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)

by Suwardi, Agus Salim, Raden Rara Fadhila Kirana Nugrahani dan Yolanda Amalia

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*