

ABSTRACT

Most people consume various chemicals throughout their lives such as medicines, household cleaning products and food. In some cases, these chemicals can be harmful and have toxic effects on our bodies. Determining the toxicity of chemicals is essential to minimize exposure to contaminants in everyday products. Toxicity is also a major issue in new drug development, with more than 30% of drug candidates failing in clinical trials due to undetected toxic effects. However, the current toxicity detection methods that are still widely used are in vivo and in vitro which are considered the least efficient and inhumane. An alternative to the previous two methods is to use in silico methods to save time and money in toxicity detection. One of the commonly used in silico methods is Deep Learning. Therefore, the purpose of this research is to implement Deep Learning with the Long Short-Term Memory (LSTM) method optimized by Grey Wolf Optimization (GWO) in predicting toxicity in the case study of Nuclear Receptor-Androgen Receptor (NR-AR) toxicity type. The dataset used in this study is provided by Tox21 Data Challenge. In this study, LSTM will be used to predict NR-AR toxicity, while GWO is used to optimize the hyperparameters of LSTM.

Keywords: LSTM, GWO, NR-AR, Tox21 Data Challenge, Deep learning, in silico