ABSTRACT

Mangosteen pericarpium and cat's whiskers have the potential to be developed as anti-diabetic herbal medicine, it is necessary to study molecular modeling of major compounds and markers found in plants, namely α-, β-, γ-mangostin and sinensetin. In this study, in-silico testing with molecular docking method and prediction of physicochemical properties, pharmacokinetics, and toxicity of α-, β-, γ-mangostin and sinensetin compounds.

Predict the physicochemical properties, pharmacokinetics, and toxicity of compounds using online tools such as admetSAR online tool and pkCSM online tool. For molecular docking use AutoDockTools 4.2.6. Before conducting molecular docking of test compounds, it is necessary to validate the docking method. If the cocrystal ligand redocking result has an RMSD value < 2Å, then the docking protocol can be accepted or declared valid and can be used for further docking processes.

The results of the predictions of physicochemical, pharmacokinetics and toxicity properties show that the test compound easily absorbed and has good permeability, ADME profile and is not a carcinogen and does not cause hepatotoxicity. In molecular docking, the interaction with the SUR1-Pancreatic K_{ATP} Channel receptor it was found that α-mangostin had the most negative ΔG (-6.29 kcal/mol) and the lowest K_i (24.38 μM) compared to other test compounds. For interaction with the Human Maltase-Glucoamylase receptor, γ-mangostin most negative ΔG (-8.88 kcal/mol) and the lowest Ki (0.31 μM). From this, it can be predicted that α-, and γ-mangostin have a high affinity as antidiabetic at the receptors used.

Keywords: Mangostin, Sinensetin, Molecular docking, SUR1-Pancreatic K_{ATP} Channel, Human Maltase-Glucoamylase.