

ABSTRACT

NADYA NURFITRIA SARI. 2025. ***IN SILICO ANALYSIS STUDY OF SOURSOP (Annona muricata L.) LEAVES AS ANTIDIABETES GUIDE FOR BIOLOGICAL STUDY SOURCE***. Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University, Tasikmalaya.

Diabetes mellitus is a metabolic disease with an increasing prevalence globally, including in Indonesia. The development of natural-based alternatives is important, given the side effects and limitations of available synthetic drugs. This study aims to analyze in silico the potential of secondary metabolite compounds from soursop leaves (Annona muricata L.) for biology learning resources. The research was conducted from December 2024 to January 2025. The research method used was descriptive qualitative method in silico using molecular docking method with PyRx software and Biovia Discovery Studio Visualizer 2024 and hardware in the form of laptop. Test compounds from the flavonoid group used include quercetin, isoquercetin, rutin, and kaempferol, while alkaloid compounds include anonaine, coclaurine, isolaureline, norcorydine, reticuline, and xylopine. The selection of compounds was based on a literature review, while Docosahexaenoic acid (DHA) was used as a control ligand to compare the strength of the interaction. The docking results of the ten compounds showed that almost all flavonoid and alkaloid compounds had lower binding affinity to the GPR120 receptor than DHA as the control ligand, indicating a stronger interaction with the GPR120 receptor. Xylopine compound had the lowest binding affinity value, which was -9.2 kcal/mol, making it the most potential candidate in activating the GPR120 receptor. The interaction between the test compounds and the receptor was characterized by the formation of hydrogen bonds and other non-covalent interactions, which strengthened the affinity of the ligand to the receptor. Activation of the GPR120 receptor by the test compounds could potentially stimulate insulin secretion through cellular signaling mechanisms, thereby contributing to the control of blood glucose levels. These findings suggest that secondary metabolites of soursop leaves have potential as early candidates for antidiabetic agents.

Keywords: Antidiabetes; GPR120; Molecular docking; Secondary metabolite compounds; Soursop leaf (*Annona muricata L.*).