# ABSTRAK

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Judul : *Molecular Docking* Senyawa Saponin dan Flavonoid Daun Sirsak (*Annona Muricata* Linn.) Terhadap Reseptor Siklooksigenase (COX-2) Sebagai Analgetik-Antiinflamasi

Daun sirsak mengandung senyawa flavonoid dan saponin yang mempunyai aktivitas penghambatan secara molekuler sebagai antiinflamasi. Penelitian ini bertujuan untuk memahami aktivitas *molecular docking* senyawa saponin dan flavonoid daun sirsak (*Annona Muricata* L.) terhadap reseptor siklooksigenase-2 (COX-2) sebagai antiinflamasi. Penelitian diawali dengan memprediksi sifat fisikokimia yang mengacu pada parameter *Lipinski's Rule of Five*. Model protein yang digunakan adalah 4COX. Preparasi reseptor dan *ligand* menggunakan aplikasi YASARA. *Docking* dilakukan menggunakan PLANTS, cmd, wingwm.dll, dan notepad. Reseptor 4COX dinyatakan valid karena memiliki nilai RMSD <2Å. Hasil dari penelitian ini senyawa bioaktif saponin, yaitu Beta-Amyrine, 2,3-Epoxydasqualene, Gypsogenin, Annoionol A, Annionol B, dan Annoionol C dan senyawa bioaktif flavonoid yaitu, Apigenin-6-C-Glucoside, Argentinine, Catechin, Daidzein, Epicatechin, Gallocatechin, Genistein, Glycitein, Isoferulic Acid, Kaempferol, Quercetin, Robinetin, dan Tengeretin dari tanaman daun sirsak (*Annona muricata* Linn.) mempunyai sifat *druglikeness* sebagai kandidat obat baru, senyawa 2,3-epoxydasqualene memiliki skor *docking* yaitu -120.208 yang dapat berpotensi sebagai antiinflamasi terhadap protein (PDB ID: 4COX) dibanding dengan obat Indomethacin (IMN) skor *docking* -106.541, sifat farmakokinetik dari senyawa 2,3-epoxydasqualene sangat baik, untuk dijadikan kandidat senyawa obat baru dengan sifat farmakokinetik absorpsi yaitu 91,045%, distribusi 0,422 L/kg, di metabolisme substrat CYP3A4, ekskresi dengan nilai 1,396 log/kg, dan toksisitas yang rendah dengan nilai 1,622 mol/kg.

Kata Kunci: *Annona Muricata* L., Antiinflamasi, Flavonoid, *Molecular Docking*, Saponin

## ABSTRACT

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Study : Pharmacy

Title : Molecular Docking of Saponin and Flavonoid Compounds in Soursop Leaves (*Annona Muricata* Linn.) Against Cyclooxygenase (COX-2) Receptors as Analgetic-AntiInflammation

Soursop leaves contain flavonoid and saponin compounds that have molecular inhibitory activity as anti-inflammatory. This study aims to understand the molecular docking activity of saponin and flavonoid compounds of soursop leaves (*Annona Muricata* L.) against cyclooxygenase-2 (COX-2) receptor as anti-inflammatory. The research began by predicting physicochemical properties that refer to Lipinski's Rule of Five parameters. The protein model used was 4COX. Preparation of receptor and ligand using YASARA application. Docking was done using PLANTS, cmd, wingwm, and notepad. The 4COX receptor was declared valid because it had an RMSD value <2Å. The results of this study are bioactive saponin compounds, namely Beta-Amyrine, 2,3-Epoxydasqualene, Gypsogenin, Annoionol A, Annionol B, and Annoionol C and bioactive flavonoid compounds namely, Apigenin-6-C-Glucoside, Argentinine, Catechin, Daidzein, Epicatechin, Gallocatechin, Genistein, Glycitein, Isoferulic Acid, Kaempferol, Quercetin, Robinetin, and Tengeretin from soursop leaves (*Annona muricata* Linn. ) has druglikeness as a new drug candidate, compound 2,3-epoxydasqualene has a docking score of -120. 208 which can have potential as an anti-inflammatory against protein (PDB ID: 4COX) compared to the drug Indomethacin (IMN) docking score of -106. 541, the pharmacokinetic properties of the compound 2,3-epoxydasqualene are very good, to be used as a candidate for new drug compounds with pharmacokinetic properties of absorption which is 91.045%, distribution of 0.422 L/kg, in the metabolism of CYP3A4 substrates, excretion with a value of 1.396 log/kg, and low toxicity with a value of 1.622 mol/kg.



Keywords: *Annona Muricata* L., Molecular Docking, Flavonoids, Saponins, Anti-inflammatory