INTISARI

ILMIAWAN, F, 2019, MOLEKULAR DOCKING DAN PREDIKSI PROFIL FARMAKO KINETIK KANDUNGAN KIMIA *Cucurbita moschata, Momordica charantia,* DAN *Luffa acutangula* SEBAGAI ANTI DIABETES, SKRIPSI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA.

Ekstrak *Cucurbita moschata, Momordica charantia* dan *Luffa acutangula* dari *Cucurbitaceae* dilaporkan memiliki aktivitas sebagai antidiabetes. Penelitian ini bertujuan untuk memprediksi sifat aktivitas antidiabetes dari kandungan kimia *Cucurbita moschata, Momordica charantia* dan *Luffa acutangula* dan juga pola interaksi terhadap beberapa makromolekul target antidiabetes yaitu Dipeptidyl-Peptidase 4 enzyme (DPP4), Protein tyrosine phospahatase-1B (PTP1B), Glucokinase, Alpha glucosides menggunakan molekular docking.

AutoDock Vina dalam PyRx telah digunakan dan hasilnya dituangkan dalam binding affinity values (kcal/mol). Program PyMOL digunakan untuk visualisasi gambar 3D molekular dari konformasi hasil docking dan interaksi antara ligan-protein. Juga kami melakukan penelitian terhadap profil farmakokinetik menggunakan SwissADME dari tiap kandungan senyawa kimia.

Hasilnya menunjukkan pada target DPP4 binding score terbaik terdapat pada Acutoside D (*Luffa acutangula*), Momordicosides D (*Momordica charantia*), and Auroxanthin *(Cucurbita moschata)*. Glucokinase menunjukkan binding score terbaik pada Alpha carotene *(Cucurbita moschata),* Carotene (*Luffa acutangula*) and Omargliptine (*Momordica charantia*). PTP1B menunjukkan binding score terbaik pada Acutoside G *(Luffa acutangula),* Auroxanthin (*Cucurbita moschata*) and Kuguacin B (*Momordica charantia*). *Alpha glucosides* menunjukkan binding score terbaik pada Acutoside B (*Luffa acutangula),* Kuguacin B (*Momordica charantia*) and Auroxanthin (*Cucurbita moschata*).. Namun hanya Kuguacin B yang memiliki pola interaksi dan profil farmakokinetik terbaik.

Kata kunci: Cucurbitaceae, Antidiabetic, Macromolecular target, Molecular Docking, Pharmacokinetic profil

ABSTRACT

ILMIAWAN, F, 2019, DOCKING MOLECULAR AND PREDICT PHARMACOKINETIC PROFIL CHEMICAL CONSTITUENT OF *Cucurbita moschata, Momordica charantia,* DAN *Luffa acutangula* AS ANTIDIABETIC, SKRIPSI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA.

Luffa acutangula, Cucurbita moschata, and *Momordica charantia* herbs extract from Cucurbitaceae have been reported to have antidiabetic activity from various studies. This study aimed to predict antidiabetic properties of phytochemical constituents of *Luffa acutangula, Cucurbita moschata,* and *Momordica charantia* as well as to study their interaction to various macromolecular targets of antidiabetic agent *Dipeptidyl-Peptidase 4 enzyme* (DPP4), *Protein tyrosine phospahatase-1B* (PTP1B), *Glucokinase, Alpha glucosides* using molecular docking.

AutoDock Vina in PyRx was used and the results were presented as binding affinity values (kcal/mol). Program PyMOL was used to visualize the 3D molecular of docked conformation and ligand-protein interactions. Also we were study the pharmacokinetic profil of extract by SwissADME of its chemical compound.

The result showed that DPP4 had the best binding score on Acutoside D (*Luffa acutangula*), Momordicosides D (*Momordica charantia*), and Auroxanthin *(Cucurbita moschata)*. Glucokinase showed the best binding score on Alpha carotene *(Cucurbita moschata),* Carotene (*Luffa acutangula*) and Omargliptine (*Momordica charantia*). PTP1B gave the best binding score on Acutoside G *(Luffa acutangula),* Auroxanthin (*Cucurbita moschata*) and Kuguacin B (*Momordica charantia*). *Alpha glucosides* showed the best antidiabetic binding score on Acutoside B (*Luffa acutangula),* Kuguacin B (*Momordica charantia*) and Auroxanthin (*Cucurbita moschata*). But only Kuguacin B that has a good interaction patern and pharmacokinetic profil.

Keywoard: Cucurbitaceae, Antidiabetic, Macromolecular target, Molecular Docking, Pharmacokinetic profil