ABSTRAK

YOSEF SABATUDUNG, 2025, ANALISIS MOLECULAR *DOCKING* DAN PREDIKSI ADME SENYAWA DALAM TANAMAN KOPASSANDA (*CHROMOLAENA ODORATA*) SEBAGAI INHIBITOR ENZIM α -GLUKOSIDASE DAN DPP-4 UNTUK AKTIVITAS ANTIABETES, PROPOSAL SKRIPSI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA. Dibimbing oleh Dr. apt. Rina Herowati, S.Si., M.Si dan apt. Ismi Puspitasari, S. Farm., M.Farm.

Diabetes melitus tipe 2 merupakan gangguan metabolik kronis yang ditandai oleh resistensi insulin dan penurunan fungsi sel β pankreas sehingga menyebabkan hiperglikemia persisten. Penghambatan enzim α-glukosidase dan dipeptidil peptidase-4 (DPP-4) menjadi salah satu strategi terapeutik yang menjanjikan dalam pengendalian kadar glukosa postprandial dan peningkatan aktivitas incretin. Penelitian ini bertujuan untuk mengeksplorasi potensi senyawa metabolit sekunder dari tanaman *Chromolaena odorata* sebagai inhibitor α-glukosidase dan DPP-4 melalui pendekatan in silico.

Metode yang digunakan meliputi molecular *docking* menggunakan perangkat lunak PLANTS versi 1.2 dengan fungsi scoring ChemPLP serta prediksi sifat farmakokinetik menggunakan ADMETlab 3.0. Struktur tiga dimensi ligan diperoleh dari basis data PubChem dan KNApSAcK, sedangkan struktur protein target α-glukosidase (PDB ID: 2QMJ) dan DPP-4 (PDB ID: 1X70) diambil dari RCSB Protein Data Bank. Hasil docking dianalisis berdasarkan skor afinitas pengikatan dan persentase kesamaan residu asam amino pada situs aktif protein target.

Hasil penelitian menunjukkan bahwa *chlorogenic acid*, *kaempferol-3-O-rutinosida*, *persicogenin,* dan *rhamnetin* memiliki interaksi yang baik terhadap enzim α-glukosidase dan DPP-4 serta menunjukkan profil ADME yang memadai. Secara keseluruhan, senyawa metabolit sekunder dari *Chromolaena odorata* berpotensi dikembangkan sebagai kandidat antidiabetes alami, namun masih memerlukan konfirmasi melalui uji eksperimental lanjutan.

Kata kunci: *Chromolaena odorata*, α-glukosidase, DPP-4, molecular *docking*, ADME, antidiabetes.

ABSTRACT

YOSEF SABATUDUNG, 2025, MOLECULAR *DOCKING* ANALYSIS AND ADME PREDICTION OF COMPOUNDS IN KOPPASANDA LEAVES (*CHROMOLAENA ODORATA*) AS α-GLUCOSIDASE AND DPP-4 ENZYME INHIBITORS FOR ANTIDIABETIC ACTIVITY, RESEARCH PROPOSAL, BACHELOR OF PHARMACY STUDY PROGRAM, FACULTY OF PHARMACY, SETIA BUDI UNIVERSITY, SURAKARTA. Supervised by Dr. apt. Rina Herowati, S.Si., M.Si and apt. Ismi Puspitasari, S.Farm., M.Farm.

Type 2 diabetes mellitus is a chronic metabolic disorder characterized by insulin resistance and progressive dysfunction of pancreatic β-cells, resulting in persistent hyperglycemia. Inhibition of α-glucosidase and dipeptidyl peptidase-4 (DPP-4) represents a promising therapeutic strategy for controlling postprandial glucose levels and enhancing incretin activity. This study aimed to investigate the potential of secondary metabolites from *Chromolaena odorata* as dual inhibitors of α-glucosidase and DPP-4 using an in silico approach.

Molecular docking was performed using PLANTS version 1.2 with the ChemPLP scoring function, while pharmacokinetic properties were predicted using ADMETlab 3.0. Three-dimensional structures of the ligands were obtained from PubChem and KNApSAcK databases, whereas protein structures of α-glucosidase (PDB ID: 2QMJ) and DPP-4 (PDB ID: 1X70) were retrieved from the RCSB Protein Data Bank. Docking results were evaluated based on binding affinity scores and the percentage of shared amino acid residues at the active sites of the target proteins.

The results demonstrated that *chlorogenic acid*, *kaempferol-3-O-rutinoside*, *persicogenin,* and *rhamnetin* exhibited favorable interactions with both α-glucosidase and DPP-4. These compounds also showed acceptable pharmacokinetic profiles based on ADME predictions. Overall, the findings suggest that secondary metabolites from *Chromolaena odorata* have potential as natural antidiabetic candidates targeting α-glucosidase and DPP-4, warranting further experimental validation.

Keywords: *Chromolaena odorata*, α-glucosidase, DPP-4, molecular *docking*, ADME, antidiabetic.