ABSTRAK

AYU PUTRI AGUSTIN, 2026. **ANALISIS *IN SILICO* POTENSI SENYAWA METABOLIT SEKUNDER DAUN HARENDONG (*Melastoma malabathricum*) SEBAGAI INHIBITOR TUBERKULOSIS UNTUK SUPLEMEN BAHAN AJAR BIOLOGI**. Jurusan Pendidikan Biologi, Fakultas Keguruan dan Ilmu Pendidikan, Universitas Siliwangi, Tasikmalaya.

Tuberkulosis merupakan penyakit yang masih menjadi permasalahan kesehatan global, terutama dengan munculnya kasus resistensi terhadap obat lini pertama seperti *isoniazid*, sehingga diperlukan pengembangan kandidat obat baru, salah satunya melalui pemanfaatan senyawa metabolit sekunder dari tumbuhan harendong. Penelitian ini bertujuan untuk menganalisis potensi senyawa metabolit sekunder daun harendong sebagai kandidat inhibitor protein target tuberkulosis menggunakan pendekatan *in silico*. Metode yang digunakan meliputi identifikasi senyawa melalui studi literatur, analisis *molecular docking*, serta evaluasi sifat fisikokimia berdasarkan *Lipinski's Rule of Five*, farmakokinetik (ADME), dan toksisitas. Berdasarkan hasil studi literatur, terdapat 13 senyawa metabolit sekunder pada daun harendong yang berpotensi sebagai antituberkulosis, diantaranya yaitu *gallocatechin, epigallocatechin, catechin, caffeic acid, quercetin, p-coumaric acid, betulinic acid, kaempferol, gallic acid, ursolic acid, ellagic acid, digiprolactone* dan *myricetin*. Senyawa tersebut dianalisis secara *in silico* sebagai ligan uji dengan ligan kontrol isoniazid dan reseptor *enoyl-acyl carrier* (InhA)(PDB ID: 5W07). Hasil *molecular docking* menunjukkan bahwa seluruh ligan uji memiliki nilai *binding affinity* yang lebih baik dibandingkan ligan kontrol *isoniazid* (-5,7 kcal/mol), namun tidak semua ligan uji memenuhi kriteria untuk dijadikan kandidat obat berdasarkan evaluasi sifat fisikokimia, farmakokinetik dan toksisitas. Adapun senyawa yang paling berpotensi sebagai kandidat obat antituberkulosis yaitu *caffeic acid* karena memiliki afinitas ikatan yang lebih kuat dari ligan kontrol, yaitu -7,2 kcal/mol, memenuhi seluruh kriteria Lipinski, profil farmakokinetik yang baik, serta berada pada kelas toksisitas 5 dan LD50 sebesar 2980 mg/kg yang menunjukkan tingkat toksisitas yang rendah. Penelitian ini memberikan informasi awal mengenai potensi senyawa metabolit sekunder daun harendong sebagai kandidat inhibitor alami InhA melalui pendekatan bioinformatika.

Kata Kunci: bioinformatika, harendong, *in silico*, *molecular docking*, tuberkulosis

ABSTRACT

AYU PUTRI AGUSTIN, 2026. ***IN SILICO ANALYSIS OF THE POTENTIAL OF SECONDARY METABOLITES FROM HARENDONG LEAVES (Melastoma malabathricum) AS TUBERCULOSIS INHIBITORS FOR BIOLOGY LEARNING SUPPLEMENT***. *Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University of Tasikmalaya.*

Tuberculosis remains a major global health problem, particularly with the emergence of resistance to first-line drugs such as isoniazid, highlighting the need for the development of new drug candidates, including those derived from secondary metabolites of harendong plants. This study aimed to analyze the potential of secondary metabolites from harendong leaves (Melastoma malabathricum) as candidate inhibitors of tuberculosis target proteins using an in silico approach. The methods employed included compound identification through literature studies, molecular docking analysis, and evaluation of physicochemical properties based on Lipinski's Rule of Five, pharmacokinetics (ADME), and toxicity. Based on literature studies, 13 secondary metabolites from harendong leaves were identified as potential antituberculosis compounds, including gallocatechin, epigallocatechin, catechin, caffeic acid, quercetin, p-coumaric acid, betulinic acid, kaempferol, gallic acid, ursolic acid, ellagic acid, digiprolactone, and myricetin. These compounds were analyzed in silico as test ligands using isoniazid as the control ligand and enoyl-acyl carrier protein reductase (InhA) (PDB ID: 5W07) as the target receptor. Molecular docking results showed that all test ligands exhibited better binding affinity values than isoniazid (−5.7 kcal/mol). However, not all ligands fulfilled the criteria to be considered drug candidates based on physicochemical, pharmacokinetic, and toxicity evaluations. Among all compounds, caffeic acid demonstrated the highest potential as an antituberculosis drug candidate because it showed stronger binding affinity (−7.2 kcal/mol), fulfilled all Lipinski criteria, exhibited good pharmacokinetic properties, and belonged to toxicity class 5 with an LD50 value of 2980 mg/kg, indicating low toxicity. This study provides preliminary information regarding the potential of secondary metabolites from harendong leaves as natural InhA inhibitor candidates through a bioinformatics approach.

Keywords**:** *bioinformatics, harendong, in silico, molecular docking, tuberculosis*