ABSTRACT

Naca Sabelia. *24020222140086. **Molecular Identification and In Silico Analysis of Secondary Metabolites from Teloschistes* sp. *and Ramalina* sp. *as Anti-Acne Candidates Targeting Inflammatory and Bacterial Proteins***. *Supervised by* Arina Tri Lunggani and Nurina Tahta Afwi Maulina

The use of conventional acne therapies, particularly antibiotics, has raised concerns regarding the development of antimicrobial resistance, highlighting the need for safer and more effective natural alternatives. Lichens such as Teloschistes sp. and Ramalina sp. are known to produce various bioactive secondary metabolites, including usnic acid, depsidones, and phenolic compounds, which possess potential antibacterial and anti-inflammatory activities. This study aimed to identify and compare the effectiveness of secondary metabolites from Teloschistes sp. and Ramalina sp. in inhibiting the growth of Cutibacterium acnes and suppressing inflammatory responses, as well as to analyze the phylogenetic relationships of the lichens. The study employed molecular identification using the MtSSU primer to determine phylogenetic relationships and an in silico approach, including molecular docking using PyRx, phylogenetic analysis using MEGA, pharmacokinetic prediction using SwissADME and pkCSM, and toxicity assessment using ProTox-III. The results showed that the Teloschistes sample was closely related to Teloschistes sieberanus with a bootstrap value of 79%, while the Ramalina sample clustered with Ramalina thrausta, Ramalina farinacea, and Ramalina peruviana, also with a bootstrap value of 79%. Among the tested compounds, α-patchoulene exhibited the lowest binding affinity toward the C. acnes receptor -8.9 kcal/mol, indicating the strongest antibacterial potential. Meanwhile, sekikaic acid methyl ester showed the lowest binding affinity toward the inflammatory receptor -7.5 kcal/mo), suggesting superior anti-inflammatory potential. Both compounds also demonstrated favorable pharmacokinetic properties and fulfilled drug-likeness criteria. These findings provide preliminary evidence supporting the potential of lichen secondary metabolites as promising natural candidates for anti-acne drug development.

KeyWords: Antibacterial, Antiinflamasi, Lichen, Molecular Docking, Pharmacokinetics