Molecular Docking and Biological Evaluation of Synthesized Compounds for Prospective Biomedical Applications

K Gour
Department of Chemistry, Priyadarshini J L College of Engineering, Nagpur, Maharashtra, India

Sampda Payal
Department of Chemistry, Institute of Science, Nagpur, Maharashtra, India

Neera Raghav
Department of Chemistry, Kurukshetra University Kurukshetra, Haryana

Prabhjot Kaur
Department of Chemistry, Kurukshetra University Kurukshetra, Haryana

Damodar Y. Maskare
Department of Chemistry, Institute of Science, Nagpur, Maharashtra, India

Abstract

A novel Schiff base ligand was obtained by the reaction of p-anisidine (4-methoxy aniline) and 3-ethoxy salicylaldehyde (3-ethoxy-2-hydroxy benzaldehyde) and their complexes with the metal Ni ++ and Zn ++ were obtained. Characterization of the ligand and metal complexes were done by elemental analysis, molar conductance and magnetic susceptibility measurements and spectroscopies methods.

Furthermore, the in vitro & in silico activity of the ligand and its metal complexes was assessed by different biological assays. The results of the study show that the binding energies are (-96.9 -110.09 kcal/mol) in trypsin activity. Among them, 5(c) compound had the least energy values, which suggests the most stable binding. In the process of pepsin docking, the binding energies are -67.9 to -73.4 kcal/mol, 5(b) having the best binding ability. In the case of lipase, the binding energy of compounds is -77.5 to -99.115 kcal/mol, where 5(c) exhibited the best affinity. The docking results shows good binding energies together with the establishment of strong intermolecular interactions, such as hydrogen bonding and hydrophobic contacts, which comprise the main features of enzyme ligand binding. The results of these computations study (Insilco) show a good correlation with the in-vitro laboratory results.

Keywords

Schiff base, Ligands-Metal Complexes, Anti enzymatic, Characterization Molecular docking.