ABSTRACT

Heterocyclic compounds are essential in the design and development of pharmaceuticals, due to their structural versatility. A library of compounds (LOCs), **6s- 6w,** was analyzed using advanced computational methods. Drug discovery methods are significantly enhanced in accuracy and efficiency through computational investigations, providing a robust foundation for predicting molecular behaviour and interactions. These techniques not only accelerate the process of discovering new drugs but also provide an economical approach to targeting specific enzymes associated with diseases. Utilizing an array of computational tools enhances our ability to predict molecular characteristics, evaluate toxicity, and determine ADME, facilitating a more efficient drug discovery process for medicinal chemists. Computational studies of oxadiazole derivatives 6s-6w were conducted using various tools. Docking scores and binding interactions with the lipoxygenase enzyme were evaluated using Discovery Studio, AutoDock, and AutoDock Vina tools. The structural parameters of the selected derivatives were calculated using Density Functional Theory (DFT) studies with the B3LYP/631G(d, p) basis set. To investigate the chemical stability and reactivity of compounds **6s-6w**, their geometries were optimised, and then a Frontier Molecular Orbital (FMO) evaluation was performed at the same theoretical level. To identify the reactive sites, the Molecular Electrostatic Potential (MEP) was also evaluated throughout the stabilised molecular geometries. To predict molecular properties, bioactivity scores, pharmacokinetic, and pharmacodynamic properties, several tools were utilised, including Molinspiration, PreADMET, SwissADME, and DataWarrior. The results showed that compound 6w exhibited a good binding affinity with the lipoxygenase enzyme, indicating that it can be used as a lipoxygenase inhibitor. DFT analysis and in silico ADMET screening also suggested that 6w can be us lipoxygenase inhibitor. These investigations are expected to enhance our understanding of molecular recognition, thereby providing vital data that will aid medicinal chemists in the future when crafting novel drug candidates. The NBO results provide enhanced insight into electron delocalisation and intramolecular charge transfer, which are pivotal in the compound's binding affinity and interaction with biological targets.