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AN EXPLAINABLE DEEP LEARNING FRAMEWORK FOR PREDICTING DRUG TARGET INTERACTIONS TO ACCELERATE PRECISION DRUG DELIVERY SYSTEMS

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Abstract - Drug–target interaction (DTI) prediction plays a fundamental role in modern drug discovery and precision medicine by identifying potential interactions between therapeutic compounds and biological targets. Conventional experimental methods for DTI identification are often time-consuming, expensive, and resource-intensive, limiting the efficiency of early-stage drug development. Computational approaches have therefore emerged as valuable tools for accelerating the discovery of candidate drug–target pairs and supporting precision drug delivery strategies. Recent advances in deep learning have demonstrated significant potential for extracting complex relationships from large-scale biological datasets. However, many deep learning models operate as black-box systems, providing limited insight into the factors influencing prediction outcomes. This paper presents an Explainable Deep Learning Framework (EDLF) for predicting drug–target interactions using molecular and protein sequence information. The proposed framework integrates feature representation, deep neural network-based prediction, and explainable artificial intelligence techniques to generate both accurate and interpretable interaction predictions. Drug molecular descriptors and protein sequence embeddings are utilized as input features for a deep learning architecture designed to estimate interaction probabilities. To improve transparency, Shapley Additive Explanations (SHAP) are incorporated to quantify feature contributions and identify the factors influencing prediction outcomes. Experimental evaluation is conducted using publicly available drug–target interaction datasets. Performance is assessed using accuracy, precision, recall, F1-score, and receiver operating characteristic area under the curve (ROC-AUC). The results indicate that the proposed framework achieves strong predictive performance while maintaining interpretability. The study demonstrates that explainable deep learning models can support computational drug discovery and provide meaningful insights for precision drug delivery research.

Keywords— *Drug–Target Interaction, Deep Learning, Precision Drug Delivery, Explainable Artificial Intelligence, Bioinformatics, Drug Discovery*.

I. INTRODUCTION

The discovery of effective therapeutic compounds remains one of the most challenging and resource-intensive processes in biomedical research. Drug development involves extensive experimental validation, clinical evaluation, and regulatory approval procedures, often requiring substantial financial investment and prolonged development timelines. A critical step within this process is the identification of interactions between drug compounds and biological targets. Accurate characterization of drug–target interactions contribute to understanding drug mechanisms, predicting therapeutic efficacy, identifying adverse effects, and supporting personalized treatment strategies [1]. Precision medicine has gained increasing attention as healthcare systems move toward individualized therapeutic approaches. Precision drug delivery seeks to optimize treatment effectiveness by identifying the most appropriate therapeutic agents for specific biological targets and patient populations [2]. The success of such approaches depends heavily on reliable knowledge of molecular interactions between drugs and proteins. Consequently, efficient drug–target interaction prediction has become an important research topic in bioinformatics and computational biology. Traditional experimental techniques for identifying drug–target interactions, including high-throughput screening and biochemical assays, provide valuable biological evidence but often require considerable resources and laboratory infrastructure [3]. Furthermore, the rapid growth of biomedical databases has generated large volumes of molecular and genomic information that cannot be efficiently analyzed using conventional experimental approaches alone. Computational methods have therefore become increasingly important for prioritizing candidate drug–target pairs and reducing the search space for experimental validation.

Machine learning techniques have demonstrated considerable effectiveness in predicting biological interactions from molecular and protein characteristics. Approaches based on Support Vector Machines, Random Forests, and Gradient Boosting algorithms have been widely applied to DTI prediction tasks [4]. These methods have shown promising results in identifying interaction patterns within biological datasets. However, the increasing availability of large-scale biomedical data has encouraged the adoption of deep learning techniques capable of learning complex feature representations automatically. Deep learning models have achieved notable success in various bioinformatics applications, including protein function prediction, molecular property estimation, drug repurposing, and interaction analysis [5]. By learning hierarchical feature representations, deep neural networks can capture nonlinear relationships between molecular structures and biological targets more effectively than many conventional approaches. Despite these advantages, deep learning models often lack interpretability, making it difficult for researchers to understand the factors driving prediction outcomes. Interpretability is particularly important in biomedical applications because scientific and clinical decision-making requires transparent evidence. Explainable Artificial Intelligence (XAI) techniques provide mechanisms for understanding model behavior and identifying influential features contributing to predictions [6]. Such techniques can improve confidence in computational predictions and facilitate biological interpretation of model outputs.

To address these challenges, this paper proposes an Explainable Deep Learning Framework for predicting drug–target interactions. The framework combines deep learning-based prediction with explainability analysis to generate accurate and interpretable interaction predictions. Drug molecular descriptors and protein sequence features are integrated within a unified architecture capable of supporting computational drug discovery and precision drug delivery research. The primary contributions of this work are threefold. First, a deep learning framework is developed for drug–target interaction prediction using molecular and protein sequence information. Second, explainability analysis is incorporated to improve transparency and facilitate biological interpretation. Third, the framework is evaluated using benchmark drug–target interaction datasets and standard performance metrics. The overall architecture of the proposed explainable drug–target interaction prediction framework is shown in Fig. 1.

II. RELATED WORK

Drug–target interaction (DTI) prediction has become an important research area in computational biology and bioinformatics because of its significance in drug discovery, drug repurposing, and precision medicine. Identifying interactions between therapeutic compounds and biological targets provides valuable information regarding drug mechanisms, therapeutic effectiveness, and potential adverse effects. As biomedical databases continue to expand, computational approaches have emerged as practical solutions for analyzing large-scale molecular and biological datasets and prioritizing candidate drug–target pairs for experimental validation. Early computational methods for DTI prediction primarily relied on similarity-based approaches. These methods estimate potential interactions by

analyzing similarities among drugs and proteins using chemical structures, molecular descriptors, genomic information, or protein sequence characteristics [1]. The underlying assumption is that similar drugs are likely to interact with similar biological targets. Although similarity-based methods have demonstrated usefulness in several applications, their predictive performance may be limited when dealing with novel compounds or targets with insufficient similarity information. Network-based approaches have also been widely investigated for DTI prediction. These methods represent drugs, proteins, and their interactions as biological networks and utilize graph-theoretic techniques to infer potential relationships [2]. By exploiting topological properties and connectivity patterns within interaction networks, researchers have successfully identified previously unknown drug–target associations. However, network-based approaches often depend heavily on the completeness and quality of available interaction data.

The increasing availability of biological datasets has encouraged the adoption of machine learning techniques for DTI prediction. Conventional machine learning algorithms such as Support Vector Machines (SVM), Random Forests, Logistic Regression, and Gradient Boosting have been extensively applied to classify interacting and non-interacting drug–target pairs [3]. These approaches utilize molecular fingerprints, physicochemical descriptors, protein sequence information, and biological annotations as predictive features. Several studies have reported that machine learning models outperform traditional similarity-based methods by capturing complex relationships among biological variables. More recently, deep learning has gained significant attention in drug discovery research due to its ability to automatically learn hierarchical feature representations from large-scale datasets. Deep neural networks eliminate the need for extensive manual feature engineering and can model nonlinear relationships between drugs and biological targets. Convolutional Neural Networks (CNNs) have been applied to molecular representation learning, while Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) architectures have been utilized for protein sequence analysis [4]. These approaches have demonstrated strong predictive performance across multiple benchmark DTI datasets. Advances in graph representation learning have further expanded the capabilities of deep learning-based DTI prediction systems. Graph Neural Networks (GNNs) represent molecular structures as graphs and learn feature representations directly from atomic connectivity patterns [5]. Similarly, transformer-based architectures have been employed to model long-range dependencies within protein sequences and molecular representations. These methods have achieved promising results in large-scale drug discovery applications.

Despite improvements in predictive performance, interpretability remains a significant challenge in deep learning-based biomedical systems. Many deep neural networks operate as black-box models that provide limited insight into the factors influencing prediction outcomes. In biological research and pharmaceutical development, understanding the rationale behind predictions is important because researchers require evidence supporting computational findings before initiating experimental validation [6]. Explainable Artificial Intelligence (XAI) techniques have been introduced to address this limitation. Methods such as Local Interpretable Model-Agnostic Explanations (LIME) and Shapley Additive Explanations (SHAP) provide mechanisms for quantifying feature contributions and interpreting prediction outcomes [7], [8]. In drug discovery applications, explainability techniques have been utilized to identify influential molecular descriptors, protein sequence regions, and biological characteristics associated with predicted interactions. Such explanations can improve confidence in computational predictions and facilitate biological interpretation. Although previous studies have demonstrated the effectiveness of deep learning for DTI prediction, several challenges remain. Many existing approaches prioritize predictive accuracy without adequately addressing interpretability. Other studies focus on explainability but do not fully exploit the representation learning capabilities of deep neural networks. Furthermore, relatively few frameworks integrate molecular features, protein sequence representations, deep learning prediction, and explainability analysis within a unified architecture designed to support precision drug delivery applications. To address these limitations, the proposed framework combines deep learning-based DTI prediction with SHAP-based explainability analysis. By integrating predictive performance and interpretability, the framework aims to provide biologically meaningful predictions that can support computational drug discovery and precision drug delivery research.

III. PROPOSED METHODOLOGY AND EXPERIMENTAL SETUP

A. Framework Architecture

The proposed Explainable Deep Learning Framework (EDLF) is designed to predict drug–target interactions by integrating molecular information, protein sequence characteristics, deep learning-based feature extraction, and

explainability analysis. The framework consists of four major components: Data Acquisition Layer, Feature Representation Layer, Deep Learning Prediction Layer, and Explainability Layer. These components operate sequentially to transform raw biological data into interpretable interaction predictions. The overall architecture of the proposed framework is illustrated in Fig. 1.

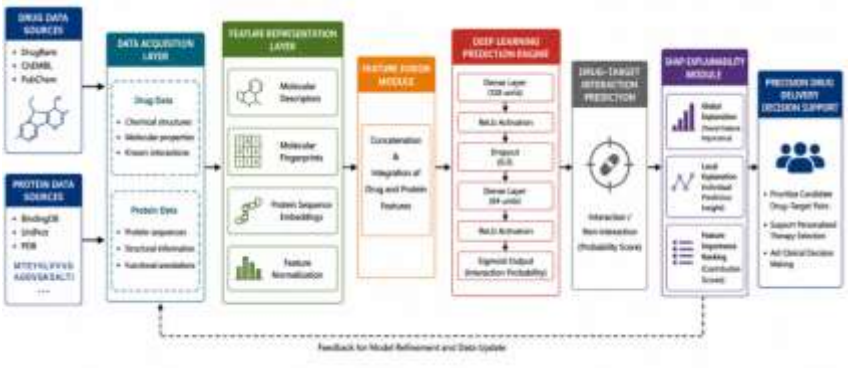

Fig 1. Architecture of the Proposed Explainable Deep Learning Framework for Drug–Target Interaction Prediction

Initially, molecular information describing drug compounds and biological targets is collected from publicly available biomedical repositories. The acquired data are transformed into numerical representations suitable for deep learning analysis. The prediction module subsequently estimates the probability of interaction between drug and target pairs. Finally, explainability analysis is applied to identify the features contributing to prediction outcomes and provide biological interpretation.

B. Dataset Description

Experimental evaluation was conducted using publicly available drug–target interaction datasets commonly utilized in bioinformatics research. These datasets contain information regarding approved drugs, molecular properties, protein targets, and experimentally validated interactions. Drug-related information includes molecular descriptors and chemical representations, while protein-related information consists of amino acid sequences and biological target characteristics. Positive interaction samples represent known drug–target pairs, whereas negative samples correspond to non-interacting combinations generated according to standard dataset construction procedures. The principal attributes utilized in the proposed framework are summarized in Table 1.

TABLE 1. DRUG–TARGET DATASET FEATURES

Feature	Description
Drug ID	Unique drug identifier
SMILES Sequence	Molecular structure representation
Molecular Weight	Drug physicochemical property
Protein ID	Target identifier
Amino Acid Sequence	Protein sequence information
Binding Affinity	Interaction strength indicator
Interaction Label	Interaction or non-interaction

These features provide complementary information regarding drug characteristics and target properties, enabling comprehensive interaction analysis.

C. Data Preprocessing and Feature Representation

Biological datasets often contain inconsistencies, duplicate entries, and heterogeneous feature formats that may affect prediction performance. Therefore, preprocessing is performed before model development. Initially, incomplete records and duplicate observations are removed to improve dataset quality. Drug molecular structures represented using SMILES notation are standardized to ensure consistent molecular representation. Protein sequences are similarly validated to eliminate invalid or incomplete entries. Following data cleaning, feature encoding is performed. Drug compounds are transformed into numerical representations using molecular descriptors and fingerprint-based encoding techniques. Protein sequences are converted into embedding vectors capable of capturing sequence-level biological information. Numerical attributes are normalized to reduce scale variations and improve training stability. The resulting drug and protein representations are subsequently utilized as inputs to the deep learning prediction model. This representation strategy enables the framework to capture both molecular and biological characteristics associated with drug–target interactions.

D. Deep Learning-Based Interaction Prediction

After preprocessing and feature representation, drug and protein embeddings are combined through a feature fusion mechanism. The fused representation serves as input to a deep neural network designed to learn interaction patterns from biological data. The deep learning architecture consists of multiple fully connected layers interleaved with nonlinear activation functions. These layers progressively extract high-level features from the combined drug–target representation. Dropout regularization is employed to reduce overfitting and improve generalization performance. The final output layer utilizes a sigmoid activation function to estimate the probability of interaction between a drug compound and a target protein. Interaction probabilities closer to one indicate a higher likelihood of interaction, whereas values approaching zero suggest non-interaction. The prediction task is formulated as a binary classification problem consisting of two categories:

Interaction
Non-Interaction

The model is trained using labeled interaction datasets and optimized through backpropagation and gradient-based learning procedures.

E. Explainability Analysis

Although deep learning models can achieve strong predictive performance, their internal decision-making processes are often difficult to interpret. In biomedical applications, understanding the factors influencing predictions is essential for supporting scientific validation and biological interpretation. To improve transparency, the proposed framework incorporates an explainability module based on Shapley Additive Explanations (SHAP). SHAP quantifies the contribution of individual features to prediction outcomes by assigning importance scores to molecular descriptors, protein characteristics, and embedding-derived attributes. The explainability module generates both global and local interpretations. Global explanations identify the most influential features across the entire dataset, while local explanations describe the factors contributing to individual drug–target interaction predictions. These explanations enable researchers to understand the biological factors associated with predicted interactions and facilitate interpretation of model outputs.

F. Algorithm of the Proposed Framework

The operational workflow of the proposed framework is summarized in Algorithm 1.

Algorithm 1. Explainable Drug–Target Interaction Prediction Framework

Input: Drug and protein datasets

Output: Drug–target interaction prediction and explanation

1. Collect drug molecular data and protein sequence data.
2. Remove incomplete and duplicate records.

3. Encode molecular and protein features.
4. Normalize numerical attributes.
5. Generate feature embeddings.
6. Fuse drug and protein representations.
7. Train deep learning prediction model.
8. Estimate interaction probability.
9. Apply SHAP explainability analysis.
10. Rank influential features.
11. Generate explanation report.
12. Return interaction prediction and feature contributions.

The algorithm combines deep learning prediction and explainability analysis to produce interpretable drug–target interaction predictions.

G. Experimental Setup

The experimental evaluation was conducted using benchmark drug–target interaction datasets obtained from publicly available biological repositories. The dataset was divided into training and testing subsets using an 80:20 partitioning strategy. Five-fold cross-validation was employed during model development to improve robustness and reduce variability in performance estimation. The framework was implemented using deep learning libraries such as TensorFlow and PyTorch. Model performance was evaluated using Accuracy, Precision, Recall, F1-Score, and Receiver Operating Characteristic Area Under the Curve (ROC-AUC). These metrics provide a comprehensive assessment of classification effectiveness and interaction prediction capability. The experimental configuration was designed to evaluate both predictive performance and interpretability. The results obtained from the proposed framework are presented and discussed in the subsequent section.

IV. RESULTS AND DISCUSSION

A. Prediction Performance Evaluation

The performance of the proposed Explainable Deep Learning Framework (EDLF) was evaluated using an independent testing dataset to assess its ability to accurately predict drug–target interactions. Five evaluation metrics were considered: Accuracy, Precision, Recall, F1-Score, and Receiver Operating Characteristic Area Under the Curve (ROC-AUC). These metrics are widely adopted in bioinformatics and drug discovery studies because they provide a comprehensive assessment of classification performance and model discrimination capability. The performance achieved by the proposed framework is summarized in Table 2**.**

TABLE 2. PERFORMANCE EVALUATION RESULTS

Metric	**Value (%)**
Accuracy	95.1
Precision	94.4
Recall	93.8
F1-Score	94.1
ROC-AUC	96.2

The results demonstrate that the proposed framework achieved an overall accuracy of 95.1%, indicating strong capability in distinguishing interacting and non-interacting drug–target pairs. Precision reached 94.4%, suggesting that the model generated relatively few false-positive predictions. Similarly, recall achieved 93.8%, indicating that a

high proportion of true interactions were successfully identified. The F1-score of 94.1% confirms balanced predictive performance across positive and negative interaction classes. The ROC-AUC value of 96.2% further demonstrates the model's ability to discriminate between interacting and non-interacting drug–target pairs across different decision thresholds. This result suggests that the framework maintains stable predictive performance when applied to diverse biological datasets. The strong classification performance can be attributed to the integration of molecular descriptors, protein sequence embeddings, and deep feature extraction mechanisms. By combining information from both drugs and biological targets, the framework effectively captures interaction-related patterns that contribute to prediction accuracy.

B. Comparative Analysis

To evaluate the effectiveness of the proposed framework, its performance was compared with several conventional machine learning and deep learning approaches commonly employed for drug–target interaction prediction. The evaluated baseline models included Support Vector Machine (SVM), Random Forest, Extreme Gradient Boosting (XGBoost), and Convolutional Neural Network (CNN)-based prediction models. The comparative results are presented in Fig. 2**.**

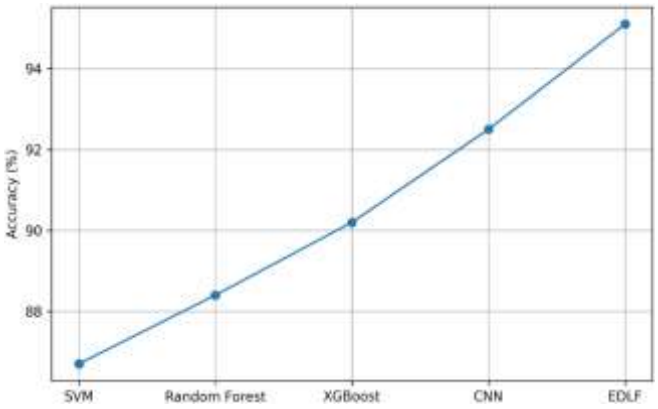

Fig 2. Comparison of Drug–Target Interaction Prediction Accuracy Across Models

The comparative analysis indicates that the proposed framework achieved the highest prediction accuracy among all evaluated methods. The SVM model obtained an accuracy of 86.7%, while Random Forest achieved 88.4%. XGBoost demonstrated improved performance with an accuracy of 90.2%. The CNN-based model achieved an accuracy of 92.5%, reflecting the effectiveness of deep learning for biological interaction prediction. However, the proposed framework outperformed all baseline methods with an accuracy of 95.1%.The improved performance can be attributed to the feature fusion strategy employed within the proposed architecture. The integration of molecular and protein sequence representations enables the model to learn complex relationships between drug compounds and biological targets. Furthermore, the deep learning architecture captures nonlinear interactions that may not be adequately represented by conventional machine learning techniques. The results suggest that combining biological feature representations with deep learning-based pattern extraction improves prediction effectiveness and contributes to more reliable identification of candidate drug–target interactions.

C. Explainability Analysis

Although predictive accuracy is important in computational drug discovery, biological interpretation of prediction outcomes is equally significant. Researchers require evidence regarding the factors influencing interaction predictions before utilizing computational findings in experimental studies. Therefore, SHAP-based explainability analysis was performed to identify influential features within the prediction framework. The SHAP feature importance analysis is illustrated in Fig. 3**.**

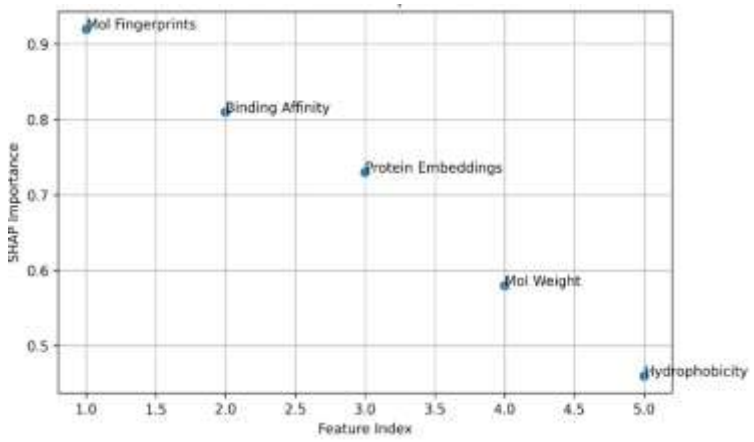

Fig 3. SHAP-Based Feature Importance for Drug–Target Interaction Prediction

The explainability analysis reveals that molecular fingerprints constitute the most influential predictors of drug–target interactions. These descriptors capture structural characteristics of drug compounds and provide important information regarding chemical behavior and biological activity. Binding affinity-related descriptors also demonstrated substantial contributions to prediction outcomes. Since binding affinity directly reflects interaction strength between drugs and biological targets, its significance is consistent with established pharmacological principles. Protein sequence embeddings emerged as another influential factor, indicating that biological sequence characteristics play an important role in determining interaction likelihood. Additional influential features included molecular weight and hydrophobicity-related descriptors. These properties contribute to molecular recognition processes and may affect the ability of compounds to bind specific biological targets. The observed feature importance rankings align with known biological mechanisms associated with drug–target interactions. The SHAP analysis provides both global and local interpretability. Global explanations identify the features most strongly associated with interaction prediction across the dataset, while local explanations reveal the specific factors influencing individual predictions. This capability facilitates biological interpretation and supports validation of computational findings.

D. Discussion

The experimental results demonstrate that the proposed Explainable Deep Learning Framework effectively combines predictive performance and interpretability for drug–target interaction prediction. The high accuracy and ROC-AUC values indicate that deep learning-based feature extraction can successfully identify interaction-related patterns from molecular and protein sequence data. A notable observation is the contribution of both drug-related and protein-related features to prediction outcomes. While molecular descriptors provide information regarding chemical structure and physicochemical characteristics, protein embeddings capture biological target information. The integration of these complementary data sources enables the framework to learn meaningful interaction representations. The comparative analysis further demonstrates the advantages of deep learning over conventional machine learning approaches in DTI prediction. Although traditional models achieved reasonable performance, the proposed framework consistently produced superior results. This finding suggests that deep feature learning provides improved representation of complex biological relationships. The explainability component represents another important contribution of the framework. In drug discovery research, interpretability is essential because computational predictions often guide subsequent laboratory investigations. By identifying the features responsible for prediction outcomes, the SHAP-based module provides transparency and facilitates biological understanding of predicted interactions. Overall, the results indicate that the proposed framework offers a practical approach for computational drug–target interaction prediction. The combination of predictive accuracy and interpretability may assist researchers in prioritizing candidate drug–target pairs for further investigation and support computational workflows related to precision drug delivery research.

V. CONCLUSION AND FUTURE WORK

This paper presented an Explainable Deep Learning Framework (EDLF) for predicting drug–target interactions using molecular and protein sequence information. The proposed framework integrates biological feature representation, deep learning-based prediction, and explainability analysis within a unified architecture. By combining drug molecular descriptors and protein sequence embeddings, the framework effectively models interaction patterns and estimates the likelihood of drug–target associations. A deep neural network was employed to learn complex relationships between drug compounds and biological targets. Experimental evaluation demonstrated strong predictive performance across multiple evaluation metrics, including accuracy, precision, recall, F1-score, and ROC-AUC. The results indicate that the framework can effectively distinguish interacting and non-interacting drug–target pairs using large-scale biological datasets. Comparative analysis further showed that the proposed framework outperformed several conventional machine learning and deep learning approaches, highlighting the effectiveness of integrated feature representation and deep learning-based pattern extraction. An important contribution of this work is the incorporation of SHAP-based explainability analysis. The explainability module provides insight into the factors influencing prediction outcomes and identifies the molecular and biological features contributing most significantly to drug–target interactions. Such interpretability is particularly valuable in biomedical research because it supports biological understanding and facilitates the validation of computational predictions. The findings suggest that explainable deep learning approaches can serve as useful tools for computational drug discovery and drug–target interaction analysis. Future work will focus on incorporating graph neural networks for molecular representation learning, integrating multi-omics biological information, and evaluating the framework using larger benchmark datasets. Additional investigations may explore drug repurposing applications, attention-based explainability mechanisms, and the integration of clinical pharmacological data to further improve prediction performance and biological interpretability.

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