabolite profiling results in this study, we identified 33 compounds in the leaf extract of *Syzygium cumini* var. *album*, with myricetin as the dominant compound (15.88%, see Table 2). In the bark extract of *Syzygium cumini* var. *album*, 26 compounds were identified, with N-[(9Z)-9-Octadecen-1-yl]-2-oxohexadecanamide as the dominant compound (31.46%, see Table 3). Among the identified compounds, two compounds, morin and alnusiin, were found to be characteristic/identical to *Syzygium cumini* var. *album*, as they were present in both the leaves and bark.

The identical compounds from *Syzygium cumini* var. *album* were further tested for PASS activity. Morin had the highest Pa value of 0.979, with activity as a Chlordecone reductase inhibitor. Meanwhile, **Table 5** shows that alnusiin had the highest Pa value of 0.953, with antioxidant activity. The PASS online test provides information on the Pa (Potential activity) and Pi (Potential inhibitory) values.[16] The Pa value represents the likelihood that a compound will exhibit biological activity in laboratory experiments, while the Pi value represents the opposite. If a compound has a Pa > Pi, it is likely to possess that activity.[17] A PASS test result with Pa > 0.7 indicates that the compound is highly biologically active, and the results are not significantly different from laboratory-scale testing. Conversely, if the Pa value is between 0.5 and 0.7, the compound has fairly high bioactivity, making it a bioactive compound with a high likelihood of success in in vitro or in vivo experimental testing.[16,18] Biological targets are identified based on Pa

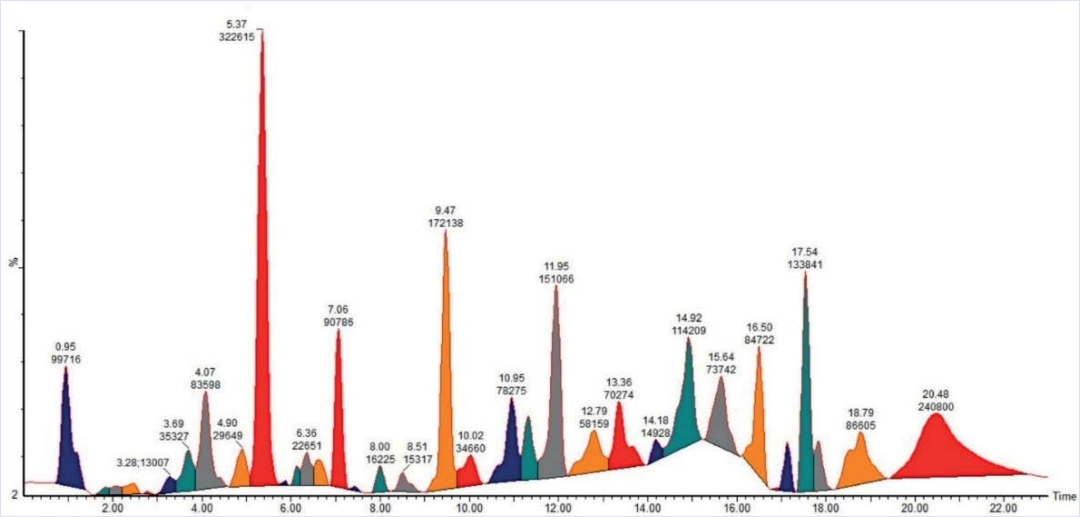


Figure 1. TIC of the Ethanolic Extract from the Leaves of *Syzygium cumini* var. *album* (Andhiarto *et al*., 2022).

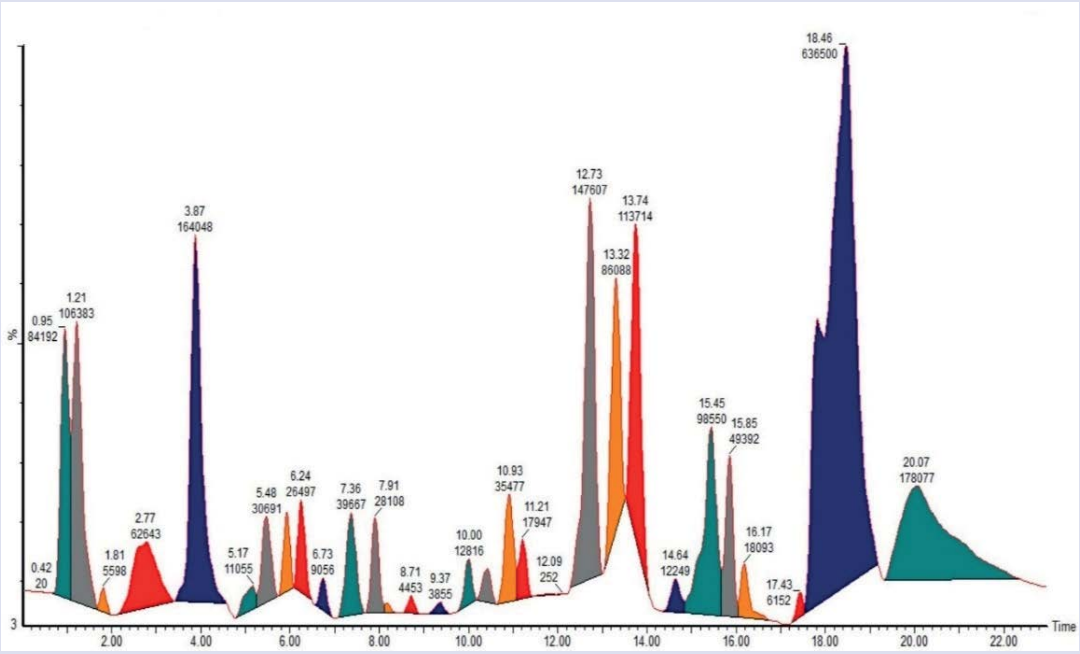


Figure 2. Metabolite profiling of the Ethanolic Extract from the bark of *Syzygium cumini* var. *album* using the UPLC-QToF-MS/MS.

values close to 1 and Pi values close to 0. Among the screening results, protein targets with Pa > 0.9 and associated with human diseases were selected for further analysis.[19]

After obtaining the PASS activity predictions, physicochemical and toxicity analyses were conducted for morin and alnusiin. The results showed that morin meets Lipinski's rule of five, with a molecular weight of 302.24 g/mol, a log P value of 1.20, HBA 7, HBD 5, "yes" for Lipinski's parameters, and a TPSA value of 131.36 Å^2. Meanwhile, alnusiin does not meet Lipinski's rule of five because its molecular weight, HBA, and HBD exceed the limits; a compound can penetrate the cell membrane if it meets at least 2 of Lipinski's rules.[20] Additionally, the toxicity test results showed that morin is less toxic than alnusiin, as it falls into toxicity class 5, while alnusiin is in toxicity class 4.

Chlordecone is an organochlorine insecticide that was intensively used in the French West Indies, Guadeloupe, and Martinique from 1973 to 1993 to control the banana root borer.[21,22] Its use led to contamination of soil, river water, wildlife, and vegetables, with contaminated soil and water becoming the primary sources of ongoing exposure.[22] Chlordecone (Kepone) is excreted in human bile as a reduced metabolite (chlordecone alcohol) and as a glucuronide conjugate. Bioreduction is catalyzed by a liver cytosolic enzyme known as chlordecone reductase. However, only 5% of the pesticide excreted in bile is found in feces each day, suggesting that the pesticide may undergo enterohepatic cycling (intestinal reabsorption and recirculation to the liver).[21]

Chlordecone is recognized as a potential carcinogen and has been shown to cause liver tumors in rodents. Its carcinogenic properties and long biological half-life increase the risk of long-term effects, such as prostate cancer.[23] These enzymes are also involved in xenobiotic metabolism and have been implicated in the pathogenesis of diabetic cataracts and muscular dystrophy.[23] Furthermore, chlordecone exhibits

prolonged toxicity involving the central nervous system (tremors, oculomotor dysfunction, ataxia, mood disturbances, and memory loss), liver enlargement, and reduced sperm count and motility.[22]

CONCLUSION

This study reveals that the leaf and bark extracts of *Syzygium cumini* var. *album* are rich in phytochemical compounds that play crucial roles in pharmacological activities, such as anti-inflammatory and antioxidant effects. Through metabolite profile analysis, morin and alnusiin were identified as identical compounds in both extracts, with morin showing strong potential as a Chlordecone reductase inhibitor, according to PASS activity results, and meeting the physicochemical and toxicity safety criteria. Therefore, morin has significant potential for further development as a safe and effective therapeutic agent, particularly in combating the adverse effects of chlordecone, which is known as a potential carcinogen with prolonged toxicity.

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