Jurnal Jamu Indonesia (2024) 9(2): 52–54

ISSN 2407-7178
eISSN 2407-7763

Editorial

DOI: https://doi.org/10.29244/jji.v9i2.333

Modernization of Herbal Medicine (Jamu): Integrating Indonesian Herbal Compounds in Drug Design Through Structural-Based Techniques

Modernisasi Obat Herbal (Jamu): Mengintegrasikan Senyawa Herbal Indonesia dalam Desain Obat Melalui Teknik Berbasis Struktural

Inda Setyawati*

Department of Biochemistry, Faculty of Mathematics and Natural Sciences, IPB University, Bogor, Indonesia

**Corresponding author: inda_setyawati@apps.ipb.ac.id; (+62) 82259348663*

Received April 27, 2024; **Accepted** April 28, 2024; **Available online** May 03, 2024

Indonesia has the second-highest biodiversity in the world, as reflected in its extensive variety of indigenous medicinal plants. Of these, approximately 9,600 species have been used for health improvement and disease treatment (Haniarti et al., 2019). A significant portion of the Indonesian population, particularly in rural areas, relies on these medicinal plants to prepare traditional herbal remedies known as jamu. Herbal medicine has long been a vital part of Indonesia's cultural heritage and natural resources, with over 50% of Indonesians reported to have consumed herbal medicine according to the 2010 Basic Health Research (Prabawani, 2017).

Furthermore, traditional healthcare systems are gaining popularity worldwide as people become more interested in herbal medicines, and their widespread acceptance is due to minimal or nonexistent side effects when used to treat various health issues. However, their widespread use is largely because of their easy accessibility, low cost, and cultural acceptance. However, there is a significant lack of pre-clinical and clinical evidence supporting the safety, efficacy, and quality of these traditional treatments. While they are embraced for their perceived benefits, there is a notable gap in proving their effectiveness, especially when dealing with more advanced medical conditions. In other words, scientific evidence for many herbal treatments is limited, often causing skepticism among medical professionals and presenting regulatory challenges.

One of the key challenges in traditional herbal medicine is the lack of scientific corroboration and standardized protocols. Many herbal remedies are based on anecdotal evidence or cultural traditions, resulting in inconsistent results. This inconsistency poses a potential risk to public health and complicates the integration of traditional practices into modern medical frameworks. To address these issues, more rigorous scientific research is needed to validate these treatments, standardize protocols, and ensure their safe application in contemporary healthcare.

On the other way around, the drug discovery process typically involves four stages: discovery, development, clinical trials, and registration (Batool et al., 2019). In the initial discovery stage, researchers identified a potential therapeutic target and its actively binding ligands. This stage typically begins with gene cloning, followed by expression of the target protein, isolation, purification, and experimental prediction of the three-dimensional (3D) structure of the target protein. Having a 3D model of medical target proteins is essential for identifying binding sites, forming the basis of structure-based drug design (SBDD). This systematic approach to drug discovery highlights the need for similar rigor in validating traditional herbal medicine to integrate it effectively into modern medical practices.

Structure-based drug design (SBDD) is a modern approach that uses computational techniques to identify and develop novel drugs. It relies on the structures of biomolecules, such as proteins, which serve as therapeutic targets, along with

bioinformatics, to design compounds that effectively target specific proteins or pathways in the human or pathogen body, as illustrated in **Figure 1**. Computational analysis using algorithms or machine learning is central to SBDD, allowing researchers to virtually dock large databases of small molecules or compound fragments into the binding site of the target protein (Batool et al., 2019). Once docked, these small molecules were ranked using a scoring system that evaluated their affinity and other key interactions within the binding site.

By leveraging the 3D structure of the therapeutic protein, researchers can conduct a detailed analysis of the electrostatic properties of the binding site, including cavities, clefts, and allosteric pockets. This analysis informs the design of compounds that fit these regions, enhancing the likelihood of successful drug development. In addition, the completion of the human genome project, along with the beginnings of proteomics and structural genomics, as well as advances in information technology, have collectively created greater opportunities for SBDD to become a significant contributor to the discovery of new drug leads (Anderson, 2003).

Structural-based techniques offer distinct advantages over conventional experimental methods for drug discovery. By focusing on molecular interactions, these techniques enable researchers to identify promising compounds with greater efficiency, reducing the need for resource-intensive (Lavecchia & Giovanni, 2013; Moore et al., 2018) and time-consuming wet lab experiments (Song et al., 2009). This approach opens new avenues for drug development, allowing scientists to explore Indonesia's abundant herbal resources more effectively.

Historically, drug candidate searches from Indonesia's indigenous plant sources have relied on traditional experimental approaches, such as high-throughput laboratory experiments. While these methods are useful for exploring the therapeutic potential and maintaining Indonesia's herbal biodiversity, they often require significant resources and have a limited screening scope. To overcome these limitations, this study employed cost-effective computational techniques grounded in rational drug design and reverse pharmacology. Using structure-based methods to identify potential target proteins allows for more efficient ligand screening. This strategy streamlines the process, reducing reliance on resource-intensive experiments while increasing the likelihood of discovering promising drug candidates.

Indonesia has a rich tradition of using indigenous medicinal plant species in herbal remedies known as jamu, with over half of the population consuming them regularly. However, despite their widespread popularity, there is a notable lack of scientific evidence supporting the safety and efficacy of these treatments, posing significant challenges for integrating them into modern healthcare. To address this, researchers are exploring the combination of Indonesia's herbal resources with SBDD to identify and develop new drug candidates more efficiently, offering a promising pathway to integrate traditional medicine into advanced pharmaceutical research. However, to ensure the safety and effectiveness of these newly developed treatments, more rigorous scientific research and standardized protocols are needed.

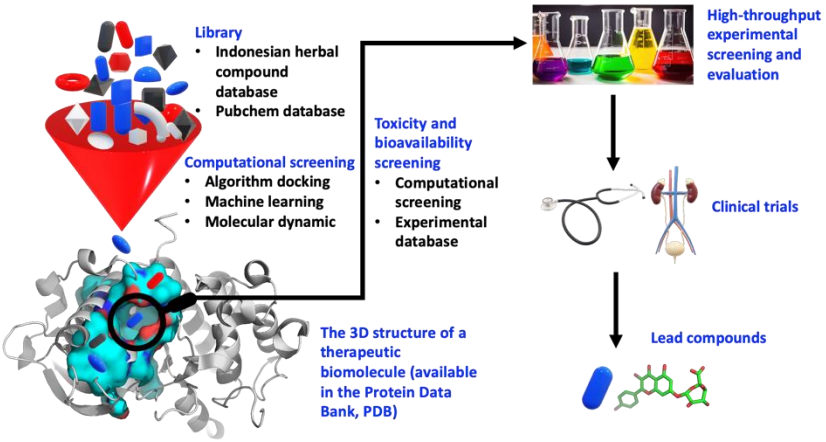

Figure 1. A workflow diagram of the structure-based drug design (SBDD) process

REFERENCES

Anderson, A. C. (2003). The Process of Structure-Based Drug Design. *Chemistry & Biology*, *10*(9), 787–797. https://doi.org/10.1016/j.chembiol.2003.09.002

Batool, M., Ahmad, B., & Choi, S. (2019). A Structure-Based Drug Discovery Paradigm. *International Journal of Molecular Sciences*, *20*(11). https://doi.org/10.3390/ijms20112783

Haniarti, Munir, Akib, M. A., Ambar, A., Rusman, A. D. P., & Abdullah, A. (2019). Herbal for increasing immunity and weight of poultry. *IOP Conference Series: Earth and Environmental Science*, *247*, 012056. https://doi.org/10.1088/1755-1315/247/1/012056

Lavecchia, A., & Giovanni, C. (2013). Virtual Screening Strategies in Drug Discovery: A Critical Review. *Current Medicinal Chemistry*, *20*(23), 2839–2860. https://doi.org/10.2174/09298673113209990001

Moore, T. J., Zhang, H., Anderson, G., & Alexander, G. C. (2018). Estimated Costs of Pivotal Trials for Novel Therapeutic Agents Approved by the US Food and Drug Administration, 2015-2016. *JAMA Internal Medicine*, *178*(11), 1451. https://doi.org/10.1001/jamainternmed.2018.3931

Prabawani, B. (2017). Jamu brand Indonesia: consumer preferences and segmentation. *Archives of Business Research*, *5*(3). https://doi.org/10.14738/abr.53.2841

Song, C. M., Lim, S. J., & Tong, J. C. (2009). Recent advances in computer-aided drug design. *Briefings in Bioinformatics*, *10*(5), 579–591. https://doi.org/10.1093/bib/bbp023

Citation Format: Setyawati, I. (2024). Modernization of Herbal Medicine (Jamu): Integrating Indonesian Herbal Compounds in Drug Design Through Structural-Based Techniques. *Jurnal Jamu Indonesia, 9*(2), 52–54. https://doi.org/10.29244/jji.v9i2.333