

ABSTRACT

Adzra Salsabila Kirana, 24020121140181, In Silico Study of the Interaction Between Black Rice (*Oryza sativa* L.) Anthocyanin Compounds and the ATP-Binding Cassette Transporter A1 (ABC-A1) as an Anti-Hypercholesterolemic Agent. Under the guidance of Sunarno and Rizki Sandhi Titisari.

Hypercholesterolemia is a condition characterized by elevated blood cholesterol levels, which can lead to an increased risk of cardiovascular disease. The ABC-A1 protein is important for moving cholesterol from cells to HDL in the reverse cholesterol transport process. Research on how anthocyanins interact with the ABC-A1 protein in hypercholesterolemia is limited; therefore, this study will focus on the interaction between the ligand and the ABC-A1 protein. This study aims to analyze the mechanism of interaction between black rice (*Oryza sativa* L.) anthocyanin compounds that bind to the ABC-A1 protein in terms of binding affinity and binding pockets based on in silico studies. Research methods included data collection of ligands and proteins from PubChem and the RSCB Protein Data Bank, screening based on Lipinski's rules, pharmacokinetic and toxicity analysis, and molecular docking simulations using PyRx. The results showed that all test compounds met Lipinski's parameters, had good pharmacokinetic profiles, and exhibited low toxicity levels. All ligands act alike at the TYR 159 amino acid, which helps stabilize the bond between the protein and ligand. The cyanidin-3-O-glucoside compound demonstrated the best interaction based on a higher number and stability of bonds compared to other compounds. The delphinidin-3-O-glucoside compound has a good *binding affinity* value of -8.2 kcal/mol. Overall, anthocyanin compounds have the potential to be used as candidates for anti-hypercholesterolemic drugs by increasing ABC-A1 protein activity.

Keywords: Hypercholesterolemia, anthocyanins, black rice, molecular docking.