ABSTRACT

In Silico Study on Interaction of Bioactive Compounds in Aqueous Extract of Roselle's Calyx (*Hibiscus sabdariffa* L.) with Xanthine Oxidase as Potensial Antioxidant and Its ADMET Prediction

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The aqueous extract of roselle's calyx (*Hibiscus sabdariffa* L.) has antioxidant activity which has been proven through *in vitro* and *in vivo* studies. This antioxidant activity occurs by the mechanism of inhibition to xanthine oxidase so the superoxide anion radicals are not formed. This study aims to explore which of the bioactive compounds in aqueous extract of roselle's calyx have antioxidant activity based on their *in silico* interaction with xanthine oxidase (XO) and predict the pharmacokinetics and toxicity (ADMET) profile of the selected high affinity compounds against XO. The interactions were performed by docking simulation of test ligands to XO (PDB code: 3NVY) using AutodockTools program. Docking results showed that 8 compounds have lower free energy than quercetin (ΔG^o= -9,783 kcal/mol). Quercetin-3-rutinoside, cyanidin-3-glucoside, and delphinidin-3-glucoside have higher binding affinity than the other compounds. Eight compounds did not show high absorption and distribution but quercetin-3-rutinoside, cyanidin-3-glucoside, and delphinidine-3-glucoside were neither hepatotoxic nor carcinogenic. It concluded that there were three compounds are potential as antioxidants.

Keywords: Roselle's bioactive compound, Antioxidant, Xanthine oxidase, Docking, ADMET