ABSTRACT

Nisrinaa Syarifah Yusuf, 24020121140121, In Silico Study of Anthocyanins Phytochemical Activity from Black Rice (*Oryza sativa* L.) as an Inhibitor of Diacylglycerol O-transferase 1 (DGAT1) in Reducing Triglyceride Levels. Under the guidance of Sunarno and Rasyidah Fauzia Ahmar.

Hypertriglyceridemia is a disorder of the vascular system caused by triglyceride levels above normal range. Diacylglycerol O-transferase 1 (DGAT1) is one of the proteins that plays an important role in triglyceride synthesis. Previous research shows that black rice (*Oryza sativa* L.) contains anthocyanin compounds known to inhibit triglyceride metabolism activity, however, there are not many studies on the potential of anthocyanin compounds as inhibitors of DGAT1 protein. This study aimed to analyze the inhibitory potential of phytochemical anthocyanins from black rice (*Oryza sativa* L.) against the DGAT1 enzyme in triglyceride synthesis using in silico methods. The anthocyanin compounds used are delphinidin 3-O-glucoside, malvidin 3-O-glucoside, pelargonidin 3-O-glucoside, peonidin 3-O-glucoside, petunidin 3-O-glucoside, and cyanidin 3-O-glucoside, as well as the control compounds pradigastat, and inhibitor T863. The methods conducted include physicochemical and pharmacokinetics predictions, using SwissADME website, toxicity prediction using Protox website, and molecular docking simulations. The physicochemical prediction results show that all anthocyanin compounds in black rice comply with Lipinski's rules, except for the petunidin-3-O-glucoside compound. All six anthocyanin compounds are categorized as safe for consumption (toxicity class 5). The peonidin-3-O-glucoside compound has a relatively good binding affinity value (-7.21) and amino acid binding affinity (SER 312, TRP 277, TRP 280, and PHE 309) that is the same as the amino acid residues of the control compounds. The conclusion of this study is that peonidin-3-O-glucoside is a potential antihypertriglyceridemic drug candidate.

Keywords: *computational method, drug discovery, hypertriglycerides, molecular docking*