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Molecular dynamics simulation of Kaempferol from Wrightia genus against wild-type and quadruple mutant of PfDHFR

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Structured Abstract

Background: Molecular dynamics simulation is an effective approach for researching how atoms and molecules interact over time. This study aims to evaluate the dynamic behavior, conformational changes, and binding interactions of kaempferol from Wrightia genus with wild-type and quadruple mutant PfDHFR. The results of this study will have consequences for the creation of new antimalarial medicines and help to understand how drugs interact with their targets.

Methods: The study selects compounds for molecular dynamics simulation based on binding energy and interactions with catalytic residues. Protein ligand complex preparation is performed using Maestro's protein preparation module, maximizing hydrogen bond assignment, and minimizing restrained energy. The system builder step module is applied to optimize and minimize the protein complex. MD simulation and MM-GBSA analysis are performed to determine binding free energy.

Results: The observation revealed that there were subtle differences in the binding patterns and stability between the two types of protein. Quadruple mutant protein displayed slightly weaker interactions with kaempferol in certain regions, which could suggest a reduced affinity when compared to the wild type.

Conclusion: Further in vivo research is advised to assess the efficacy and safety of kaempferol as an anti-malarial drug.

Keywords: Wild-type *pf*DHFR, quadruple mutant *pf*DHFR, MD simulation

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