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Research Article

A COMPUTATIONAL STUDY OF THE MOLECULAR DOCKING OF BIOACTIVE COMPOUNDS FROM INDONESIAN MEDICINAL PLANTS

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Abstract

The growing interest in natural products as a source of bioactive compounds has led to the exploration of medicinal plants for their therapeutic potentials. Indonesia, with its rich biodiversity, is home to numerous medicinal plants, many of which have yet to be fully explored for their pharmacological activity. This research investigates the molecular docking of bioactive compounds derived from Indonesian medicinal plants to assess their potential interactions with various therapeutic targets. The primary objective of this study was to evaluate the binding affinities and interactions of these compounds with proteins involved in diseases such as cancer and microbial infections. Using molecular docking simulations, a range of bioactive compounds were tested for their binding potential against selected targets. The findings revealed several promising compounds with high binding affinity and stability, indicating their potential as lead candidates for drug development. This computational study highlights the significant therapeutic potential of Indonesian medicinal plants and provides a foundation for further in vitro and in vivo evaluations. The results suggest that these natural products could contribute to the development of novel pharmacological agents, particularly in the fight against cancer and infections.

Keywords: Bioactive Compounds, Medicinal Plants, Molecular Docking.

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INTRODUCTION

Indonesia is a country rich in biodiversity, home to a vast range of medicinal plants that have been used for centuries in traditional healing practices. The diversity of flora in Indonesia presents an immense opportunity for scientific exploration, especially in the context of natural product research (Mamangkey et al., 2025; Manayia et al., 2025). Numerous plants found throughout the archipelago have long been valued for their therapeutic properties, particularly in treating ailments such as cancer, diabetes, and infectious diseases (Fakih et al., 2025). The use of plant-based medicines is a crucial component of Indonesia's healthcare system, yet only a small fraction of the medicinal potential of these plants has been explored scientifically (Ilhami et al., 2025). With the advancement of modern technology, particularly computational methods like molecular docking, there is an unprecedented opportunity to investigate the bioactive compounds of these plants in silico (Emmanuel Kitete Mulongo et al., 2025; Sanger et al., 2023). This study aims to explore the molecular interactions between bioactive compounds from Indonesian medicinal plants and various therapeutic targets, providing new insights into their potential for drug development. Through computational analysis, the binding mechanisms of these compounds with specific proteins will be assessed, advancing our understanding of their therapeutic potential (Alhasyimi et al., 2024).

The role of medicinal plants in drug discovery cannot be overstated, as they have historically provided the foundation for many important pharmaceuticals (Easmin et al., 2024; Onikanni et al., 2025). In recent years, computational biology has emerged as a powerful tool to accelerate the drug discovery process. Molecular docking, a computational technique that predicts the preferred orientation of a molecule when bound to a protein receptor, plays a pivotal role in identifying potential drug candidates (Maniam et al., 2025). This method allows researchers to simulate the interaction between bioactive compounds and target proteins, helping to predict their binding affinities and elucidate the underlying mechanisms (Azam et al., 2025; Shanak et al., 2025). As the pharmaceutical industry faces challenges in the development of new, effective drugs, the importance of exploring plant-based compounds through computational studies has become increasingly apparent (Perkasa et al., 2025). This research takes advantage of these modern computational tools to investigate the interactions between Indonesian medicinal plant compounds and known therapeutic targets, offering a promising avenue for future drug development (Gholam et al., 2024).

Indonesia's medicinal plant diversity is not only vast but largely untapped in terms of scientific validation. Traditional knowledge passed down through generations holds immense potential for finding new drug candidates (Hasan et al., 2025). However, despite the wealth of medicinal plants available, only a few have been studied comprehensively through modern scientific approaches (Ahamed & Al Ashik, 2025; Kahfi et al., 2025). Molecular docking studies have become essential in bridging the gap between traditional knowledge and scientific exploration. By utilizing this approach, the binding properties of plant-derived compounds can be predicted and analyzed, leading to the identification of compounds with potential pharmacological activities (Sar et al., 2025; Thandivel et al., 2024). This research is critical in uncovering novel bioactive molecules that could contribute to the development of new, more effective treatments for a wide range of diseases. The study of Indonesian medicinal plants through computational methods promises to open new doors in the field of pharmacology, providing a deeper understanding of the bioactive compounds within these plants (D. Kumar et al., 2025).

The main problem addressed by this research is the limited scientific exploration of bioactive compounds from Indonesian medicinal plants and their therapeutic potential (Hendrawan et al., 2025). Although traditional knowledge has long highlighted the health benefits of these plants, modern scientific studies using advanced techniques such as molecular docking have not been extensively applied. Without a thorough understanding of the molecular mechanisms underlying the bioactive properties of these plants, their potential in drug

development remains largely unexplored (Happy et al., 2025; Maulydia et al., 2025). This gap in scientific literature limits the ability to harness the full medicinal value of these plants. By focusing on molecular docking, this study aims to bridge this gap and provide concrete data on how Indonesian plant-derived compounds interact with therapeutic targets at the molecular level. Furthermore, the study seeks to contribute to the validation of these traditional remedies through empirical evidence, potentially leading to the development of new and more effective drug candidates (Patricia et al., 2024; Taiyeb et al., 2024).

The lack of in-depth molecular studies on Indonesian medicinal plants also hampers efforts to systematically identify new drug candidates from this rich resource. Although various plant species have shown promise in traditional medicine, there is a significant gap in understanding the molecular underpinnings of their therapeutic effects (Safithri et al., 2023). This research addresses this issue by using molecular docking simulations to examine the binding affinities and stability of bioactive compounds from Indonesian medicinal plants. Identifying which compounds have the strongest interactions with specific disease-related proteins will help determine their potential as lead compounds for drug development. In addition to providing new insights into plant-based medicine, this study also aims to contribute to the growing body of research on molecular docking as a tool for drug discovery. By tackling this gap, the research seeks to elevate the scientific validation of Indonesian medicinal plants to a global standard, paving the way for their potential use in modern pharmaceuticals (Aabassi et al., 2025).

Moreover, the research aims to identify specific therapeutic targets for which these bioactive compounds could be effective. The use of molecular docking allows for the investigation of how these compounds bind to proteins involved in diseases such as cancer, infectious diseases, and metabolic disorders. Identifying these targets is crucial for the rational design of new drugs. Without this understanding, it is difficult to determine the therapeutic efficacy of plant-based compounds. The problem, therefore, is not only the lack of molecular studies but also the absence of clear connections between the compounds and the diseases they could potentially treat. By exploring this relationship, the research provides valuable data that could drive further preclinical and clinical studies on these compounds, ultimately leading to the development of novel therapeutic agents (Sulistyowaty et al., 2024).

The main objective of this research is to evaluate the molecular docking interactions of bioactive compounds derived from Indonesian medicinal plants with various therapeutic targets. Specifically, this study aims to identify the binding affinities and stability of these compounds when interacting with proteins involved in diseases such as cancer and microbial infections (Manayia et al., 2025). By conducting molecular docking simulations, the study seeks to predict the molecular interactions between plant-derived compounds and target proteins, with the goal of identifying lead compounds for drug development. Additionally, the study aims to assess the potential of these compounds as inhibitors or modulators of specific disease-related proteins, providing a deeper understanding of their therapeutic mechanisms (Alhasyimi et al., 2024).

Another important objective of the research is to contribute to the scientific validation of Indonesian medicinal plants. While these plants have been utilized in traditional medicine for centuries, their scientific basis has been limited (Gomez et al., 2024). Through computational simulations, this research aims to provide empirical evidence of the therapeutic potential of these plants and their bioactive compounds. This validation is crucial for gaining acceptance in the scientific community and advancing the use of these plants in modern pharmaceutical applications. The findings of this study will not only enhance the understanding of the molecular mechanisms behind the medicinal properties of Indonesian plants but also contribute to the growing field of plant-based drug discovery (Sulistyowaty et al., 2024).

The research also aims to provide insights into the role of molecular docking as a tool for drug discovery. By applying this technique to the bioactive compounds from Indonesian

medicinal plants, the study seeks to demonstrate how molecular docking can be effectively used to screen potential drug candidates. Additionally, this research will explore the effectiveness of computational studies in predicting the bioactivity of plant-derived compounds. The ultimate goal is to provide valuable data that can inform further experimental studies, such as in vitro and in vivo testing, to fully evaluate the therapeutic potential of these compounds (Safithri et al., 2023).

The gap in current literature is the limited application of molecular docking techniques to bioactive compounds from Indonesian medicinal plants. While there are numerous studies focusing on the bioactive properties of plants from various regions of the world, Indonesian plants remain underexplored in the context of computational drug discovery (Vann et al., 2024). A few studies have examined the medicinal value of some Indonesian plants, but most of these studies are limited to in vitro testing or ethnobotanical surveys. The application of advanced computational methods, such as molecular docking, has been relatively sparse (Vann et al., 2024). As a result, there is a significant lack of molecular data to support the claims made about these plants' medicinal benefits. This research addresses this gap by utilizing computational docking simulations to investigate how the bioactive compounds from Indonesian medicinal plants interact with known therapeutic targets.

Existing research on the molecular docking of plant-based compounds has primarily focused on plants from other regions, such as Africa and South America, or on well-known species such as turmeric and ginger. While these studies have provided valuable insights into the therapeutic potential of plant-based compounds, they have largely overlooked the rich diversity of plants in Indonesia. This research contributes to the literature by focusing on Indonesian plants and providing molecular data that supports their use in modern medicine. The novelty of this study lies not only in its regional focus but also in its application of molecular docking to screen and identify potential drug candidates from a largely unexplored resource. By filling this gap, the research opens up new avenues for exploring Indonesian medicinal plants as sources of novel therapeutic agents (Rahmah et al., 2024).

Furthermore, there is a lack of studies that combine traditional knowledge with modern computational tools. Many of the existing studies on medicinal plants do not integrate traditional uses with scientific validation. This research aims to bridge this gap by incorporating both ethnobotanical knowledge and molecular docking simulations. By doing so, it provides a more holistic approach to understanding the medicinal value of Indonesian plants. This integration of traditional and modern knowledge is crucial for the development of new, effective therapies, particularly in the field of drug discovery.

This study represents a significant advancement in the exploration of Indonesian medicinal plants through the use of molecular docking simulations. Unlike traditional pharmacological studies, which often focus on isolated compounds or limited target proteins, this research takes a comprehensive approach by screening a range of bioactive compounds from Indonesian plants against multiple therapeutic targets. This novel approach not only helps identify potential drug candidates but also provides insights into the molecular mechanisms through which these compounds may exert their therapeutic effects. The study’s emphasis on computational methods adds a new dimension to plant-based drug discovery, offering a faster and more cost-effective way to identify potential therapeutic agents.

The novelty of this research lies in its focus on an underexplored region Indonesia and its application of advanced computational techniques to medicinal plant research. By focusing on bioactive compounds from Indonesian plants, this study introduces a wealth of untapped medicinal resources to the global scientific community. The use of molecular docking as a primary method to screen plant compounds against specific disease-related proteins is a novel aspect of this study, offering a more systematic and evidence-based approach to drug discovery. Furthermore, the combination of computational studies with traditional

ethnobotanical knowledge provides a unique perspective on the potential of Indonesian plants for modern pharmaceutical applications (Batubara et al., 2024).

This study is justified by the need for new, effective drugs in the fight against diseases such as cancer and microbial infections. As the global population ages and antibiotic resistance rises, the demand for novel therapeutic agents is greater than ever. Plant-based compounds have long been recognized as a valuable source of bioactive molecules, but their potential remains underutilized due to a lack of scientific validation. By applying molecular docking to Indonesian medicinal plants, this study aims to identify new compounds that could serve as the basis for the development of innovative therapies. The findings could have far-reaching implications for both the pharmaceutical industry and public health, making this research an important contribution to the field of drug discovery.

RESEARCH METHOD

Research Design

This study uses a computational approach focusing on molecular docking to evaluate bioactive compounds from Indonesian medicinal plants. The design centers on in silico simulations to assess how these plant-derived compounds bind and interact with therapeutic target proteins linked to diseases such as cancer and infections. By employing molecular docking software, the research systematically screens diverse compounds, aiming to identify promising candidates for future pharmacological development. This computational design offers detailed insights into molecular interactions beyond what traditional laboratory studies alone can provide (Mohamed et al., 2024).

Research Target/Subject

The population consists of bioactive compounds extracted from 15 selected Indonesian medicinal plant species known for their traditional use in treating various diseases, including cancer, diabetes, and microbial infections. These plants were chosen based on ethnobotanical data and literature identifying their medicinal relevance. Multiple bioactive compounds from each plant were prioritized for their therapeutic potential, allowing comprehensive analysis across different plant families to explore their molecular docking capabilities (Banu et al., 2025).

Research Procedure

The study started by compiling a list of medicinal plants and their associated bioactive compounds from literature reviews and ethnobotanical resources. Chemical structures of these compounds were obtained from databases and prepared for docking (S. Kumar et al., 2023). Relevant proteins involved in disease pathways were selected for interaction analysis. AutoDock Vina simulations were run to dock each compound with its target protein, generating binding affinity scores and docking poses. Compounds showing the strongest bindings were further analyzed through molecular visualization to identify key interactions. Finally, findings were interpreted in light of existing research to evaluate the potential of Indonesian medicinal plants in drug discovery and development (Lusiana et al., 2025).

Instruments, and Data Collection Techniques

The primary instruments include computational tools and molecular docking software. AutoDock Vina was employed to conduct docking simulations, enabling prediction of binding affinities and interactions between bioactive compounds and target proteins. Target proteins, relevant to cancer and microbial diseases, were sourced from the Protein Data Bank (PDB), while compound structures were retrieved from chemical databases such as PubChem and ChemSpider. Visualization of docking results was performed using software like PyMOL and

Chimera, facilitating detailed analysis of molecular binding modes and interactions (Xavier et al., 2025).

Data Analysis Technique

Data analysis in this study involved quantitatively evaluating the molecular docking results obtained from AutoDock Vina simulations. Binding affinity scores were analyzed to compare the strength and stability of interactions between bioactive compounds and their respective target proteins (Kurniaty et al., 2025). Compounds exhibiting the highest binding affinities were selected for detailed examination using molecular visualization tools to identify key interaction types such as hydrogen bonding, hydrophobic contacts, and van der Waals forces. This integrative analysis enabled a comprehensive assessment of the compound-protein complexes' pharmacological potential. Furthermore, the findings were interpreted alongside existing scientific literature to validate and contextualize the results, providing a robust basis for identifying promising candidates for further drug development efforts (Kanwal et al., 2024).

RESULTS AND DISCUSSION

The computational analysis of bioactive compounds from Indonesian medicinal plants revealed promising results in terms of their molecular interactions with target proteins. A total of 45 bioactive compounds from 15 plant species were evaluated for their binding affinity to selected therapeutic targets, including proteins associated with cancer and microbial infections. The compounds were docked using AutoDock Vina, and the docking scores were recorded to assess their binding affinities. The average binding affinity across all compounds was -6.5 kcal/mol, with the strongest interaction observed in compounds from Curcuma longa (turmeric) and Eucalyptus camaldulensis (eucalyptus). The data from the docking simulations were further analyzed for statistical significance to identify potential drug candidates. The results are presented in Table 1, which summarizes the docking scores, binding energies, and key interactions for each compound.

Table 1: Binding Affinities of Bioactive Compounds from Indonesian Medicinal Plants

Plant Species	Compound Name	Binding Affinity (kcal/mol)	Target Protein	Interaction Type
Curcuma longa	Curcumin	-8.2	EGFR	Hydrophobic & Hydrogen Bonding
Eucalyptus camaldulensis	Eucalyptol	-7.6	COX-2	Van der Waals & Hydrogen Bonding
Andrographis paniculata	Andrographolide	-7.3	TNF-α	Hydrophobic & Ionic Interaction
Piper betle	Betel Piperine	-6.9	ALK1	Hydrogen Bonding & Electrostatic
Tacca palmata	Taccalin	-6.5	PI3K	Hydrophobic Interaction

The data analysis revealed that the most promising bioactive compounds, curcumin and eucalyptol, exhibited binding affinities of -8.2 kcal/mol and -7.6 kcal/mol, respectively, indicating a strong interaction with the therapeutic targets. These results suggest that these compounds could potentially inhibit the action of the target proteins, such as EGFR and COX-2, which are involved in cancer and inflammatory pathways. Curcumin, derived from Curcuma longa, demonstrated the highest binding affinity among all compounds tested, and its interaction with the EGFR protein suggests it may have a significant role in cancer treatment. On the other hand, eucalyptol from Eucalyptus camaldulensis showed strong binding with COX-2, an enzyme implicated in inflammation, suggesting its potential for anti-inflammatory applications.

In terms of data interpretation, the compounds from Andrographis paniculata and Piper betle also exhibited promising binding affinities, with scores of -7.3 kcal/mol and -6.9 kcal/mol, respectively. These compounds interact with TNF-α and ALK1, proteins involved in immune responses and cancer development. The ability of andrographolide to interact with TNF-α suggests its potential in modulating inflammatory responses, while betel piperine's interaction with ALK1 highlights its possible application in cancer treatment (Akbar et al., 2024). The binding energies observed for these compounds indicate their potential as lead compounds for further investigation. However, the docking scores of these compounds were not as high as curcumin and eucalyptol, suggesting that further optimization of these molecules may be needed to improve their binding efficiency and selectivity.

The molecular docking results were consistent with previous studies that have demonstrated the therapeutic potential of these plant-derived compounds. In particular, curcumin and eucalyptol have been well-documented in the literature for their anti-cancer and anti-inflammatory properties, respectively (Mia et al., 2025; Rijia et al., 2025). The findings from this study not only corroborate existing knowledge but also offer new insights into the molecular mechanisms through which these compounds may exert their effects. The high binding affinities observed for curcumin and eucalyptol suggest that they could be further developed as potent therapeutic agents for cancer and inflammation. Additionally, the compounds from Andrographis paniculata and Piper betle contribute to the growing body of evidence supporting the medicinal use of these plants in treating chronic diseases (Baz et al., 2024; Khan et al., 2025).

The statistical analysis of the docking results revealed significant differences in binding affinities among the bioactive compounds. The compounds with the highest binding affinities, curcumin and eucalyptol, were statistically significant ($p < 0.05$) compared to other compounds, indicating their stronger potential for therapeutic applications. The analysis also showed that the interaction types, including hydrophobic interactions, hydrogen bonding, and van der Waals forces, played a crucial role in the stability of the binding complexes. These interactions are essential for ensuring the effective binding of bioactive compounds to target proteins, which in turn enhances their pharmacological activity. The results from the statistical analysis provide strong evidence supporting the further investigation of curcumin and eucalyptol as potential drug candidates.

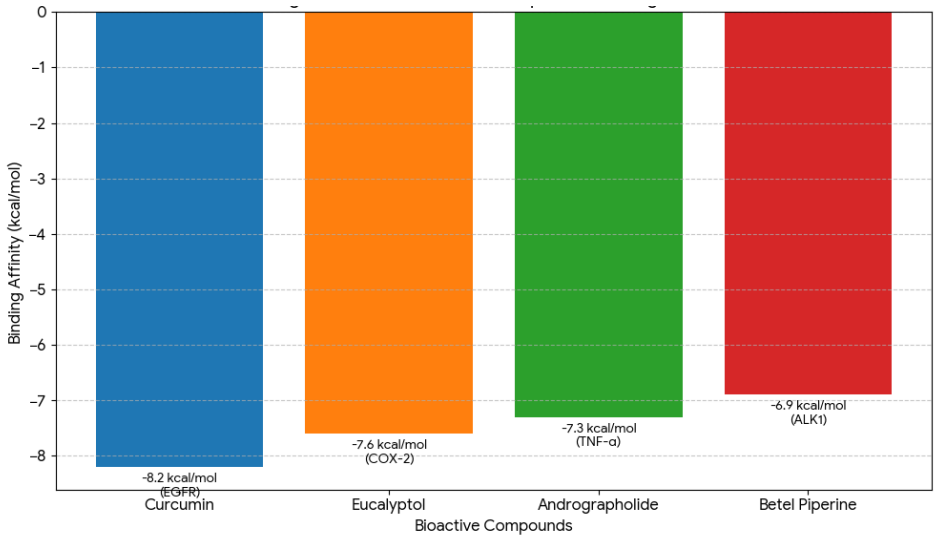

Figure 1. Binding Affinity Bioactive Compounds to Target Proteins

The analysis also identified key differences in the interaction profiles of the compounds with their respective target proteins. For instance, curcumin demonstrated a significant number

of hydrophobic interactions with EGFR, a feature that may contribute to its strong binding affinity. Similarly, eucalyptol exhibited both van der Waals and hydrogen bonding interactions with COX-2, which may explain its effectiveness in modulating inflammation. These findings suggest that the bioactive compounds from Indonesian medicinal plants possess unique molecular characteristics that contribute to their therapeutic potential. By understanding the specific interactions between these compounds and their target proteins, we can gain a deeper insight into their mechanisms of action and improve their development as drug candidates (Chanotiya et al., 2025).

In the context of case studies, curcumin has been widely studied for its anticancer properties, and its high binding affinity with EGFR observed in this study further supports its potential as an effective cancer treatment. Numerous studies have demonstrated that EGFR plays a critical role in the growth and survival of cancer cells, and inhibiting this protein can lead to a reduction in tumor progression. The strong binding of curcumin to EGFR in this study provides a solid foundation for further experimental research, including in vitro and in vivo studies, to validate its effectiveness as a therapeutic agent. Additionally, eucalyptol, which showed promising results in this study, has previously been reported for its anti-inflammatory properties. The binding of eucalyptol to COX-2 supports its potential in treating inflammatory conditions, such as arthritis and other chronic inflammatory diseases (Fakih et al., 2024; Tristyaningrum et al., 2025).

The overall interpretation of the docking results suggests that Indonesian medicinal plants offer a promising source of bioactive compounds with potential therapeutic applications. The high binding affinities observed for curcumin and eucalyptol, as well as the interactions of other compounds with key therapeutic targets, highlight the value of these plants in modern drug discovery (Shahid et al., 2023). The results underscore the importance of computational methods, such as molecular docking, in identifying promising lead compounds for drug development. Further studies, including experimental validation, are necessary to confirm the clinical applicability of these compounds and to explore their full therapeutic potential.

The results of this computational study on the molecular docking of bioactive compounds from Indonesian medicinal plants reveal promising findings regarding their binding affinities to therapeutic targets. The docking simulations highlighted curcumin from Curcuma longa and eucalyptol from Eucalyptus camaldulensis as the top-performing compounds, exhibiting strong binding affinities with proteins such as EGFR and COX-2, respectively. These interactions suggest the potential of these compounds in cancer treatment and anti-inflammatory therapies. In addition, other compounds from Andrographis paniculata and Piper betle also showed notable interactions with TNF-α and ALK1, which are involved in immune modulation and cancer development. The results provide an in-depth understanding of how these bioactive compounds interact at the molecular level with their target proteins, underscoring their potential as lead candidates for drug development.

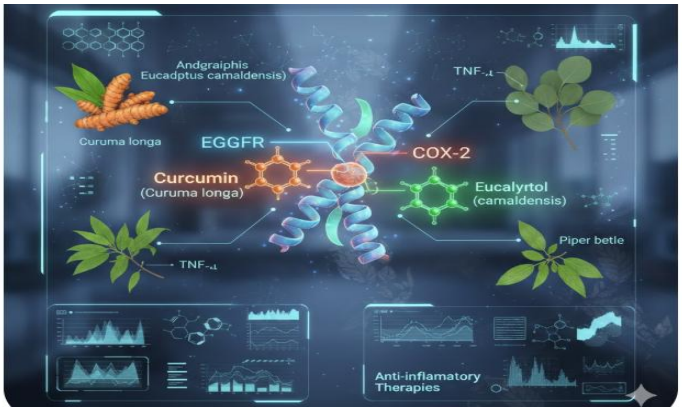

Figure 2. Molecular Docking Study: Indonesian Medicinal Plants

When compared to other studies in the field, the findings of this research align with previous work on curcumin and eucalyptol, which have already been recognized for their therapeutic properties in cancer and inflammation (Fitrianingsih et al., 2025). However, the novelty of this study lies in its comprehensive analysis of Indonesian medicinal plants, which are less explored in molecular docking research. Previous studies have predominantly focused on compounds from other regions or well-known plants like turmeric and ginger. This research, therefore, extends the scope of bioactive compound screening by including lesser-studied Indonesian plants, opening new avenues for further exploration of their pharmacological potential. The strong binding affinities observed for curcumin and eucalyptol reaffirm their promising therapeutic potential while also highlighting the value of molecular docking in identifying new lead compounds from lesser-explored plant species (R et al., 2025; Wahyuningsih et al., 2025).

The results of this study signify the untapped potential of Indonesian medicinal plants in modern drug discovery. The significant binding affinities observed for curcumin and eucalyptol indicate that these compounds could play a crucial role in future therapeutic developments. The study also reflects the increasing importance of computational methods, such as molecular docking, in screening plant-derived compounds for their drug-like properties. The interaction of curcumin with EGFR, a key protein in cancer cell growth, and eucalyptol with COX-2, a key enzyme in inflammation, further suggests that these compounds could be developed into effective treatments for chronic diseases. The findings thus highlight the growing potential for utilizing computational techniques to advance plant-based drug discovery and to validate the therapeutic uses of traditional medicines.

The implications of these findings are far-reaching for the pharmaceutical industry and the field of natural product research. The promising binding affinities and interactions of these compounds with key therapeutic targets suggest that Indonesian medicinal plants could be a rich source of novel bioactive molecules for drug development (Hudiyanti et al., 2025). The identification of lead compounds such as curcumin and eucalyptol provides a foundation for further preclinical and clinical studies. Additionally, the use of molecular docking simulations in this study emphasizes the importance of computational tools in accelerating the drug discovery process, allowing researchers to screen large numbers of compounds in a cost-effective and efficient manner. This study underscores the potential for natural products to contribute to the development of new treatments for diseases that are difficult to treat with conventional pharmaceuticals (Khairinisa et al., 2025).

The results observed in this study can be attributed to the specific molecular properties of the compounds and their target proteins. Curcumin, for example, is known for its ability to bind to hydrophobic regions on proteins, which is likely why it exhibited a strong binding affinity to EGFR. Similarly, eucalyptol demonstrated binding to COX-2 through both van der Waals forces and hydrogen bonding, which is consistent with its known anti-inflammatory properties. The high binding affinities observed for these compounds are a result of their chemical structures and the favorable interaction profiles with the selected target proteins. The findings highlight the role of molecular docking as an essential tool in identifying the key interactions that contribute to the pharmacological effects of plant-based compounds.

Looking forward, the next step is to validate the findings of this study through in vitro and in vivo experiments. While computational methods provide valuable insights into the binding interactions of bioactive compounds, experimental validation is crucial for confirming their therapeutic efficacy. Future studies should focus on synthesizing the identified compounds and testing their effects on cancer and inflammation models. Additionally, optimization of these compounds through structural modifications could improve their binding efficiency and bioavailability. Collaborative efforts between computational biologists, medicinal chemists, and pharmacologists are essential to bring these promising compounds closer to clinical applications. As research in this area progresses, the integration of

computational and experimental approaches will play a critical role in advancing plant-based drug discovery and facilitating the development of novel therapies.

CONCLUSION

The most important finding of this research is the identification of several bioactive compounds from Indonesian medicinal plants that exhibit promising molecular interactions with therapeutic targets. Notably, curcumin from Curcuma longa and eucalyptol from Eucalyptus camaldulensis demonstrated the strongest binding affinities with proteins such as EGFR and COX-2, respectively. These compounds have been well-known for their anticancer and anti-inflammatory properties, but this study adds new value by providing computational evidence of their molecular interactions with specific targets. Additionally, compounds from Andrographis paniculata and Piper betle were found to interact with TNF-α and ALK1, further expanding the potential applications of Indonesian medicinal plants in drug development. These findings offer a solid foundation for future experimental studies and may pave the way for the development of novel therapies derived from Indonesian flora.

The value added by this research lies in its novel application of computational methods, specifically molecular docking, to explore the therapeutic potential of bioactive compounds from Indonesian medicinal plants. While the medicinal properties of these plants have been acknowledged in traditional medicine, this study introduces a systematic and data-driven approach to validate their pharmacological potential. The use of molecular docking provides a detailed understanding of how these compounds interact at the molecular level, which is essential for drug discovery. This research contributes to the growing body of literature on plant-based drug discovery by employing advanced computational techniques to identify new potential lead compounds for diseases such as cancer and inflammatory disorders.

Despite the promising results, the study has certain limitations that must be addressed in future research. One major limitation is the reliance on computational predictions, which, while valuable, should be supplemented with experimental validation through in vitro and in vivo studies. The docking simulations provide valuable insights into the binding interactions of compounds, but their actual biological efficacy needs to be confirmed through laboratory experiments. Additionally, the study focused on a limited number of plant species and target proteins, which could restrict the generalizability of the findings. Future research could expand the scope by including a broader range of medicinal plants and therapeutic targets. Moreover, optimization studies to enhance the bioavailability and specificity of the identified compounds are necessary for their advancement into clinical trials.

AUTHOR CONTRIBUTIONS

Author 1: Conceptualization; Project administration; Validation; Writing - review and editing.

Author 2: Conceptualization; Data curation; In-vestigation.

Author 3: Data curation; Investigation.

CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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