SKRIPSI SARJANA FARMASI

POTENSI MINYAK ATSIRI BANGLE (*Zingiber cassumunar*) SEBAGAI ANTI-AGING SECARA IN SILICO

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ABSTRAK

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(Program Studi Sarjana Farmasi)

Penuaan dini pada kulit merupakan masalah umum yang sering terjadi akibat paparan sinar UV berlebihan, polusi udara, merokok, dan konsumsi alkohol. Salah satu mekanisme penuaan kulit yaitu degradasi komponen struktural kulit yang dipicu oleh aktivitas enzim kolagenase, elastase, hialuronidase, dan tirosinase. Penelitian ini bertujuan untuk mengevaluasi potensi minyak atsiri bangle (*Zingiber cassumunar*) sebagai agen anti-aging dengan pendekatan in silico. Metode penelitian melibatkan molecular docking antara senyawa minyak atsiri bangle dengan enzim kolagenase, elastase, hialuronidase, dan tirosinase. Senyawa minyak atsiri bangle diperoleh dari Pubchem, sedangkan protein target diperoleh dari Protein Data Bank (PDB) dengan kode 5UWK (kolagenase), 5A8Y (elastase), 5DIY (hialuronidase), dan 5M8P (tirosinase). Validasi protokol docking menunjukkan nilai RMSD < 2Å yang menandakan keakuratan metode yang digunakan. Hasil docking menunjukkan bahwa α-terpineol memiliki skor docking terbaik terhadap enzim kolagenase (-7,146 kcal/mol), terpinen-4-ol terhadap enzim elastase (-5,31 kcal/mol), cis-piperitol terhadap enzim hialuronidase (-6,38 kcal/mol), dan p-menth-2-en-1-ol terhadap enzim tirosinase (-5,984 kcal/mol). Akan tetapi hasil docking senyawa minyak atsiri bangle terhadap empat enzim tersebut memiliki afinitas lebih rendah dibandingkan *native ligand*. Analisis Lipinski menunjukkan bahwa senyawa minyak atsiri bangle memenuhi kriteria kandidat obat yang mencakup berat molekul ≤ 500 g/mol, Log P ≤ 5, jumlah akseptor ikatan hidrogen (HBA) ≤ 10, dan jumlah donor ikatan hidrogen (HBD) ≤ 5. Prediksi ADMET terhadap senyawa minyak atsiri bangle menunjukkan profil farmakokinetik yang baik. Dapat disimpulkan bahwa minyak atsiri bangle diprediksi sedikit berpotensi sebagai agen anti aging.

Kata kunci : *Zingiber cassumunar*, in silico, molecular docking, binding affinity

ABSTRACT

POTENTIAL OF BANGLE (*Zingiber cassumunar*) ESSENTIAL OIL AS IN SILICO ANTI-AGING

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Premature aging of the skin is a common issue that often occurs due to excessive exposure to UV rays, air pollution, smoking and alcohol consumption. One of the mechanisms of skin aging involves the degradation of skin structural components which is triggered by the activity of the collagenase, elastase, hyaluronidase, and tyrosinase enzymes. This study aims to evaluate the potential of bangle (*Zingiber cassumunar*) essential oil as an anti-aging agent using in silico approach. The research method involved molecular docking between the compounds in bangle essential oil with collagenase, elastase, hyaluronidase, and tyrosinase enzymes. The bangle essential oil compounds were obtained from Pubchem, while the target proteins were retrieved from the Protein Data Bank (PDB) with codes 5UWK (collagenase), 5A8Y (elastase), 5DIY (hyaluronidase), and 5M8P (tyrosinase). Docking protocol validation showed an RMSD value of < 2Å which indicate the accuracy of the applied method. The docking results showed that α-terpineol had the best docking score against the collagenase enzyme (-7.146 kcal/mol), terpinen-4-ol against the elastase enzyme (-5.31 kcal/mol), cis-piperitol against the hyaluronidase enzyme (-6.38 kcal/mol), and p-menth-2-en-1-ol against the tyrosinase enzyme (-5.984 kcal/mol). However, the docking results of bangle essential oil compounds against the four enzymes have a lower affinity compared to the native ligand. Lipinski analysis showed that bangle essential oil compounds met the drug candidate criteria which include molecular weight ≤ 500 g/mol, Log P ≤ 5, number of hydrogen bond acceptors (HBA) ≤ 10, and number of hydrogen bond donors (HBD) ≤ 5. ADMET prediction of bangle essential oil compounds showed a good pharmacokinetic profile. It can be concluded that bangle essential oil is predicted to have less potential as an anti-aging agent.

Keywords: *Zingiber cassumunar*, in silico, molecular docking, binding affinity