ABSTRACT

Heterocyclic compounds make up about 50% of global organic research chemical experience. A significant part of pharmaceuticals, agrochemicals, pesticides, biomolecules, veterinary products, and other valuable chemicals are heterocyclic. These are all over the place in drug molecules because of the structural flexibility. Heterocyclic moiety comprises about 56% of the existing drugs. Finding and developing new drugs is a complicated, drawn-out, and interdisciplinary process. The application of molecular modelling and *in-silico* chemistry in computer-aided drug creation has recently increased. Applications of *in-silico* drug design knowledge are found in molecular biology, biochemistry, nanotechnology, and other fields. Cost-effectiveness in medication research and development is the main benefit of *in-silico* drug design. In the biomedical field, *in-silico* design is being used to minimize safety concerns, optimize the ADMET profile, and speed up and facilitate hit discovery and hit-to-lead selection. For this purpose, Oxadiazole derivatives **6i–6m** were computationally studied utilizing a variety of instruments. AutoDock, Discovery Studio, and the AutoDock Vina program were used to find the binding affinity; against the lipoxygenase enzyme. B3LYP/6-31G (d, p) basis set was used to determine the structural properties of selected derivatives by Density Functional Theory (DFT). Optimal geometry of the title compound, molecule electrostatic potential (MEP), intricacy of quantum molecular descriptors, frontier molecular orbitals (FMO), and NBO were also calculated. The HOMO, LUMO, and optimal molecular structures surface view were presented using GaussView 06. To the examination of charge delocalization and hyperconjugative interactions, the electronic structure of the title chemical was studied using the Natural Bond Orbital (NBO) analysis. Numerous technologies, including Molinspiration, PreADMET, SwissADME, pkCSM, molsoft, Pass Online analysis, and DataWarrior, were used to predict molecular characteristics, bioactivity score, pharmacokinetic, and pharmacodynamic parameters. According to the findings, compound 6k exhibited a high binding affinity of **-8.7 kcal/mol** for the lipoxygenase enzyme, meaning it might be employed as a lipoxygenase inhibitor. The attempt to enter into an experimental verification and optimization of computationally predicted heterocyclic compounds that can be considered as part of future research aimed at their future application in therapeutic purposes.