

ABSTRACT

IN SILICO STUDY OF FLAVONOID AND ALKALOID COMPOUNDS ON *Justicia gendarussa* *Burm. f.* FOR PREDICTION OF VOMITING ACTIVITY

Based on previous researches, *Justicia gendarussa* Burm. f had been used for male contraception and anti-HIV. But, it had a minor side effects which are nausea and vomit. *Justicia gendarussa* Burm. f contains the derivative compounds of gendarusins, amino-benzyl alcohols and justidrusamides. The aim of this research was to investigate the prediction of absorption and activity the 13 compounds of *Justicia gendarussa* on vomiting receptors (5HT₃ and Dopamine type 2) by in silico study. The prediction of absorption used the Lipinski's rule of five and ACD/I-Lab online program, while the prediction of activity used docking simulation with Molegro Virtual Docker (MVD) program. Results showed from docking simulation using MVD, it can be identified by presence of interaction between vomiting receptors (PDB ID : 4PIR and 2YOU) and all compounds of *Justicia gendarussa* as well as lowest free energy of binding (rerank score). Gendarusin B had highest vomit activity on 5HT₃ receptor and gendarusin E had highest vomit activity on Dopamin type 2 as well as smallest rerank score compared to all compounds of *Justicia gendarussa* by in silico study.

Keyword : *in silico*, *Justicia gendarussa*, Molegro Virtual Docker, Vomiting receptor, Gendarusin, Amino-benzyl alcohols, Justidrusamides