ABSTRACT

Kartika Septiana Puspitaningsih, 24020222130051, **Molecular Characterization and In Silico Studies of *Aloe* sp. Leaf Extracts as a Treatment for Type 2 Diabetes**, supervised by Hermin Pancasakti Kusumaningrum and Parwa Oryzanti.

Type 2 diabetes mellitus is a chronic metabolic disorder characterized by insulin resistance and impaired pancreatic β-cell function. Adenosine Monophosphate-Activated Protein Kinase (AMPK) plays an important role in increasing glucose uptake through GLUT4 translocation, making it a potential target for antidiabetic therapy. This study aimed to characterize *Aloe* sp. originating from Semarang and Bogor, identify bioactive compounds using Gas Chromatography-Mass Spectrometry (GC-MS), and evaluate their antidiabetic activity through molecular docking against the AMPK protein. Morphological characterization was conducted based on leaf size and color pattern, while molecular characterization was performed using ITS markers and BLAST analysis. The compounds identified by GC-MS were docked to the AMPK protein using PyRx and visualized with Discovery Studio. The results showed morphological differences between *Aloe* sp. from Semarang and Bogor. Molecular analysis revealed the highest homology with *Aloe vera* isolate BPTPS162, with similarity values of 88.06% for *Aloe* sp. Semarang and 84.4% for *Aloe* sp. Bogor. Molecular docking results demonstrated that palmitic acid and methyl oleate from *Aloe* sp. Semarang had binding affinity values of -4.8 kcal/mol, while 5-Cyclohexadecen-1-one from *Aloe* sp. Bogor showed a binding affinity of -6.3 kcal/mol. Lipinski and ADMET analyses indicated that most compounds possessed good drug-likeness characteristics and favorable pharmacokinetic profiles as oral drug candidates. Based on the binding affinity values and in silico analysis, *Aloe* sp. Bogor has greater potential as a candidate for type 2 antidiabetic therapy.

Keywords: AMPK, molecular docking, insulin resistance, bioactive compounds