POTENTIAL OF CURRY LEAF COMPOUNDS AS *Pf*AP4AH INHIBITORS: *IN SILICO* STUDY

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ABSTRACT

NADINE AYU ALEYDA RUDIYANA. Potential of Curry Leaf Compounds as *Pf*AP4AH Inhibitors: *In Silico* Study. Supervised by INDA SETYAWATI and I MADE ARTIKA.

Diadenosine tetraphosphate hydrolase of *Plasmodium falciparum* (*Pf*Ap4AH) catalyzes the hydrolysis of diadenosine tetraphosphate into adenosine monophosphate (AMP). Curry leaf (*Murraya koenigii*) is a plant species rich in carbazole alkaloids and possesses antimalarial properties. This study aims to identify potential inhibitors for the *Pf*Ap4AH enzyme from the screening of 156 active compounds derived from curry leaves, *in silico*. The molecular docking tools used were Google Colab, AutoDock 4, and AutoDock Vina to assess the Gibbs free energy (ΔG) and ligand interactions with the target amino acid residues (Tyr87, Pro133, and Ser135) that can interact with the ATP adenine ring. The analysis results identified ten active compounds with the best ΔG values and stability in binding to *Pf*Ap4AH. The compound 1-(2-hydroxy-3-methyl-9H-carbazole-1-yl)-3-methyl-9H-carbazole-2-ol is the most promising ligand, with a ΔG value of -8.0 kcal/mol. Bikoeniquinone A and 3,3'-[Oxybis(methylene)]bis(9-methoxy-9H-carbazole) demonstrated effective interaction with key target residues, thereby underscoring the potential of compounds derived from the curry leaf tree as promising inhibitors of *Pf*Ap4AH. These findings provide a significant foundation for further investigation and development of these compounds as potential antimalarial agents.

Keywords: malaria, *Murraya koenigii*, molecular docking, *Pf*Ap4AH

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The author acknowledges the limitations of this thesis and welcomes constructive feedback and suggestions for its improvement from fellow researchers and critics. It is the author's hope that this work will contribute meaningfully to the field and prove valuable to others.

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Nadine Ayu Aleyda Rudiyana

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