ABSTRAK

STUDI BIOINFORMATIKA DAN *MOLECULAR DOCKING* SENYAWA GALANGIN TERHADAP KANKER SERVIKS

Iffah Hasmo Nur Septianing[1], Nur Amalia Choironi[2], Sarmoko[3]

Latar Belakang : Kanker serviks menduduki peringkat keempat kanker paling umum pada wanita secara global. Pengobatan kemoradioterapi disebut paling efektif tetapi banyak mengalami resistensi. Galangin secara *in vitro* diketahui mempunyai aktivitas antikanker serviks pada sel hela. Penelitian in silico ini bertujuan untuk mengetahui target molekuler, energi ikatan dan jenis ikatan senyawa galangin pada kanker serviks.

Metodologi : Analisis bioinformatika dilakukan melalui NCBI, STITCH, STRING, venny 2.1 hingga didapatkan PTTGs yang kemudian dianalisis menggunakan webgestalt dan dicari *top 10 hub gene* melalui cytoscape. Protein potensial dilakukan *molecular docking* dengan galangin menggunakan AutoDock Vina dan divisualisasikan menggunakan DS BIOVIA.

Hasil Penelitian : *Top 10 hub gene* yaitu VEGFA, AKT1, MMP2, CD44, TNF, STAT3, CYP1A1, TGFB1, IL6, dan FN1. AKT1 dan MMP2 berhasil memenuhi parameter validasi *molecular docking* dengan RMSD ≤ 2 Å. MMP2 menjadi protein target terpilih karena memiliki energi ikatan lebih rendah dari kontrol positif marimastat dengan energi ikatan sebesar -8.3 kkal/mol dengan jenis ikatan hidrogen dan hidrofobik.

Kesimpulan : Senyawa galangin memiliki potensi sebagai antikanker serviks pada penambatan protein MMP2 dengan jenis ikatan hidrogen dan hidrofobik dan energi sebesar -8.3 kkal/mol.

Kata Kunci : Kanker serviks, galangin, bioinformatika, *molecular docking*

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ABSTRACT

BIOINFORMATICS AND MOLECULAR DOCKING STUDY OF GALANGIN COMPOUNDS ON CERVICAL CANCER

Iffah Hasmo Nur Septianing[1], Nur Amalia Choironi[2], Sarmoko[3]

Background : Cervical cancer maintains its fourth-place ranking in women globally. Chemoradiotherapy treatment is called the most effective but many experience resistance. Galangin has potential as an anticancer agent in Hela cells. This study aims to identify molecular targets, binding energy, and type of attachment of galangin compound in cervical cancer.

Methods : Bioinformatics analysis was carried out using NCBI, STITCH, STRING, Venny 2.1 until PTTGs were obtained which were then analyzed using webgestalt, and the top 10 hub genes were searched for via Cytoscape. Potential proteins were subjected to molecular docking with galangin using AutoDock Vina and visualized using DS BIOVIA.

Results : The top 10 hub genes are VEGFA, AKT1, MMP2, CD44, TNF, STAT3, CYP1A1, TGFB1, IL6, and FN1. AKT1 and MMP2 successfully fulfilled the molecular docking validation parameters with RMSD ≤ 2 Å. MMP2 was the chosen target protein because it has a lower binding energy than the positive control marimastat with a binding energy of -8.3 kcal/mol with hydrogen and hydrophobic bond types.

Conclusion : Galangin compound has the potential as a cervical anticancer by binding to the MMP2 with hydrogen and hydrophobic bonds and binding energy -8.3 kcal/mol.

Keywords : Cervical cancer, galangin, bioinformatic, molecular docking

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