

## ABSTRAK

Berdasarkan data *World Health Organization* (WHO), di seluruh dunia, ada sekitar 11,9 juta. Organisasi Kesehatan Dunia (WHO) menganjurkan pengobatan tradisional yang memanfaatkan bahan alami yang potensial. Metode yang digunakan dalam penelitian ini yaitu secara *in silico*. Penelitian ini bertujuan untuk menganalisis turunan flavonoid yang terkandung dalam daun sambung nyawa mempunyai interaksi yang stabil terhadap enzim *cyclooxygenase-1* (COX-1) dan enzim *cyclooxygenase-2* (COX-2) sehingga dapat diprediksi mempunyai aktivitas sebagai kandidat anti-inflamasi. Hasil *Virtual screening* pada turunan flavonoid daun sambung nyawa yang berinteraksi dengan reseptor 1EQG terdapat satu senyawa yang memiliki *energy bebas Gibbs* terendah yaitu senyawa homoorientin dengan *energy Gibbs* terendah -9,3 kcal/mol, lalu untuk senyawa yang memiliki *energy Gibbs* terendah saat berinteraksi dengan reseptor 3LN1 yaitu senyawa apigenin dengan *energy Gibbs* terendah -9,9 kcal/mol. Hasil *molecular dynamic* pada senyawa homoorintin terhadap reseptor COX-1 memiliki nilai RMSD 2,400748 1,095145 dan nilai RMSF 1,095145, untuk senyawa apigenin terhadap reseptor COX-2 yaitu memiliki nilai RMSD 3,255918 dan nilai RMSF 1,368337. Berdasarkan hasil simulasi molekular dinamik dari interaksi senyawa flavonoid terhadap reseptor *cyclooxygenase-1* dan *cyclooxygenase-2* terlihat bahwa turunan flavonoid (homoorientin) memiliki interaksi yang cukup stabil terhadap reseptor *cyclooxygenase-1* (1EQG) dibandingkan dengan interaksi antara *cyclooxygenase-2* (3LN1) dan turunan apigenin.

**Kata Kunci :** *Cyclooxygenase-1*, *Cyclooxygenase-2*, Anti-Inflamasi, *Gynura procumbens*, *Molecular Docking*.

KARAWANG

## ABSTRACT

*Based on data from the World Health Organization (WHO), worldwide, there are around 11.9 million. The World Health Organization (WHO) advocates traditional medicine that utilizes potential natural ingredients. The method used in this study is in silico. This study aims to analyze the flavonoid derivatives contained in the leaves of the life connection have a stable interaction with the enzyme cyclooxygenase-1 (COX-1) and the enzyme cyclooxygenase-2 (COX-2) so that it can be predicted to have activity as an anti-inflammatory candidate. The results of the Virtual screening on the flavonoid derivatives of the leaves of life that interact with the 1EQG receptor there was one compound that had the lowest Gibbs free energy, namely homoorientin compounds with the lowest Gibbs energy of -9.3 kcal/mol, then for compounds that had the lowest Gibbs energy when interacting with the 3LN1 receptor, namely apigenin compounds with the lowest Gibbs energy of -9.9 kcal/mol. The molecular dynamic results of homoorintin compounds against COX-1 receptors had an RMSD value of 2.400748 1.095145 and an RMSF value of 1.095145, for apigenin compounds against COX-2 receptors, which had an RMSD value of 3.255918 and an RMSF value of 1.368337. Based on the results of dynamic molecular simulation of the interaction of flavonoid compounds with cyclooxygenase-1 and cyclooxygenase-2 receptors, it was seen that flavonoid derivatives (homoorientin) had fairly stable interactions with cyclooxygenase-1 receptors (1EQG) compared to the interactions between cyclooxygenase-2 (3LN1) and apigenin derivatives.*

**Keyword :** Cyclooxygenase-1, Cyclooxygenase-2, Anti-Inflammatory, *Gynura procumbens*, Molecular Docking.