

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

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**DEPARTMENT OF BIOCHEMISTRY
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BOGOR
2025**



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ABSTRACT

NADINE AYU ALEYDA RUDİYANA. Potential of Curry Leaf Compounds as *PfAP4AH* Inhibitors: *In Silico* Study. Supervised by INDA SETYAWATI and I MADE ARTIKA.

Diadenosine tetraphosphate hydrolase of *Plasmodium falciparum* (*PfAp4AH*) 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 *PfAp4AH* 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 *PfAp4AH*. 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. Bikoquinone 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 *PfAp4AH*. These findings provide a significant foundation for further investigation and development of these compounds as potential antimalarial agents.

Keywords: malaria, *Murraya koenigii*, molecular docking, *PfAp4AH*



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

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Thesis
as one of the requirements to obtain the
Bachelor degree
Biochemistry Study Program

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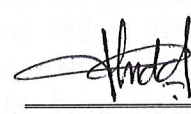
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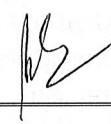
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ACKNOWLEDGMENT

Praise Allah SWT for the blessings that have facilitated the completion of this thesis. The thesis titled “Potential of Curry Leaf Compounds as *Pf*AP4AH Inhibitors: *In Silico* Study” was conducted from December 2022 to January 2025. This research was compiled as a prerequisite for obtaining a Bachelor of Science degree in the Biochemistry Department, at IPB University.

The author would like to thank the mentors, Dr. Inda Setyawati, S.TP, M.Si and Prof. Dr. Ir. I Made Artika, M.App.Sc who acted as supervisors, for their indispensable mentorship and recommendations throughout the process of thesis completion. The author thanks the author’s family and fellow Biochemistry classmates from the 2019 class. The author would also like to thank Aisyah, Rizal, Alfari, Farina, Gisella and Gibran as true friends, who have extended their hospitality and provided their support that keeps the author motivated. In addition, gratitude is extended towards Mr. Ghiyas, who contributed to both the instruction and mentorship of the author. The author would also like to express gratitude to Mr. Khrisna, who made valuable contributions to the teaching and guidance provided.

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.

Bogor, January 2025

Nadine Ayu Aleyda Rudiyan



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