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ISOLATION, CHARACTERIZATION, AND BIOLOGICAL ACTIVITY EVALUATION OF BIOACTIVE COMPOUNDS FROM HERBAL PLANTS AS DRUG CANDIDATES

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Abstract
Research on herbal plants in the field of medicinal chemistry aims to explore the potential of bioactive compounds as drug candidates. Herbal plants are known to contain secondary metabolites such as flavonoids, alkaloids, and phenolic compounds that exhibit various biological activities. This study aims to evaluate the potential of active compounds derived from herbal plants through a medicinal chemistry approach, including isolation, characterization, and biological activity evaluation based on literature studies. The method used in this study was a literature review of relevant scientific journals, including publications from lecturers and other supporting articles. The results indicate that bioactive compounds from herbal plants possess antioxidant, antibacterial, antidiabetic, and anticancer activities. Furthermore, medicinal chemistry approaches such as structural modification and molecular docking have been shown to enhance the effectiveness and selectivity of compounds toward biological targets. In conclusion, herbal plants have great potential as sources of new drug candidates that can be further developed through medicinal chemistry approaches.

Keywords: *herbal plants, medicinal chemistry, bioactive compounds, biological activity, flavonoids*

INTRODUCTION

Indonesia is one of the countries with the highest levels of biodiversity in the world, offering significant potential as a source of bioactive compounds for drug development. Various medicinal plants are known to contain secondary metabolites such as alkaloids, flavonoids, terpenoids, saponins, and phenolics, which have been reported to possess various pharmacological activities, including antioxidants, anti-inflammatory, antimicrobial, anticancer, and antidiabetic properties. This wealth of natural resources offers ample opportunities to discover new drug candidates derived from natural ingredients and with relatively fewer side effects compared to some synthetic drugs (Newman & Cragg, 2020).

Natural products, particularly those derived from herbal plants, continue to be an important source for the discovery and development of new drugs. The diverse bioactive compounds produced by plants have made significant contributions to the development of modern therapies due to their diverse chemical structures and broad biological activities. According to Chihomvu et al. (2024), phytochemicals from medicinal plants serve as a bridge between traditional medicine and modern pharmaceutical innovation because they provide novel molecules with the potential to be developed into drug candidates. Therefore, the exploration and characterization of bioactive compounds from herbal plants are crucial steps in supporting a more effective and sustainable drug discovery process (Chihomvu et al., 2024).

However, the use of bioactive compounds from herbal plants as modern medicines still faces various challenges. Many natural compounds demonstrate excellent biological activity in initial testing, but suffer from limitations such as low bioavailability, poor chemical stability, and suboptimal selectivity for specific biological targets. These conditions reduce the compounds' therapeutic

effectiveness when applied to more complex biological systems, necessitating various optimization efforts to enhance their pharmacological potential (Naeem et al., 2022).

Advances in medicinal chemistry have opened up new opportunities to overcome these limitations through structural modification approaches. Modifying specific functional groups in bioactive compounds can increase affinity for biological targets, improve pharmacokinetic properties, and enhance the resulting biological activity. This approach allows natural compounds to be used not only in their original form but also to be developed into various derivatives with improved efficacy and safety as future drug candidates (Al-Karmalawy et al., 2025).

In addition to structural modification approaches, advances in computational technology have also made significant contributions to the natural product-based drug discovery process. Various in silico methods enable faster and more efficient identification and evaluation of drug candidates, thereby accelerating the research process and reducing drug development costs. The combination of natural compound exploration, medicinal chemistry approaches, and computational technology is currently a widely used strategy in the development of new drug candidates from natural products (Amin et al., 2025).

The use of plants for medicinal purposes has been practiced for thousands of years and is an essential part of traditional health systems in many countries, including Indonesia. Indonesia's rich biodiversity offers significant potential for developing herbal plants as raw materials for medicines. With the growing demand for safer, more effective medicines with minimal side effects, research into the active compounds found in herbal plants continues to expand. Various herbal plants are known to contain secondary metabolites that play a crucial role in providing pharmacological effects, thus offering potential for use in the development of modern medicines.

Advances in pharmaceutical science and technology have encouraged the use of natural ingredients not only as traditional medicines but also as primary sources of compounds in the discovery and development of new drugs. Many drugs currently in use are derived from natural compounds or modified natural compounds that have undergone various stages of scientific research. Therefore, exploring the chemical constituents of herbal plants is a crucial strategy in discovering drug candidates with specific biological activity against various diseases.

Herbal plants have long been used as a source of traditional medicine due to their diverse bioactive compounds with pharmacological activity. In medicinal chemistry, secondary metabolites such as flavonoids, alkaloids, tannins, and phenolics are of primary interest due to their potential for development as new drug candidates. Various studies have shown that these compounds possess biological activities such as antioxidant, antibacterial, antidiabetic, and anticancer properties, which play a crucial role in the prevention and treatment of degenerative diseases (Rahman *et al*., 2021).

The biological activity of herbal plants is closely related to their bioactive compounds, which interact with specific biological targets. Flavonoids are known to act as antioxidants by scavenging free radicals and inhibiting oxidative stress, the primary cause of cell damage (Sari *et al*., 2021). Furthermore, alkaloids and phenolic compounds are also known to possess antibacterial activity by inhibiting the growth of pathogenic microorganisms (Abass *et al*., 2024). This demonstrates that herbal plants have great potential as sources of therapeutic compounds in modern drug development.

Current developments in medicinal chemistry research focus not only on the isolation and characterization of active compounds but also on modifying their chemical structures to increase the effectiveness and selectivity of their biological activity. Based on research conducted by Rio Anggi Setiawan (2023), computational approaches and the synthesis of flavonoid derivatives showed that modifying the compound's structure can increase affinity for protein targets that play a role in type 2 diabetes mellitus. This research shows that the molecular docking approach can be used to predict interactions between active compounds and biological receptors, thus supporting the development of natural product-based drug candidates.

Furthermore, another study by Anggi Setiawan and Amin (2026) on the modification of natural compounds for anticancer activity showed that changes in chemical structure can increase cytotoxic activity and selectivity against cancer cells. The relationship between chemical structure and biological activity, or Structure–Activity Relationship (SAR), is an important aspect in drug development, because small changes in molecular structure can have a significant impact on the pharmacological activity of a compound (Thomford *et al*., 2024). Therefore, a medicinal chemistry approach plays a crucial role in optimizing the potential of active compounds from herbal plants.

The increasing prevalence of degenerative diseases such as diabetes mellitus, cancer, cardiovascular disease, and other metabolic disorders poses a major challenge to the healthcare world. The use of currently available synthetic drugs often leads to various side effects, drug resistance, and relatively high treatment costs. This situation has prompted researchers to seek alternative therapies derived from natural ingredients, particularly herbal plants, which are considered to be safer and more readily available. Therefore, the exploration of active compounds from herbal plants has become a primary focus in pharmaceutical and medicinal chemistry research.

In modern drug development, identifying and understanding the relationship between a compound's chemical structure and its biological activity is essential. Advances in chemical analysis and computational technology have enabled researchers to identify active compounds more quickly and accurately. Methods such as compound isolation, spectroscopy, molecular docking, and the Structure–Activity Relationship (SAR) approach are widely used to evaluate a compound's potential as a drug candidate. Through this approach, natural product-based drug development can be carried out more systematically, resulting in compounds with greater effectiveness and selectivity toward disease targets.

Based on this description, this research was conducted to assess the potential of active compounds from herbal plants through a medicinal chemistry approach, including isolation, characterization, and evaluation of biological activity as drug candidates. This research is expected to provide scientific information regarding the use of herbal plants in the development of more effective and safe natural-based medicines.

RESEARCH METHODS

This study employed a literature review with a qualitative descriptive approach to assess the potential of active compounds in herbal plants in the field of medicinal chemistry. Data were obtained from national and international scientific journals accessed through Google Scholar, PubMed, and ScienceDirect using the keywords "herbal plants," "bioactive compounds," "medicinal chemistry," "flavonoids," and "biological activity." The literature used was published within the last five years (2021–2025) and had full-text access and was relevant to the research topic (El-Saadony *et al*., 2025).

The selected journals were then analyzed based on their active compound content, biological activity, and the medicinal chemistry approach used. Research by Rio Anggi Setiawan (2022; 2023) on the modification of natural compounds and flavonoid derivatives served as the primary reference in this study. The obtained data were analyzed descriptively and qualitatively to determine the relationship between compound structure and biological activity (Structure–Activity Relationship/SAR) in the development of drug candidates (Thomford *et al*., 2024).

RESULTS AND DISCUSSION

The success of developing herbal-based medicines depends heavily on the quality of the extraction and purification processes for the active compounds they contain. Different extraction methods can produce different compositions of bioactive compounds, thus affecting the resulting biological activity. The use of appropriate solvents and optimal extraction conditions are crucial for obtaining the maximum amount of active compounds. Furthermore,Factors such as temperature, extraction time, particle size of the herbal ingredients, and the type of solvent used can also affect the quantity and quality of the compounds successfully extracted. Bioactive compounds obtained through improper extraction processes can potentially degrade, reducing their biological activity. Therefore, standardization of extraction

methods is necessary to maintain the consistent quality and effectiveness of herbal-based products. This standardization is also important to ensure the reproducibility of research results, ensuring that the resulting active compounds have uniform characteristics and can be used as raw materials in the development of safe and effective pharmaceutical products.

In addition to the extraction process, characterizing the structure of active compounds is also a crucial step in medicinal chemistry research. Various analytical techniques such as UV-Vis spectroscopy, Fourier Transform Infrared (FTIR), Nuclear Magnetic Resonance (NMR), and Mass Spectrometry (MS) are widely used to identify the chemical structure of isolated compounds. Information about molecular structure is essential for understanding the relationship between structure and biological activity of a compound, thus providing a basis for molecular modification and the design of new drugs. Accurate characterization allows researchers to identify the functional groups responsible for a compound's biological activity, enabling structure optimization to improve therapeutic effectiveness. Furthermore, structural identification also ensures the purity of the compounds used in research, allowing biological testing results to more accurately reflect the compound's activity. With comprehensive structural data, the process of developing natural-based drugs can be conducted in a more focused and scientific manner.

Advances in computational technology have significantly contributed to the development of bioactive compounds from herbal plants. Molecular docking methods enable researchers to quickly and efficiently predict interactions between active compounds and protein targets. This approach can reduce research costs and time, as only compounds with high affinity for biological targets are prioritized for further testing. In addition to molecular docking, advances in bioinformatics and molecular modeling also provide opportunities to evaluate the pharmacokinetic properties, toxicity, and stability of compounds before laboratory testing. The use of computational technology can accelerate the drug discovery process, allowing researchers to screen thousands of candidate compounds in a relatively short time. Therefore, molecular docking and other computational approaches are crucial for more effective and efficient natural-based drug discovery.

Advances in computational technology have made significant contributions to the discovery and development of natural-based drugs. Computational approaches enable the identification, selection, and evaluation of bioactive compounds to be carried out more quickly, efficiently, and economically than conventional experimental methods. In recent years, various computational methods such as molecular docking, molecular dynamics simulation, and pharmacokinetic and toxicity prediction (ADMET) have been increasingly used to aid the screening of drug candidates from natural sources. These approaches can provide an initial overview of a compound's ability to interact with a specific biological target, thus providing a basis for developing more effective and safe drugs (Amin *et al*., 2025).

Molecular docking is one of the most widely applied computational methods in medicinal chemistry research because it can predict the orientation and strength of interactions between ligands and target proteins. Through this method, researchers can identify the amino acid residues involved in the binding process and estimate the stability of the resulting complex. The lower the binding energy obtained, the higher the affinity of a compound for the target protein being analyzed. Therefore, molecular docking is a crucial method in the initial screening of natural product-based drug candidates before further in vitro and in vivo testing (Amin *et al*., 2025).

In addition to molecular docking, ADMET analysis also plays a crucial role in the development of herbal drug candidates. Not all compounds with high biological activity can be developed into drugs because they must meet various pharmacokinetic and safety requirements. ADMET predictions are used to evaluate the absorption, distribution, metabolism, excretion, and toxicity of a compound, thus assisting researchers in selecting drug candidates with a higher chance of success in subsequent development stages. The integration of molecular docking and ADMET analysis can improve the efficiency of the research process by enabling more rational and targeted compound selection (Amin *et al*., 2025).

In medicinal chemistry, compound structure optimization is a crucial step in enhancing the biological activity of a molecule. Various studies have shown that structural modification through the addition or substitution of specific functional groups can increase a compound's affinity for biological targets. The

addition of halogen, methoxy, triazole, or certain aromatic substituents is known to enhance hydrophobic interactions and hydrogen bonds between ligands and target proteins, resulting in enhanced biological activity. This structural modification strategy has been widely applied to various classes of natural compounds, particularly flavonoids, due to their relatively easy structural framework without compromising their primary biological activity (Zhu & Zhong, 2022).

The relationship between chemical structure and biological activity, or Structure-Activity Relationship (SAR), is the primary basis for optimizing drug candidates. Through SAR analysis, researchers can understand which functional groups play a significant role in pharmacological activity, allowing for more targeted modifications. This information is crucial because it allows for the development of derivative compounds with higher activity than their parent compounds. Therefore, the drug development process relies not only on the search for new natural compounds but also on the ability to modify the structures of compounds already known to possess promising biological activity (Amin *et al*., 2025).

Literature reviews also show that the combination of several bioactive compounds in herbal plants can produce synergistic effects that enhance pharmacological activity. The interaction between compounds such as flavonoids, alkaloids, phenolics, and saponins can produce stronger biological effects than the use of a single compound. This phenomenon is one of the advantages of herbal plants because they can produce various mechanisms of action that support each other in treating a disease. This synergistic effect can increase the effectiveness of therapy through various biological pathways simultaneously, for example, the combination of antioxidant, anti-inflammatory, and antibacterial activities in a single plant extract. In addition to increasing effectiveness, the combination of bioactive compounds also has the potential to reduce the dosage of each compound, thereby reducing the risk of side effects. Therefore, research on the interactions between active compounds needs to be continued to gain a deeper understanding of the effectiveness of herbal plants and their potential to produce more optimal drug formulations.

In general, the results of the study indicate that herbal plants have excellent prospects as sources of bioactive compounds in the field of medicinal chemistry. Their various biological activities, such as antioxidant, antibacterial, antidiabetic, anti-inflammatory, and anticancer properties, indicate great potential for development into new drug candidates. Supported by modern technology through compound isolation, structural characterization, structure-activity relationship (SAR) analysis, and molecular docking further strengthens the opportunities for utilizing herbal plants in the development of more effective, selective, and safe drugs for the public. Furthermore, the growing interest in the use of natural ingredients as alternative treatments has also driven the development of research on herbal plants in various countries. The availability of abundant biological resources, especially in tropical countries like Indonesia, presents a significant opportunity for the development of a natural-based pharmaceutical industry. With the support of continuous research and the use of modern technology, herbal plants have the potential to become a primary source for the discovery of innovative medicines to treat various diseases in the future.

Table 1. Bioactive Compounds and Biological Activities of Terbal Plants

No	Bioactive Compounds	Biological Activity	Working Mechanism	Reference
1.	Flavonoid	Antioxidants	Capture free radicals	Sari *et al*., 2021
2.	Phenolic	Antioxidants	Electron donor	Dewi *et al*., 2022
3.	Alkaloid	Antibacterial	Damages bacterial cell membranes	Abbas *et al*., 2024
4.	Tannin	Antibacterial	Inhibits bacterial metabolism	Wijaya *et al*., 2022
5.	Flavonoid Derivatives	Antidiabetic	Interaction with target protein	Amin *et al*., 2023

6.	Modified natural compounds	Anticancer	Increase target cell selectivity	Amin *et al*., 2022
7.	Saponin	Anti-inflammatory	Inhibits inflammatory mediators	Lestari *et al*., 2023

Research results indicate that herbal plants have great potential as sources of bioactive compounds that can be developed into new drug candidates. Flavonoids are among the most abundant compounds and possess various important biological activities, particularly as antioxidants. The antioxidant activity of flavonoids is related to their ability to donate electrons or hydrogen atoms to stabilize free radicals, thereby preventing cell damage caused by oxidative stress (Sari *et al*., 2021). Oxidative stress is known to be a major factor in degenerative diseases such as diabetes mellitus, cancer, and cardiovascular disease.

In addition to flavonoids, phenolic compounds also have high antioxidant activity. Research by Dewi *et al*. (2022) showed that the higher the phenolic content in a plant extract, the stronger its antioxidant activity. This suggests a relationship between active compound content and the biological properties of an herbal plant. Therefore, the isolation and characterization of active compounds are crucial steps in natural-based medicinal chemistry research.

Phenolic compounds act as antioxidants by donating hydrogen atoms or electrons to neutralize free radicals, thereby inhibiting cell-damaging oxidation reactions. This activity plays a crucial role in protecting the body from various diseases associated with oxidative stress, such as cardiovascular disease, diabetes, cancer, and premature aging. Furthermore, several classes of phenolic compounds have also been reported to possess other pharmacological activities, such as anti-inflammatory, antimicrobial, antidiabetic, and hepatoprotective properties. The presence of phenolic compounds in plants is influenced by various factors, including plant species, growing conditions, maturity level, and extraction method. Therefore, analysis of total phenolic content is often used as a parameter to evaluate the quality and potential bioactivity of a plant extract. By understanding the phenolic content and its biological activity, the development of herbal plants as raw materials for medicines and health products can be carried out more effectively and scientifically. Furthermore, in-depth identification and characterization of phenolic compounds can provide important information regarding the mechanisms of action of these compounds in producing therapeutic effects, thus supporting the development of safe, effective, and economically valuable natural-based medicines.

The antibacterial activity of herbal plants suggests that secondary metabolites can be used as alternative natural antimicrobial agents. Alkaloids and tannins work by damaging bacterial cell membranes, inhibiting protein synthesis, and disrupting microbial metabolism, thereby suppressing bacterial growth (Abass *et al*., 2024). The use of herbal plants as antibacterials is becoming increasingly important due to the increasing incidence of antibiotic resistance in pathogenic bacteria.

Medicinal chemistry approaches through structural modification of compounds have a significant impact on increasing biological activity. Research by Saeful Amin *et al*. (2023) demonstrated that modifying the structure of flavonoids can increase the compound's affinity for antidiabetic protein targets. A molecular docking approach was used to predict interactions between ligands and receptors, thus facilitating more effective and efficient drug design. The results of this study indicate that changes in molecular structure can enhance the effectiveness of a compound's pharmacological activity.

Furthermore, research by Saeful Amin *et al*. (2022) demonstrated that modifying natural compounds can enhance cytotoxic activity against cancer cells by increasing selectivity toward target cells. This demonstrates that the relationship between structure and biological activity, or Structure–Activity Relationship (SAR), is a crucial aspect in the development of natural-based drugs. According to Thomford *et al*. (2024), small changes in molecular structure, such as the addition of hydroxyl groups or substitution of certain functional groups, can significantly impact a compound's pharmacological activity.

The development of herbal-based drugs has several advantages, such as the abundant availability of natural ingredients, relatively low production costs, and a tendency to have fewer side effects compared

to synthetic drugs (El-Saadony *et al*., 2025). However, the development of herbal compounds still requires further research regarding toxicity, bioavailability, and effectiveness both in vivo and clinically for safe and effective use in therapy. Overall, the study results indicate that the combination of herbal plant utilization and modern medicinal chemistry approaches offers significant opportunities for the development of new drug candidates. Approaches such as active compound isolation, structural characterization, molecular modification, and molecular docking are important strategies for increasing the effectiveness and selectivity of bioactive compounds from herbal plants.

The success of herbal-based drug development depends heavily on the quality of the extraction and purification processes for active compounds. Different extraction methods can produce varying compositions of bioactive compounds, thus affecting the resulting biological activity. The use of appropriate solvents and optimal extraction conditions are crucial for obtaining the maximum amount of active compounds. Therefore, standardization of extraction methods is necessary to consistently maintain the quality and effectiveness of herbal-based products.

In addition to the extraction process, characterizing the structure of active compounds is also a crucial step in medicinal chemistry research. Various analytical techniques such as UV-Vis spectroscopy, Fourier Transform Infrared (FTIR), Nuclear Magnetic Resonance (NMR), and Mass Spectrometry (MS) are widely used to identify the chemical structure of isolated compounds. Information on molecular structure is essential for understanding the relationship between a compound's structure and biological activity, thus providing a basis for molecular modification and the design of new drugs.

Characterization of active compounds aims to ensure the identity, purity, and physicochemical properties of the obtained compounds (Amin *et al*., 2025). Through UV-Vis spectroscopy analysis, researchers can determine the presence of chromophore groups that play a role in absorbing light at certain wavelengths. Meanwhile, FTIR is used to identify functional groups present in a molecule based on the resulting infrared absorption pattern. NMR techniques provide more detailed information regarding the arrangement of carbon and hydrogen atoms in molecules, thus allowing for more accurate determination of compound structures. On the other hand, Mass Spectrometry (MS) is used to determine molecular mass and fragmentation patterns that can aid in identifying the structure of complex compounds.

The development of increasingly sophisticated analytical instrument technology has increased the accuracy and speed of characterizing active compounds. The use of combined techniques such as LC-MS (Liquid Chromatography-Mass Spectrometry) and GC-MS (Gas Chromatography-Mass Spectrometry) allows for the separation and identification of various components in complex mixtures. These techniques are very useful in natural product research because plant extracts generally contain many secondary metabolites with different structures and biological activities. Furthermore, the use of High Performance Liquid Chromatography (HPLC) is also widely applied to determine the levels of active compounds and evaluate the purity of isolated results.

Structural information obtained from various characterization methods can be used to elucidate the mechanism of action of a compound at the molecular level. The relationship between chemical structure and biological activity, or Structure-Activity Relationship (SAR), is a crucial aspect of modern drug development. Through the SAR approach, researchers can identify the parts of a molecule responsible for producing a specific pharmacological activity and then modify the structure to improve the effectiveness, selectivity, stability, and safety of the compound. This approach enables the development of more potent drug candidates than the original natural compounds.

In addition to supporting the drug discovery process, active compound characterization also plays a role in the standardization of herbal medicinal raw materials. Standardization is necessary to ensure consistent quality, safety, and effectiveness of the resulting products (Abass *et al*., 2024). By knowing the complete chemical profile, manufacturers can ensure that each product contains the appropriate amount of active compounds and is free from contaminants that could potentially harm health. Therefore, active compound characterization is not only a crucial part of basic research but also plays a strategic role in the development of a sustainable pharmaceutical, phytopharmaceutical, and natural product-based health industry. Furthermore, the integration of modern characterization techniques, molecular biology

approaches, and computational methods such as molecular docking and computer-based drug design further accelerates the process of identifying bioactive compounds with the potential to be developed into new drugs for various diseases. Therefore, active compound structural characterization is a key foundation in medicinal chemistry research, which aims to produce effective, safe, and high-quality therapeutic products.

Advances in computing technology have significantly contributed to the development of bioactive compounds from herbal plants. Molecular docking methods enable researchers to quickly and efficiently predict interactions between active compounds and protein targets. This approach can reduce research costs and time, as only compounds with high affinity for biological targets are prioritized for further testing. Therefore, molecular docking is a crucial method in the natural product-based drug discovery process.

Literature reviews also show that the combination of several bioactive compounds in herbal plants can produce synergistic effects that enhance pharmacological activity. The interaction between compounds such as flavonoids, alkaloids, phenolics, and saponins can produce stronger biological effects than the use of a single compound. This phenomenon is one of the advantages of herbal plants, as they can produce various mutually supportive mechanisms of action in treating a disease. Therefore, research into the interactions between active compounds needs to be further developed to gain a deeper understanding of the effectiveness of herbal plants.

In general, the study results indicate that herbal plants have excellent prospects as sources of bioactive compounds in medicinal chemistry. Their diverse biological activities, such as antioxidant, antibacterial, antidiabetic, anti-inflammatory, and anticancer properties, demonstrate significant potential for development as new drug candidates. Modern technological support through compound isolation, structural characterization, structure-activity relationship (SAR) analysis, and molecular docking further strengthens the potential for utilizing herbal plants in the development of more effective, selective, and safe drugs for the public.

Although various studies have shown that herbal plants are potential sources of secondary metabolites as drug candidates, their development into modern pharmaceutical products still faces various challenges. One major obstacle is the low bioavailability of some natural compounds due to their low solubility, poor chemical stability, and limited ability to penetrate biological membranes. This condition results in suboptimal concentrations of active compounds reaching therapeutic targets, which can reduce their pharmacological effectiveness when used in complex biological systems (Amin & Pratama, 2025).

Besides bioavailability, compound stability is also a crucial factor in the successful development of herbal drug candidates. Many bioactive compounds undergo degradation during storage, distribution, and metabolism in the body. Consequently, biological activity demonstrated in laboratory tests cannot always be reproduced in in vivo or clinical trials. Therefore, structural optimization strategies and the development of drug delivery systems capable of protecting active compounds from degradation are necessary to maintain their therapeutic effectiveness (Amin & Pratama, 2025).

Another common challenge is the variation in secondary metabolite content in herbal plants. Active compound content can be influenced by various factors such as environmental conditions, growing location, soil type, climate, harvest age, and raw material processing methods. These variations can lead to differences in biological activity, making the standardization process a crucial aspect in the development of herbal-based medicines. Standardization is necessary to ensure the quality, safety, and effectiveness of the resulting products, ensuring they meet applicable scientific and regulatory standards (Amin & Pratama, 2025).

The development of modern formulation technology offers significant opportunities to overcome these limitations. One widely developed approach is the use of nanoparticle-based drug delivery systems. Nanoparticle technology can improve the solubility, stability, bioavailability, and penetration of active compounds into target tissues. Furthermore, nanoparticle-based delivery systems can also reduce side effects by allowing more selective distribution of compounds to target tissues. Therefore, the combination

of bioactive herbal compounds and modern formulation technology can produce more effective and safe drug candidates (Amin & Pratama, 2025).

Although in vitro and in silico research results show promising potential, validation through in vivo studies and clinical trials remains a crucial step. Many candidate compounds exhibit high biological activity in early research, but experience reduced effectiveness when tested in living organisms due to more complex metabolic factors, distribution, and biological interactions. Therefore, further research involving various disciplines such as pharmacology, medicinal chemistry, molecular biology, and pharmaceutical technology is needed to ensure the safety and effectiveness of these compounds before their widespread use in the health sector (Amin & Pratama, 2025).

Going forward, the integration of natural resource exploration, computational approaches, chemical structure optimization, and modern drug delivery technologies is expected to accelerate the process of discovering new drugs from natural sources. Indonesia's vast biodiversity provides ample opportunities to discover various new bioactive compounds with the potential to be developed as drug candidates. With the support of ongoing research, multidisciplinary collaboration, and the application of modern technology, bioactive compounds from herbal plants have the potential to become an important source in the development of more effective, safe, and affordable future drugs (Amin & Pratama, 2025).

CONCLUSION

Based on the results of the literature review, it can be concluded that herbal plants have great potential as sources of bioactive compounds in the field of medicinal chemistry. Secondary metabolites such as flavonoids, alkaloids, phenolics, tannins, and saponins have been shown to possess various biological activities, including antioxidants, antibacterials, antidiabetic, anti-inflammatory, and anticancer properties. These biological activities are influenced by the compound's chemical structure and its ability to interact with specific biological targets.

Medicinal chemistry approaches through isolation, characterization, structural modification, and molecular docking play a crucial role in increasing the effectiveness and selectivity of a compound's biological activity. The reviewed research results indicate that structural modification of flavonoids and other natural compounds can enhance their antidiabetic and anticancer potency. Therefore, herbal plants are a promising source of natural ingredients for development as new, more effective and safe drug candidates to support the development of modern therapies.

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