ABSTRAK

Pada Desember 2019, kasus pertama COVID-19 dilaporkan terjadi di Wuhan, China. Kasus ini menjadi perhatian dunia dan menjadi ancaman bagi kesehatan masyarakat. Berdasarkan penelitian sebelumnya, dengan metode *Molecular Docking* ditemukan bahwa Flavonoid menunjukkan aktivitas penghambatan yang kuat pada SARS-CoV-2 *Main Protease*. Penelitian ini bertujuan untuk menentukan senyawa flavonoid daun jamblang (*Syzygium cumini* (L.) Skeels) yang dapat berinteraksi dengan reseptor SARS-CoV-2 *Main Protease* dan dapat digunakan sebagai kandidat terapi COVID-19 dengan *virtual screening*. Hasil *Molecular Docking* 15 senyawa turunan flavonoid daun jamblang terhadap reseptor *Main Protease* (7C6S), didapatkan senyawa Myricetin 4″-O-acetyl-2-O-gallate memiliki energi bebas Gibbs (ΔG) terendah sebesar -9.82 kkal/mol. Hasil dinamika molekul senyawa terbaik Myricetin 4″-O-acetyl-2-O-gallate, nilai RMSD dan RSMF cukup stabil. Hasil *drug scan*, senyawa terbaik memenuhi 2 dari 5 aturan Lipinski. Hasil prediksi farmakokinetik dan toksisitas, senyawa terbaik memiliki profil farmakokinetik yang cukup baik, dan tidak toksik. Dari hasil ini didapatkan bahwa senyawa Myricetin 4″-O-acetyl-2-O-gallate daun jamblang diprediksi berinteraksi dengan reseptor SARS-CoV-2 *Main Protease* (7C6S) berpotensi sebagai kandidat obat pada terapi COVID-19.

Kata Kunci: SARS-CoV-2 *Main Protease*, COVID-19, Flavonoid daun Jamblang, *Virtual Screening*.

ABSTRACT

In December 2019, the first case of COVID-19 was reported in Wuhan, China. Subsequently, this case became a global concern and a threat to public health. Based on previous research, the Molecular Docking method found that flavonoids showed strong inhibitory activity on SARS-CoV-2 Main Protease. This study aims to determine flavonoid compounds of jamblang leaves (Syzygium cumini (L.) Skeels) that can interact with SARS-CoV-2 Main Protease receptors and can be used as COVID-19 therapeutic candidates by virtual screening. The Molecular Docking results of 15 flavonoid-derived compounds of jamblang leaves against the Main Protease receptor (7C6S), obtained the compound Myricetin 4"-O-acetyl-2-O-gallate has the lowest Gibbs free energy (ΔG) of -9.82 kcal/mol. The results of the molecular dynamics of the best compound Myricetin 4"-O-acetyl-2-O-gallate show that the RMSD and RSMF values are quite stable. Drug scan results, the best compound fulfills 2 out of 5 Lipinski rules. Pharmacokinetic and toxicity prediction results, the best compound has a fairly good pharmacokinetic profile, and is not toxic. From these results, it was found that the Myricetin 4"-O-acetyl-2-O-gallate compound of jamblang leaves is predicted to interact with the SARS-CoV-2 Main Protease (7C6S) receptor as a potential drug candidate in COVID-19 therapy.

Keyword : SARS-CoV-2 *Main Protease, COVID-19, Flavonoids of Jamblang Leaves, Virtual Screening*