ABSTRAK

KHOIRONI, A. 2021. STUDI BIOKEMOINFORMATIKA KANDUNGAN KIMIA DAUN KELOR (*Moringa oleifera,* Lam) TERHADAP TARGET ANTIDIABETES, SKRIPSI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA.

Daun kelor secara empiris telah diketahui memiliki khasiat yang dapat mengurangi resiko penyakit diabetes. Tujuan penelitian ini mengetahui interaksi target molekul antidiabetes berdasarkan skor konformasi, mengetahui farmakokinetika dari senyawa daun kelor dan untuk melihat kestabilan senyawa daun kelor terhadap target terapi antidiabetes.

Interaksi senyawa aktif daun kelor dengan reseptor target antidiabetes dilakukan dengan metode penambatan molekular menggunakan perangkat lunak *AutoDock4, AutoDockTools, MarvinSketch, Pymol*, yang kemudian divisualisasikan menggunakan *Discovery Studio Visualizer* lalu dianalisis hasil ikatan energinya dan profil farmakokinetiknya, setelah itu dilakukan uji simulasi molekular dinamik untuk mengetahui kestabilan ligan uji berikatan dengan reseptor.

Hasil penelitian menunjukkan bahwa senyawa daun kelor yaitu N-α-L-Rhamnopyranosyl Vincosamide memiliki nilai afinitas pengikatan yang lebih baik pada DPP4 dan α-G serta 4-(α-L-Rhamnopyranosyloxy) benzyl glucosinolate pada protein GK dan PTP-1B. Berdasarkan prediksi interaksi yang terbaik untuk masing-masing target yaitu 2-Methylpropyl Glucosinolate, 4-(α-L-Rhamnopyranosyloxy)benzyl Glucosinolate, 4-Hydroxybenzyl Glucosinolate, Benzyl glucosinolate, Kaempferol, N-α-L-Rhamnopyranosyl Vincosamide, O-ethyl-4-(α-l-rhamnosyloxy)benzyl carbamate, Quercetin, Rhamnetin, dan β-sitosterol 3-O-β-D-glucuronopyranoside. Prediksi ADME menunjukkan senyawa dari daun kelor yaitu kaempferol, kuersetin dan rhamnetin , karena memiliki nilai absorpsi yang tinggi dan tidak menembus sawar darah otak serta dapat dimetabolisme dengan baik sehingga ketiga senyawa tersebut dapat diprediksi memiliki profil farmakokinetik terbaik serta ligan 4-(α-L-Rhamnopyranosyloxy) benzyl glucosinolate stabil berikatan dengan PTP1B melalui uji simulasi dinamika molekular.

Kata Kunci: *Moringa oleifera*, Penyakit Antidiabetes, Molekuler *Docking*, Simulasi Molekular Dinamik.

ABSTRACT

KHOIRONI, A. 2021. BIOCHEMOINFORMATICS STUDY OF THE CHEMICAL CONTENT OF KELOR LEAVES (Moringa oleifera, Lam) FOR ANTIDHIABETIC DISEASES, FACULTY OF PHARMACY, UNIVERSITY OF SETIA BUDI, SURAKARTA.

Moringa leaves have been empirically known to have properties that can reduce the risk of diabetes. The purpose of this study was to determine the protein that became the molecular target, to determine the interaction of the molecular target of antidiabetic based on the conformation score and to determine the pharmacokinetics of the compounds of moringa leaves.

Modeling of the interaction of the active compound of Moringa leaves with antidiabetic target receptors was carried out using the molecular docking method using Autodock4 software, autodock tools, MarvinSketch, Pymol, which were then visualized using the Discovery Studio Visualizer then analyzed the results of their energy bonds and pharmacokinetic profiles, after which a dynamic molecular simulation test was carried out. to see the stability of the test ligand bind to the receptor.

The results showed that the moringa leaf compound, namely N- α -L-Rhamnopyranosyl Vincosamide, had better binding affinity values for DPP4 and α-G and 4- (L-L-Rhamnopyranosyloxy) benzyl glucosinolate on GK and PTP-1B proteins. Based on the best predicted interactions for each target 2-Methylpropyl Glucosinolate,4- (α-L-Rhamnopyranosyloxy) benzyl Glucosinolate, 4-Hydroxybenzyl Glucosinolate, Benzyl glucosinolate, Kaempferol, N- α -L-Rhamnopyranosyl α -l-rhamnosyloxy) benzyl carbamate, Quercetin, Rhamnetin, and β-sitosterol 3-O-β-D-glucuronopyranoside. ADME prediction shows that the compounds from moringa leaves, namely kaempferol, quercetin and rhamnetin, have high absorption values and do not cross the blood-brain barrier and can be metabolized properly so that the three compounds can be predicted to have the best pharmacokinetic profile and ligand 4- (α -L- Rhamnopyranosyloxy) is stable to bind benzyl glucosinolate with PTP1B through molecular dynamics simulation tests.

Keywords: *Moringa oleifera, Antidiabetic Disease, Molecular Docking, Molecular Dynamic Simulation.*