ABSTRACT

Traditional drug discovery is a challenging and costly process, necessitating the development of more efficient and precise computer methods. Cyclooxygenase-2 (COX-II) is an important and established target for anticancer therapy, but estimating the bioactivity of possible pharmacologic inhibitors remains a major difficulty. Traditional machine learning models sometimes fail to take full advantage of molecules' inherent graph structure, limiting their predictive effectiveness. This study creates and tests a Graph Convolutional Network (GCN), a deep learning model that extracts characteristics directly from chemical graphs, to reliably categorize the bioactivity of prospective COX-II inhibitors. A dataset of 2,646 chemicals was obtained from the ChEMBL database, preprocessed, and classified as active or inactive based on IC50 values. Molecules were transformed into graph representations to be fed into a GCN architecture, which was enhanced using both systematic grasp modifying and automated hyperparameter optimization with Particle Swarm Optimization (PSO) and the Hybrid Bat Algorithm (HBA). The GCN models' performance was carefully evaluated against traditional Artificial Neural Network (ANN), Long Short-Term Memory (LSTM), and Convolutional Neural Network (CNN) baselines. The findings show that the GCN-based strategy is clearly superior. The final model optimized with PSO (GCN-PSO) performed the best, with an Accuracy of 0.9121, an F1-Score of 0.9378, and a Matthews Correlation Coefficient (MCC) of 0.7878. This study supports the concept that GCNs offer a more effective framework for bioactivity prediction by learning from molecular topology. The resulting high-performance model is a verified tool for virtual screening, which helps speed up the vital early phases of discovering potential anti-cancer drugs.

Keywords: Graph Convolutional Network, COX-II Inhibitor, Bioactivity Prediction, Hyperparameter Optimization, Drug Discovery, Anti-cancer