ABSTRACT

OXALYL AMINOBENZOIC ACID COMPOUND Garcinia cowa AS ANTIHYPERCHOLESTEROLEMIA STUDY In Silico

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Hypercholesterolemia can be a factor in several diseases in the human body, one of which is thickening of the blood vessel walls. Garcinia cowa fruit contains chemical compounds that can treat several diseases such as antipyretic, antimicrobial, can improve blood circulation, expectorant, laxative, and can lower cholesterol. One of the compounds from Garcinia cowa that is effective in lowering cholesterol levels in the body is oxalyl aminobenzoic acid. Therefore, in silico testing with molecular docking approach is needed. The first step in this research is sample preparation assisted by Pyrx 0.8 software to stabilize the compound in PDB form. Then, HMG-CoA Reductase protein preparation is carried out with the help of Discovery Studio software to remove ligands and water. The final step is to conduct in silico studies between the ligand and the prepared protein using the molecular docking approach with HEX Cuda tools. The results show that oxalyl aminobenzoic acid compound in Garcinia cowa has 6 amino acid residues bound and a binding affinity value of -232.29. Based on the results of in silico studies, Garcinia cowa plants have the potential as antihypercholesterolemia drugs.

Keywords : Garcinia cowa, in silico, anti-hypercholesterolemia, HMG-CoA Reductase