ABSTRAK

ANALISIS BIOINFORMATIKA DAN *MOLECULAR DOCKING* SENYAWA ETIL P-METOKSI SINAMAT (EPMS) PADA PROTEIN-PROTEIN YANG TERLIBAT DALAM JALUR PERSINYALAN KANKER PAYUDARA LUMINAL

Latar Belakang : Kanker payudara luminal menyumbang sekitar 70% dari semua jenis kanker payudara, namun terapi pengobatannya banyak mengalami resistensi. Sehingga diperlukan eksplorasi senyawa berkhasiat dari bahan alam, salah satunya yaitu Etil P-Metoksi Sinamat (EPMS) yang memiliki aktivitas sitotoksik terhadap sel MCF-7. Penelitian ini bertujuan untuk mengetahui protein target potensial dan profil *molecular docking* senyawa EPMS terhadap kanker payudara luminal

Metodologi : Analisis bioinformatika menggunakan *database* GeneCards, Swiss Target Prediction dan dicari *Potential Target Theurepatic Genes (*PTTGs*)* melalui Venny 2.1. PTTGs dianalisis menggunakan WebGestalt untuk didapatkan informasi terkait ontologi gen, jalur KEGG, dan asosiasi obat serta diolah menggunakan Cytoscape untuk mendapatkan *top 10 hub gene*. Analisis *molecular docking* menggunakan ChemDraw, AutoDock Tools, PyMol, AutoDock Vina untuk mendapatkan energi ikatan dan divisualisasikan menggunakan DS Biovia

Hasil Penelitian : Hasil analisis bioinformatika didapatkan *top 10 hub gene* yaitu EGFR, CYP3A4, AKR1C3, ESR1, JAK2, AR, MMP9, ABL1, MAPK14, dan PTPN1. Analisis *molecular docking* senyawa EPMS terhadap ESR1, AR, MMP9, ABL1 dan PTPN1 menghasilkan energi ikatan yang lebih kecil daripada kontrol positif. Selain itu, EPMS juga mengikat residu asam amino pada sisi aktif masing masing protein.

Kesimpulan : Protein ESR1, AR, MMP9, ABL1, dan PTPN1 menghasilkan energi ikatan yang lebih kecil daripada kontrol positif sehingga memiliki potensi sebagai target aksi obat senyawa EPMS terhadap kanker payudara luminal

Kata Kunci : EPMS, Etil P- Metoksi Sinamat, Bioinformatika, *Molecular Docking*, Antikanker Payudara Luminal

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ABSTRACT

ANALYSIS OF BIOINFORMATICS AND MOLECULAR DOCKING OF ETHYL P-METHOXYCINNAMATE (EPMC) COMPOUND ON PROTEINS INVOLVED IN LUMINAL BREAST CANCER SIGNALING PATHWAYS

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Background: Luminal breast cancer accounts for 70% of all breast cancer types, yet many of its treatment therapies have shown resistance. Therefore, it is necessary to explore efficacious compounds derived from natural materials, one of which is Ethyl P-Methoxycinnamate (EPMC), which has cytotoxic activity against MCF-7 cells. This study aims to determine the potential target proteins and the molecular docking profile of the EPMC compound against luminal breast cancer.

Methodology: Bioinformatics analysis using the GeneCards, Swiss Target Prediction, and Venny 2.1 was used to find Potential Target Theurepatic Genes (PTTGs). PTTGs were analyzed using WebGestatl to obtain information related to gene ontology, KEGG pathways, and drug associations and then processed using Cytoscape to obtain the top 10 hub genes. Molecular docking analysis using ChemDraw, Autodock Tools, Pymol, AutoDock Vina to obtain information about bond energy and visualization using Biovia.

Research Results: Bioinformatics analysis results is Top 10 hub genes included EGFR, CYP3A4, AKR1C3, ESR1, JAK2, AR, MMP9, ABL1, MAPK14, and PTPN1. The molecular docking of the EPMC compound to ESR1, AR, MMP9, ABL1 and PTPN1 produced a lower bond energy than the positive control. They bind to amino acid residues on the active site of each protein.

Conclusion: The ESR1, MMP9, AR, ABL1, and PTPN1 proteins produce lower binding energy than the positive control, making them potential targets for the action of EPMC compound drug against luminal breast cancer.

Keywords: EPMS, Ethyl P-Methoxycinnamate, Bioinformatics, Molecular Docking, Luminal Breast Anticancer.

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