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BiFormerDTA: Structural Embedding of Protein in Drug Target Affinity Prediction Using BiFormer

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Abstract : Predicting the interaction between drugs and their molecular targets is pivotal for advancing drug development processes. Due to the time and cost limitations, computational approaches have emerged as an effective approach to drug-target interaction (DTI) prediction. Most of the introduced computational based approaches utilize the drug molecule and protein sequence as input. This study does not only utilize these inputs, it also introduces a protein representation developed using a masked protein language model. In this representation, for every individual amino acid residue within the protein sequence, there exists a corresponding probability distribution that indicates the likelihood of each amino acid being present at that particular position. Then, the similarity between each pair of amino acids is computed to create a similarity matrix. To encode the knowledge of the similarity matrix, Bi-Level Routing Attention (BiFormer) is utilized, which combines aspects of transformer-based models with protein sequence analysis and represents a significant advancement in the field of drug-protein interaction prediction. BiFormer has the ability to pinpoint the most effective regions of the protein sequence that are responsible for facilitating interactions between the protein and drugs, thereby enhancing the understanding of these critical interactions. Thus, it appears promising in its ability to capture the local structural relationship of the proteins by enhancing the understanding of how it contributes to drugprotein interactions, thereby facilitating more accurate predictions. To evaluate the proposed method, it was tested on two widely recognized datasets: Davis and KIBA. A comprehensive series of experiments was conducted to illustrate its effectiveness in comparison to cutting edge techniques.

Keywords : BiFormer, transformer, protein language processing, self-attention mechanism, binding affinity, drug target interaction, similarity matrix, protein masked representation, protein language model
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