ABSTRAK

Skrinning Virtual dari Permodelan Farmakofor berbasis Ligan dari Turunan Germacranolide, dan Penambatan Molekul untuk Mengidentifikasi Inhibitor dari Topoisomerase

Oleh :

Jessica Aulia

191FF03062

Kanker adalah suatu kondisi dimana sel-sel abnormal tumbuh di luar kendali pada bagian tubuh tertentu dan dapat menyerang jaringan lain sehingga membentuk sel kanker lainnya. Sel kanker bersifat ganas dan bisa menyebabkan kematian. Jenis kanker payudara dan kanker serviks menjadi kematian terbanyak pada wanita di negara maju dan berkembang. Pengobatan kanker serviks yang dilakukan antara lain pembedahan, radioterapi, dan kemoterapi. Pengobatan yang dilakukan penderita kanker serviks memberikan dampak fisik secara langsung bagi penderitanya yakni mudah lelah, perubahan warna kulit, maupun penurunan berat badan secara drastis. Berbagai bahan alam dikembangkan sebagai terapi alternatif untuk kanker serviks, salah satunya yang berpotensi yaitu tanaman anviella garcinii yang mengandung senyawa germacranolide yang berpotensi sebagai anti kanker serviks. Tujuan penelitian ini untuk memperoleh hits yang berpotensi sebagai anti kanker serviks. Metode yang digunakan yaitu penelitian secara *in silico* dimulai dari preparasi bahan yang diperlukan, Virtual Screening (VS), dan dilanjutkan penambatan molekul. Hasil preparasi bahan digunakan sebanyak 5 training set isolat germacranolide, diperoleh dataset aktif sebanyak 32 senyawa, 1.152 decoys, dan database ZINC Natural Product sebanyak 270.547 senyawa. Hits hasil VS berbasis farmakofor dihasilkan sebanyak 1000 senyawa, sedangkan hits VS berbasis docking diperoleh sebanyak 224 senyawa. Berdasarkan hasil analisis interaksi, diperoleh tiga hits terbaik yaitu ZINC000252515534, ZINC000079216817, dan ZINC000085594035. Senyawa ZINC000252515534 memiliki energi ikatan lebih negatif dibandingkan dengan hits lainnya sehingga dapat disimpulkan memiliki potensi paling tinggi sebagai anti kanker serviks

Kata kunci: Kanker Serviks, Germacranolide, Anviella Garcinii, Virtual Screening, Penambatan molekul

ABSTRACT

Virtual Screening of Ligand-Based Pharmacophore Modeling of Germacranolide Derivatives, and Molecular Anchoring to Identify Topoisomerase Inhibitors

By :

Jessica Aulia

191FF03062

Cancer is a condition in which abnormal cells grow out of control in certain parts of the body and can invade other tissues to form other cancer cells. Cancer cells are malignant and can cause death. Types of breast cancer and cervical cancer are the most common causes of death for women in developed and developing countries (Dewi, 2017). Treatment for cervical cancer includes surgery, radiotherapy, and chemotherapy. Treatment performed by cervical cancer sufferers has a direct physical impact on sufferers, namely fatigue, changes in skin color, and drastic weight loss. Various natural products have been developed as alternative therapies for cervical cancer, one of which has the potential to be the Anviella garcinii plant which contains a germacranolide compound which has the potential to act as an anti-cervical cancer. The purpose of this study is to obtain hits that have the potential as an anti-cervical cancer. The method used is *in silico* research starting from the preparation of the required materials, Virtual Screening (VS), and continuing with molecular docking. The results of the material preparation used 5 training sets of germacranolide isolates, obtained an active dataset of 32 compounds, 1,152 decoys, and the ZINC Natural Product database of 270,547 compounds. Pharmacophore-based VS hits resulted in 1000 compounds, while docking-based VS hits resulted in 224 compounds. Based on the results of the interaction analysis, the three best hits were ZINC000252515534, ZINC000079216817, and ZINC000085594035. The ZINC000252515534 compound has more negative bond energy compared to other hits, so it can be concluded that it has the highest potential as an anti-cervical cancer.

Keywords: Cervical Cancer, Germacranolide, Anviella Garcinii, Virtual Screening, Molecular docking