Abstract

In recent years, research on absorption, distribution, metabolism, excretion, and toxicity (ADMET) has increased significantly. This is due to the high rate of drug discovery failures during the drug developmentstage. More than 90% of drug compounds fail during their development process, and the major contributor to this failure is the poor performance of ADMET parameters. One key ADMET parameter isHuman Oral Availability (HOB), crucial in determining the fate of new drugs in clinical trials. Human Oral Bioavailability (HOB) is a pharmacokinetic parameter that measures the extent to which a drug, when taken orally, can be absorbed and reach systemic circulation within the human body. However, conventional experiments on HOB are time-consuming and costly. An alternative is the use of in-silico approaches. In-silico approaches can be enhanced with machine learning to provide more accurate HOB predictions. The goal of this study is to implement the Grey Wolf Optimization (GWO) metaheuristic algorithm in an architecture of Long Short-Term Memory (LSTM) to predict HOB. The selection ofGWO and LSTM is driven by their potential to optimize and enhance the accuracy of HOB predictions, addressing the challenges posed by conventional experimental approaches. Based on the study results, we obtained the best model with 3 hidden layers, a relu activation function, and an SGD optimizer. For the test data, the model achieved F1-score and accuracy values on of 0.776 and 0.722 respectively.

Keywords: ADMET, HOB prediction, LSTM, GWO