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MOLECULAR DOCKING STUDIES OF EPIFRIEDELANOL FROM GUAZUMA ULMIFOLIA AS A NATURAL ANTIHYPERLIPIDEMIC AGENTS

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Abstract

Objective: *Natural compounds derived from plants have been known to have activity on our body's metabolism, one of which is the Guazuma ulmifolia (Jati Belanda plant). This plant is known empirically by the people of Indonesia has an activity to reduce obesity and LDL cholesterol value in the body. The character of natural compounds that have low toxicity, and high specificity has become the focus of research. This study aims to investigate the mechanism of antihyperlipidemic activity of Epifriedelanol compounds from Guazuma ulmifolia with three molecular targets; Niemann Pick C1 Like1 protein (NPC1L1), Lanosterol 14α-Demethylase (LDM), and Squalene Synthase (SqS) known to be implicated in the physiology of hyperlipidemia. The interactions of Epifriedelanol were compared with the interactions of their respective co-crystallized native ligands at the active sites of these receptors.*

Materials and Methods: *Molecular docking studies began by downloading the receptor file as a target on the Protein Data Bank (PDB). The ligand structure was obtained from pubchem and zinc.docking. The receptor and ligand setup was done with discovery studio software, pyrx, MgTool, followed by docking and visualization processes using AutoDock Vina and Discovery Studio Visualizer.*

Results: *Molecular docking obtained the value of binding affinity of Epifriedelanol against Niemann Pick C1 Like1 protein (NPC1L1) -2.5 kcal/mol receptors, Lanosterol 14α-Demethylase (LDM) receptor -11.2 kcal/mol, and with the Squalene Synthase (SqS) reseceptor -10.3 kcal/mol.*

Conclusions: *Molecular docking studies show that epifriedelanol from the Guazuma ulmifolia plant has a strong affinity and potential as an antihyperlipidemic through the mechanism of inhibiting LDM and SqS receptors.*

Author Keywords

Molecular Docking, Antihyperlipidemic, Guazumae Ulmifolia, Epifriedelanol, NPCL1, LDM, SqS

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