PENAMBATAN MOLEKULER SENYAWA DERIVAT BRAZILIN SEBAGAI ANTIKANKER PAYUDARA

SKRIPSI

MOCH MULKY APRIANSYAH
A233013

SEKOLAH TINGGI FARMASI INDONESIA
YAYASAN HAZANAH
BANDUNG
2025

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Sebagai salah satu syarat untuk memperoleh gelar Sarjana Farmasi

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Disetujui oleh :

Pembimbing	Pembimbing
Dr. apt. Adang Firmansyah, M.Si.	**Dr. Syarif Hamdani, M.Si.**

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ABSTRAK

Kanker merupakan penyakit yang ditandai dengan adanya sel abnormal yang bisa berkembang tanpa terkendali dan memiliki kemampuan untuk berpindah antar sel dan jaringan tubuh. Salah satu jenis kanker yang memiliki prevalensi kejadian paling banyak adalah kanker payudara. Brazilin diketahui memiliki aktivitas antikanker. Penelitian ini bertujuan untuk mengetahui aktivitas antikanker brazilin dan derivatnya, yaitu tetra-asetil brazilin (senyawa A), tri-benzil brazilin (senyawa B), tri-metoksi brazilin (senyawa C), dan 5-propan-brazilin (senyawa D) terhadap beberapa reseptor pada kanker payudara menggunakan metode penambatan molekuler. Reseptor yang digunakan adalah estrogen alfa dengan ligan asli hidroksitamoksifen, progesteron dengan ligan asli progesteron, HER2 dengan ligan asli pirolopirimidin, androgen dengan ligan asli androstenedion, siklooksigenase-2 dengan ligan asli indometasin, PD-1/PD-L1 dengan ligan asli etilenetanamid, FGFR dengan ligan asli ponatinib, dan IGF-1R dengan ligan asli hidantoin. Reseptor, brazilin, dan derivatnya dipreparasi menggunakan aplikasi *Biovia Discovery Studio 2021*, kemudian validasi dan penambatan molekuler dilakukan menggunakan *AutoDockTools* 1.5.7. Hasil penambatan molekuler menunjukkan bahwa brazilin memiliki hasil penambatan yang paling baik terhadap reseptor estrogen alfa; senyawa A memiliki hasil penambatan yang paling baik terhadap reseptor progesteron, androgen, dan PD-1/PD-L1; senyawa B memiliki hasil penambatan yang paling baik terhadap reseptor HER2; senyawa C; dan D tidak memiliki hasil penambatan yang paling baik dari semua reseptor.

Kata kunci: brazilin, derivat, kanker payudara, penambatan molekuler

ABSTRACT

Cancer is a disease characterized by the presence of abnormal cells that can grow uncontrollably and can move between cells and body tissues. One type of cancer that has the highest prevalence of occurrence is breast cancer. Brazilin is known to have anticancer activity. This study aims to determine the anticancer activity of brazilin and its derivatives, namely tetra-acetyl brazilin (compound A), tri-benzyl brazilin (compound B), tri-methoxy brazilin (compound C), and 5-propane-brazilin (compound D) against several receptors in breast cancer using molecular docking methods. The receptors used were estrogen alpha with native ligand hydroxytamoxifen, progesteron with native ligand progesteron, HER2 with native ligand pyrrolopyrimidine, androgen with native ligand androstenedione, cyclooxygenase-2 with native ligand indomethacin, PD-1/PD-L1 with native ligand ethylethanamide, FGFR with native ligand ponatinib, and IGF-1R with native ligand hydantoin. Receptors, brazilin, and its derivatives were prepared using the Biovia Discovery Studio 2021, then validation and molecular docking were carried out using the AutoDockTools 1.5.7. The molecular docking results showed that brazilin had the best docking results against the estrogen alpha receptor; compound A had the best docking results against the progesteron, androgen, and PD-1/PD-L1 receptors; compound B had the best docking results against the HER2 receptor; compound C; and D does not have the best docking results of all the receptors.

Keywords: *brazilin, derivative, breast cancer, molecular docking*

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