

ABSTRACT

The drug development process requires accurate drug-target interaction (DTI) information to evaluate a drug's potential. However, existing traditional methods for estimating DTI are slow and expensive. Deep learning offers an efficient and effective alternative by leveraging sequence data for prediction. Nevertheless, the DTI binary classification approach suffers from a large number of non-interacting pairs, resulting in data imbalance and has a negative impact on performance. To address this issue, DTI is modeled as a regression problem known as drug-target affinity (DTA), which predicts the strength of interactions. While various deep learning methods show competitive results in DTA prediction, they face a challenge in capturing specific drug-target patterns with limited data. To overcome the problem, this study leverages pre-trained language models for enhanced representation. Also, we utilize gated multi-head attention (GMHA), which modifies multi-head attention by including dynamic scaling and a gate process to capture the mutual interactions better. The results show that our proposed method exceeds the benchmark and baseline in all evaluation metrics, with CI of 0.893 and 0.872 and r_m^2 of 0.673 and 0.723 in Davis and KIBA. Our findings further suggest that pre-trained language models for drug and target receptor representation improve DTA prediction model performance. Also, the GMHA method generally outperforms the simple concatenation method, with more obvious advantages in more complex datasets like KIBA.

Keywords: drug target affinity, pre-trained language model, gated multi-head attention, deep learning, regression