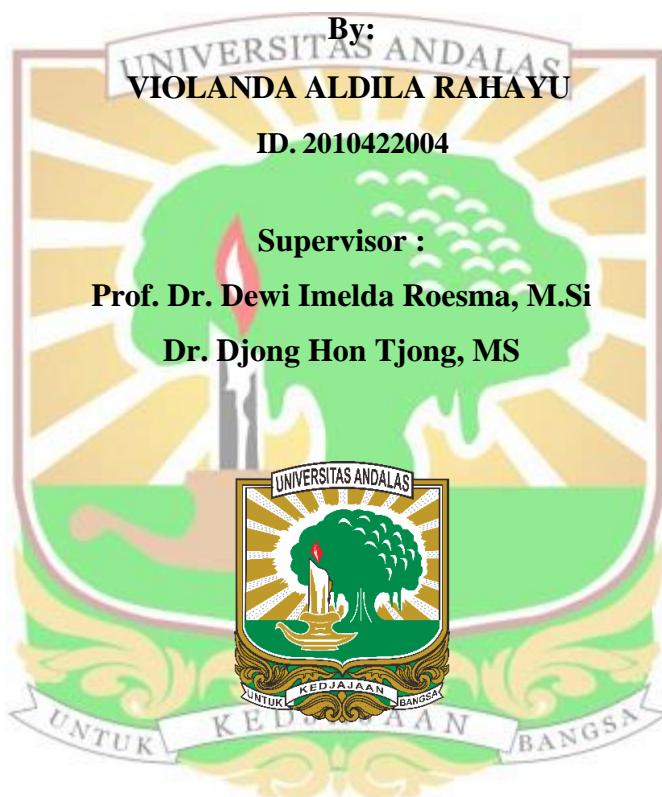


**IN SILICO STUDIES OF CAROTENOID ANTIOXIDANTS IN SAND
LOBSTER (*Panulirus homarus*) AS CANDIDATE ANTI-BREAST CANCER
COMPOUNDS**

UNDERGRADUATE THESIS



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ABSTRAK

Kanker payudara merupakan jenis kanker dengan tingkat diagnosa dan kematian tertinggi yang dialami oleh wanita di seluruh dunia. Di Indonesia, kanker payudara menempati peringkat teratas dalam data statistik kanker dengan 58.256 kasus dan jumlah kematian sebesar 22.692 kasus. Riset ini bertujuan untuk menganalisis potensi kandungan antioksidan karotenoid yang terkandung pada lobster pasir (*Panulirus homarus*) sebagai antikanker payudara secara *in silico*. Dalam riset ini digunakan enam senyawa karotenoid yaitu dinoxanthin, diadinoxanthin, zeaxanthin, lutein, astaxanthin, dan violaxanthin. Data struktur 3D kristal protein diperoleh dari Protein Data Bank (PDB) yaitu estrogen alfa (Kode PDB: 3ERT), estrogen beta (Kode PDB: 1X7J) dan aromatase (Kode PDB: 3S7S) sebagai reseptor antikanker. Kemudian, dilakukan analisis bioaktivitas dan analisis bioavailabilitas senyawa uji. Setelah itu, protein dan senyawa uji dipreparasi dan dilakukan docking terhadap reseptor estrogen alfa, estrogen beta dan aromatase yang divisualisasikan menggunakan Discovery Studio. Selanjutnya untuk melihat kestabilan ikatan melalui simulasi dinamika molekuler menggunakan software YASARA dynamics. Lalu, prediksi toksisitas menggunakan Protox Web Server (https://tox-new.charite.de/protox_II/). Hasil riset menunjukkan bahwa dua dari enam yaitu senyawa uji lutein dan violaxanthin menunjukkan aktivitas yang stabil sebagai inhibitor terhadap reseptor estrogen alfa, estrogen beta, dan aromatase serta tidak bersifat toksisitas terhadap tubuh sehingga berpotensi dijadikan sebagai kandidat senyawa anti kanker payudara.

Kata Kunci : Bioaktivitas, Bioavailabilitas, Lutein, Toxicity, Violaxanthin

ABSTRACT

Breast cancer is the most diagnosed and deadliest type of cancer among women worldwide. In Indonesia, breast cancer ranks at the top of cancer statistics with 58,256 cases and 22,692 deaths. This research aims to analyze the potential of carotenoid antioxidants found in the sand lobster (*Panulirus homarus*) as a breast cancer treatment candidate through an in silico approach. In this study, six carotenoid compounds were used: dinoxanthin, diadinoxanthin, zeaxanthin, lutein, astaxanthin, and violaxanthin, alongside natural ligands such as 4-hydroxytamoxifen, genistein, and exemestane, and controls like tamoxifen, metformin, and letrozole. The 3D crystal protein structures used for molecular docking were obtained from the Protein Data Bank (PDB), including estrogen alpha (PDB ID: 3ERT), estrogen beta (PDB ID: 1X7J), and aromatase (PDB ID: 3S7S) as anti-cancer receptors. Subsequently, bioactivity and bioavailability analyses of the test compounds were performed. The proteins and test compounds were prepared, followed by molecular docking against the estrogen alpha, estrogen beta, and aromatase receptors, with visualization performed using Discovery Studio. Molecular dynamics simulations were conducted using YASARA dynamics software to evaluate the stability of binding interactions. Toxicity prediction was carried out using the Protox Web Server (https://tox-new.charite.de/protox_II/). The research results indicate that two out of the six tested compounds, lutein and violaxanthin, exhibit stable inhibitory activity against estrogen receptor alpha, estrogen receptor beta, and aromatase. Additionally, these compounds demonstrate non-toxic properties, making them potential candidates for breast cancer treatment.

Keywords: Bioactivity, Bioavailability, Lutein, Toxicity, Violaxanthin