

ANALISIS INTERAKSI MOLEKULER SENYAWA AKTIF BAKTERI ENDOFIT AKAR KELAPA SAWIT SEBAGAI KANDIDAT ANTIFUNGI TERHADAP *Ganoderma boninense* SECARA IN SILICO

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ABSTRAK

Penyakit busuk pangkal batang yang disebabkan oleh *Ganoderma boninense* merupakan ancaman utama pada budidaya kelapa sawit. Pengendalian penyakit ini masih bergantung pada fungisida kimia sehingga diperlukan alternatif yang lebih ramah lingkungan. Pendekatan *in silico* melalui *molecular docking* dapat dimanfaatkan sebagai metode penyaringan awal dalam mengidentifikasi kandidat senyawa antifungi. Penelitian ini bertujuan menganalisis interaksi molekuler senyawa aktif bakteri endofit akar kelapa sawit terhadap protein target *Ganoderma boninense*, yaitu lakase (Lac), mangan peroksidase (MnP), dan lignin peroksidase (LiP) yang berperan dalam proses infeksi. Senyawa uji diperoleh dari hasil identifikasi GC-MS ekstrak bakteri endofit, sedangkan struktur 3D protein dimodelkan menggunakan *homology modeling* dan divalidasi sebelum dilakukan *molecular docking*. Simulasi *docking* dilakukan menggunakan AutoDock Vina dengan heksakonazol sebagai kontrol positif, kemudian dianalisis berdasarkan energi afinitas (ΔG), konstanta inhibisi (K_i), dan interaksi residu asam amino. Hasil menunjukkan bahwa 3,7-dimethyl-1-phenylsulfonyl-2,6-octadiene dan 1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester memiliki energi afinitas yang lebih rendah dibandingkan heksakonazol pada ketiga protein target. Nilai energi yang lebih rendah mengindikasikan afinitas pengikatan yang lebih kuat dan kestabilan kompleks ligan-protein lebih tinggi, sehingga kedua senyawa tersebut diprediksi memiliki potensi penghambatan yang lebih baik terhadap *Ganoderma boninense*. Hasil penelitian ini menunjukkan bahwa kedua senyawa tersebut berpotensi dikembangkan sebagai kandidat antifungi hayati terhadap *Ganoderma boninense* dan layak dikaji lebih lanjut melalui pengujian *in vitro* maupun *in vivo*.

Kata Kunci: Antifungi, bakteri endofit, *Ganoderma boninense*, *in silico*, *molecular docking*

IN SILICO MOLECULAR INTERACTION ANALYSIS OF ACTIVE COMPOUNDS FROM OIL PALM ROOT ENDOPHYTIC BACTERIA AS ANTIFUNGAL CANDIDATES AGAINST *Ganoderma boninense*

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ABSTRACT

Basal stem rot caused by *Ganoderma boninense* is one of the major threats to oil palm cultivation. Disease management still relies heavily on chemical fungicides, highlighting the need for more environmentally friendly alternatives. An *in silico* approach using molecular docking can serve as a preliminary screening method for identifying potential antifungal compounds. This study aimed to analyze the molecular interactions of active compounds derived from oil palm root endophytic bacteria with the target proteins of *G. boninense*, namely laccase (Lac), manganese peroxidase (MnP), and lignin peroxidase (LiP), which play important roles in the infection process. The tested compounds were obtained from GC-MS identification of endophytic bacteria extract, while the three-dimensional protein structures were constructed using homology modeling and validated prior to molecular docking. Docking simulations were performed using AutoDock Vina with hexaconazole as the positive control, and the resulting complexes were evaluated based on binding affinity (ΔG), inhibition constant (K_i), and amino acid residue interactions. The results showed that 3,7-dimethyl-1-phenylsulfonyl-2,6-octadiene and 1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester exhibited lower binding affinity values than hexaconazole against all three target proteins. Lower binding affinity values indicate stronger binding affinity and greater ligand–protein complex stability, suggesting that both compounds have a higher predicted inhibitory potential toward the target proteins of *G. boninense*. These findings indicate that both compounds have the potential to be developed as bio-based antifungal candidates against *G. boninense* and warrant further investigation through *in vitro* and *in vivo* studies.

Keywords: antifungal, endophytic bacteria, *Ganoderma boninense*, in silico, molecular docking