SKRIPSI SARJANA FARMASI

STUDI *MOLECULAR DOCKING* DAN PREDIKSI PROFIL FARMAKOKINETIKA SENYAWA KANDUNGAN JAMBU BIJI (*Psidium guajava* L.) SEBAGAI ANTIBAKTERI

Oleh:

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ABSTRAK

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Infeksi bakteri merupakan masalah kesehatan global yang signifikan, dengan dampak yang luas terhadap morbiditas dan mortalitas di seluruh dunia. Peningkatan resistensi terhadap antibiotik memerlukan pengembangan strategi baru untuk penanganan dan pencegahan penyakit infeksi bakteri. Hal ini mendorong pencarian sumber obat baru dari alam, salah satunya tanaman jambu biji (*Psidium guajava* L.) yang telah lama digunakan secara turun- temurun sebagai antibakteri. Penelitian ini mengkaji afinitas ikatan (kkal/mol), interaksi, dan profil farmakokinetika senyawa kandungan jambu biji terhadap protein target antibakteri melaui simulasi *molecular docking*. Terdapat empat protein target antibakteri yang mewakili mekanisme kerja antibakteri di antaranya protein *DNA gyrase B inhibitor* (PDB ID: 5L3J), protein *dihydrofolate reductase* (PDB ID: 2W9G), *penicillin-binding protein* (PDB ID: 5OJ0), dan protein 30S *ribosom synthesis inhibitor* (PDB ID: 6YPU). Protokol *docking* ini menggunakan perangkat lunak Schrödinger dan prediksi ADMET menggunakan pkCSM. Hasil simulasi *docking* menunjukkan terdapat dua belas senyawa jambu biji yang potensial dalam pengembangan terapi antibakteri baru yaitu myrciaphenone B, kaempferol-3-o-rutinoside, chlorogenic acid, catechin, myricetin, (-)-epicatechin 8-C-galactoside, 3-[2,6-Bis-O-(3,4,5-trihydroxybenzoyl)-beta-D-glucopyranosyl] 2,4,6 trihydroxyphenyl methanone, sesamolinol 4"-O-β-D-glucosyl (1-6)-O-β-D-glucoside, quercetin 3,7-diglucoside, quercetin 3-(2G-xylosylrutinoside), 2-amino-1,4-naphthoquinone, dan corynan-17-ol,18,19-didehydro-10-methoxy-acetate. Hasil prediksi ADMET menunjukkan Corynan-17-ol,18,19-didehydro-10-methoxy-acetate merupakan kandidat senyawa antibakteri yang paling potensial karena menunjukkan sifat absorpsi, distribusi, ekskresi, dan toksisitas yang signifikan. Dari hasil di atas, senyawa kandungan jambu biji dapat berpotensi pada empat mekanisme kerja antibakteri.

Kata kunci: Jambu biji (*Psidium guajava* L.), *molecular docking*, antibakteri, dan ADMET

ABSTRACT

MOLECULAR DOCKING STUDIES AND PHARMACOKINETIC PROFILE PREDICTION OF COMPOUNDS FROM GUAVA (*Psidium guajava* L.) AS ANTIBACTERIALS

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Bacterial infections are a significant global health issue, with widespread impacts on morbidity and mortality worldwide. The increasing resistance to antibiotics requires the development of new strategies for managing and preventing bacterial infections. This encourages the search for new sources of drugs from nature, one of which is the guava plant (*Psidium guajava* L.) which has long been used for generations as an antibacterial. This study examines the binding affinity (kcal/mol), interactions, and pharmacokinetic profiles of guava compounds against antibacterial target proteins through molecular docking simulations. There are four bacterial target proteins that represent the mechanism of antibacterial mechanisms were used, including DNA gyrase B inhibitor (PDB ID: 5L3J), dihydrofolate reductase (PDB ID: 2W9G), penicillin-binding protein (PDB ID: 5OJ0), and 30S ribosome synthesis inhibitor (PDB ID: 6YPU). The docking protocol employed Schrödinger software, and ADMET predictions were performed using pkCSM. The docking simulation result identified twelve guava compounds with potential for developing new antibacterial therapies, including myrciaphenone B, kaempferol-3-o-rutinoside, chlorogenic acid, catechin, myricetin, (-)-epicatechin8-C-galactoside, 3-[2,6-Bis-O-(3,4,5 trihydroxybenzoyl)-beta-D-glucopyranosyl] 2,4,6 trihydroxyphenyl methanone, sesamolinol 4"-O-β-D-glucosyl (1-6)-O-β-D-glucoside, quercetin 3,7-diglucoside, quercetin 3-(2G-xylosylrutinoside), 2-amino-1,4-naphthoquinone, and corynan-17-ol,18,19-didehydro-10-methoxy-acetate. The ADMET prediction result indicated that corynan-17-ol,18,19-didehydro-10-methoxy-acetate is the most promising antibacterial candidate due to its significant absorption, distribution, excretion, and toxicity properties. These result suggest that guava compounds have potential against four antibacterial mechanisms.

Keywords: Guava (*Psidium guajava* L.), molecular docking, antibacterial, and ADMET.