ABSTRAK

MOLECULAR DOCKING SENYAWA DARI GENUS ALPHITONIA TERHADAP _MYCOBACTERIUM TUBERCULOSIS_ MENGGUNAKAN _PLANTS_® (Oleh Imanda Asya Noor Rajih; Pembimbing Hafiz Ramadhan dan Nafila; 2024; 165 Halaman)

Mycobacterium tuberculosis merupakan agen penyebab penyakit tuberkulosis yang menyerang organ paru pada manusia. Penghambat keberhasilan pengobatan tuberkulosis yakni obat antituberkulosis tidak adekuat dalam terapi dan dapat meningkatkan risiko resistensi seperti *Multiple Drug Resistance Tuberculosis* (MDR-TB). Sehingga penemuan kandidat obat baru perlu dilakukan yaitu salah satunya berasal dari senyawa bioaktif yang terkandung dalam genus Alphitonia karena diketahui memiliki potensi khasiat sebagai antibakteri. Tujuan penelitian ini yaitu untuk mengetahui potensi aktivitas dan interaksi senyawa genus Alphitonia terhadap reseptor InhA dan RNA polimerase dari *Mycobacterium tuberculosis* dibandingkan dengan dengan *native ligand* serta obat Isoniazid dan Rifampicin menggunakan *molecular docking* PLANTs. Metode yang digunakan adalah eksperimental eksploratif dengan *computational experiment* senyawa marker dan senyawa pilihan sebanyak 30 struktur 3D dari genus Alphitonia terhadap protein target *Enoyl Acyl Carrier Protein Redictase/*InhA (PDB ID: 2X23) dan *RNA Polimerase/*RNAP (PDB ID: 1YNN) menggunakan aplikasi *docking* PLANTs. Senyawa yang memiliki skor *docking* terbaik terhadap protein 2X23 sebanyak 14 senyawa potensial dan terhadap 1YNN sebanyak 15 senyawa potensial. Senyawa yang memiliki kemiripan ikatan residu asam amino dengan *native ligand* adalah *6'-Heptadecanoyl-3-O-β-D-glucopyranosylsitosterol* terhadap protein 2X23 dan *Quercetin 3-O-α-L-rhamnopyranosyl (1→2)-α-L arabinopyranosyl (1→2)-α-L-rhamnopyranoside* terhadap protein 1YNN.

Kata Kunci: *Molecular Docking, Mycobacterium tuberculosis,* Alphitonia, PLANTs

ABSTRACT

MOLECULAR DOCKING OF COMPOUNDS FROM THE GENUS ALPHITONIA AGAINST MYCOBACTERIUM TUBERCULOSIS USING PLANTS® (By Imanda Asya Noor Rajih; Advisor Hafiz Ramadhan and Nafila; 2024; 165 Pages)

Mycobacterium tuberculosis is the causative agent of tuberculosis disease that attacks the lung organ in humans. The obstacle to the success of tuberculosis treatment is that antituberculosis drugs are inadequate in therapy and can increase the risk of resistance such as Multiple Drug Resistance Tuberculosis (MDR-TB). So the discovery of new drug candidates needs to be done, one of which comes from bioactive compounds contained in the Alphitonia genus because it is known to have potential efficacy as an antibacterial. The purpose of this study was to determine the potential activity and interaction of Alphitonia genus compounds against InhA and RNA polymerase receptors from Mycobacterium tuberculosis compared to native ligands and Isoniazid and Rifampicin drugs using PLANTs molecular docking. The method used is an exploratory experiment with the computational experiment of marker compounds and selected compounds as many as 30 3D structures from the genus Alphitonia against target proteins Enoyl Acyl Carrier Protein Reductase/InhA (PDB ID: 2X23) and RNA Polymerase/RNAP (PDB ID: 1YNN) using PLANTs docking application. Compounds that have the best docking score against protein 2X23 are 14 potential compounds and against 1YNN are 15 potential compounds. Compounds that have similar amino acid residue bonds with native ligands are 6'-Heptadecanoyl-3-O-β-D-glucopyranosylsitosterol against protein 2X23 and Quercetin 3-O-α-L-rhamnopyranosyl (1→2)-α-L arabinopyranosyl (1→2)-α-L-rhamnopyranoside against protein 1YNN.

Keywords: Molecular Docking, Mycobacterium tuberculosis, Alphitonia, PLANTs