IN SILICO SCREENING OF CHEMICAL COMPOUND ACTIVITY AS AN A-GLUCOSIDASE INHIBITOR FROM SWEET FLAG RHIZOME (*ACORUS CALAMUS* L.)

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Abstract.

The research on screening in silico of the chemical of *Acorus calamus* L. as the inhibitor α-glucosidase has been conducted. The aim of this research to obtain an active chemical compound towards Acorus calamus L. which is potentially to be inhibitor of α-glucosidase using the screening method in silico The docking process was employed using 28 chemical compounds in the *Acorus calamus* L. as the ligand to the inhibitor α-glucosidase becoming the target receptor using PyRx and ArgusLab programs. The chemical compound model of *Acorus calamus* L was obtained from Take Out "Jamu" KnapSack. Whereas the enzyme model of α-glucosidase obtained from Protein Data Bank (PDB) with the enzyme code ILWJ. Each compound which has been docked using enzyme α-glucosidase taken from the free energy changing ΔG as the docking result and visualization of the docking result was conducted using PyMol program. The evaluation result of AG indicated that 28 chemical compounds of *Acarus calamus* have potential as the inhibitor of α-glucosidase where Delta-Cardinene as the lowest change had the most potential compound. The approximate free energy change (ΔG) was -8.50 kcaI/mol in the PyRx and -9.53 kcal/mol in the ArgusLab program.

Keywords: *Acorus calamus* L, α-glucosidase, *In silico* Screening