Integrated Model for Drug–Target Interaction Prediction Leveraging Multiple Protein Language Embeddings

Shasha Tao, Jin Liu, and Xiaolin Ning, Xin Ma

***Abstract*—The prediction of drug-target interactions (DTIs) plays a crucial role in drug design, significantly reducing research and development costs. However, the accuracy of DTI predictions is still below expectations. We present a deep learning model, IM-DTI. First, we utilize a topology-based feature extraction method alongside multiple pretrained protein language models (PLMs) to provide encoded features for drugs and targets. Subsequently, the feature embedding structure yields component predictions corresponding to the three respective protein language models. Finally, a Bayesian Optimization-enhanced Random Forest (BO_RF) algorithm fuses these three component predictions to enhance prediction accuracy and improve generalization capability. Moreover, we introduce a residual structure within the feature embedding framework to accelerate the model's convergence process and effectively address overfitting issues. Experimental results demonstrate that IM-DTI surpasses six compare against other state-of-the-art (SOTA) works, achieving performance improvements of 4% to 10%.**

***Index Terms*— Drug-Target Interactions, Feature Embedding, Protein Language Models.**

I. Introduction

The accurate prediction of drug-target interactions (DTIs) is considered crucial in the drug development process, as it not only accelerates drug development but also plays a central role in drug repurposing and the discovery of new therapies [1–3].

Traditional biochemical experimental methods, widely employed in wet laboratories, are often time-consuming and costly, while also facing challenges related to insufficient generalization capabilities [4-5]. Consequently, an increasing number of researchers have begun to focus on the application of computational methods [6-7] to identify drug-target interactions. This shift has significantly reduced development costs and shortened the drug development cycle [8]. Computational methods for drug-target interaction can be categorized into four fields: ligand-based approaches, molecular docking techniques, feature-driven methods, and network analysis strategies.

Ligand-based approaches assume that drugs can predict interactions relying on existing knowledge [9], even in the absence of the three-dimensional structure of the target. However, when the number of known ligands that bind to the target protein is small, the values obtained from these methods may become unreliable.

Molecular docking techniques utilize the chemical composition of drugs and the three-dimensional (3D) structure of proteins to predict the binding patterns of drugs with known 3D proteins. This approach relies on the availability of 3D structures for simulations. However, in cases involving a large number of proteins, such as G-protein-coupled receptors and ion channels [11-12], it is challenging to obtain the required structural data due to their structural complexity. Keizer et al. identified potential DTIs through grouping and quantitative analysis based on the chemical similarity of proteins [13]. Nevertheless, the lack of accurate 3D protein structures significantly impacts the performance of molecular docking techniques.

Feature-driven methods [14], commonly referred to as feature engineering, aim to represent the relationship between drugs and targets as fixed-length feature vectors, typically accompanied by binary labels. By classifying these vectors according to their labels, it is feasible to effectively distinguish between positive interactions and negative interactions. These features are applied to various machine learning models, such as support vector machines, tree-based algorithms, and other kernel methods, to identify DTIs [15]. However, such methods overlook heterogeneous types and face challenges when adding long indirect connections between two vertices.

Network analysis strategies illustrate the interactions between multiple biological entities through heterogeneous networks, while homogeneous networks describe the associations within specific biological entities. Various network-based models have been developed to predict

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interactions between drugs and targets. Considering the possibility of information loss, Li et al. [16] employed a node perspective, network pattern perspective, and semantic perspective for modeling, proposing a heterogeneous graph neural network (MHGNN) that integrates multi-perspective information to extract interactions between multiple semantics. Similarly, Cheng et al. [17] obtained structural features of drugs and targets, as well as their interaction features, by extending connection fingerprints and knowledge graph embedding models. In the graph neural network constructed by Zhao et al. [18], modeling was performed from the node perspective, network pattern perspective, and semantic perspective to information of multiple granularities within the heterogeneous graph. By extracting detailed information about nodes from multiple perspectives, heterogeneous interactions between adjacent nodes, and the mutual influences between multiple semantics, predictions of drug-target interactions can be made.

In the task of predicting DTIs, it is crucial to consider the complex relationships between drugs and targets [19-20]. Although significant progress has been made in the association studies of multiple entities or drug-protein pairs, a common limitation of these methods is their reliance on a small number of modalities [21]. Such perspectives fail to capture abundant information and do not fully utilize the existing knowledge of the relationships between molecules and proteins. To enhance the effectiveness of drug-target prediction, it is particularly necessary to explore additional sources of information. The integration of multiple features not only provides a comprehensive perspective but also reveals the potential complex relationships between drugs and targets, thereby improving the accuracy and reliability of predictions.

In recent years, significant progress has been made in the field of protein research with Transformer-based models that utilize protein datasets for pre-training [22]. By pre-training on large-scale protein sequence data, these models have greatly enhanced the performance of protein-related tasks and enabled effective learning of protein language representations. Although pre-trained protein language models such as ProtTrans and the ESM-1b series [23] have demonstrated excellent performance across various protein tasks, the differences in their model architectures and pre-training datasets lead to distinct advantages in the features they extract, showcasing unique capabilities in multiple aspects.

Inspired by the abundance of feature expression capabilities of Protein Language Models (PLMs) and their outstanding performance in DTIs prediction tasks, we propose an integrated deep learning model named IM-DTI. This model fuses three PLMs from the ProtTrans and ESM-1b series to facilitate the identification of DTI. IM-DTI is a rapid and purely sequence-based DTI prediction model that fully leverages the abundant features provided by pre-trained PLMs. Furthermore, the model avoids the challenges associated with constructing complex graph structures required by Graph Neural Networks (GNNs). PLMs, through unsupervised learning, capture the distributional features of amino acid sequences from millions of proteins and generate sequence-based representations that encode hierarchical structure information. However, due to differences in model architecture and pre-training datasets, the features extracted by each PLM have distinct advantages, showcasing unique capabilities in various aspects. Therefore, we select multiple pre-trained PLMs for feature extraction and employ two feature embedding modules on the output of each PLM to learn high-dimensional features of drug and target segments, respectively. These high-dimensional features are subsequently compressed into a low-dimensional feature embedding space to enable binding affinity prediction that transcends binary classification. In this space, distances can effectively reflect the binding affinity between drugs and targets. Next, we combine distance features and utilize a Bayesian Optimization-enhanced Random Forest (BO_RF) algorithm for DTIs prediction. Additionally, to address the overfitting issues associated with complex models, we introduce residual modules in the feature embedding module and further accelerate the model's convergence speed through skip connections.

II. Methods and Materials

In this section, we detail the definition of the DTIs prediction problem and its modeling framework. We propose the IM-DTI model, which integrates higher-order information from multiple Protein Language Models to achieve effectiveness and accuracy in DTIs prediction. The architecture of IM-DTI is illustrated in Figure 1, and the overall design can be divided into three main modules: feature encoding module , feature embedding module and BO_RF module. First, four feature encoding modules are responsible for mapping the structural information of drug and protein segments into embedding feature vectors. Second, three feature embedding modules are utilized for feature mapping, calculating the cosine distances between features, and extracting interaction features between drug segments and protein segments. In this process, we introduce residual structures to accelerate model convergence and effectively alleviate overfitting issues. Finally, a BO_RF serves as the final layer of the ensemble learning framework, aiming to learn and integrate the features from each embedding space.

In the feature encoding module, for a given drug-target pair, we first apply the Morgan algorithm to extract various fragment types of the drug, and utilize Probert [24], ESM-1b [25], and ProtT5[24] to extract the functional segments of the protein, respectively. Subsequently, this fragment information is encoded and input into the embedding layer to generate the corresponding embedding feature vectors.

In the feature embedding module, the embedded feature vectors are used as input to generate feature representations for multiple targets and drugs through the corresponding embedding blocks. The features are then non-linearly compressed into the embedding space Leveraging cosine similarity, effectively representing the interactions between the drug and the target.

BO_RF module serves as the final layer of the ensemble learning framework, taking the three sets of interaction component prediction values as feature inputs. This model aims to integrate the feature information learned by the front-end models, ultimately yielding the aggregated prediction values for drug-target interactions.

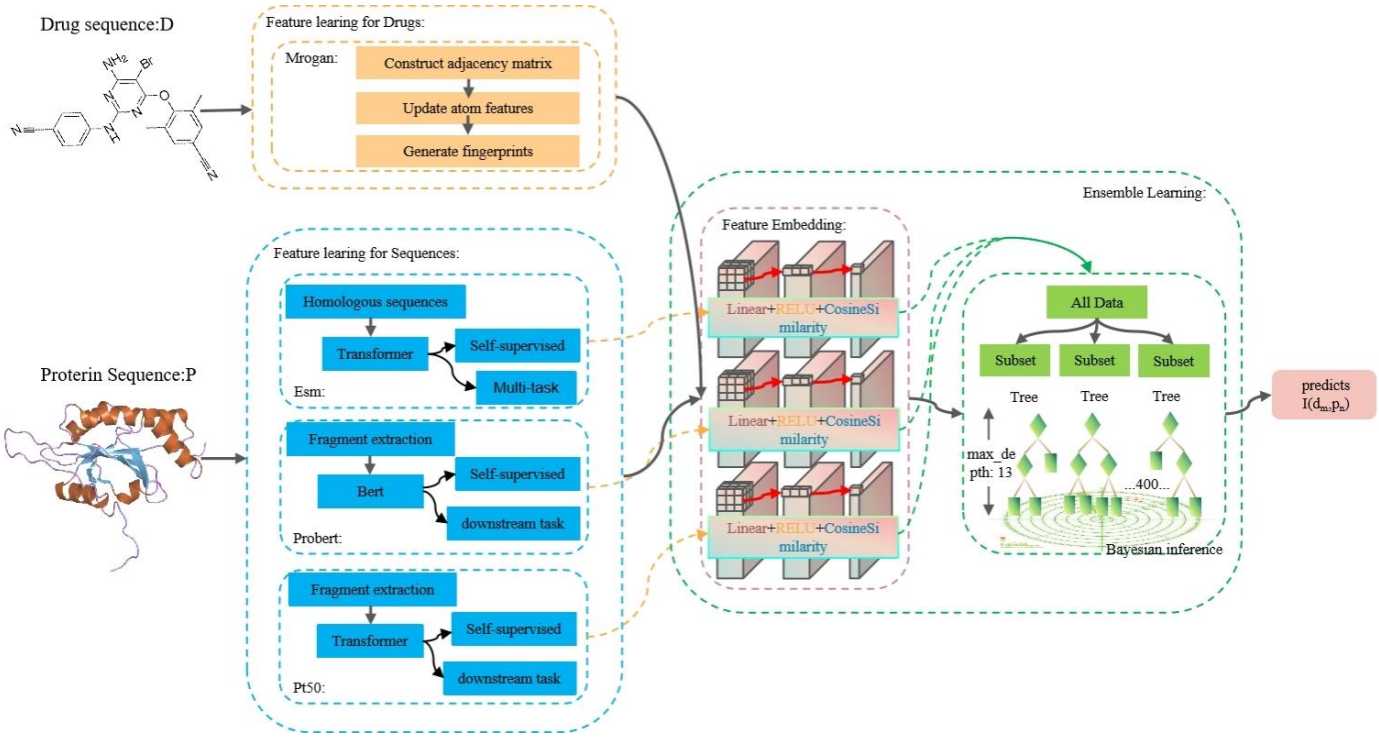

Fig. 1. IM-DTI Framework. First, the drug and target sequences is encoded Leveraging multiple protein language models to obtain embedding feature vectors. Then, the feature embedding module extracts features from drug fragments and protein fragments, projecting them non-linearly into the embedding space. Finally, a BO_RF module extracts learning information from the three embedding spaces, ultimately producing the aggregated prediction.

III. Results and Discussion

A. Datasets and Experimental Conditions

TABLE I
DATASET

Dataset	Drugs	Targets	Positive	Negative	Interactions
BIOSNAP	4510	2181	13836	13647	27483
DAVIS	68	379	1506	9597	11103
BindingDB	10	665	9166	23435	32601

TABLE II
TRAINING PARAMETERS

Parameter	Setting
Optimizer	AdamW
Initial Learning Rate	10^{-3}
Weight Decay (L2 Regularization)	10^{-4}
Cosine Annealing Learning Rate Scheduler	Ture
T_0 (Initial Cycle Length)	10
T_mult (Cycle Length Multiplication Factor)	2
eta_min (Minimum Learning Rate)	10^{-6}

We utilize three public datasets, namely BioSNAP [26], DAVIS [27], and BindingDB [28], to train and evaluate our IM-DTI model. These datasets are widely employed in DTIs prediction research and contain a range of samples and features, which facilitate effective training and validation of the model. In Table 1, we provide a detailed enumeration of the number of drugs, proteins, and both positive and negative samples contained within each dataset. The diversity and quantity of these samples not only offer a robust foundation for model training but also provide a reliable basis for subsequent performance evaluation and comparison. Regarding the configuration of training parameters, we list all key parameters and their settings in Table2.

B. Comparative Analysis

In this subsection, we evaluate the IM-DTI model and compare against other state-of-the-art (SOTA) works. These methods include a single PLM as well as some protein feature extraction techniques that do not use PLM, such as ConPLex, EnzPred-CPI, MolTrans, GNN CPI, DeepConv-DTI, and a single-task Ridge regression model. Our experiments are based on three low-coverage public datasets: BIOSNAP, BindingDB, DAVIS, Unseen Drugs and Unseen Targets.

In Table 3, we present the average area under the precision-recall curve (AUPR) for each model across five Monte Carlo Methods, a metric that is particularly important for evaluating imbalanced datasets. The results indicate that IM-DTI outperforms other methods in terms of accuracy, achieving an overall improvement of over 4%. Notably, on the DAVIS dataset, the AUPR improvement reached as high as 10%.

Moreover, IM-DTI also performs exceptionally well on two subsets, Unseen Drugs and Unseen Targets, which are not included in the training set but are part of the test set. This result

further validates the effectiveness of IM-DTI in zero-shot prediction tasks. In summary, this study demonstrates that the IM-DTI model exhibits outstanding performance in drug-target interaction prediction, showcasing its excellent generalization capability and good adaptability in handling large-scale, low-coverage prediction tasks.

TABLE III
IM-DTI VS. SIX STATE-OF-THE-ART WORKS

Dataset	ConPLex+	EnzPred-CPI+	MolTrans+	GNN-CPI*	DeepConv-DTI*	Ridge+	IM-DTI
BIOSNAP	0.897 ± 0.001	0.866 ± 0.003	0.885 ± 0.005	0.890 ± 0.004	0.889 ± 0.005	0.641 ± 0.000	0.940±0.000
BindingDB	0.628 ± 0.012	0.602 ± 0.006	0.598 ± 0.013	0.578 ± 0.015	0.611 ± 0.015	0.516 ± 0.000	0.705±0.001
DAVIS	0.458 ± 0.016	0.277 ± 0.009	0.335 ± 0.017	0.269 ± 0.020	0.299 ± 0.039	0.320 ± 0.000	0.560±0.003
Unseen Drugs	0.874 ± 0.002	0.844 ± 0.005	0.863 ± 0.005	–	0.847 ± 0.009	N/A	0.916±0.001
Unseen Targets	0.842 ± 0.006	0.795 ± 0.004	0.668 ± 0.045	–	0.766 ± 0.022	0.617 ± 0.000	0.891±0.000

+cited from (29), *cited from (30)

C. Affinity aggregated prediction

In this subsection, we aim to evaluate the performance of the IM-DTI model, trained for affinity prediction, on the TDC-DG dataset. This research employs a combination of dot product and GELU activation function, endowing the IM-DTI model with the capability for real-valued aggregated prediction value, which are interpreted as binding affinity. This approach underscores the importance of the model's out-of-domain generalization ability, aiming to simulate scenarios for predicting unrecorded interactions in real-world environments while being trained on known interactions. In contrast to previous studies where binary interaction predictors utilized a ReLU activation function in the final step to convert the cosine distances between projections in the DTI space into probability values, our method provides a flexible prediction mechanism. We train the IM-DTI model Leveraging five random training/validation splits and evaluate its performance on a held-out test set, resulting in an average Pearson correlation coefficient (PCC) of 0.596±0.000 between the true affinities and predicted affinities. This result indicates that the IM-DTI model excels in the affinity prediction task, effectively capturing the complex interactions between unknown drugs and targets. Notably, our research surpasses the current top-ranking model, Otter-Knowledge-Ensemble, highlighting the significant advantages of the IM-DTI model in drug-target interaction prediction.

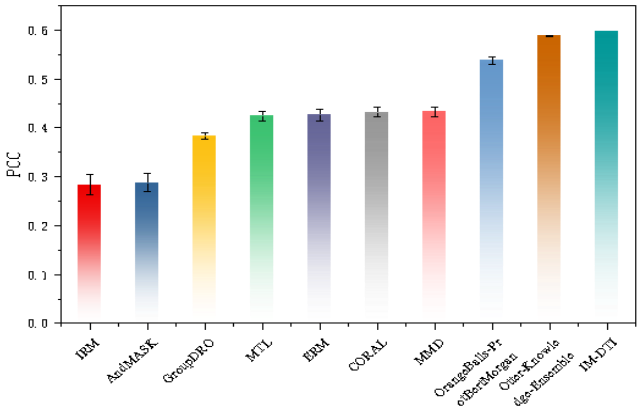

Fig. 2. Affinity aggregated prediction.

D. Ablation Study

In this study, we conduct ablation experiments to analyze the contribution of multiple pre-trained models to overall performance, with a particular focus on the combined effects of PerBERT, ESM-1b, and ProtT5. By incrementally adding one or two models, we are able to systematically evaluate the impact of each model on the aggregated prediction. This approach enables us to gain a deeper understanding of the role each model plays in overall performance.

Table 4 clearly presents the performance of individual models across various datasets. The experimental results indicate that PerBERT and ESM-1b exhibit the best overall performance, particularly demonstrating high predictive accuracy across multiple datasets. This finding suggests that PerBERT and ESM-1b possess significant advantages in capturing sequence information and understanding protein structures. Subsequently, we combine PerBERT and ESM-1b to form the ProBERT+ESM-1b model, and the experimental results show that this combination led to significant improvements across multiple datasets. This outcome further validates the effectiveness of model integration, indicating that

the combination of these two models can capture the complexity of drug-target interactions. Following this, we attempt to add a third model, ProtT5, to the combination, resulting in the IM-DTI model. The experimental results reveal that IM-DTI shows a slight improvement over ProBERT+ESM-1b, but does not significantly surpass its performance. This suggests that after the introduction of the ProtT5 model, the model is unable to capture additional features or information, leading to a diminished marginal effect on performance improvement. This is attributed to ProtT5's relatively accurate prediction values for certain negative interactions, while its performance in identifying positive interactions remains insufficient. Therefore, we do not pursue further model integration.

Overall, the IM-DTI model demonstrates superior performance across various datasets, particularly in prediction tasks involving low coverage and unseen samples, showcasing its strong generalization ability and adaptability. These results indicate that the IM-DTI model not only effectively integrates the advantages of multiple models but also delivers accurate aggregated prediction values in the complex prediction of drug-target interactions.

TABLE IV
MODEL EFFICACY COMPARISON MATRIX

Dataset	Perbert	ESM-1b	ProtT5	Probert+ESM-1b	ESM-1b+ProtT5	Probert+ProtT5	IM-DTI
BIOSNAP	0.935±0.000	0.939±0.000	0.713±0.000	0.940±0.000	0.937±0.001	0.933±0.000	0.940±0.000
BindingDB	0.689±0.000	0.683±0.000	0.562±0.000	0.694±0.001	0.686±0.001	0.696±0.002	0.705±0.001
DAVIS	0.530±0.000	0.532±0.000	0.260±0.000	0.525±0.009	0.535±0.004	0.532±0.006	0.560±0.003
Unseen Drugs	0.912±0.000	0.913±0.000	0.671±0.000	0.918±0.000	0.911±0.001	0.908±0.001	0.916±0.001
Unseen Targets	0.686±0.000	0.886±0.000	0.675±0.000	0.883±0.001	0.888±0.001	0.871±0.001	0.891±0.000
TDC-DG	0.592±0.000	0.568±0.000	0.488±0.000	0.598±0.000	0.568±0.000	0.591±0.000	0.596±0.000
Mean Accuracy	0.724	0.754	0.562	0.759	0.754	0.755	0.768

IV. Conclusion

In this study, we propose the IM-DTI model, designed to effectively predict drug-target interactions (DTI). By integrating high-order information from multiple pre-trained protein language models, IM-DTI demonstrates exceptional capability in identifying the complex interactions between drugs and targets. The model's design emphasizes the effectiveness of feature encoding and embedding, combining BO_RF algorithm ensemble learning to fully leverage fragment information from both drugs and proteins. We validate the importance of each pre-trained model in contributing to overall performance, highlighting the critical role of multi-model integration in drug-target prediction tasks. In summary, the IM-DTI model provides a novel and effective framework for predicting drug-target interactions, showcasing its potential in this field.

Future research focusses on further optimizing model performance and exploring its applications in broad biomedical contexts to advance drug discovery and development processes.

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