# Molecular Docking and Dynamics Simulation for Searching Anti-Cancer Compounds of Piperlongumine Derivatives that Have Potential As An Inhibitor Against MAO-B (Monoamin Oxidase B)

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ABSTRACT

The docking of the piperlongmine molecule and its derivatives has been carried out with the aim of finding molecules that have potential as anti-cancer. A total of 18 ligands were docked to the 2v5z protein using the autodock4 and autodock vina programs. The binding energies of piperlongumine and piperlongumine derivatives [R1 = CH3 and R2 = H] were -8.6 kcal/mol and -9.3 kcal/mol, respectively. Based on molecular dynamics simulations, the hydrogen bond interaction fraction was dominated by GLN 206 residue in both the SAG (88%) and piperlongumine derivatives ((R1=CH3, R2 = H)(93%) ligand, for this reason this piperlongumine derivative molecule is predicted to have potential as MAO B inhibitor.

Kata Kunci: *molecular docking, piperlongumine and its derivatives, molecular dynamics simulation*