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Utilization of Artificial Intelligence in the Discovery of Indonesian Herbal Medicines: Opportunities and Challenges

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Abstract

This study examines the potential use of artificial intelligence (AI) in the development of Indonesian herbal medicine. Indonesia, as a megabiodiversity country with more than 6,000 species of medicinal plants, has great potential in the development of herbal medicine, but is constrained by a long research process, high costs, and low success rates. The research method uses a descriptive qualitative approach through literature studies with content analysis techniques. The results of the study indicate that AI integration can accelerate the drug development process, reducing the time from 10-15 years to a few months, and reducing costs from USD 2.8 billion to USD 500 million - 1 billion. The ConvNeXt model achieved 92.8% accuracy in the classification of Indonesian medicinal plants, proving its effectiveness as a tool for documentation and preservation of biodiversity. The AI-based virtual screening technique successfully predicted the pharmacological potential of bioactive compounds without requiring early in vitro/in vivo tests. Challenges in implementing AI include limitations of integrated local databases, gaps in multidisciplinary collaboration, inadequate computing infrastructure, and ethical aspects related to indigenous peoples' rights and Intellectual Property Rights. This study recommends strategies to strengthen the AI research ecosystem through the development of a national database, strengthening multidisciplinary collaboration, increasing infrastructure and human resource capacity, strengthening regulations, and public advocacy and education.

Keywords: Artificial intelligence, herbal medicine, Indonesia, biodiversity, virtual screening

1. Introduction

Indonesia is known as a megabiodiversity country rich in biodiversity, including medicinal plants that have been used for generations in traditional medicine. More than 6,000 plant species have been empirically utilized as a source of natural medicine by nearly 40 million Indonesians. One form of popular traditional medicine is herbal medicine, which has become an integral part of the nation's culture and health heritage (Rustandi et al., 2023).

Despite its great potential, the development of herbal medicine in Indonesia faces various challenges. The long research process, high costs, and low success rates are the main obstacles in transforming herbal medicine into standardized herbal medicine or phytopharmaceuticals. It takes 10–15 years and costs around US$ 2.8 billion to develop one type of new drug, with a failure rate of 80–90% when entering the clinical trial stage (Rustandi et al., 2023).

In the era of the Industrial Revolution 4.0, artificial intelligence (AI) has emerged as an innovative solution to overcome these obstacles. AI has the ability to analyze large-scale data, identify patterns, and predict outcomes with high accuracy, thus accelerating the process of herbal medicine discovery and development (Tripathi et al., 2021). By utilizing AI, processes that previously took years can be shortened to months, saving costs and increasing the chances of success.

One application of AI in herbal medicine development is through virtual screening techniques, which allow researchers to simulate the interaction between bioactive compounds and biological targets in silico (Lin et al., 2022). This method can identify potential compounds with certain pharmacological activities, such as anti-inflammatory or anticancer, without the need for expensive and time-consuming initial laboratory tests (Erlina et al., 2022).

In addition, AI can also be used in the identification and classification of medicinal plants through computer vision technology. By utilizing machine learning algorithms, such as Convolutional Neural Networks (CNN), AI can recognize plant species based on digital images with high accuracy. Recent studies have shown that the ConvNeXt

model is capable of achieving up to 92.8% accuracy in classifying Indonesian medicinal plants (Musyaffa et al., 2024).

However, the implementation of AI in herbal medicine discovery in Indonesia is not without challenges. One of them is the limited availability of integrated and high-quality local databases. AI requires big data for model training, so building a national herbal database that includes morphological descriptions, phytochemical content, and empirical data on traditional use is an urgent priority (Jacob et al., 2024).

Another challenge is the lack of multidisciplinary collaboration between botanists, pharmacologists, bioinformaticians, and AI experts. The development of AI-based herbal medicines requires cross-field synergy to ensure the scientific validity and practical relevance of research results (Leng et al., 2024). Therefore, efforts are needed to build an inclusive and collaborative research ecosystem.

Ethical issues and protection of intellectual property rights (IPR) are also important concerns. The use of AI to explore the traditional knowledge of indigenous peoples must be done by respecting their rights and ensuring fair compensation (Hossain & Ballardini, 2021). This is important to prevent exploitation and maintain the sustainability of biological resources and local knowledge.

Limited technological infrastructure, such as access to high-performance computing, is also a barrier to the large-scale data processing required by AI (Gathu, 2024). Investment in infrastructure and human resource training in the fields of AI, bioinformatics, and molecular pharmacy is key to overcoming these challenges (Subha et al., 2024).

By overcoming these challenges, the use of artificial intelligence in the discovery of Indonesian herbal medicines has great potential to accelerate innovation, improve research accuracy, and streamline development costs. This will strengthen national health sovereignty based on its own natural resources and make Indonesia a center for modern AI-based herbal medicine research in Southeast Asia.

2. Literature Review

Indonesia is known as a megabiodiversity country that is rich in biodiversity, including medicinal plants that have been used for generations in traditional medicine. More than 6,000 plant species have been empirically utilized as a source of natural medicine by almost 40 million Indonesians (Rustandi et al., 2023). These plants, such as Clinacanthus nutans (ki tajam), have been used in traditional medicine for various diseases, including diabetes and skin infections. This biodiversity provides great opportunities for the development of herbal medicines based on local and traditional knowledge.

Despite its great potential, the development of herbal medicines in Indonesia faces various challenges. The long research process, high costs, and low success rates are the main obstacles in transforming herbal medicine into standardized herbal medicines or phytopharmaceuticals. It takes 10–15 years and costs around US$ 2.8 billion to develop one type of new drug, with a failure rate of 80–90% when entering the clinical trial stage (Rustandi et al., 2023). In addition, the lack of standardized scientific data and limited research infrastructure are also obstacles in developing effective and safe herbal medicines.

Artificial Intelligence (AI) has emerged as an innovative solution to overcome these obstacles. AI has the ability to analyze large-scale data, identify patterns, and predict outcomes with high accuracy, thereby accelerating the process of herbal medicine discovery and development. By leveraging AI, processes that previously took years can be shortened to months, saving costs and increasing the chances of success (Tripathi et al., 2021).

AI can be used in the identification and classification of medicinal plants through computer vision technology. By utilizing machine learning algorithms, such as Convolutional Neural Networks (CNN), AI can recognize plant species based on digital images with high accuracy. A recent study showed that the ConvNeXt model was able to achieve an accuracy of up to 92.8% in classifying Indonesian medicinal plants. In addition, AI can also be used in the analysis of bioactive compound content from plant extracts. Through deep learning techniques, AI can predict molecular structures and their pharmacological potential, helping researchers prioritize compounds with the most promising biological activities (Musyaffa et al., 2024).

The implementation of AI in herbal medicine discovery in Indonesia is not without its challenges. One of them is the limited integrated and high-quality local database. AI requires big data for model training, so the development of a national herbal database that includes morphological descriptions, phytochemical content, and empirical data on traditional use is an urgent priority (Jacob et al., 2024). Another challenge is the lack of multidisciplinary collaboration between botanists, pharmacologists, bioinformaticians, and AI experts. The development of AI-based herbal medicine requires cross-field synergy to ensure the scientific validity and practical relevance of research results (Magare & Patil, 2025). Ethical issues and protection of intellectual property rights (IPR) are also important concerns. The use of AI to explore the traditional knowledge of indigenous peoples must be carried out by respecting their rights and ensuring fair compensation. Limited technological infrastructure, such as access to high-performance computing, is also an obstacle to the large-scale data processing required by AI. Investment in infrastructure and human resource training in AI, bioinformatics, and molecular pharmacy is key to addressing these challenges.

3. Methods

The research flow in this study is designed systematically to achieve the research objectives, starting from determining the type of research, data collection, data analysis, to drawing conclusions. Each stage is structured to

support the validity and relevance of the research results to the issue of developing artificial intelligence-based herbal medicine in Indonesia. The stages in this study can be seen in Figure 1.

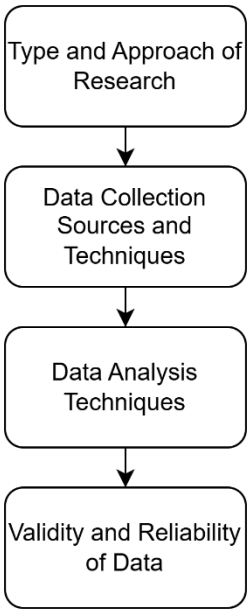

Figure 1: Research Flow

This study uses a descriptive qualitative research type with a literature study approach (library research). This approach was chosen because it is in accordance with the research objectives which focus on in-depth exploration of the use of artificial intelligence (AI) in the process of discovering herbal medicine in Indonesia. Descriptive qualitative research allows researchers to systematically describe the phenomena, patterns, and challenges that arise in the integration of AI with the development of traditional herbal medicine. The literature study approach is used to collect secondary data from various scientific sources, allowing for a comprehensive analysis without collecting primary data directly in the field. This research is directed at exploring the thoughts and findings of experts, comparing the results of previous studies, and analyzing current trends in the application of AI to support innovation in herbal medicine based on Indonesian biodiversity.

The data sources in this study are secondary, obtained through systematic searches of various scientific publications, policy documents, research reports, and other credible sources relevant to the research topic. Primary sources include reputable international journals such as Frontiers in Artificial Intelligence, BMC Complementary Medicine and Therapies, and Scientific Reports, which discuss the application of artificial intelligence technology in the health sector, especially the discovery of herbal medicines. In addition, data is also obtained from official reports and documents published by government agencies, such as the Ministry of Health of the Republic of Indonesia, and international organizations such as WHO regarding the development of herbal medicine and health innovation policies. Searches are also carried out through online databases such as PubMed, ScienceDirect, Google Scholar, and ResearchGate using relevant keywords, including "Artificial Intelligence", "herbal medicine discovery", "Indonesia", "machine learning", and "virtual screening". Every data obtained will be strictly selected by considering aspects of relevance, credibility, and up-to-dateness to support the validity of the research results.

The collected data were analyzed using the content analysis method which was carried out in a hierarchical and systematic manner. This analysis begins with data reduction, which is the process of filtering relevant information according to the focus of the research, such as data on the application of AI in identifying medicinal plants, virtual screening, classification of bioactive compounds, to the challenges faced in implementing this technology in Indonesia. After the data is summarized, the next step is to present the data in the form of a structured descriptive narrative, equipped with tables, diagrams, or other visualizations that support data interpretation. This presentation aims to make it easier for readers to understand the relationship between variables and the information found. The final stage is drawing conclusions, which is an in-depth interpretation of the data that has been presented to answer the problem formulation and achieve the research objectives. The conclusions produced not only describe the phenomenon, but also provide strategic recommendations that can be implemented in the development of AI-based herbal medicine in Indonesia.

This research flow also pays attention to the aspects of data validity and reliability through the application of several verification strategies. One of the main strategies is source triangulation, which is comparing data from various sources to ensure consistency of information. For example, the results of a study related to the effectiveness of the CNN model in classifying medicinal plants are compared with national policies regarding biodiversity data management. Researchers also conduct peer debriefing with experts or colleagues in the fields of AI, bioinformatics,

and pharmacy, to obtain input, clarification, and avoid subjective bias. The entire research process is documented through an audit trail, so that each step can be traced and re-verified by other parties. This approach is expected to increase the credibility, objectivity, and accountability of research results.

This research flow is also carried out by paying attention to the principles of research ethics, especially regarding the use of secondary data and traditional knowledge. Researchers uphold intellectual property rights by including appropriate citations for each use of literature. In addition, researchers ensure that all data used is not manipulative, discriminatory, or violates the rights of indigenous peoples. The research recommendations are designed to support the protection of local communities' rights to their biological resources and traditional knowledge. By applying the principles of justice and sustainability, this research is expected to contribute ethically, scientifically, and practically to the development of AI-based herbal medicine in Indonesia.

4. Results and Discussion

4.1. Potential of AI in Accelerating Herbal Medicine Discovery

The results of the study show that the application of Artificial Intelligence (AI) can significantly accelerate the process of herbal medicine discovery. Previously, the development of a new drug required a lengthy process spanning 10–15 years, with estimated costs reaching up to USD 2.8 billion and a relatively low success rate of around 10–20% (Rustandi et al., 2023). These challenges are attributed to the complexity of identifying active compounds, conducting various testing phases, and complying with regulatory requirements.

However, by integrating AI into the drug discovery pipeline, these processes can be significantly streamlined. AI enables faster identification of potential bioactive compounds through computational screening, predictive modeling, and machine learning algorithms capable of analyzing vast chemical and biological data. As a result, the overall timeline of drug development can be reduced to just several months, while operational costs are also significantly lowered, and the probability of success increases due to more targeted and data-driven approaches.

Table 1: Comparison of Drug Development Time and Costs

Development Stage	Without AI	With AI
Compound Discovery	5–7 years	1–2 years
Preclinical Trials	2–3 years	6–12 months
Clinical Trials	3–5 years	1–2 years
Cost	USD 2.8 billion	USD 500 million – 1 billion

Table 1 illustrates a clear comparison between conventional drug development processes and those assisted by AI. It shows that the compound discovery stage, which typically takes 5–7 years using traditional methods, can be reduced to just 1–2 years with AI assistance. Similarly, preclinical trials that usually last 2–3 years can be shortened to 6–12 months, while clinical trials can be reduced from 3–5 years to only 1–2 years. Moreover, the application of AI not only reduces the duration of each stage but also significantly cuts costs, from an average of USD 2.8 billion down to approximately USD 500 million to 1 billion.

These findings demonstrate that AI does not merely act as a complementary tool but represents a transformative innovation capable of optimizing time, resources, and success rates in herbal medicine discovery. The integration of AI technologies such as deep learning, natural language processing, and molecular docking simulations provides pharmaceutical researchers with a more efficient pathway to identify, validate, and develop novel herbal compounds for therapeutic use.

In addition to accelerating timelines and reducing costs, AI also enables researchers to explore broader chemical spaces, predict molecular interactions more accurately, and identify potential side effects earlier in the development process. This highlights the strategic role of AI in addressing the long-standing challenges of drug discovery, particularly in the field of herbal medicine, where natural product complexity and biodiversity richness often pose significant barriers to conventional research methods.

4.2. Application of ai in identification and classification of medicinal plants

The application of AI, especially the Convolutional Neural Networks (CNN) algorithm, has been successfully used to identify and classify Indonesian medicinal plants. A study by Musyaffa et al. (2023) showed that the ConvNeXt model achieved the highest accuracy of 92.8% in classifying Indonesian medicinal plants. This shows that AI can be an effective tool in documenting and preserving Indonesia's biodiversity.

Table 2: Comparison of CNN Model Accuracy in Classifying Medicinal Plants

CNN Models	Accuracy (%)
ResNet	85%

DenseNet	89%
VGG	84%
ConvNeXt	92.8%
Swin Transformer	65%

4.3. The Role of AI in virtual screening of bioactive compounds

AI also plays a role in the virtual screening stage, which is the process of simulating in silico molecular interactions between bioactive plant compounds and biological targets of disease. This method is able to predict the pharmacological potential of compounds without the need for early in vitro/in vivo testing (Lin et al., 2022). AI analyzes chemical structures, structure-activity relationships (SAR), and automatically models molecular docking.

The results of the study found that the use of AI in virtual screening was able to expand the exploration of bioactive compounds from thousands of candidates to dozens of priority compounds in a short time. This has positive implications for accelerating the development of phytopharmaceuticals based on local biodiversity. Several studies have also reported the success of AI in predicting the anticancer, anti-inflammatory, and antimicrobial activities of Indonesian plant extracts (Erlina et al., 2022).

4.4. Challenges of implementing AI in herbal drug discovery in Indonesia

Despite its great potential, the results of the study show significant challenges in implementing AI in Indonesia. One of the main challenges is the limited availability of integrated and high-quality local databases (Jacob et al., 2024). AI requires big data for model training, while data related to phytochemistry, morphology, and empirical use of Indonesian medicinal plants are still scattered and unstandardized.

In addition, there is a gap in multidisciplinary collaboration between botanists, pharmacologists, bioinformaticians, and AI experts. The lack of cross-disciplinary synergy causes herbal-based AI research to tend to be fragmented and unsustainable. Another obstacle is the lack of sophisticated computing infrastructure in national research centers, which hinders large-scale data processing (Gathu, 2024).

Ethical aspects are also an important concern, especially regarding the protection of indigenous peoples' rights and intellectual property rights (IPR). The use of AI to explore traditional knowledge must be carried out by respecting the principles of prior informed consent (PIC) and access and benefit-sharing (ABS) to ensure sustainability and fairness.

4.5. Strengthening strategy for the AI research ecosystem for herbal medicine development

Based on the results of the analysis, this study recommends several strategies to overcome existing challenges. First, the development of a national database of Indonesian medicinal plants that includes morphological, phytochemical, genomic, and traditional use data in an integrated manner. This database can be a valid and representative source of AI model training. Second, strengthening multidisciplinary collaboration through the establishment of integrated research centers involving various disciplines. The involvement of indigenous communities also needs to be integrated from the start to ensure the sustainability and bias of research. Third, increasing the capacity of infrastructure and human resources (HR) in the fields of bioinformatics, AI, and pharmacy through training, international partnerships, and technology investment. Fourth, the need to strengthen regulations related to data protection and intellectual property rights that are adaptive to the development of AI. This policy must support innovation while protecting the collective rights of local communities as owners of traditional knowledge. Fifth, the importance of advocacy and public education regarding the benefits, risks, and ethics of using AI in the development of herbal medicines, in order to create a shared understanding and public acceptance of this technology.

5. Conclussion

Based on the results of the studies that have been conducted, it can be concluded that the use of artificial intelligence (AI) in the discovery of Indonesian herbal medicines has a very significant potential to accelerate the research and development process. The integration of AI technology can substantially reduce the time and cost of drug development, from 10-15 years to just a few months, and reduce costs from USD 2.8 billion to USD 500 million - 1 billion. The use of the Convolutional Neural Networks (CNN) algorithm, especially the ConvNeXt model, has been proven to achieve an accuracy of up to 92.8% in the classification of Indonesian medicinal plants, demonstrating its effectiveness as an instrument for the documentation and preservation of Indonesian biodiversity.

AI-based virtual screening techniques also play an important role in in silico simulations of molecular interactions between bioactive plant compounds and biological targets of disease. This approach allows prediction of pharmacological potential without the need for in vitro/in vivo tests at an early stage, thus expanding the exploration of bioactive compounds from thousands of candidates to dozens of priority compounds in a short time. Several studies have also reported the success of AI in predicting anticancer, anti-inflammatory, and antimicrobial activities of Indonesian plant extracts.

However, the implementation of AI in herbal medicine discovery in Indonesia still faces various challenges. The limited availability of integrated and high-quality local databases is a major obstacle, considering that AI requires big data for model training. In addition, the gap in multidisciplinary collaboration between botanists, pharmacologists, bioinformatics, and AI experts, as well as inadequate computing infrastructure in national research centers, also hamper large-scale data processing. Ethical aspects, especially related to the protection of indigenous peoples' rights and intellectual property rights (IPR), are also important concerns in the use of AI for traditional knowledge exploration. To overcome these challenges, several strategies are needed to strengthen the AI research ecosystem for herbal medicine development. These strategies include: (1) development of a national database of Indonesian medicinal plants that includes integrated morphological, phytochemical, genomic, and traditional use data; (2) strengthening multidisciplinary collaboration through the establishment of integrated research centers involving various disciplines and indigenous peoples; (3) increasing the capacity of infrastructure and human resources (HR) in the fields of bioinformatics, AI, and pharmacy; (4) strengthening regulations related to data protection and intellectual property rights that are adaptive to the development of AI. and (5) advocacy and public education on the benefits, risks, and ethics of using AI in herbal medicine development.

With the implementation of this strategy, the use of AI in the discovery of Indonesian herbal medicine has the potential to strengthen national health sovereignty based on its own natural resources and make Indonesia a center for modern AI-based herbal medicine research in Southeast Asia. Further research is needed to develop AI models that are more specific to the characteristics of Indonesian medicinal plants and integrate traditional knowledge with modern technology ethically and sustainably.

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