

ABSTRACT

Drug-target affinity (DTA) prediction is crucial in drug discovery research because traditional methods are costly and time-consuming. Yet, recent computational approaches often struggle with limitations in representing the structural and sequential complexities of drugs and proteins, resulting in inferior prediction performance. Therefore, this study proposes enhancing DTA prediction accuracy using Dynamic Graph Attention Networks (GATv2) and Bidirectional Long Short-Term Memory (BiLSTM). The model incorporates multi-scale features, which include drug motif graphs, and a three-way multi-head attention mechanism to capture complex interactions between drug and protein representations. Tested on Davis and KIBA datasets, the proposed model outperformed baseline and existing benchmark methods across three evaluation metrics achieving MSE of 0.3209 and 0.1864, CI of 0.8646 and 0.8616, and r_m^2 of 0.5046 and 0.6672, respectively. This approach addresses limitations in static attention mechanisms, lack of multi-scale representation, and simplified interaction modeling in existing methods, offering a more robust process for DTA prediction.

Keywords: drug-target affinity, drug graph, protein sequences, dynamic graph attention network, multi-scales features, attention mechanism