ANALISIS *IN SILICO* SENYAWA GENISTEIN KEDELAI (*Glycine max* L.) SEBAGAI INHIBITOR VEGFR-2 TERHADAP KANKER PAYUDARA

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ABSTRAK

ANALISIS *IN SILICO* SENYAWA GENISTEIN KEDELAI (*Glycine max* L.) SEBAGAI INHIBITOR VEGFR-2 TERHADAP KANKER PAYUDARA

Vascular Endothelial Growth Factor Receptor (VEGFR) adalah sekelompok reseptor yang memainkan peran penting dalam proses angiogenesis, yang merupakan mekanisme kunci dalam perkembangan kanker payudara. Terdapat tiga jenis utama VEGFR, yaitu VEGFR-1, VEGFR-2, dan VEGFR-3. Salah satu pendekatan terapeutik dalam pengobatan kanker payudara adalah pengembangan obat alami yang dapat menghambat angiogenesis dengan menargetkan VEGFR-2. Tivozanib sebagai salah satu penghambat angiogenesis telah digunakan dalam pengobatan kanker, penggunaan obat ini sering kali disertai dengan efek samping yang signifikan. Oleh karena itu, penelitian untuk menemukan alternatif pengobatan yang lebih aman dan efektif sangat diperlukan untuk meningkatkan terapi kanker payudara. Genistein dari kedelai (*Glycine max* L.) muncul sebagai kandidat potensial untuk pengembangan terapi kanker payudara yang lebih aman dan efektif. Metode yang digunakan adalah observasional deskriptif secara *in silico* melalui *molecular docking* menggunakan perangkat lunak PyRx (*Autodock Vina*, Open Babel), BIOVIA *Discovery Studio Visualizer*, dan PyMOL. Protein target yang digunakan adalah VEGFR-2 dengan kode PDB ID: 4ASE. Ligan natif (kontrol) yang digunakan adalah senyawa tivozanib (CID: 9911830) dan ligan uji senyawa genistein (CID: 5280961). Hasil penelitian menunjukkan senyawa genistein mampu berikatan pada protein reseptor VEGFR-2 dengan posisi yang sama dengan ligan natif. Afinitas pengikatan genistein sebesar -8,6 kkal/mol dengan standar deviasi 0,377 menunjukkan bahwa hasil ini lebih baik dibandingkan dengan ligan natif (kontrol). Senyawa genistein memenuhi syarat hukum lima Lipinski, uji toksisitas, uji permeabilitas membran, dan uji bioaktivitas. Berdasarkan hasil tersebut dapat dinyatakan bahwa senyawa genistein berpotensi sebagai kandidat obat kanker payudara secara *in silico*. Diperlukan penelitian secara *in vitro* dan *in vivo* untuk memastikan efektivitas genistein dalam menghambat angiogenesis pada kanker payudara.

Kata kunci: Antikanker, genistein, kanker payudara, kedelai, *in silico*, VEGFR-2, *molecular docking*

ABSTRACT
IN SILICO ANALYSIS OF SOYBEAN GENISTEIN (*Glycine max* L.) AS A VEGFR-2 INHIBITOR AGAINST BREAST CANCER

Vascular Endothelial Growth Factor Receptor (VEGFR) is a group of receptors that play a crucial role in the process of angiogenesis, a key mechanism in breast cancer development. There are three main types of VEGFR: VEGFR-1, VEGFR-2, and VEGFR-3. Therapeutic approach in breast cancer treatment is the development of natural compounds that can inhibit angiogenesis by targeting VEGFR-2. Tivozanib, as an angiogenesis inhibitor, has been used in cancer treatment, but its use is often accompanied by significant side effects. Therefore, research to find safer and more effective treatment alternatives is essential to improve breast cancer therapy. Genistein from soybeans (*Glycine max* L.) has emerged as a potential candidate for the development of safer and more effective breast cancer therapies. The method used is a descriptive observational approach through in silico molecular docking using the PyRx software (Autodock Vina, Open Babel), BIOVIA Discovery Studio Visualizer, and PyMOL. The target protein used is VEGFR-2 with the PDB ID: 4ASE. The native ligand (control) used is the tivozanib compound (CID: 9911830), and the test ligand is the genistein compound (CID: 5280961). The results show that genistein can bind to the VEGFR-2 receptor protein at the same position as the native ligand. The binding affinity of genistein is -8,6 kcal/mol with a standard deviation of 0,377 indicating that this result is better than the native ligand (control). Genistein meets the requirements Lipinski's rules of five, toxicity test, membrane permeability test, and bioactivity test. Based on these results, it can be concluded that genistein has the potential to be a breast cancer drug candidate in silico. In vitro and in vivo studies are needed to confirm the effectiveness of genistein in inhibiting angiogenesis in breast cancer.

Key words: Anticancer, genistein, breast cancer, soybean, in silico, VEGFR-2, *molecular docking*

DAFTAR ISI

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