Abstract

Heterocyclic compounds, due to their structural diversity, are of prime importance in the design and development of medicinal drugs. A library of compounds (LOCs), **6n-6r** was analyzed using advanced bioinformatic methodologies. Drug discovery process is made more efficient and accurate by employing computational investigation, offering a powerful foundation for predicting molecular interaction and behavior. These techniques speed up the process of drug discovery as well as present an economical approach to focus on the particular enzyme responsible for a particular ailment. Various computational tools have been utilized enhancing ability to predict molecular characteristics, determine ADMET and discover more efficient process of drug discovery. Analysis of docking scores and binding interactions was done using Discovery Studio, AutoDock and AutoDock Vina tool. Density Functional Theory (DFT) studies were performed to calculate structural parameters using B3LYP/6- 31G (d, p) basis set. Geometries were optimized and Frontier Molecular Orbital (FMO) analysis was done to study chemical stability and reactivity. Molecular Electrostatic Potential (MEP) was performed throughout the optimized geometries in order to find the reactive sites. Various tools which include molinspiration, PreADMET, SwissADME and DataWarrior were utilized in the prediction of molecular properties, bioactivity score, pharmacokinetics and pharmacodynamics properties. The findings indicated that the compound **6n** and **6r** exhibited good binding with lipoxygenase enzyme and hence they can be employed as lipoxygenase inhibitors. DFT calculation and *in silico* ADMET screening also indicated that **6n** and **6r** can be employed as lipoxygenase inhibitor. These studies are likely to further our understanding of molecular recognition, hence providing critical information that will aid medicinal chemists in the future while designing new drug candidates.