Junior Science Communications
Faculty of Applied Sciences, UiTM Shah Alam
https://journal.uitm.edu.my/ojs/index.php/JSC

E-ISSN 2637-0689
Vol 45 2025

Colloquium on Applied Sciences 2 2024
8-14 July 2024, Faculty of Applied Sciences, UiTM Shah Alam, Malaysia

Molecular docking study of compounds from *Dryobalanops aromatica* as the anti-MRSA agent

Nur Shasha Iwani Mohd Isa[a], Latifah Munirah Bakar[a*], Mohamad Zakkirun Abdullah[b]

Structured Abstract

Background: The emergence of antibiotic-resistant microorganisms poses a significant global health threat, particularly Methicillin-resistant *Staphylococcus aureus* (MRSA), which resists several antibiotics, including oxacillin, amoxicillin, and penicillin. Despite advancements in antimicrobial drugs, resistance continues to rise, necessitating alternative treatments. This study investigates the potential of compounds from *Drayobalanops aromatica* as anti-MRSA agents using molecular docking techniques. *D. aromatica*, known for its valuable timber and non-timber products like camphor, is indigenous to Southeast Asia. It has been historically used for its medicinal properties, making it a promising candidate for new antibacterial compounds.

Methods: A comprehensive literature review identified potential anti-MRSA compounds from *D. aromatica*. Molecular docking studies were conducted using *AutoDock Vina, Discovery Studio Biovia 2021*, and *PyMol* to evaluate the binding affinity of these compounds with the MRSA PBP2a protein. The quinazolinone ligand, known for interacting with PBP2a's allosteric sites, was used as a reference due to its established antibacterial properties.

Results: Results indicated that quinazolinone exhibited the highest binding affinity to PBP2a at -7.1 kcal/mol, supported by strong hydrogen and hydrophobic interactions. Among the *D. aromatica* phytochemicals, *β*-caryophyllene, curcumene, and caryophyllene oxide demonstrated notable binding affinities at -5.2 kcal/mol. However, their interactions were primarily hydrophobic with fewer hydrogen bonds, indicating less specificity and binding strength compared to quinazolinone.

Conclusion: The study concludes that *D. aromatica* phytochemicals show potential as anti-MRSA agents, although less effective than quinazolinone. The findings underscore the need for further in vivo and in vitro research to validate these compounds' efficacy and explore a broader range of phytochemicals. Additionally, future studies should consider automated docking techniques to streamline the evaluation process. By integrating these approaches, researchers can expedite the discovery of new antibacterial agents to combat MRSA effectively.

Keywords: Antibiotic resistance, Methicillin-resistant *Staphylococcus aureus* (MRSA), *Drayobalanops aromatica*, Anti-MRSA agents, Molecular docking studies

*Correspondence: latifahmunirah@uitm.edu.my

[a] School of Biology, Faculty of Applied Sciences, Universiti Teknologi MARA, Shah Alam, Malaysia

[b] Department of Fundamentals in Dental and Medical Science, Kulliyyah of Dentistry, International Islamic University Malaysia