Abstrak

STUDI BIOINFORMATIKA SENYAWA AKTIF RIMPANG BANGLE HANTU (*Zingiber ottensii*) TERHADAP PROTEIN PROINFLAMASI SEBAGAI KANDIDAT AGEN ANTIINFLAMASI ALAMI

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Latar Belakang: Inflamasi merupakan respon imun terhadap rangsangan berbahaya seperti patogen dan toksin, yang dapat memicu penyakit degeneratif seperti artritis dan penyakit kardiovaskular. Terapi inflamasi umumnya melibatkan obat antiinflamasi steroid dan nonsteroid. Penggunaan bahan alam dengan aktivitas antiinflamasi kini berkembang sebagai terapi komplementer yang berpotensi mendukung efektivitas pengobatan konvensional. Rimpang *Zingiber. ottensii* mengandung senyawa bioaktif seperti flavonoid, terpenoid, dan fenolik yang diketahui memiliki aktivitas antiinflamasi. Penelitian ini bertujuan mengetahui potensi senyawa aktif rimpang *Z. ottensii* terhadap protein target proinflamasi melalui pendekatan bioinformatika.

Metodologi: Penelitian dilakukan secara *in silico* melalui seleksi ADMET, prediksi target molekuler, dan analisis *molecular docking* untuk mengevaluasi interaksi senyawa aktif dengan protein proinflamasi.

Hasil Penelitian: Delapan senyawa memenuhi parameter ADMET, yaitu α-terpineol, trans sabinene hydrate, elemol, β-eudesmol, 1-terpineol, terpinen-4-ol, γ-eudesmol, dan 7-epi-α-eudesmol. Senyawa tersebut berinteraksi dengan protein target proinflamasi meliputi EGFR, HIF1A, ESR1, MAPK1, PTGS2, PGR, RELA, PPARG, MAPK3, dan MAPK8. Hasil *docking* menunjukkan bahwa β-eudesmol, γ-eudesmol, dan elemol memiliki afinitas pengikatan terbaik, dengan nilai energi ikatan masing-masing sebesar -8,4 kkal/mol (MAPK1), -7,7 kkal/mol (MAPK8), dan -7,1 kkal/mol (HIF1A), yang lebih rendah dibandingkan kontrol positif. Interaksi yang terbentuk meliputi ikatan hidrogen pada residu kunci serta interaksi hidrofobik (alkil dan π-alkil), yang berperan dalam meningkatkan stabilitas kompleks ligan–protein.

Kesimpulan: Senyawa aktif rimpang *Z. ottensii* berpotensi sebagai agen antiinflamasi melalui penghambatan protein proinflamasi, dengan β-eudesmol, γ-eudesmol, dan elemol sebagai kandidat utama.

Kata Kunci: antiinflamasi, bioinformatika, *molecular docking*, *Zingiber ottensii*

Abstract

BIOINFORMATICS STUDY OF ACTIVE COMPOUNDS ON BANGLE HANTU (*Zingiber ottensii*) RHIZOME ON PROINFLAMMATORY PROTEINS AS CANDIDATES FOR NATURAL ANTI-INFLAMMATORY AGENTS

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Background: Inflammation is the body's immune response to harmful stimuli such as pathogens and toxins, which can lead to degenerative diseases like arthritis and cardiovascular disorders. Conventional anti-inflammatory therapies include steroidal and nonsteroidal drugs; however, natural compounds with anti-inflammatory activity are increasingly explored as complementary treatments. The rhizome of *Zingiber ottensii* contains bioactive compounds, including flavonoids, terpenoids, and phenolics, known for their anti-inflammatory potential. This study aimed to evaluate the interaction of *Z. ottensii* active compounds with proinflammatory target proteins using a bioinformatics approach.

Methodology: This study was conducted *in silico* through ADMET screening, molecular target prediction, and molecular docking analysis to evaluate the interaction between active compounds and proinflammatory proteins.

Results: Eight compounds met the ADMET criteria, namely α-terpineol, trans-sabinene hydrate, elemol, β-eudesmol, 1-terpineol, terpinen-4-ol, γ-eudesmol, and 7-epi-α-eudesmol. These compounds interacted with proinflammatory targets proteins, including EGFR, HIF1A, ESR1, MAPK1, PTGS2, PGR, RELA, PPARG, MAPK3, and MAPK8. Docking results revealed that β-eudesmol, γ-eudesmol, and elemol exhibited the best binding affinities, with binding energies of −8.4 kcal/mol (MAPK1), −7.7 kcal/mol (MAPK8), and −7.1 kcal/mol (HIF1A), respectively, which were lower than those of the positive controls. The interactions involved hydrogen bonds at key residues as well as hydrophobic interactions (alkyl and π-alkyl), contributing to the stability of the ligand–protein complexes.

Conclusion: Active compounds from *Z. ottensii* rhizome have potential as natural anti-inflammatory agents through inhibition of proinflammatory proteins, with β-eudesmol, γ-eudesmol, and elemol identified as the most promising candidates.

Keywords: anti-inflammatory, bioinformatics, molecular docking, *Zingiber ottensii*