ABSTRACT

ANITA PUTRI NINGRUM. 2025. ***IN SILICO ANALYSIS OF THE POTENTIAL COMPOUNDS IN SECANG (CAESALPINIA SAPPAN L.) AS BLOOD GLUCOSE REGULATORS FOR BIOLOGY LEARNING RESOURCES***. *Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University,* Tasikmalaya.

Diabetes is a chronic degenerative disease characterized by abnormally elevated blood glucose levels resulting from impaired insulin secretion. The long-term use of conventional drugs such as acarbose may lead to adverse side effects, thereby necessitating alternative treatments utilizing safe, natural compounds. Caesalpinia sappan L. is known to contain bioactive compounds with potential biological activity as pancreatic alpha-amylase inhibitors. This study aimed to evaluate the interaction of 11 bioactive compounds as potential inhibitors of the target protein through in silico analysis using molecular docking methods. The analysis employed three primary parameters: RMSD, binding affinity, and ligand–protein interaction profiles, using Discovery Studio and PyRx software. These evaluation tools were applied to determine the accuracy and stability of the compounds in binding to the target protein. The compound Spirost-8-en-11-one, 3-hydroxy-, (3ß,5a,14ß,20ß,22ß,25R) exhibited the highest binding affinity (-10.4 kcal/mol), surpassing that of acarbose as the control compound (-7.8 kcal/mol). Further analyses were conducted to predict drug-likeness properties, including physicochemical characteristics, pharmacokinetics, and toxicity, to assess the compound's potential efficacy in vivo. The findings indicate that the compound may be suitable for oral administration with minimal side effects. In conclusion, the bioactive compounds in Caesalpinia sappan L. demonstrate potential as blood glucose regulation.

Keywords*:* Diabetes; *in silico*; *Alpha-Amylase*; *Caesalpinia sappan* L.