ABSTRAK

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Program Studi : Farmasi
Judul : Uji Aktivitas Antibakteri Ekstrak *n*-heksana Fuli Pala (*Myristica fragrans* Houtt.) Terhadap Bakteri *Cutibacterium acnes* Secara *In Silico* Dan *In Vitro*

Fuli pala (*Myristica fragrans* Houtt.) berpotensi sebagai agen antibakteri terhadap *Cutibacterium acnes* karena mengandung berbagai senyawa bioaktif, terutama fenilpropanoid dan terpenoid. Penelitian ini bertujuan untuk mengidentifikasi senyawa aktif dalam ekstrak *n*-heksana fuli pala melalui pendekatan *in silico* serta menguji aktivitas antibakterinya secara *in vitro*. Studi *in silico* dilakukan dengan menggunakan beberapa protein target penting *C. acnes*, yaitu lipase, *exo-β-1,4-mannosidase*, dan *β-ketoacyl-ACP synthase* III (KAS III), dengan klindamisin HCl sebagai kontrol positif. Analisis *in silico* mencakup prediksi Lipinski's Rule of Five, evaluasi sifat farmakokinetik dan toksisitas menggunakan pkCSM dan ProTox, serta simulasi *molecular docking* menggunakan perangkat lunak PyRx. Hasil menunjukkan miristisin memiliki afinitas ikatan paling kuat terhadap seluruh protein target, ditandai dengan energi ikatan yang lebih negatif dibandingkan *native ligand* dan kontrol positif. Uji farmakokinetik *in silico* menunjukkan bahwa miristisin memiliki profil ADMET yang baik, meskipun diprediksi berpotensi mutagenik dan hepatotoksik pada dosis tinggi. Uji *in vitro* menunjukkan bahwa ekstrak *n*-heksana fuli pala pada konsentrasi 12,5%, 25%, dan 50% menghasilkan rata-rata Diameter Daya Hambat (DDH) masing-masing sebesar 8,44 ± 1,65 mm (kategori sedang), 12,14 ± 0,84 mm (kategori kuat), dan 13,03 ± 0,62 mm (kategori kuat). Analisis statistik menunjukkan adanya perbedaan signifikan antara konsentrasi ekstrak terhadap aktivitas antibakteri ($p < 0,05$) yang menegaskan peningkatan konsentrasi ekstrak secara signifikan meningkatkan aktivitas antibakteri ekstrak fuli pala terhadap *C. acnes.*

Kata kunci:
Cutibacterium acnes, fuli pala (*Myristica fragrans* Houtt.), *in silico*, *in vitro,* miristisin.

ABSTRACT

Name : Kurnia Djayanti Yunus
Study Program : Pharmacy
Title : Antibacterial Activity Test Of *n*-hexane Extract of Nutmeg Mace (*Myristica fragrans* Houtt.) Against *Cutibacterium acnes In Silico* and *In Vitro.*

Nutmeg mace (*Myristica fragrans* Houtt.) has potential as an antibacterial agent against *Cutibacterium acnes* due to its content of various bioactive compounds, particularly phenylpropanoids and terpenoids. This study aimed to identify the active compounds in the *n*-hexane extract of nutmeg mace through an *in silico* approach and to evaluate its antibacterial activity *in vitro*. The *in silico* study employed several essential protein targets of *C. acnes*, including lipase, *exo-β-1,4-mannosidase*, and *β-ketoacyl-ACP synthase III* (KAS III), with clindamycin HCl used as a positive control. The analysis included prediction of Lipinski's Rule of Five, evaluation of pharmacokinetic and toxicity profiles using pkCSM and ProTox, and molecular docking simulations conducted with PyRx. The docking results demonstrated that myristicin exhibited the strongest binding affinity toward all protein targets, indicated by lower binding energy values compared to the native ligands and the positive control. *In silico* ADMET evaluation revealed that myristicin possesses favorable pharmacokinetic properties, although it may have mutagenic and hepatotoxic potential at high doses. The in vitro antibacterial assay showed that the *n*-hexane extract of nutmeg mace at concentrations of 12.5%, 25%, and 50% produced mean inhibition zone diameters of 8.44 ± 1.65 mm (moderate category), 12.14 ± 0.84 mm (strong category), and 13.03 ± 0.62 mm (strong category), respectively. Statistical analysis indicated a significant difference among extract concentrations ($p < 0.05$), confirming that increasing extract concentration significantly enhances the antibacterial activity of nutmeg mace extract against *C. acnes.*

Keywords:
Cutibacterium acnes, nutmeg mace (*Myristica fragrans* Houtt.), *in silico, in vitro,* myristicin.