

ABSTRACT

The interaction of drugs with target proteins is an important basis in the treatment and prevention of disease. However, unexpected side effects resulting from these interactions remain a serious problem. Approximately 35% of drugs interact with multiple protein targets, causing significant negative impacts and a large burden on healthcare. Traditional ways to predict drug side effects, such as tests on living organisms (in-vivo) and trials in a laboratory environment (in-vitro), are often hampered by high costs and low accuracy. In situations like these, in-silico methods, especially those using machine learning, provide a more cost-effective and efficient alternative for predicting side effects. This research presents a new way of using a lightweight molecular representation called SMILES2Vec, which is better than conventional methods. This approach not only overcomes computational constraints, but also improves prediction accuracy. Deep learning techniques with the Gated Recurrent Unit (GRU) model are used to understand patterns in sequential data. Additionally, an automatic approach with the Bat Algorithm is used to optimize parameter settings and improve prediction performance. The results showed an increase in the prediction performance of drug side effect. By auto tuning the GRU model with 3 layers (G3) and applying automatic tuning with the Bat algorithm to the Convolution Layer and GRU layer (CG) schemes, we managed to achieve good results. The G3 model has an F1-Score of 75.61%, while automatic tuning with the Bat Algorithm on the CG scheme outperforms with an F1-Score of 77.64%. This automatic approach succeeded in finding a more optimal combination of parameters in predicting drug side effects. In addition, an increase in the performance of drug side effect prediction occurred by using a dataset that uses the SMILES2Vec Chemical representation and a deep learning approach with GRU, especially for the Blood and Lymphatic System organs.

Keywords: drug side effects, blood and lymphatic system, smile2vec, gru, optimization algorithm, bat algorithm