

## ABSTRACT

RESA SOHIB PUTRI. 2025. **IN SILICO ANALYSIS OF KERSEN (*Muntingia calabura* L.) LEAVES AS ANTIHYPERTENSIVE CANDIDATES FOR BIOLOGY LEARNING RESOURCES.** *Department of Biology Education, Faculty of Teacher Training and Education, Siliwangi University, Tasikmalaya.*

*Kersen (*Muntingia calabura* L.) is a plant that has various benefits and has been widely used as a medicine by boiling or soaking in water. The boiled water of kersen leaves is believed by the community as one of the antihypertensive herbal medicines. This study aims to determine the in silico analysis of kersen leaves (*Muntingia calabura* L.) as an antihypertensive candidate. This research uses descriptive qualitative methods in silico by utilizing quantitative data from molecular docking results as the basis of its research.. Leaves are the organ that contains the most flavonoid compounds in kersen plants. The results of literature analysis show that kersen leaves contain secondary metabolite compounds including flavonoid compounds that have the potential as antihypertensives, namely kaempferol-3-o-galactoside (Trifolin), myricetin, quercetin-3-o-galactoside (Hyperoside), kaempferol-3-O-glucoside (Astragalin), quercetin-3-o-glucuronide (Querciturone), quercetin, quercetin dimer, rhamnetin, pinobaksin, pinocembrin, kaempferol, and genistein. The compounds were analyzed in silico as test compounds with control ligands lisinopril and Angiotensin Converting Enzyme (ACE) receptor (PDB ID: 1O86). The results showed that all test compounds have binding affinity with ACE, almost all test compounds have better binding affinity than lisinopril where lisinopril has a binding affinity of -7.8 kcal/mol. The best binding affinity was shown by the quercetin dimer compound which was -12.0 kcal/mol, but quercetin dimer did not meet several indicators to be used as a drug. The most potential compounds as antihypertensives in kersen leaves are kaempferol and quercetin, because both have a lower binding affinity than the control ligand, molecular bond similarity and better bond complexity than the control ligand, fulfill the Lipinski Rule of Five, can be absorbed well by the body, and have a relatively low level of toxicity.*

**Keywords:** ACE Receptor; Antihypertensive; Flavonoids; Kersen Leaf.