# PENAMBATAN MOLEKUL DAN SIMULASI DINAMIKA MOLEKUL SENYAWA KIMIA DARI TANAMAN ALGA COKELAT (*Dictyota dichotoma*) TERHADAP RESEPTOR ANDROGEN SEBAGAI ANTIKANKER PROSTAT

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## ABSTRAK

Kanker prostat merupakan salah satu penyebab utama kematian akibat kanker pada pria. *Androgen Deprivation Therapy* (ADT) yang digunakan saat ini sering menimbulkan efek samping serius, sehingga diperlukan alternatif terapi yang lebih aman dan efektif. Penelitian ini bertujuan untuk mengevaluasi potensi senyawa dari alga cokelat (*Dictyota dichotoma*) sebagai inhibitor reseptor androgen (AR) menggunakan pendekatan *in silico*. Sebanyak 122 senyawa diunduh dari basis data PubChem dan diseleksi berdasarkan *Lipinski's Rule of Five*, menghasilkan 93 senyawa yang lolos kriteria *drug-likeness*. Proses *docking* dilakukan menggunakan AutoDock, sedangkan stabilitas kompleks dianalisis melalui simulasi dinamika molekul dengan GROMACS. Hasil *docking* menunjukkan bahwa senyawa S116, S100, dan S77 memiliki afinitas ikatan terbaik berdasarkan nilai ΔG dan Ki. Visualisasi interaksi molekul memperlihatkan pembentukan ikatan hidrogen dan hidrofobik pada residu kunci seperti Thr877, Gln711, dan Leu704. Berdasarkan perhitungan MMGBSA, senyawa S100 dan S116 memiliki energi pengikatan total terendah, menunjukkan potensi kuat sebagai kandidat antikanker prostat. Studi ini menyimpulkan bahwa senyawa dari *Dictyota dichotoma*, khususnya S100 dan S116, memiliki prospek sebagai inhibitor reseptor androgen.

**Kata kunci:** Androgen, kanker prostat, penambatan molekul, simulasi dinamika molekul, *Dictyota dichotoma*, *in silico*

# MOLECULAR DOCKING AND MOLECULAR DYNAMICS SIMULATION OF CHEMICAL COMPOUNDS FROM BROWN ALGAE (*Dictyota dichotoma*) AGAINST ANDROGEN RECEPTOR AS A PROSTATE CANCER INHIBITOR

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## ABSTRACT

Prostate cancer is one of the leading causes of cancer-related deaths in men. Current therapies such as Androgen Deprivation Therapy (ADT) often result in severe side effects, prompting the need for safer and more effective alternatives. This study aims to evaluate the potential of compounds derived from the brown algae *Dictyota dichotoma* as androgen receptor (AR) inhibitors through an in silico approach. A total of 142 compounds were obtained from the PubChem database and screened using Lipinski's Rule of Five, resulting in 93 drug-like candidates. Molecular docking was conducted using AutoDock, and the stability of the complexes was further analyzed via molecular dynamics simulation using GROMACS. Docking results identified compounds S116, S100, and S77 as top candidates with strong binding affinity based on ΔG and Ki values. Molecular interaction visualization revealed the formation of hydrogen and hydrophobic bonds with key residues such as Thr877, Gln711, and Leu704. MMGBSA calculations indicated that compounds S100 and S116 exhibited the lowest total binding free energy, highlighting their potential as anti-prostate cancer agents. This study concludes that *Dictyota dichotoma* compounds, particularly S100 and S116, are promising candidates for androgen receptor inhibition.

**Keywords:** Androgen, prostate cancer, molecular docking, molecular dynamics simulation, *Dictyota dichotoma*, in silico