Exploration Ketapang (*Terminalia catappa* L.) Leaf Compounds Using *Swiss*ADME and *Toxtree*

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ABSTRACT

Background: The ketapang plant (*Terminalia catappa* L.) has been used traditionally across generations as a medicinal remedy, particularly its leaves. Ketapang leaves contain active compounds that have the potential to treat gastrointestinal disorders, reduce high blood pressure, and act as antidiabetic and anticancer agents. The exploration phase of natural compounds requires adequate assessment of absorption, distribution, metabolism, excretion, and toxicity (ADMET) according to standard parameters. **Objective:** This study aims to explore the ADMET profiles of 70 active compounds from ketapang leaves using *Swiss*ADME and Toxtree. **Methods:** This research was conducted *in silico*, utilizing *Swiss*ADME for ADME screening, *Toxtree* for toxicity evaluation, *VegaZZ* for compound structure optimization, and ChemDraw for 2D and 3D structural preparation. **Results:** A total of 52 compounds complied with *Lipinski's Rule of Five* and pharmacokinetic parameters, while 18 compounds failed to meet Lipinski's criteria. 17 compounds were classified the Low Toxicity category (Class I). 41 compounds were found to be non-carcinogenic and non-mutagenic, whereas 29 compounds exhibited carcinogenic and mutagenic properties. Additionally, 44 compounds showed no mutagenicity alerts against *Salmonella typhimurium*. **Conclusion:** Methyl Gallate and Hemipic acid were identified as compounds that satisfy *Lipinski's Rule of Five*, Low Toxicity category (Class I), and exhibit neither carcinogenic nor mutagenic properties.

Keywords: *ADME; Ketapang Leaf; SwissADME; Toxicity; Toxtree.*

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INTRODUCTION

Ketapang has been traditionally used across generations as a medicinal plant to treat cardiovascular, skin, hepatic, and respiratory, as well as insomnia; Ketapang leaves contain active compounds that have the potential to treat gastrointestinal disorders, reduce high blood pressure, and act as antidiabetic and anticancer agents (1). Ketapang leaves contain secondary metabolites such as alkaloids, flavonoids, tannins, saponins, steroids, triterpenoids, phenols, coumarins, and glycosides (2). This is supported by a study (3) showing that the ethanolic extract and methanol fraction of ketapang leaves can reduce blood glucose levels in alloxan-induced white rats due to their flavonoid content. However, these studies remain limited to in vivo testing without mapping out the pharmacokinetic and toxicity profiles of the leaf's active compounds.

The in silico method in drug discovery and development processes allows for a faster and more efficient identification of potential drug candidates before undergoing further testing (4). The success of a compound as a drug candidate is determined not only by its biological activity but also by its absorption, distribution, metabolism, and excretion (ADME) parameters, alongside its toxicological safety (5). This study aims to explore the ADMET profiles of 70 active compounds from ketapang leaves and identify compounds that conform to *Lipinski's Rule of Five* while remaining non-carcinogenic and non-mutagenic.

METHODS

This study employs a computational experimental design to determine the pharmacokinetic profiles (absorption, distribution, metabolism, and excretion) via *Lipinski's Rule of Five*, as well as toxicity profiles via *Cramer Rules, Carcinogenicity (genotoxic and non-genotoxic), and the mutagenicity rulebase by ISS*, alongside *in vitro* Mutagenicity (*Ames test*) alerts *by ISS* on 70 active compounds from ketapang (*Terminalia catappa* L.) leaves.

Research Stages Flowchart

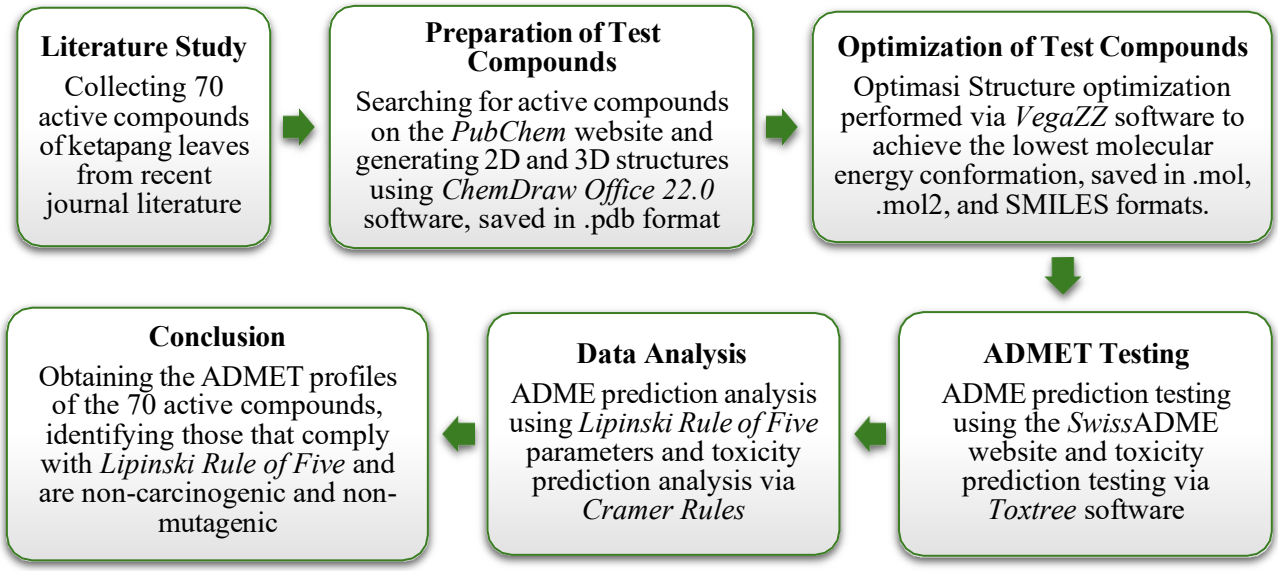

Figure 1. Research Stages Flowchart

Tools and Materials

This study utilized 70 active compounds of ketapang (*Terminalia catappa* L.) leaves in 2D and 3D structures. The hardware used was a LAPTOP-224BT2N7 VivoBook ASUS Laptop Model X415DAP_M415D (AMD Ryzen 3 3250U with Radeon Graphics 2.60 GHz, 8.00 GB RAM, and a 477 GB NVMe SSD). The software suite included Windows 11 Version 24H2, Microsoft Office Home and Student 2019, *ChemDraw Ultra 22.0*, *Chem 3D Ultra 15.0*, *VegaZZ 3.2.3.28*, and *Toxtree.* Online web tools accessed were *PubChem* and *Swiss*ADME.

Preparation of Test Compounds

The 2D structures of the 70 test compounds were sourced from the *PubChem* database. The canonical SMILES strings were copied and inputted into ChemDraw Ultra 22.0 via *Edit* → *Paste Special* → *SMILES*, and saved. They were subsequently converted into 3D models using Chem 3D Ultra 22.0 via *View* → *Show Chem 3D* and exported into .pdb format (6)

Optimization of Test Compounds

The 3D structures saved in .pdb format were optimized using *VegaZZ* software through the following sequence: Open *VegaZZ*, click *File* → *Open* to load the .pdb structure. Go to *View* → *Display* → *Ball and stick solid* to visualize the confirmation. Hydrogen atoms were added, and partial charges were assigned via *Calculate* → *Charge & Pot*, selecting *Gasteiger* charges to fix the compound's electrostatic profile, followed by applying the AutoDock force field. Energy minimization was performed for 3000 steps to yield the most stable conformation via *Calculate* → *AMMP* → *Minimization*, setting minimum steps to 3000, tolerance to 1000, checking the 'Trust' option, and saving the output in .pdb, .mol, and .mol2 formats (7).

ADME Screening

ADME values were predicted using the online *Swiss*ADME web server (http://www.swissadme.ch). The 2D structures of the ketapang leaf constituents were imported into the molecular sketcher interface, then transferred into the SMILES list box (one molecule per line) by clicking the double-arrow button. Once the molecular list was queued, calculations were initiated by clicking "*Run*" (7).

Toxicity Screening

Toxicity prediction was conducted via Toxtree software to identify structural alerts signaling potential *in vitro* mutagenicity (Ames Test) based on the ISS rulebase, which categorizes chemical structures into mutagenic and non-mutagenic classes (8). The operational steps were: *Open Toxtree* → *File* → *Open* to import the .pdb or .mol2 files. Select parameters using *Method* → *Select Decision Tree* to view specific criteria, then click *Estimate*. The toxicity classifications were displayed in the *Classification Area* (7).

Data Analysis

Data analysis for this study was structured into two core screenings. The ADME evaluation monitored *Lipinski's Rule of Five* parameters that included the hydrogen donor bond is no more than 5; The hydrogen acceptor bond is no more than 10; Molecular mass less than 500 Da; partition coefficient is not more than 5. Rule of Five because all parameter values are multiples of five (9). Concurrently, the toxicity evaluation mapped out the safety profile of the compounds, focusing on parameters that included *Cramer rules classification*, *carcinogenicity (genotoxic and non-genotoxic),* and *mutagenicity rulebases by the ISS.* The classification of cramer rules is divided into 3, namely the Low category (Class I) has a low level of toxicity, Intermediate (Class II) has medium toxicity and High (Class III) has a high toxicity (7).

RESULTS

The 70 active compounds of ketapang (*Terminalia catappa* L.) leaves were compiled from literature studies published between 2020 and 2026. The results of a literature study of 70 active compounds of ketapang leaves (*Terminalia catappa* L.) can be seen in table 1.

Table 1. Literature Study of Active Compounds of Ketapang Leaves

No	Title	Ketapang leaf compound
1.	Chemical Composition and Antidiabetic Activity of the Leaves of Terminalia catappa Linn. Grown in Dutsin-Ma	Dibutyl Phthalate; Bis(2-ethylhexyl) phthalate; 1,2-benzenedicarboxylic acid; Lup-20(29)-en-3-one; SH-3,5-Epoxynaphth [2,1, -0] ox (Linolenic Acid); Palmitic acid; Euphol; Lanosterol; Methylprednisolone; dan 2-Dodecan-1-ylsuccinic anhydride (2).
2.	Chemical Constituents From The Leaves of *Terminalia Catappa* L. (Combretaceae)	Tectochrysin; Luteolin, Gallic acid; Kaempferol 3, 7, 4' - trimethyl ether; dan Kaempferol (10).
3.	Pharmacognostic, Phytochemical, and Multianalytical Profiling of the Leaves and Fruit of Terminalia Catappa Integrated With in-silico Docking Studies	Ellagic acid dan Quercetin (11)
4.	Identifikasi Komponen Kimia Ekstrak Daun Katapangg (*Terminalia catappa* L.) Berdasarkan Perbandingan Metode Ekstraksi	Furfural, 5-(Hydroxymethyl) furfural; Levoglucosan; 1,6-Anhydro-Beta-D-Glucofuranose; Octahydro-Naphthalene; 2-Hexenoic acid 5-hydroxy-3,4,4- trimethyl; dan 2-Furancarboxaldehyde, 5- (hydroxymethyl) (12).
5.	Elusidasi Awal Daya Hambat Ekstrak Etanol Daun Ketapang (*Terminalia Catappa* L.) Terhadap	Alpha Terpinolene dan Cyclohexanol 5-methyl (13).

	Pertumbuhan Staphylococcus Aureus ATCC25923 Penyebab Gingivitis	
6.	Uji Aktivitas Antioksidan *Syzygium Polyanthum* Dan *Terminalia Catappa* L. Secara In Vitro dan In Silico	1,2,3,3a,4,6a-hexahydropentalen; Hydroxychavicol; B-Sesquiphellandrepene; Caryophyllene; Geranial; Muurola-4,10(14)-dien1-beta-ol; 2-phenyloctahydro-2H-chromene; Alpha-phinen; dan B-phinene (14).
7.	Understanding the Seasonal Effect of Metabolite Production in Terminalia catappa L. Leaves through a Concatenated MS- and NMR-Based Metabolomics Approach	Apigenin-6-C-(-O-galloyl)-hexose; Apigenin-6-C-hexose (isovitexin); Hydroxyursolic acid; Trihydroxyurs-12-en-28-oic acid (Asiatic acid); Tetrahydroxyolean-12-en-28-oic acid (Protobassic acid); Luteolin-6-C-hexose (isoorientin); Trihydroxyursadien-28-oic acid (Quillaic acid); dan 3-oxo-urs-12,18-dien-28-oic acid (Ganoderic acid) (15).
8.	Polyphenol-Rich Purified Bioactive Fraction Isolated from Terminalia catappa L.: UHPLC-MS/MS-Based Metabolite Identification and Evaluation of Their Antimicrobial Potential	1-O-Galloyl fructose (1-O-Galloyl-beta-D-glucose); 2,6-Digalloyl glucose ; 1,3,6,Trigalloyl glucose; Kaempferol 3-O-galactoside; Gallic acid 3-O-(6- galloylglucoside); Rutin; Apigenin 7-glucoside; Myricetin 7-rhamnoside; Astragalin 7-rhamnoside; Melitric acid A; Methyltrihydroxy benzoate (Methyl Gallate); (8R,80R)- Secoisorlariciresinol 9-glucoside; 2-O-Feruloyl hydroxycitric acid; Kaempferol 7-O glucoside; Cynaroside; Tricin 7-(6-malonyl glucoside); 6-C-Fucosyl luteolin (Vitexin); Hyperoside; Nogalonic acid methyl ester; Hispidulin 7-glucuronide; 3-Oxo-12,18- ursadien-28-oic acid; (3S,4S)-3- Hydroxytetradecane 1,3,4-tricarboxylic acid; 5,6,7,3',4' – Pentahydroxy isoflavone; dan Hemipic acid (16).
9.	Phytochemical Evaluation of Terminalia catappa L. Extracts with Antibacterial and Antibiotic Potentiation Activities Against β-Lactam Drug-Resistant Bacteria	Chalcone; Flavan-3-ol; dan Flavone (17).

Lipinski's Rule of Five (Ro5) is a vital benchmark for evaluating orally administered active compounds. A compound is considered acceptable if it violates no more than one Ro5 parameter (18). The results of a ADME predictions of 70 active compounds of ketapang leaves (*Terminalia catappa* L.) can be seen in table 2 and toxicity predicitions in table 3.

Table 2 ADME Prediction Results

Parameter	Criteria	Compound Count
Molecular Weight	≤ 500 g/mol	62
HBA (*Hydrogen Bond Acceptors*)	≤ 10	54
HBD (*Hydrogen Bond Donors*)	≤ 5	52
LogP	≤ 5	65
Water Solubility	*Soluble*	61
GI *Absorption*	*High*	37
BBB *permeant*	*No*	49
Pgp *substrate*	*No*	47
CYP1A2 *inhibitor*	*No*	60
CYP2C19 *inhibitor*	*No*	64
CYP2C9 *inhibitor*	*No*	56
CYP2D6 *inhibitor*	*No*	65
CYP3A4 *inhibitor*	*No*	64
Bioavailability score	≥ 0.55	53

Table 3 Toxicty Prediction Results

Parameter	Criteria	Compound Count
Cramer Rules	*Low (Class I)*	17
	Intermediate (Class II)	0
	High (Class III)	53
Carcinogenicity and mutagenicity	*Structural alert for genotoxic carcinogenicity*	24
	Structural alert for non genotoxic carcinogenicity	5
	Negative for genotoxic carcinogenicity	42
	Negative for nongenotoxic carcinogenicity	66
	Unlikely to be a S.typhimurium TA100 mutagen based on QSAR	1
In vitro mutagenicity	*Structural alert for S. typhimurium mutagenicity*	26
	No alert for S. typhimurium mutagenicity	43
	Unlikely to be a S.typhimurium TA100 mutagen based on GSAR	1

DISCUSSION

ADME (Absorption, Distribution, Metabolism, Excretion)

The in silico approach via pharmacokinetic parameters aims to characterize the active components of Ketapang (*Terminalia catappa* L.) leaves in determining their oral bioavailability (5). Based on the results of the study, 70 active compounds of ketapang leaves showed varied ADME test results. In the molecular weight parameters, 62 compounds exhibit a molecular weight of ≤ 500 g/mol so they have good permeability. This aligns with a study by (19) that small molecular weights are generally positively correlated with diffusion ability through cell membranes. In compounds with HBA values ≤ 10 and HBD ≤ 5, they showed good potential interactions with enzyme targets through hydrogen bonding without compromising their pharmacokinetic stability (19). This aligns with a study by (20) that the compound has the ability to penetrate the bi-layer membrane and affect drug permeability and absorption in the body.

In the logarithmic parameters of the octanel/water partition coefficient (LogP), 7 compounds were obtained that did not meet the LogP ≥ 5 requirements so that they were less soluble and unable to reach the surface of the membrane. This aligns with a study by (21) that compounds that have a logP value of ≥ 5 will be difficult to absorb and have low permeability. Water-soluble compounds show success in achieving the active side of the enzyme target. This aligns with a study by (22) that if a compound is difficult, water (hydrophilic) is easily dissolved but difficult to penetrate the membrane composed of lipid layers, and if the compound is too hydrophobic, it will be difficult to be circulated by body fluids

In the GI absorption parameters, 37 compounds were obtained that showed high gastrointestinal absorption so that they had good oral bioavailability potential. This aligns with a study by (20) that test compounds that show high gastrointestinal are able to carry out the absobanization process in the intestinal organs. The Blood Brain Barrier parameter is used to predict the ability of a compound to penetrate the blood barrier of the brain and reach the central nervous system. Compounds that are able to penetrate the blood-brain barrier have the potential to have effects on the central nervous system (23). In the P-glycoprotein parameters, 47 compounds were obtained showing P-glucoprotein susbtrats that cannot penetrate the brain, making it difficult to treat diseases involving the central nervous system (6). This aligns with a study by (23) that compounds that are not easily pumped out of cells by P-glucoproteins can increase intracellular concentration and their effectiveness

The cytochrome enzyme P450 is used as a primary source of variability in pharmacokinetics and drug responses (24). Compounds that exhibit non-inhibitory CYP1A2 do not have the ability to inhibit the activity of the CYP1A2 enzyme (20). Compounds that show non inhibitors CYP2C19 show no donor hydrogen bonds with CYP2C19 enzymes. This aligns with a study by (25) that the compound does not inhibit the activity of CYP2C19 enzymes. Compounds that show non-inhibitory CYP2C9 indicate that the properties of the compound do not form a substrate that can be ionized into the CYP2C9 enzyme because its characteristics must be acidic (nonionized). This aligns with a study by (26) that compounds that do not inhibit the activity of the CYP2C9 enzyme may reduce the potential

for concurrent drug interactions. In compounds that show non-inhibitors, CYP2D6 does not have ionizing properties. This aligns with a study by (25) that non-inhibitory compounds CYP2D6 are indicated not to inhibit the activity of the CYP2D6 enzyme. In the parameters of compounds that show non-inhibitory CYP3A4, it indicates that the compound has alkaline properties or that there is a molecular size that is not the same as the CYP3A4 enzyme. This aligns with a study by (25) that non-inhibitory compounds of CYP3A4 do not inhibit the activity of the enzyme CYP3A4. In compounds that have a bioavailability score of ≥ 0.55, it indicates that the compound is available systemically after oral administration. aligns with a study by (23) the higher the score, the better the bioavailability.

Toxicity

Toxicity predictions of the test compound of ketapang leaf (*Terminalia catappa* L.) using *Toxtree* software showed mixed results. Based on the results of the toxicity test, the compounds that obtained the Low category (Class I) are compounds with a simple form, easily absorbed, and if consumed orally have a low level of toxicity (27). This aligns with a study by (20) that compounds with the Low category have chemical characteristics that are guaranteed to be safe or likely not to have high toxicity. Meanwhile, compounds in the High category (Class III) show compounds that have high toxicity and do not provide a guarantee of safety if consumed (20). This aligns with a study by (28) that High category compounds indicate chemical structures that are unsafe or have significant toxicity or have reactive functional groups

In the parameters of the C*arcinogenicity (genetox and nongenotox) and mutagenicity rulebase by ISS*, compounds that show "*Structural alert for genotoxic carcinogenicity*" are structural warnings that have the potential to be genotoxic carcinogenicity (28). Meanwhile, "*Negative for genotoxic carcinogencity*" shows that no harmful functional groups are found as triggers for DNA mutations in compounds and the results "*Negative for nongenotoxic carcinogenicity*" show that compounds are not classified as cancer triggers through non-DNA pathways such as hormonal disorders or uncontrolled proliferation (27). This aligns with a study by (28) that compounds that show "*Negative for genotoxic and nongenotoxic carcinogenic*" are non-carcinogenic compounds.

In the *in vitro mutagenicity (Ames test) alert by ISS* parameters, the compound indicating "*Structural alert for S.typhimurium mutagenicity*" is a test compound that has the potential to cause mutagenicity against S.Typhimurium bacteria and the result "*No alert for S.Typhimurium mutagenicity*" shows no warning for mutagenicity against S.Typhimurium. This aligns with a study by (28) that compounds that show "*No alert for S.typhimurium mutagenicity*" are non-mutagenic compounds and there is no warning of mutagenicity against S.Typhimurium or vice versa.

CONCLUSION

This study concludes that 52 out of 70 compounds satisfy *Lipinski's Rule of Five*, 17 belong to the Low Toxicity category (Class I), 41 score negative for both genotoxic and non-genotoxic carcinogenicity, and 44 compounds exhibit no mutagenicity alerts against *S. typhimurium*. Notably, Methyl Gallate and Hemipic acid stand out as the premier candidates, as they comply fully with *Lipinski's Rule of Five*, fall into the safe Low Toxicity Class I bracket, and display entirely non-carcinogenic and non-mutagenic profiles.

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