PENAMBATAN MOLEKUL DAN SIMULASI DINAMIKA MOLEKUL SENYAWA TERPENOID GENUS AMOMUM PADA TARGET RESEPTOR ESTROGEN ALFA SEBAGAI AGEN ANTIKANKER PAYUDARA

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ABSTRAK

Kanker payudara merupakan kanker paling umum pada wanita dengan angka kematian tinggi. Terapi kanker seperti kemoterapi sering menimbulkan efek samping dan resistansi, sehingga diperlukan alternatif terapi yang lebih efektif dan selektif. Reseptor estrogen alfa (ERα) berperan penting dalam perkembangan kanker payudara hormonal. Genus Amomum dari famili Zingiberaceae diketahui mengandung senyawa terpenoid yang berpotensi sebagai agen antikanker. Penelitian ini bertujuan mengevaluasi potensi senyawa terpenoid dari Amomum sebagai inhibitor ERα melalui pendekatan *in silico* menggunakan metode penambatan molekul dan simulasi dinamika molekul. Hasil penambatan molekul menunjukkan ligan uji T31 dan T35 memiliki afinitas yang baik dengan energi bebas ikatan dan konstanta inhibisi mendekati performa ligan alami Tamoxifen. T31 dan T35 membentuk ikatan hidrogen dengan residu penting ARG394 dan GLU353 serta membentuk interaksi hidrofobik dengan residu LUE387, MET388 dan LEU391. Berdasarkan perhitungan energi bebas pengikatan dengan MMGBSA menunjukkan T35 memiliki afinitas pengikatan kuat sebesar −49,32 kcal/mol. Namun T31 memiliki stabilitas paling baik berdasarkan grafik nilai RMSD dan nilai RMSF yang lebih stabil serta fluktuasi yang rendah di situs aktif ERα. Maka, dapat dikatakan ligan uji T31 (*Kravanhin A*.) dan T35 (*4-(2-((1S,4aR,5R,6S,8aR)-6-hydroxy-5-(hydroxymethyl)-5,8a dimethyl l-2-methylenedecahydronaphthalen-1-yl)ethyl)furan-2(5H)-one*) dari genus Amomum berpotensi sebagai kandidat agen antikanker payudara dan layak dikembangkan lebih lanjut.

Kata kunci: antikanker payudara, reseptor estrogen alfa, terpenoid, penambatan molekul, simulasi dinamika molekul.

Molecular Docking and Molecular Dynamics Simulation of Terpenoid Compounds from Amomum Genus on Estrogen Receptor Alpha Target as Breast Cancer Anticancer Agents

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ABSTRACT

Breast cancer is the most common cancer in women and is associated with a high mortality rate. Conventional therapies such as chemotherapy often cause side effects and resistance, highlighting the need for more effective and selective alternatives. Estrogen receptor alpha (ERα) plays a crucial role in the progression of hormone-dependent breast cancer. The Amomum genus from the Zingiberaceae family is known to contain terpenoid compounds with potential anticancer activity. This study aims to evaluate the potential of terpenoid compounds from Amomum as ERα inhibitors through an in silico approach using molecular docking and molecular dynamics simulation methods. The molecular docking results showed that test ligands T31 and T35 exhibited good binding affinity, with binding free energy and inhibition constants comparable to the natural ligand, Tamoxifen. T31 and T35 formed hydrogen bonds with key residues ARG394 and GLU353, as well as hydrophobic interactions with LEU387, MET388, and LEU391. Binding free energy calculations using the MMGBSA method indicated that T35 had strong binding affinity with a value of −49.32 kcal/mol. However, T31 demonstrated the best stability based on the RMSD and RMSF plots, showing more consistent values and lower fluctuations at the ERα active site. Therefore, T31 (*Kravanhin A.*) *and T35* (*4-(2-((1S,4aR,5R,6S,8aR)-6-hydroxy-5-(hydroxymethyl)-5,8a dimethyl l-2-methylenedecahydronaphthalen-1-yl)ethyl)furan-2(5H)-one*) *from the Amomum genus show potential as candidate breast cancer agents and warrant further development.*

Keywords: *breast anticancer, estrogen receptor alpha, terpenoids, molecular docking, molecular dynamics simulation.*