

ABSTRACT

Louis Abisha Tzurriel Simanjuntak, 24020222140070. ***Molecular Identification and Analysis Of Potential Metabolites Of In Silico Compounds Of Teloschistes sp. And Ramalina sp. As Antifungal Drug Candidates Against Candida albicans.*** Supervised by Arina Tri Lunggani and Puspa Hening.

Candida albicans is the primary causative agent of candidiasis, with a mortality rate approximately 40% higher than that of sepsis caused by other bacteria or fungi. The increasing resistance to conventional antifungal drugs has become a serious medical challenge, necessitating the development of more effective alternative therapeutic agents. Lichens are symbiotic associations between fungi and algae or cyanobacteria that are known to produce a wide variety of secondary metabolites with diverse biological activities and have been traditionally utilized by various cultures worldwide. This study aimed to identify the potential of metabolites derived from Ramalina sp. and Teloschistes sp. as antifungal drug candidates against Candida albicans using bioinformatics and computational (in silico) approaches. The methods included lichen sample identification through both morphological and molecular analyses, followed by molecular docking, visualization, and prediction of pharmacokinetic and toxicity profiles. Molecular identification results revealed that the lichen samples used in this study were Teloschistes sp. and Ramalina peruviana. Molecular docking analysis showed that the compound o-Pyrocatechuic acid, 4-methoxy-6-propyl-, methyl ester, 3-(2-hydroxy-6-propyl-p-anisate) exhibited the strongest binding affinity, with a binding energy of -8.4 kcal/mol. Furthermore, four potential antifungal drug candidates were identified as occupying the active site of the native ligand. Based on pharmacokinetic and toxicity predictions, all four compounds met the criteria for absorption, distribution, metabolism, excretion, and toxicity (ADMET), indicating their potential as antifungal drug candidates.

Keywords: Antifungal, Candida albicans, Lichen, Ramalina sp., Teloschistes sp..