Antimalarial Potential of Phytochemicals from Aristolochia Albida (Duch) on Plasmodium Falciparum HSP 70-1 using Molecular Docking and In Silico Toxicity

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Abstract

Malaria remains a significant global health burden, causing approximately 409,000 deaths in 2019, according to the World Health Organization. *P. falciparum* is the deadliest plasmodium specie that causes cerebral malaria which ultimately leads to death. P. falciparum has coexisted with humans for a long time, leading to negative consequences such as drug resistance. HSPs are essential for the parasite's ability to develop drug resistance. Conventional methods for treating malaria are now developing drug resistance therefore there is need for novel antimalarial agents e.g., phytochemicals. Phytochemicals are medicinal plants that can be used as antimalarial drugs e.g., Aristolochia albida (duch). The use of computational techniques in antimalarial drug discovery has become increasingly important in the quest for effective treatments for example, molecular docking and in silico toxicity testing. A ligand and a protein were prepared using UCSF Chimera. Molecular docking using CB Dock 2 was performed, and a protein-ligand complex with a vina score of -7.3 was obtained. The protein-ligand interaction analysis performed using Discovery Studio, and the bonds between the protein and ligand were visualised. Drug likeness and toxicity testing analysis were done using data warrior, the ligand passed all the drug likeness parameters following the RO5 and for toxicity analysis the ligand was discovered that it contained high tumorigenicity and mutagenicity effects. MD Simulation was done using CABS Flex to check the stability of the complex. In conclusion, the research has identified several phytochemicals from Aristolochia albida with promising antimalarial activity against PfHSP70-1, as determined by molecular docking. The identified compounds demonstrate promising antimalarial activity however, the in silico toxicity assessment has raised significant concerns about their tumorigenicity and mutagenicity, which must be carefully considered before further development and potential clinical applications.

Index Terms

Plasmodium falciparum; Aristolochia Albida; Molecular Docking; Drug Resistance; Antimalarial Drug Resistance