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**“STUDI *IN SILICO* SENYAWA AKTIF KAYU SECANG (*CAESALPINIA
SAPPAN L.*) SEBAGAI INHIBITOR EGFR PADA KANKER PARU TIPE
NSCLC”**

Latar Belakang: Kanker paru merupakan penyebab utama kematian akibat kanker, dengan Non-Small Cell Lung Cancer (NSCLC) mencakup sekitar 85% kasus. Mutasi *Epidermal Growth Factor Receptor* (EGFR) berperan dalam proliferasi dan kelangsungan hidup sel kanker sehingga menjadi target terapi. Namun, penggunaan EGFR-TKI seperti erlotinib masih menghadapi resistensi dan efek samping. Kayu secang (*Caesalpinia sappan L.*) mengandung senyawa brazilin, butein, dan sappanchalcone yang berpotensi sebagai antikanker.

Tujuan: Menganalisis dan membandingkan potensi ikatan brazilin, butein, dan sappanchalcone terhadap protein EGFR secara *in silico*.

Metode: Penelitian eksploratif menggunakan metode *molecular docking*. Struktur EGFR (PDB ID: 1M17) diperoleh dari Protein Data Bank dan ligan dari PubChem. Preparasi dilakukan dengan BIOVIA Discovery Studio dan AutoDockTools, kemudian docking menggunakan AutoDock Vina. Parameter yang dianalisis adalah nilai *binding affinity* dan interaksi residu sisi aktif.

Hasil: Ketiga senyawa mampu berikatan dengan EGFR. Sappanchalcone menunjukkan nilai *binding affinity* paling rendah, diikuti brazilin dan butein, serta membentuk interaksi hidrogen dan hidrofobik pada sisi aktif protein.

Kesimpulan: Senyawa aktif kayu secang, terutama sappanchalcone, berpotensi sebagai inhibitor EGFR pada NSCLC berdasarkan analisis *in silico* dan memerlukan validasi lebih lanjut secara eksperimental.

Kata Kunci: NSCLC, EGFR, *molecular docking*, *Caesalpinia sappan L.*, brazilin, butein, sappanchalcone.

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**“IN SILICO STUDY OF ACTIVE COMPOUNDS FROM SAPPAN WOOD
(CAESALPINIA SAPPAN L.) AS EGFR INHIBITORS IN NON-SMALL
CELL LUNG CANCER (NSCLC)”**

Background: Lung cancer is a leading cause of cancer-related mortality, with Non-Small Cell Lung Cancer (NSCLC) accounting for approximately 85% of cases. Mutations in the Epidermal Growth Factor Receptor (EGFR) play a crucial role in cancer cell proliferation and survival, making EGFR a major therapeutic target. However, resistance and adverse effects limit the long-term use of EGFR-TKIs such as erlotinib. *Caesalpinia sappan* L. (*sappan wood*) contains bioactive compounds, including brazilin, butein, and sappanchalcone, which have potential anticancer properties.

Objective: To analyze and compare the binding potential of brazilin, butein, and sappanchalcone against EGFR protein using an *in silico* approach.

Methods: This exploratory bioinformatics study employed molecular docking. The 3D structure of EGFR (PDB ID: 1M17) was obtained from the Protein Data Bank, and ligand structures were retrieved from PubChem. Protein and ligand preparation were conducted using BIOVIA Discovery Studio and AutoDockTools, followed by docking simulation with AutoDock Vina. Binding affinity values and interactions at active site residues were analyzed.

Results: All compounds demonstrated binding interactions with EGFR. Sappanchalcone showed the lowest binding affinity, followed by brazilin and butein, forming hydrogen and hydrophobic interactions at the active site.

Conclusion: Active compounds from *Caesalpinia sappan* L., particularly sappanchalcone, show potential as EGFR inhibitors in NSCLC based on *in silico* analysis and require further experimental validation.

Keywords: NSCLC, EGFR, molecular docking, *Caesalpinia sappan* L., brazilin, butein, sappanchalcone.