ABSTRACT

The Human Epidermal Growth Factor Receptor 2 or HER2 is one of the targets of breast cancer therapy because HER2 is often overexpressed and is a transmembrane tyrosine kinase receptor that regulates cell division and growth. This study aims to predict the interaction of bioactive compounds as inhibitors on proteins and to obtain residues and groups that determine the strength of the interaction between proteins and bioactive ligands. The study used 3D protein structures, with cyanidin and peonidin-3-glucoside as bioactive compounds and lapatinib as a positive control. The steps included structure preparation and validation, ligand position confirmation, simulation at an equilibrium temperature of 300 K and pressure of 1 bar, followed by RMSD analysis and electrostatic and van der Waals interaction energy analysis. The results showed that peonidin-3-glucoside had lower interaction energy, a stable complex, and more strong bonds with active residues, including Ala-751 and Val-734. These findings indicate that peonidin-3-glucoside has higher affinity and a more effective inhibition mechanism than cyanidin, making peonidin-3-glucoside a potential inhibitor of HER2.

Keywords*: HER2, lapatinib, cyanidin, peonidin, molecular dynamics*