INTISARI

JULAIHA, 2019, STUDI BIOINFORMATIKA TANAMAN KEJI BELING (*Strobilanthes Crispus* L.) DAN SAMBILOTO (*Andrographis paniculata* Nees) SEBAGAI ANTIDIABETES

Tanaman *Strobilanthes crispus* dan *Andrographis paniculata* dilaporkan memiliki banyak aktivitas biologi, salah satunya yaitu antidiabetes. Penelitian ini bertujuan untuk memprediksi sifat aktivitas antidiabetes dari kandungan kimia *Strobilanthes crispus* dan *Andrographis paniculata* 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 digunakan untuk proses docking dan hasilnya dituangkan dalam binding affinity values (kcal/mol). Program PyMOL dan Discovery Studio Visualizer digunakan untuk melihat interaksi ligan dan makromolekul. Selain itu, prediksi ADME sangat penting karena memiliki peran dalam menilai kualitas kandidat klinis potensial obat baru. ADME Swiss digunakan untuk analisis untuk memilih senyawa obat yang kuat.

Hasil kandungan kimia *Andrographis paniculata* yang memiliki afinitas terbaik adalah glukokinase (-10,4 kkal / mol), DPP4 (9,3 kkal / mol) dan α-glukosidase (-8,8 kkal / mol) senyawa 19-tripenhyl andrographolide dan PTP1B (-9,5 kkal / mol) senyawa andrographolactone. Sedangkan kandungan kimia *Strobilanthes crispus* memiliki afinitas terbaik adalah glukokinase (-9,9 kkal / mol) senyawa stigmasterol, DPP4 (-9,7 kkal / mol) senyawa rutin, α-glukosidase (-8,8 kkal / mol) senyawa lupeol dan PTP1B (- 8,8 kkal / mol) senyawa luteolin. Prediksi ADME menunjukkan bahwa andrographolactone memiliki profil farmakokinetik sangat baik.

Kata Kunci : Bioinformatik, Swiss ADME, *Andrographis paniculata, Strobilanthes crispus,* antidiabetes

ABSTRACT

JULAIHA, 2019, STUDY BIOINFORMATICTS OF *Strobilanthes Crispus* L. AND *Andrographis paniculata* Nees CHEMICAL CONSTITUENS AS ANTIDIABETIC AGENTS

Strobilanthes crispus and *Andrographis paniculata* are known to have a wide range of biological activity, one of them is antidiabetic. This study aimed to study the molecular interaction of *Strobilanthes crispus* and *Andrographis paniculata* phytochemical constituents to the various macromolecular targets of antidiabetic agent through molecular docking. Nineteen *Andrographis paniculata* and twenty *Strobilanthes crispus* chemical constituents were docked to four 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). In this study Program PyMOL and Discovery Studio Visualizer are used to the visualizer molecular of ligand-macromolecule interactions. Other than that, ADME predictions are very important because they play a critical role in assessing the quality of potential clinical candidates a new drug. Swiss ADME used for analysis to select a potent drug compound.

The result from *Andrographis paniculata* compounds that have the best binding affinity were glucokinase (-10.4 kcal/mol), DPP4 (9.3 kcal/mol) and α-glucosidase (-8.8 kcal/mol) of 19-tripenhyl andrographolide and PTP1B (-9.5 kcal/mol) of andrographolactone. Whereas in the *Strobilanthes crispus* compounds that have the best binding affinity were glucokinase (-9.9 kcal/mol) of stigmasterol, DPP4 (-9.7 kcal/mol) of rutin, α-glucosidase (-8.8 kcal/mol) of lupeol and PTP1B -8.8 kcal/mol) of luteolin. ADME predictions indicate that andrographolactone has an excellent pharmacokinetic profile.

***Keywords*:** Bioinformatics, Swiss ADME, *Andrographis paniculata, Strobilanthes crispus,* antidiabetic