

Subsequently, Gasteiger-Marsili model (Gasteiger and Marsili 1980) was employed to assign partial charges for all prepared ligands. Tertiary amines of all ligands were set as protonated. The ligands were separately docked into the previously prepared active site using Autodock (Morris et al., 1998, Morris et al., 2009) (version 4.2). Whereas the protein structure was treated as a rigid entity, the ligand structures were treated as flexible and a conformational sampling process was carried out using Lamarckian Genetic Algorithm (Morris et al., 1998). The Autodock scoring function was then used to score all docked poses. The Autodock scoring function includes different terms for van der Waals, hydrogen bond, electrostatic interactions, and the ligand internal energy.