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Phytochemical profiling and glutathione peroxidase 1-targeted *in silico* analysis of mango mistletoe (*Dendrophthoe pentandra*) leaves: A natural antioxidant prospect

Acivrida Mega Charisma[1*], Yohanes Ardian Kapri Negara[1], Yani Ambari[2], I Ketut Sudiana[3], Win Darmanto[4], Marsellyna Rahma Gantari[1], Jessica Dewi Nur Aini[1], Aulia Umi Rohmatika[5], Ilham Kurniawan[5]

[1]Department of Medical Laboratory, Faculty of Health Sciences, Anwar Medika University, Sidoarjo, East Java, Indonesia
[2]Department of Pharmacy, Faculty of Health Sciences, Anwar Medika University, Sidoarjo, East Java, Indonesia
[3]Department of Anatomical Pathology, Faculty of Medicine, Airlangga University, Surabaya, East Java, Indonesia
[4]Department of Biology, Faculty of Science and Technology, Airlangga University, Surabaya, East Java, Indonesia
[5]Faculty of Medicine, Universitas Pembangunan Nasional "Veteran" Jawa Timur, Surabaya, East Java, Indonesia

*Corresponding to:
Acivrida Mega Charisma; Department of Medical Laboratory, Faculty of Health Sciences, Anwar Medika University, Sidoarjo, East Java, Indonesia;
acie.vrida@uam.ac.id

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ABSTRACT

Introduction: Plant-derived antioxidants are being increasingly explored for their potential in preventing oxidative stress-related diseases. Mango mistletoe (*Dendrophthoe pentandra (L.) Miq.*) is traditionally used for its potent antioxidant properties. This study aimed to characterize the phytochemical composition and explore the antioxidant potential of *Dendrophthoe pentandra* leaves using a combination of experimental and in silico approaches.
Methods: Ethanolic extracts of *Dendrophthoe pentandra* leaves were prepared by maceration and subjected to qualitative phytochemical screening for primary and secondary metabolites. Thin-layer chromatography (TLC) was used to identify quercetin-like flavonoids. Representative flavonoids reported in *D. pentandra* or suggested by TLC were then docked *in silico* against Glutathione Peroxidase 1 (GPx1) using AutoDock tools to assess binding affinity and interaction patterns, and inhibition constants (Ki) were estimated from binding energies.
Results: Phytochemical profiling revealed the presence of key secondary metabolites, predominantly flavonoids, phenolics, and tannins. TLC analysis indicated quercetin- and kaempferol-like compounds based on characteristic Rf values and UV responses. Molecular docking of representative flavonoids demonstrated strong binding affinities toward GPx1, with quercetin showing the lowest binding energy and the most favorable interaction profile. Ki calculations further supported the higher predicted inhibitory potency of quercetin and kaempferol compared with other tested compounds, suggesting their plausible role as GPx1 modulators. These integrated phytochemical and computational findings support the antioxidant prospect of *Dendrophthoe pentandra* leaves through GPx1-targeted mechanisms.
Conclusion: Mango mistletoe (*Dendrophthoe pentandra*) leaves contain bioactive phytochemicals and flavonoids with favorable predicted interactions with GPx1, indicating their potential as antioxidant candidates that warrant further in vivo validation.

Keywords: Glutathione peroxidase, mango mistletoe, molecular docking, screening phytochemistry, secondary metabolites.
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INTRODUCTION

Indonesia is one of the countries with the highest levels of biodiversity in the world, particularly in terms of medicinal plant diversity. Indonesia's tropical rainforests are the second largest globally after Brazil and are home to approximately 30,000 of the world's approximately 40,000 identified plant species. Approximately 940 species are known to have been used as traditional medicinal plants by various indigenous communities for generations, and collectively represent approximately 90% of the cultivated medicinal flora in Asia.[1]

One of the widely used traditional medicinal plants is the mango mistletoe (*Dendrophthoe pentandra* (L.) Miq.), a parasitic plant that grows on mango trees, especially in lowland areas. *Dendrophthoe pentandra* leaves are empirically utilized for their strong antioxidant activity and are traditionally used as anti-inflammatory, analgesic, antiviral, and anticancer agents.[2] However, scientific validation of its efficacy and safety is still needed, considering the report of the Indonesian Food and Drug Monitoring Agency indicating that some traditional medicines may contain

toxic compounds. Phytochemically, *Dendrophthoe pentandra* is known to contain various bioactive compounds, including flavonoids, tannins, alkaloids, saponins, amino acids, and carbohydrates. Flavonoids, as phenolic compounds, play a role in scavenging reactive oxygen species, chelating metal ions, and modulating cellular antioxidant enzymes, thus contributing to the prevention of oxidative stress that plays a role in the pathogenesis of cancer, cardiovascular disease, and neurodegenerative disorders.[3]

Phytochemical screening is an important approach to identify the presence and characteristics of secondary metabolites in natural materials, either qualitatively, semi-quantitatively, or quantitatively, using specific reagents according to the analysis objectives.[4] Thin-layer chromatography is widely used to strengthen screening results as a confirmatory method in the identification and separation of secondary metabolites in small quantities.[2,5,6] This method is a form of liquid chromatography that involves a stationary phase and a mobile phase (eluent).[7] Various previous studies have reported that *Dendrophthoe pentandra* has diverse pharmacological activities, including antimicrobial, anticancer, antidiabetic, and hypolipidemic, which are generally attributed to its flavonoid content, especially quercitrin, which is known to inhibit cancer cell growth and modulate oxidative stress-related pathways.[8,9]

The selection of glutathione peroxidase 1 (GPx1) as a molecular target is based on its central role in the cellular defense system against oxidative stress, through catalyzing the reduction of hydrogen peroxide and lipid hydroperoxides.[10] Flavonoids contained in *Dendrophthoe pentandra* have been reported to be able to modulate enzymes involved in cellular redox regulation, making their interaction with GPx1 relevant to study.[11,12] In this study, auranofin was used as a reference ligand because it is known to be a GPx1 inhibitor. Although *Dendrophthoe pentandra* has long been used traditionally and is reported to have antioxidant activity, the molecular interaction of its flavonoids with GPx1 has never been systematically evaluated. Therefore, this study aims to conduct a qualitative profiling of secondary metabolites of *Dendrophthoe pentandra* leaves and evaluate the binding affinity of representative flavonoids to GPx1 through a molecular docking approach with auranofin as a reference ligand.

METHODS

Study designs

This *in vitro* and *in silico* study was conducted through phytochemical profiling using thin-layer chromatography and docking simulations performed using AutoDock 4.2. The ligands were prepared with Avogadro 1.2.0. Receptor preparation was done using Discovery Studio Visualizer 2025, and the final visualization was performed in both Discovery Studio Visualizer 2021 and MOE 2015. The 3D structures used in this study were obtained in FASTA, PDB, and PDBQT formats. The 3D crystal structure of the selenocysteine-to-glycine mutant of human glutathione peroxidase 1, with PDB code 2F8A, was acquired from the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB). The chemical structures of the ligands, including Auranofin (PubChem CID 16667669), Quercitrin (PubChem CID 5280459), Kaempferol 3-O-α-L-rhamnopyranoside (PubChem CID 15558501), and Rutin (PubChem CID 5280805), were sourced from the PubChem Substance and Compound Database.

Preparation of Mango Mistletoe Leaves Extract

Sampling of *Dendrophthoe pentandra* (L.) Miq. was conducted in the Bojonegoro area, Bojonegoro Regency. The plant species was identified and confirmed at the Materia Medica Integrated Service Unit. Sample preparation began with cleaning the collected plants to remove soil and debris, followed by washing with clean, running water. The leaves were selected as the plant part used in this study. These leaves were then thinly chopped and air-dried indoors under shade to prevent direct exposure to sunlight. Once dried, the leaf material (simplisia) was ground into a coarse powder using a blender, sieved through an 18-mesh sieve, and stored in a sealed container to prevent moisture absorption. The dried simplisia was then used as the raw material for further phytochemical analysis. The dried and blended samples were subjected to maceration using 95% ethanol at a ratio of 1:7 (sample to solvent) for 72 hours at room temperature. The extraction process was carried out with occasional stirring to enhance compound dissolution. After maceration, the extract was filtered, and the solvent was evaporated using a rotary evaporator until a concentrated extract was obtained.

Phytochemical Test of the Extract

Phytochemical screening was conducted to identify the presence of alkaloids, flavonoids, tannins, polyphenols, and saponins in the *Dendrophthoe pentandra* extract. For alkaloid detection, 1-2 mL of extract was mixed with 2 mL of chloroform and 2 mL of ammonia, homogenized, and filtered. The filtrate was then treated with 3-5 drops of concentrated H_2SO_4, forming two distinct layers. The upper layer was transferred into three separate test tubes and tested with Mayer's, Wagner's, and Dragendorff's reagents. A positive alkaloid reaction was indicated by the formation of a white, cloudy precipitate (Mayer's), yellow to red coloration (Wagner's), or purple to orange coloration (Dragendorff's). The Flavonoid test was performed by adding a small amount of magnesium powder, 2N HCl, and 4-5 drops of ethanol to a 1-2 mL extract sample. A color change to red, yellow, or orange confirmed the presence of flavonoids. Tannin detection involved heating 1-2 mL of extract in a water bath, followed by filtration and the addition of 1% gelatin solution. The formation of a white precipitate indicated a positive result for tannins. Similarly, for the polyphenol test, 1-2 mL of extract was heated in a water bath, filtered, and treated with $FeCl_3$ solution. A color change to green, bluish-green, or blue-black, or the presence of a precipitate, confirmed the presence of polyphenols. Lastly, the saponin test was performed by adding hot water to 1-2 mL of extract, allowing it to cool, and vigorously shaking it for 10 minutes. The formation of stable foam indicated the presence of saponins.

Thin Layer Chromatography (TLC) Test

The TLC identification test was performed using a G60F254 silica plate that was

activated in an oven at 60-80°C for 30 minutes. The plate was then cut into dimensions of 5 cm × 10 cm. The mobile phase used for chromatographic separation consisted of a methanol: chloroform mixture in a 1:1 ratio (5:5). Quercetin and piperine were used as reference standards for comparison. Detection of flavonoid compounds was carried out using 1% $FeCl_3$ as a reagent. If the spots did not appear clearly, visualization was conducted under UV light at a wavelength of 254 nm.

Ligand Preparation

Three flavonoid compounds (Rutin, Quercitrine, and Kaempferol 3-O-α-L-rhamnopyranoside),[2] along with the reference inhibitor Auranofin, were selected based on their reported antioxidant and enzyme-modulating properties. The chemical structures of these ligands were obtained from the PubChem compound database (https://pubchem.ncbi.nlm.nih.gov) in SDF format using their respective CID numbers. The initial geometry optimization of all ligands was performed using Avogadro and MOE with the MMFF94 force field to ensure that the ligands were in their lowest energy conformation. After optimization, ligands were converted into PDB format and further processed into PDBQT format using AutoDock Tools (ADT) 4.2, where Gasteiger partial charges were assigned, non-polar hydrogens were merged, and rotatable bonds were defined while maintaining the planarity of aromatic rings.[13]

Protein Preparation

The three-dimensional crystallographic structure of GPx1 was downloaded from the Protein Data Bank (https://www.rcsb.org) using the PDB ID 2F8A. The protein structure was pre-processed using Discovery Studio by removing co-crystallized water molecules, ligands, and ions that might interfere with the docking process. Special attention was given to the catalytic triad of GPx1, especially Gly47 and Gly48, which are key residues involved in the redox activity of the enzyme. The cleaned structure was subsequently imported into AutoDock Tools, where all polar hydrogens were added, Kollman charges were assigned, and torsional flexibility was disabled to maintain a rigid receptor conformation. The resulting structure was saved as PDBQT for docking.[13] The selected structure represents a mutant GPx1 in which Sec47 is substituted by Gly47, resulting in Gly47/Gly48 being treated as a surrogate for the catalytic center during docking simulations.

Grid Box Configuration and Docking Protocol

Docking simulations were conducted using AutoDock Vina (v4.2). The search space was defined to comprehensively cover the active site region of GPx1 based on the catalytic site surrounding Gly47, which is a critical residue for peroxidase activity. The grid box was centered at coordinates center_x = (-3.224, center_y = 25.063, center_z = 23.659) with dimensions of 26 × 26 × 26 Å in each direction, ensuring sufficient coverage of the binding pocket and allowing the ligands to explore the interaction environment. The exhaustiveness value was set to 64, which controls the accuracy of the global search algorithm. For each ligand, nine binding poses were generated, and the conformation with the lowest binding energy (most negative ΔG) was selected for further analysis.[13]

Analysis of Docking Results and Interaction Profiling

The best docking poses (with the lowest binding energy) were visualized and analyzed using Discovery Studio Visualizer 2021 (BIOVIA), Chimera, and MOE. The focus of analysis was on hydrogen bonding, hydrophobic interactions, π-π stacking, van der Waals interactions, and salt bridges formed between ligands and active site residues. Residues involved in critical interactions, especially those in the vicinity of Gly47, Gly48, Trp143, Gln79, and Arg179, were annotated in detail. The strength and stability of interactions were inferred based on the bond distance, bond type, and geometry. 2D and 3D interaction maps supported visualization to illustrate ligand binding orientation

Inhibition Constant (Ki) Estimation

The inhibition constant (Ki) for each ligand was approximated based on the Gibbs free binding energy (ΔG) obtained from docking, using the following thermodynamic equation $\Delta G = -RT \ln Ki$, where ΔG represents the binding energy (kcal/mol), R is the gas constant (1.987 cal/mol·K). T is absolute temperature (assumed to be 298.15 K). The equation was applied in Python or spreadsheet software to calculate the estimated Ki in micromolar (μM). The calculated Ki value serves as a comparative parameter for ligand inhibitory potency, where lower Ki values suggest stronger ligand-target binding affinity.

Validation and Controls

To validate the docking protocol, the reference ligand Auranofin, a known GPx1 inhibitor, was redocked into the protein structure. The binding mode and interactions were compared to literature-reported data to ensure the reliability of docking parameters. Additionally, the reproducibility of ligand binding poses was confirmed by repeating docking procedures under identical parameters for three independent runs.

Data Analysis

The study results were analyzed descriptively by presenting the findings in tables and images. The obtained data were then compared with relevant literature to interpret and validate the results.

RESULTS

Phytochemical screening

Morphological identification confirmed that the sample used in this study was *Dendrophthoe pentandra*. Qualitative phytochemical analysis of mango mistletoe leaf extract showed the presence of various secondary metabolites (**Table 1**; **Figure 1A-1E**). The test results showed that flavonoids were detected through a red color change after the addition of zinc powder and 2N hydrochloric acid. Alkaloids were consistently identified through positive reactions with Mayer's reagent, which produced an orange color, Dragendorff's reagent, which produced a reddish-yellow color, and Wagner's reagent, which showed a green color change. Tannin compounds gave positive results, indicated by a greenish color change after the addition of gelatin. In

addition, polyphenols and flavonoids showed positive reactions with 1% iron(III) chloride reagent in the ethanol extract and ethyl acetate fraction, which was indicated by a blackish-brown color change. The presence of saponins was confirmed by the formation of stable foam after shaking.

Thin-Layer Chromatography (TLC) Profile

Phytochemical screening confirmed the presence of major antioxidant compounds, including flavonoids, alkaloids, tannins, polyphenols, and saponins. Thin-layer chromatography was used as a qualitative method to identify active constituents in mistletoe mango extract. The TLC analysis utilized a methanol: chloroform (5:5) mobile phase and polar silica gel 60 F254 plates, which had been activated at 70°C to ensure optimal separation. After bottling the ethanol extract, the TLC plate was developed, air-dried, and examined under UV light at 254 and 366 nm (Figure 1F & 1G). The TLC results showed three distinct spots in the extract. A yellow spot was observed at 254 nm, while a black spot appeared at 366 nm. One of the spots had an Rf value of 0.91, closely matching the quercetin standard (Rf 0.92), indicating the presence of flavonoids. The other spots were not further identified, as the chosen solvent system was optimized mainly for detecting tannins and evaluating the polarity of the compounds (Table 2).

Molecular docking to GPx1

Molecular docking simulations showed that three flavonoid compounds, namely rutin, quercitrin, and kaempferol 3-O-α-L-rhamnopyranoside, interact with the active site of GPx1 with higher affinity than the reference ligand auranofin. Validation of the docking protocol by redocking the malonic acid co-crystal ligand resulted in a root mean square deviation of 0.0394 Å with a binding energy of –3.9 kcal/mol and an inhibition constant (Ki) of 1.390 μM, indicating excellent ligand pose reproduction. Docking of the test compounds showed binding energies of –6.6 kcal/mol for rutin, –5.9 kcal/mol for quercitrin, and –5.5 kcal/mol for kaempferol 3-O-α-L-rhamnopyranoside, respectively, while auranofin had a binding energy of –4.9 kcal/mol. The calculated Ki values are in line with these binding energies, namely 12.2 μM for rutin, 49.4 μM for quercitrin, 97.4 μM for kaempferol 3-O-α-L-rhamnopyranoside, and 253 μM for auranofin. Ligand interactions with the active residues of GPx1 involve a combination of hydrogen bonds, van der Waals interactions, and ionic bridges, which stabilize the ligand-protein complex (Figure 2A).

Molecular docking analysis showed that auranofin binds to mutant GPx1 in the catalytic pocket with a binding energy of –4.9 kcal/mol (Figure 2B). Flavonoid docking showed lower binding energies, namely –6.6 kcal/mol for rutin, –5.9 kcal/mol for quercitrin, and –5.5 kcal/mol for kaempferol 3-O-α-L-rhamnopyranoside. Auranofin forms several hydrogen bonds with residues Gly48, Gln82, Trp160, Arg179, Arg180, and Thr143. Quercitrin interacts with GPx1 through hydrogen bonds with Gln82, Thr143, Met142, and Arg179, as well as van der Waals

Table 1. Phytochemical Screening of Mango Mistletoe (*Dendrophthoe pentandra* (L.) Miq.) Leaf Extract

No.	Chemical Compounds	Reagent	Results	Interpretation
1	Flavonoid	Zn, HCl 2N, Ethanol	Formed red color	(+)
		Meyer	Formed orange color	(+)
2	Alkaloid	Dragondorf	Formed rosewood color	(+)
		Wagner	Formed green color	(+)
3	Tannin	Gelatin	Formed green color	(+)
4	Polyphenols	$FeCl_3$ 1%	Formed brown color	(+)
5	Saponins	Aquadest	Formed stable foam (1 cm high foam for 10 minutes)	(+)

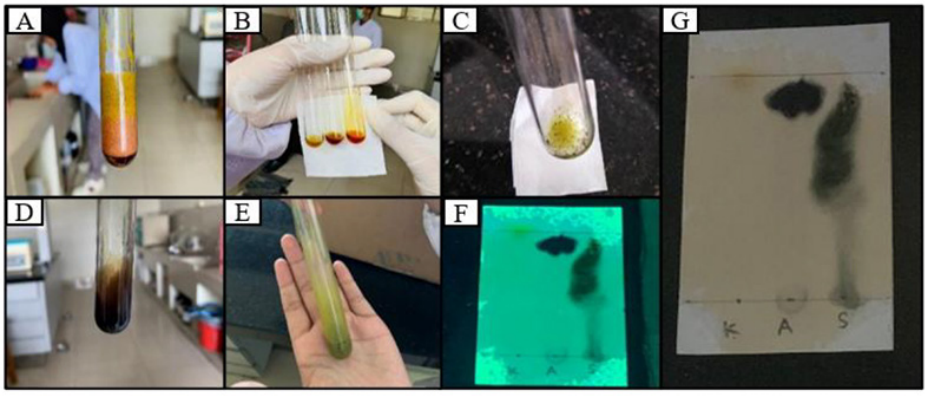

Figure 1. (A) Flavonoid Test Results (+), (B) Alkaloid Test Results (+), (C) Tannin Test Results (+), (D) Polyphenol Test Results (+), (E) Saponin Test Results (+), (F) TLC Staining Results under UV Light at 254 nm, (G) TLC Staining Results under UV Light at 366 nm

Table 2. Thin Layer Chromatography Test with Methanol and Chloroform (5:5) Mobile Phase

Sample	No	Rf Price	Ray Looks	Light (254 nm)	Light (366 nm)
Leaf Extract of Mango Mistletoe	1	0.52	Faded brown	Brown	-
	2	0.80	-	Yellow	-
	3	0.91	-	Yellow	Black

interactions with Gly47, Gly48, Trp160, Arg180, Asp144, and Lys146, accompanied by π-cation interactions with Arg179 and hydrophobic interactions with Leu142 and Met142 (Figure 2C). Rutin shows the lowest binding energy and forms six hydrogen bonds with residues Gly47, Gly48, Leu46, Arg98, Thr143, and Gly80, as well as van der Waals interactions with Thr49, Asn161, Asp144, Arg180, Met142, His81, Gln82, and Arg179, including a hydrophobic π-alkyl interaction with Leu147 (Figure 2D). Kaempferol 3-O-α-L-rhamnopyranoside binds to GPx1 through hydrogen bonds with Gly48 and Gln82, π-cation interactions with Arg179 and Arg180, and van der Waals interactions with Thr143, Thr49, Leu46, Gly47, Arg98, Leu147, and Asp144, accompanied by hydrophobic π-sigma interactions with Gly48 and T-shaped π-π interactions with Trp160 (Figure 2E).

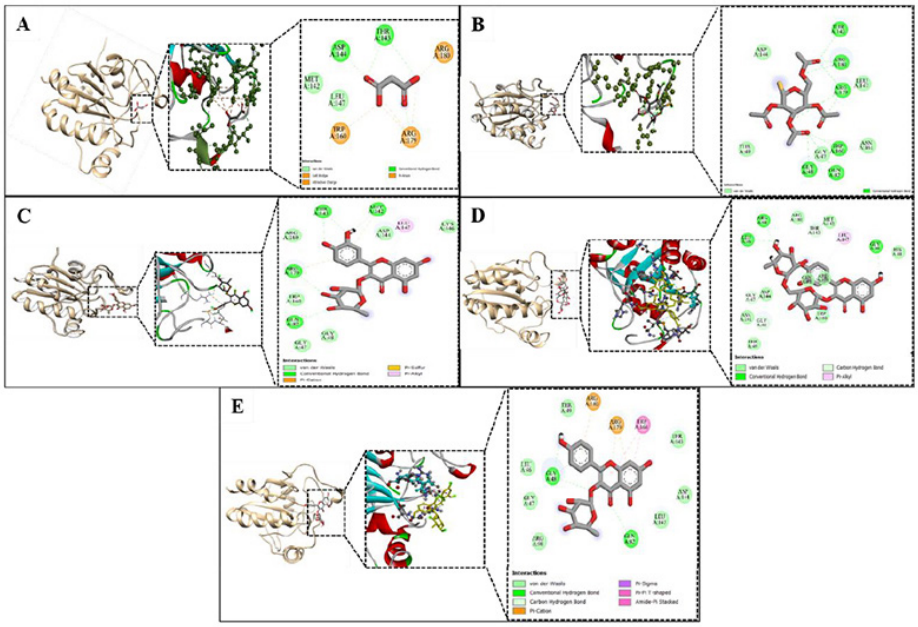

Figure 2. A) Redocking of the co-crystallized ligand, B) Docking pose of auranofin bound to the catalytic pocket of human GPx1 mutant, C) Docking pose of quercitrin bound to the catalytic pocket of human GPx1 mutant, D) Docking pose of rutin bound to the catalytic pocket of human GPx1 mutant, E) Docking pose of Kaempferol 3-O-α-L-rhamnopyranoside bound to the catalytic pocket of human GPx1 mutant

Table 3. Binding affinities and Inhibition Constant of selected ligands to GPx1 (PDB ID: 2F8A)

Ligand	Binding Affinity (Kcal/mol)	Inhibition Constant (μM)	Comparison to Auranofin
Malonic acid	-3.9	1390	Co-crystallized ligand
Auranofin (reference inhibitor)	-4.9	253	Reference
Rutin	-6.6	12.2	Stronger binding than Auranofin
Quercitrin	-5.9	49.4	Stronger binding than Auranofin
Kaempferol 3-O-α-L-rhamnopyranoside	-5.5	97.4	Stronger binding than Auranofin

DISCUSSION

This study integrated a qualitative phytochemical approach and in silico analysis based on molecular docking to explore the antioxidant potential of mango mistletoe (*Dendrophthoe pentandra*) leaves. Species identification was carried out based on morphological characters and the taxonomic framework of Southeast Asian plants as summarized in Flora Malesiana and modern plant phenotype ontology,[14] and was strengthened by reports on plastome characters and the hemiparasitic nature of *Dendrophthoe pentandra*, which is partially dependent on the host but still maintains photosynthetic activity.[15–17] The use of phytochemical screening and thin-layer chromatography as part of the standardization of natural products follows common practices in the development of medicinal plants and traditional formulations.[1,4,18,19] The molecular docking approach to GPx1 with auranofin as a reference was carried out in line with computational-based redox and cancer target exploration strategies that have been widely used in flavonoid and natural compound research.[11–13]

Phytochemical screening results showed that *Dendrophthoe pentandra* leaves contain flavonoids, tannins, polyphenols, alkaloids, and saponins, which are consistent with previous reports on *Dendrophthoe pentandra* and other *Loranthaceae* species known to be rich in protective secondary metabolites.[2,6,8,20] These findings are also in line with cross-species phytochemical studies showing the dominance of flavonoids and tannins in tropical medicinal plant extracts.[21–25] The TLC profile showing numerous spots with characteristic color reactions of flavonoids and tannins supports the high content of phenolic compounds, which ecologically play a role as a chemical defense mechanism in parasitic and semi-parasitic plants.[26] The initial detection of rutin, quercitrin, and kaempferol derivatives is also consistent with reports of phytochemicals in *Dendrophthoe pentandra* and other tropical plants with antioxidant, analgesic, and anti-inflammatory activities.[27–29] However, as emphasized in the TLC literature, common eluent systems have resolution limitations, so compound identification remains preliminary and requires further confirmation using high-resolution analytical methods.[5–7]

Molecular docking analysis showed that the tested flavonoids had a stronger

binding affinity for GPx1 than auranofin, with rutin exhibiting the lowest predicted binding energy and inhibition constant values. Protocol validation through co-crystal ligand redocking followed standard principles of modern docking accuracy evaluation, where ligand pose reproducibility is an indicator of model reliability.[30,31] Ligand interactions with key residues such as Gly47/Gly48, Arg179, Thr143, and Asp144 are consistent with previous structural reports and docking studies that emphasize the role of these residues in GPx1 stability and catalytic function.[32–35] The use of the mutant GPx1 structure (Sec47→Gly47) is a common approach in in silico studies to allow exploration of non-covalent interactions in selenocysteine-based enzymes, without losing the relevance of key catalytic residues.[36]

Biologically, these docking findings are relevant to experimental evidence showing that flavonoids such as rutin and quercitrin can increase glutathione levels and modulate cellular antioxidant systems.[37–41] GPx1 is a key enzyme in the antioxidant defense network that controls peroxide reduction and maintains intracellular redox balance.[42–44] Auranofin, known to modulate the redox system through interactions with thiol-based enzymes, has been widely used in the context of cancer and oxidative stress.[45] In addition to flavonoids, other metabolites such as tannins and saponins are also known to have broad anti-inflammatory, antimicrobial, and cytoprotective activities.[46–51] Various studies on other plants have shown that high phenolic and flavonoid contents are correlated with significant antioxidant capacity,[52–55] thus the phytochemical profile of *Dendrophthoe pentandra* provides a strong chemical basis for its empirically reported antioxidant activity.

Theoretically, targeting GPx1 in this study is based on the enzyme's central role in maintaining cellular redox homeostasis, where dysfunction in its activity contributes to oxidative stress and the progression of chronic diseases, including cancer and degenerative disorders.[42–44] Flavonoids are known to have pleiotropic mechanisms of action, ranging from free radical scavenging and metal ion chelation to modulation of antioxidant enzymes such as GPx, superoxide dismutase, and catalase.[56–58] Molecular docking serves as an exploratory tool to map possible structural interactions and formulate initial mechanistic hypotheses, rather than as direct evidence of the direction of their biological effects.

The main strength of this study lies in the integration of phytochemical profiling with a molecular docking-based structure approach, as well as the use of reference ligands to evaluate the relative performance of test compounds. This approach allows for an initial mechanistic interpretation of the potential bioactivity of *Dendrophthoe pentandra*. However, this study has limitations that should be considered. The phytochemical data are qualitative, and the TLC system used was not specifically optimized for flavonoid resolution; therefore, compound identification remains preliminary. Furthermore, the docking analysis was performed on a mutant GPx1 structure and did not consider protein dynamics, the biological environment, or experimental validation. Therefore, the findings of this study should be understood as hypothesis-generating, and further studies, including quantitative analysis, biochemical assays, and biological models, are needed to confirm their functional and therapeutic relevance.

CONCLUSION

Phytochemical screening and TLC analysis demonstrated the presence of flavonoid-rich secondary metabolites in the leaves of *Dendrophthoe pentandra*. In silico profiling indicated that rutin, quercitrin, and kaempferol 3-O-α-L-rhamnopyranoside bind to GPx1 with favorable predicted affinities, suggesting potential interaction with antioxidant defense pathways. Together with qualitative evidence of phenolic and flavonoid constituents, these findings indicate that *Dendrophthoe pentandra* leaves may represent a promising source of antioxidant flavonoids. However, these results are predictive in nature, and the functional implications remain to be confirmed. Further *in vitro* and *in vivo* studies are needed to validate the antioxidant activity, elucidate the mechanisms, and determine the physiological relevance. Previous literature has reported the ability of flavonoids to modulate oxidative stress through free radical scavenging and enhancement of endogenous antioxidant systems, which provides a rationale for future investigation of *Dendrophthoe pentandra* in this context.

DISCLOSURES

Ethical Approval

Ethical approval not applicable, as this study involved only plant material and in silico analyses without human or animal subjects.

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Conflict of Interest

The authors declare that there was no conflict of interest.

Author Contribution

AMC: Conceptualization; Methodology; Writing - Original Draft Preparation. YAKN: Data Curation; Investigation. Yani Ambari: Formal Analysis; Visualization. IKS Resources; Validation. WD: Supervision; Writing - Reviewing and Editing. MRG: Methodology; Data Curation. JDNA: Visualization; Investigation. AUR: Validation; Writing - Original Draft Preparation. IK: Formal Analysis; In Silico Analysis; Writing - Original Draft Preparation.

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