ABSTRAK

ANALISIS INTERAKSI DARI SENYAWA AKTIF DAUN JAMBU BIJI (*Psidium guajava)* TERHADAP RESEPTOR CAR dan PXR SECARA *MOLECULAR DOCKING*

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Latar Belakang : Menurut riset Kesehatan Dasar penggunaan obat herbal di indonesia pada tahun 2018 mencapai 59,12%. Daun jambu biji sering digunakan bersama obat konvensional sebagai pengobatan alternatif. Daun jambu biji dapat menginduksi aktivitas antiplatelet dan antikoagulan dan memperlambat metabolisme warfarin. Daun jambu biji memiliki senyawa aktif seperti kuerstin, asam galat, dan asam elagat yang bersifat lipofilik sehingga berkemungkinan dapat berinteraksi dengan reseptor nuclear. Reseptor CAR dan PXR berperan dalam mengatur ekspresi enzim metabolisme obat fase I dan II. Adanya interaksi antara kuersetin, asam galat, dan asam elagat dengan reseptor CAR dan PXR dapat berisko menyebabkan interaki obat-herbal. Sehingga peneliti ingin meneliti interaksi senyawa aktif daun jambu biji dengan reseptor CAR dan PXR menggunakan *molecular docking*.

Metodologi : Penelitian menggunakan metode *molecular docking* untuk mengetahui energi ikatan dan jenis ikatan. Hasil penelitian dibandingkan dengan kontrol positif yaitu fenitoin untuk reseptor CAR dan hiperforin untuk reseptor PXR.

Hasil Penelitian : Kuersetin memiliki energi ikatan terendah dibandingan asam galat, asam elagat dan kontrol positif PXR yaitu -9,2 terhadap reseptor CAR dan -8,7 terhadap reseptor PXR.

Kesimpulan : Kuersetin berinteraksi paling kuat tehadap CAR dan PXR dibandingkan asam galat dan asam elagat.

Kata Kunci : Kuersetin, Asam Galat, Asam elagat, Reseptor CAR, Reseptor PXR, *Molecular docking.*

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ABSTRACT

THE ANALYSIS OF INTERACTION IN ACTIVE COMPOUNDS OF GUAVA LEAVES (*Psidium guajava*) ON CAR AND PXR RECEPTORS BY MOLECULAR DOCKING

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Background: According to Basic Health research, the use of herbal medicines in Indonesia in 2018 reached 59.12%. Guava leaves are often used with conventional medicine as an alternative treatment. Guava leaves can induce antiplatelet and anticoagulant activity and slow down the metabolism of warfarin. Guava leaves have active compounds such as querstin, gallic acid, and elagatic acid which are lipophilic so they are likely to be able to interact with nuclear receptors. CAR receptors and PXR play a role in regulating the expression of phase I and II drug metabolizing enzymes. The interaction between quercetin, gallic acid, and ellagic acid with CAR and PXR receptors can lead to drug-herbal interactions. So researchers want to examine the interaction of active compounds in guava leaves with CAR and PXR receptors using molecular docking.

Methodology: The study used molecular docking to determine bond energies and types. The study's results were compared with positive controls, namely phenytoin for CAR receptors and hyperforin for PXR receptors.

Results: :Quercetin has the lowest binding energy compared to gallic acid, elagic acid and PXR positive control, namely -9.2 for the CAR receptor and -8.7 for the PXR receptor.

Conclusion: Quercetin interacts most strongly with CAR and PXR compared to gallic acid and ellagic acid.

Keywords: Quercetin, Gallic Acid, Ellagic Acid, CAR Receptors, PXR Receptors, Molecular docking

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