

ABSTRACT

Fajar Wicaksono, 24020121130090. Potential of Active Compounds of Temulawak (*Curcuma xanthorrhiza*) as Inhibitors of Pancreatic α -amylase Enzyme *in silico*. Supervised by Agung Janika Sitasiwi and Rizki Sandhi Titisari.

Diabetes mellitus (DM) was a chronic metabolic disorder characterized by elevated blood glucose levels due to impaired insulin secretion or action. Hyperglycemia emerged as a primary condition in individuals with DM and was exacerbated by the high activity of pancreatic α -amylase, which catalyzed the hydrolysis of complex carbohydrates into simpler sugars. Inhibition of pancreatic α -amylase served as a crucial strategy in managing blood glucose levels. Temulawak (*Curcuma xanthorrhiza*) contained various active compounds with potential antidiabetic properties, while *in silico* studies on its inhibitory effect against pancreatic α -amylase remained limited. This study aimed to predict and identify active compounds in temulawak as pancreatic α -amylase inhibitors using an *in silico* approach. The stages included bioavailability and toxicity prediction of 39 test ligands, virtual screening, molecular docking validation, 2D and 3D interaction visualization, and inhibition constant calculation. The analysis results identified demethoxycurcumin as the most promising candidate inhibitor of pancreatic α -amylase (PDB: 1B2Y). Molecular docking parameters indicated the highest binding affinity, the formation of two hydrogen bonds with residues Arg195 and His299, and a low inhibition constant (K_i) value.

Keywords: *Diabetes mellitus, pancreatic α -amylase, molecular docking, demethoxycurcumin*