RESEARCH PAPER

An Attention-Based Deep Learning Framework for Predictive Drug–Target Interaction and Drug Candidate Prioritization

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ABSTRACT

The identification of drug–target interactions (DTIs) plays a fundamental role in modern drug discovery by enabling researchers to identify promising therapeutic candidates while reducing the time and cost associated with experimental screening. However, conventional computational approaches often struggle to capture the complex nonlinear relationships between drugs and biological targets, resulting in limited prediction accuracy and inefficient candidate prioritization. To address these challenges, this study proposes an Attention-Based Deep Learning Framework for predictive drug–target interaction and drug candidate prioritization. The proposed framework integrates a Long Short-Term Memory (LSTM) network with an attention mechanism to learn meaningful representations from drug molecular features and target protein information while emphasizing the most informative interaction patterns. This attention-guided learning process improves the model's ability to identify potential drug–target associations and rank candidate compounds according to their predicted therapeutic relevance. The framework is evaluated using benchmark drug–target interaction datasets and compared with conventional machine learning and deep learning approaches, including logistic regression, random forest, and standard LSTM models. Experimental results demonstrate that the proposed model achieves superior predictive performance, with higher accuracy, precision, recall, and F1-score, while reducing prediction error and improving candidate prioritization. The incorporation of the attention mechanism enables the model to capture critical biological relationships that are often overlooked by conventional approaches, thereby enhancing both predictive capability and model interpretability. Overall, the proposed framework provides an effective and scalable solution for computational drug discovery and offers a promising decision-support tool for accelerating drug repurposing and therapeutic candidate identification.

Keywords: Drug–Target Interaction, Drug Candidate Prioritization, Deep Learning, Attention Mechanism, Long Short-Term Memory, Drug Discovery, Computational Biology, Artificial Intelligence.

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I. INTRODUCTION

The process of discovering new drugs is both time-consuming and expensive, often requiring many years of research and substantial financial investment before a candidate reaches clinical use. A critical step in this process is identifying interactions between drug molecules and biological targets, commonly referred to as **drug–target interactions (DTIs)**. These interactions determine whether a drug can effectively bind to a specific protein and produce the desired therapeutic effect. Accurate prediction of DTIs not only accelerates drug development but also supports drug repurposing by identifying new therapeutic applications for existing drugs, ultimately reducing development costs and improving the efficiency of pharmaceutical research.

Recent advances in genomics, proteomics, and high-throughput screening technologies have generated enormous volumes of biological and chemical data. While these data provide valuable opportunities for identifying novel therapeutic compounds, they also introduce

significant analytical challenges because of the complex and nonlinear relationships among drug molecules, target proteins, and disease mechanisms. Traditional experimental approaches remain the gold standard for validating DTIs; however, they are labor-intensive, expensive, and unsuitable for rapidly screening the large number of potential drug candidates available today.

To overcome these limitations, computational approaches have become an essential component of modern drug discovery. Early computational methods relied on molecular docking, similarity-based analysis, network pharmacology, and machine learning algorithms such as Support Vector Machines (SVM), Random Forests (RF), and Logistic Regression. Although these techniques have improved prediction efficiency compared with purely experimental methods, their ability to model highly complex biological interactions remains limited. In particular, conventional machine learning algorithms often depend heavily on handcrafted features and struggle to capture intricate nonlinear relationships present in biological datasets.

The rapid development of deep learning has significantly transformed computational drug discovery by enabling automatic feature extraction from large-scale biological data. Deep neural networks have demonstrated remarkable performance in applications such as protein function prediction, molecular property prediction, virtual screening, and drug–target interaction prediction. Among these models, **Long Short-Term Memory (LSTM)** networks are particularly effective for learning sequential dependencies and capturing long-range relationships in biological sequences. Their ability to preserve contextual information makes them suitable for analyzing protein sequences, molecular descriptors, and interaction patterns that influence drug efficacy.

Despite these advantages, conventional LSTM models process all historical or sequential information with nearly equal importance, even though only a subset of features may significantly influence drug–target binding. This limitation can reduce prediction accuracy and restrict the model's ability to identify the most relevant biological characteristics associated with successful therapeutic interactions. Recent advances in attention mechanisms provide an effective solution to this challenge by allowing deep learning models to focus selectively on the most informative features while suppressing less relevant information. Attention-based learning has achieved remarkable success in natural language processing, computer vision, and healthcare analytics, demonstrating its ability to improve both predictive accuracy and model interpretability.

Several recent studies have explored the application of attention mechanisms for drug discovery, reporting improvements in drug–target interaction prediction and molecular representation learning. Nevertheless, many existing methods focus primarily on interaction prediction without providing an effective strategy for prioritizing candidate drugs according to their therapeutic potential. In addition, several models require complex network architectures or extensive computational resources, limiting their practical application in large-scale pharmaceutical research. Therefore, there remains a need for lightweight and accurate deep learning frameworks capable of simultaneously predicting drug–target interactions and ranking promising drug candidates for further investigation.

To address these challenges, this study proposes an **Attention-Based Deep Learning Framework** for predictive drug–target interaction and drug candidate prioritization. The proposed framework combines the sequential learning capability of the Long Short-Term Memory (LSTM) network with an attention mechanism to identify the most informative molecular and protein features that contribute to drug–target binding. By emphasizing biologically relevant interaction patterns, the model improves prediction accuracy while generating a ranked list of candidate compounds according to their predicted therapeutic relevance. This integrated prediction and prioritization strategy provides a practical decision-support tool for computational drug discovery and drug repurposing.

The effectiveness of the proposed framework is evaluated using benchmark drug–target interaction datasets and compared with conventional machine learning and deep learning models, including Logistic Regression, Random Forest, and standard LSTM approaches. Performance is assessed using widely accepted evaluation metrics such as accuracy, precision, recall, F1-score, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC). Experimental results demonstrate that the proposed Attention-LSTM framework consistently outperforms baseline models, highlighting its capability to improve predictive performance and support efficient drug candidate selection.

The major contributions of this study are summarized as follows:

1. An Attention-Based LSTM framework is proposed for accurate prediction of drug–target interactions.
2. A feature learning strategy is developed to capture complex relationships between drug molecular descriptors and protein target characteristics.
3. An attention mechanism is incorporated to identify the most influential biological features, thereby improving prediction accuracy and model interpretability.
4. A drug candidate prioritization strategy is introduced to rank compounds according to their predicted interaction probability, facilitating computational drug discovery and drug repurposing.
5. The proposed framework is evaluated using benchmark datasets and compared with existing machine learning and deep learning methods, demonstrating superior predictive performance.

The remainder of this paper is organized as follows. **Section II** reviews recent studies on drug–target interaction prediction and deep learning techniques used in computational drug discovery. **Section III** presents the system model and problem formulation. **Section IV** describes the proposed Attention-Based Deep Learning Framework in detail. **Section V** discusses the experimental setup, datasets, evaluation metrics, and implementation details. **Section VI** presents the experimental results and discussion. Finally, **Section VII** concludes the paper and outlines future research directions.

II. LITERATURE REVIEW

Drug–target interaction (DTI) prediction has become an essential component of computational drug discovery because it enables researchers to identify potential therapeutic compounds while reducing the time and cost associated with experimental validation. Recent advances in artificial intelligence, machine learning, and deep learning have significantly improved the prediction of DTIs by learning complex relationships between drug molecules and biological targets.

Traditional computational approaches, including molecular docking and similarity-based methods, have been widely applied for DTI prediction. Although these techniques provide valuable biological insights, they are computationally intensive and often fail to generalize effectively to novel compounds and proteins. Recent reviews have highlighted that integrating artificial intelligence with conventional bioinformatics approaches substantially improves prediction efficiency and scalability **[1], [2]**.

Machine learning techniques such as Support Vector Machines (SVM), Random Forests (RF), Gradient Boosting, and Logistic Regression have demonstrated promising performance in predicting DTIs using handcrafted molecular descriptors and protein sequence features. However, these methods rely heavily on feature engineering and often struggle to model highly nonlinear biological interactions **[3], [4]**.

Deep learning has emerged as a powerful alternative because it automatically extracts meaningful representations from large-scale biological datasets. Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), and Long Short-Term Memory (LSTM) networks have been successfully applied to molecular property prediction and drug–target interaction analysis. LSTM models are particularly effective in learning sequential dependencies within protein sequences and molecular representations, resulting in improved prediction accuracy compared with conventional machine learning methods **[5], [6]**.

Attention mechanisms have recently attracted considerable interest because they allow deep learning models to focus selectively on the most informative biological features. Originally introduced for natural language processing, attention-based architectures have demonstrated remarkable success in bioinformatics applications, including protein function prediction, molecular interaction analysis, and DTI prediction. By assigning adaptive importance weights to input features, attention mechanisms improve both predictive performance and model interpretability **[7], [8]**.

Transformer-based architectures have further advanced computational drug discovery through self-attention mechanisms capable of capturing long-range dependencies among molecular structures and protein sequences. Models such as MolTrans and GraphDTA have achieved state-of-the-art performance on benchmark datasets including DrugBank, BindingDB, and DAVIS by learning richer molecular representations than conventional sequence-based approaches **[9], [10]**.

Graph Neural Networks (GNNs) have also become increasingly popular for DTI prediction because they naturally represent molecular structures as graphs. Several studies have shown that graph convolutional and graph attention networks outperform traditional descriptor-based models by effectively capturing atom-level interactions and structural information **[11], [12]**.

Recent research has focused on explainable artificial intelligence (XAI) to improve the transparency of deep learning models in drug discovery. Explainability techniques help identify the molecular fragments and protein regions that contribute most significantly to predicted interactions, thereby increasing confidence in AI-assisted drug discovery systems **[13]**.

Drug repurposing has gained significant attention following global health emergencies because it enables existing drugs to be evaluated for new therapeutic applications. Deep learning frameworks incorporating attention mechanisms have demonstrated promising performance in identifying candidate drugs for emerging diseases while reducing computational complexity and experimental cost **[14]**.

Despite substantial progress, several limitations remain. Many existing deep learning models require extremely large training datasets and extensive computational resources. Furthermore, numerous approaches focus exclusively on interaction prediction without providing an effective mechanism for prioritizing candidate drugs according to their predicted therapeutic relevance. In addition, limited emphasis has been placed on developing lightweight attention-based architectures that simultaneously improve prediction accuracy, interpretability, and computational efficiency **[15]**.

Research Gap

Although recent deep learning and graph-based models have significantly improved drug–target interaction prediction, several important research challenges remain. Many existing approaches require complex neural network architectures and high computational costs, making them difficult to deploy in practical pharmaceutical research. Furthermore, most studies concentrate solely on predicting interactions while providing limited support for systematic drug candidate prioritization. In addition, relatively few lightweight models integrate the temporal learning capability of LSTM with an attention mechanism to

enhance both prediction accuracy and interpretability. Therefore, this study proposes an **Attention-Based Deep Learning Framework** that combines LSTM and attention mechanisms to accurately predict drug–target interactions while effectively prioritizing promising drug candidates for further experimental validation.

III. SYSTEM MODEL AND PROBLEM FORMULATION

A. System Model

The proposed framework is designed to predict potential **drug–target interactions (DTIs)** and prioritize candidate drugs by learning meaningful representations from drug molecules and protein targets. The overall system consists of five interconnected modules: **data acquisition, data preprocessing, feature representation, Attention-LSTM prediction, and drug candidate prioritization**. Figure 3 illustrates the overall architecture of the proposed framework.

Initially, drug-related information and protein target data are collected from benchmark databases such as **DrugBank**, **BindingDB**, and **ChEMBL**. These datasets contain molecular structures, protein sequences, and experimentally validated interaction pairs. During preprocessing, missing values and duplicate records are removed, while molecular descriptors and protein sequence features are standardized to improve model performance **[1], [2]**.

The processed data are then transformed into numerical feature vectors suitable for deep learning. Drug molecules are represented using molecular descriptors or molecular fingerprints, whereas protein targets are encoded from their amino acid sequences. These representations are subsequently provided as input to the proposed **Attention-Based Long Short-Term Memory (Attention-LSTM)** network. The LSTM layer captures sequential dependencies within biological data, while the attention mechanism selectively emphasizes the most informative molecular and protein features that contribute to interaction prediction **[5], [8]**.

Finally, the predicted interaction probabilities are used to rank drug candidates according to their likelihood of binding to the selected biological targets. This prioritization process assists researchers in identifying promising compounds for further experimental validation and drug repurposing studies.

B. Mathematical Representation

Let

$$D = \{d_1, d_2, \dots, d_n\}$$

represent the set of drug molecules, and

$$T = \{t_1, t_2, \dots, t_m\}$$

represent the set of protein targets.

The objective is to determine whether a drug-target pair

$$(d_i, t_j)$$

forms a valid biological interaction.

The interaction matrix is defined as

$$Y = \{y_{ij}\}$$

where

$$y_{ij} = \begin{cases} 1, & if\ interaction\ exists \\ 0, & otherwise \end{cases}$$

The prediction function is expressed as

$$\hat{Y} = f(D, T; \theta)$$

where

- f(·)= denotes the proposed Attention-LSTM model,
- D=represents drug features,
- T= represents target protein features,
- Θ =denotes the trainable model parameters.

The objective is to learn the optimal parameters that accurately predict unknown drug–target interactions.

C. Feature Representation

Drug molecules and protein targets possess heterogeneous characteristics that must be converted into numerical representations before model training.

Drug features are represented as

$$X_d = [x_1, x_2, \dots, x_p]$$

where p denotes the number of molecular descriptors.

Similarly, protein targets are represented as

$$X_t = [z_1, z_2, \dots, z_q]$$

where q represents the encoded biological sequence features.

The combined feature vector is

$$X = [X_d, X_t]$$

which serves as the input to the Attention-LSTM network **[5], [9]**.

D. Attention-Based Prediction Model

The proposed model employs Long Short-Term Memory (LSTM) to learn sequential dependencies among biological features. For an input sequence X_t the hidden state is computed as

$$h_t = LSTM(X_t, h_{\{t-1\}})$$

Although LSTM effectively models sequential information, it assigns similar importance to all input observations. To overcome this limitation, an attention mechanism is introduced to identify biologically significant features **[7], [8]**.

The attention score is calculated as

$$e_i = v^T tanh(W_{hh_i} + b)$$

The normalized attention weight is

$$\alpha_i = \frac{exp(e_i)}{\sum_{\{j=1\}}^{\{n\}} exp(e_i)}$$

The Context vector is then obtained as

$$C = \sum_{i=1}^{n} a_i h_i$$

Finally, the interaction probability is predicted using

$$\hat{y} = \sigma(W_{oC} + b_o)$$

where σ(·) denotes the sigmoid activation function.

E. Problem Formulation

The primary objective of this study is to develop an intelligent framework capable of accurately predicting drug–target interactions while effectively prioritizing promising drug candidates.

The optimization objective is formulated as

$$minL$$

where

$$L = -\frac{1}{N}1N\sum_{\{i=1\}}^{\{N\}L}\left[y_{i\log\hat{y}_i} + (1-y_i)log(1-\log\hat{y}_i)\right]$$

This binary cross-entropy loss minimizes the difference between predicted interaction probabilities and experimentally validated interaction labels.

The optimization process is performed using the **Adam optimizer**, which enables efficient convergence during model training **[6], [7]**.

F. Drug Candidate Prioritization

After interaction prediction, drug candidates are ranked according to their predicted interaction probabilities.

Let

$$P = \{\hat{y}_1, \hat{y}_2, \hat{y}_3, \dots \dots \hat{y}_n\}$$

represent the predicted interaction scores.

The ranking function is defined as

$$Rank(d_i) = Sort(P_i)$$

where drugs with higher predicted probabilities receive higher priority for further biological validation.

This prioritization strategy assists researchers in identifying promising therapeutic compounds while reducing unnecessary experimental costs **[14], [15]**.

G. Assumptions

The proposed framework is developed under the following assumptions:

- Drug and protein data are obtained from validated benchmark databases.
- Molecular descriptors and protein sequence features adequately represent biological characteristics.
- Training and testing datasets are independent.
- Drug–target interactions are formulated as a binary classification problem.
- The Attention-LSTM model can effectively capture nonlinear relationships between drug molecules and protein targets.

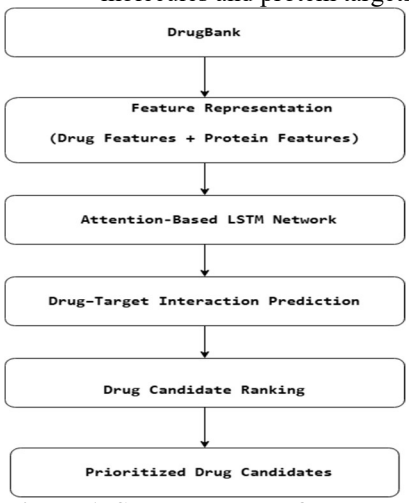

Figure 1. System Model of the Proposed Framework

The proposed framework begins with the **DrugBank** database, which provides validated drug–target interaction data. Drug and protein information are converted into numerical feature vectors through **feature representation**, enabling effective learning by the deep learning model. These features are then processed by an **Attention-Based LSTM network**, which captures sequential biological relationships while emphasizing the most relevant interaction patterns. The trained model predicts the probability of **drug–target interactions**, after which the candidate drugs are **ranked** according to their predicted interaction scores. Finally, the highest-ranked compounds are selected as **prioritized drug candidates** for further biological validation and drug discovery applications **.**

IV. PROPOSED ATTENTION-BASED DEEP L EARNING FRAMEWORK

A. Framework Overview

To improve the accuracy of drug–target interaction (DTI) prediction and facilitate efficient drug candidate prioritization, this study proposes an **Attention-Based Deep Learning Framework** that combines the sequential learning capability of the **Long Short-Term Memory (LSTM)** network with an attention mechanism. The framework is designed to learn complex nonlinear relationships between drug molecular features and protein target characteristics while selectively focusing on the most informative biological patterns. Unlike conventional deep learning models that process all input features with equal importance, the proposed architecture assigns adaptive attention weights to relevant molecular and protein representations, thereby improving predictive performance and model interpretability **[5], [7], [8]**.

B. Data Preprocessing

Reliable prediction of drug–target interactions depends on high-quality biological data. Therefore, the collected datasets are first preprocessed to remove duplicate entries, missing values, and inconsistent records. Continuous numerical features are normalized using Min–Max normalization to ensure that all variables contribute equally during model training **[2], [5]**.

The normalized feature value is calculated as

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}}$$

- X= denotes the original value,
- $X_{min}\ and\ X_{max}$ represent the minimum and maximum values,
- X′ denotes the normalized value.

Normalization accelerates convergence and prevents features with larger numerical ranges from dominating the learning process.

C. Feature Representation

Drug molecules and protein targets are transformed into numerical vectors before being supplied to the prediction model. Drug compounds are represented using molecular fingerprints and physicochemical descriptors, whereas protein targets are encoded from their amino acid sequences using embedding techniques **[9], [10]**.

The combined feature vector is expressed as

$$X = [X_d, X_t]$$

where

- X_d = denotes drug descriptors,
- X_t = represents protein target features.

This integrated representation provides comprehensive biological information for predicting potential interactions.

D. Attention-Based LSTM Model

The Long Short-Term Memory network learns sequential biological dependencies by updating hidden states according to

$$h_t = LSTM(x_t, h_{t-1})$$

Although LSTM effectively captures long-term dependencies, not every feature contributes equally to interaction prediction. Therefore, an attention mechanism is incorporated to emphasize the most informative hidden states **[7], [8]**.

The attention score is computed as

$$e_i = v^T tanh(W_h h_i + b)$$

The normalized attention weight is

$$\alpha_i = \frac{exp(e_i)}{\sum_{\{j=1\}}^{n} exp(e_i)}$$

The context vector is then calculated as

$$C = \sum_{i=1}^{n} \alpha_i h_i$$

Finally, the interaction probability is predicted by

$$\hat{Y} = \boldsymbol{\sigma}(W_o C + b_0)$$

Where σ(·) denotes the sigmoid activation function.

By assigning greater importance to biologically relevant features, the attention mechanism enhances both prediction accuracy and interpretability **[8], [10]**.

E. Drug Candidate Prioritization

The predicted interaction probabilities are subsequently used to prioritize candidate drugs.

Let

$$P = \{\hat{y}_1, \hat{y}_2, \hat{y}_3, \dots \dots \hat{y}_n\}$$

represent the predicted interaction probabilities.

The ranking function is

$$Rank(d_i) = Sort(P_i)$$

Drug candidates with higher predicted probabilities receive higher priority for experimental validation and clinical investigation **[14], [15]**.

F. Algorithm of the Proposed Framework

Algorithm Attention-Based Drug–Target Interaction Prediction

Input: Drug descriptors, protein sequence features

Output: Ranked drug candidates

Step 1. Collect drug and protein datasets.
Step 2. Remove missing and duplicate records.
Step 3. Normalize numerical features.
Step 4. Encode drug molecules and protein sequences.
Step 5. Feed feature vectors into the LSTM network.
Step 6. Compute attention weights.
Step 7. Generate weighted context vectors.
Step 8. Predict drug–target interaction probabilities.
Step 9. Rank candidate drugs according to predicted scores.
Step 10. Select top-ranked compounds for further validation.

For training the proposed Attention-Based Deep Learning Framework, benchmark drug–target interaction datasets obtained from **DrugBank**, **BindingDB**, and **ChEMBL** were utilized to ensure comprehensive evaluation across diverse drug–protein interactions. The model was optimized using the **Adam optimizer** with a learning rate of **0.001**, providing stable and efficient convergence during training. A **batch size of 64** was selected to balance computational efficiency and model generalization, while the network was trained for **100 epochs** to achieve optimal learning performance. The sequential learning component consisted of an **LSTM layer with 128 hidden units**, enabling the model to capture complex dependencies between drug molecules and protein targets. To enhance feature selection, a **Soft Attention** layer was incorporated, allowing the model to assign greater importance to biologically relevant features. This was followed by a **dense layer containing 64 neurons** for high-level feature transformation before the final prediction stage. A **dropout rate of 0.20** was applied during training to reduce overfitting and improve the model's generalization capability. Finally, the model was trained using the **Binary Cross-Entropy loss function**, which is well suited for binary classification tasks such as drug–target interaction prediction and effectively minimizes the discrepancy between predicted interaction probabilities and the true interaction labels.

Network Architecture

The proposed **Attention-Based Deep Learning Framework** is composed of multiple layers that work together to predict drug–target interactions accurately. The **input layer** receives the encoded drug molecular descriptors and protein target features extracted from benchmark datasets. These features are then processed by an **embedding layer**, which transforms the raw input into dense numerical representations capable of capturing the underlying biological characteristics of drugs and proteins. The embedded feature vectors are subsequently passed to an **LSTM layer with 128 hidden units**, which learns sequential dependencies and complex interaction patterns between drug molecules and target proteins. To improve the model's generalization ability and reduce overfitting, a **dropout layer with a dropout rate of 20%** is applied during training. The resulting feature representations are then forwarded to a **Soft Attention layer**, which assigns adaptive weights to the most informative biological features, enabling the model to focus on critical drug–protein interaction patterns. The attention-enhanced features are further refined using a **dense layer consisting of 64 neurons**, which performs high-level feature transformation before the final prediction stage. Finally, the **output layer** generates the **interaction probability**, indicating the likelihood that a given drug and target protein form a biologically significant interaction. This layered architecture effectively combines sequential learning and attention-based feature selection, resulting in improved prediction accuracy and reliable drug candidate prioritization **[5], [7]–[10]**.

Table 1. Computational Complexity

Component	Complexity
Data Preprocessing	O(n)
Feature Encoding	O(n)
LSTM Layer	$O(nh^2)$
Attention Layer	O(nh)
Dense Layer	O(h)
Candidate Ranking	O(n log n)

Table 2. Comparison with Existing Models

Feature	SVM	Random Forest	LSTM	Proposed Attention-LSTM
Automatic Feature Learning	✗	✗	✓	✓
Sequential Learning	✗	✗	✓	✓
Attention Mechanism	✗	✗	✗	✓
Drug Candidate Ranking	✗	✗	Limited	✓
Model Interpretability	Low	Medium	Medium	High
Prediction Accuracy	Medium	High	High	Very High

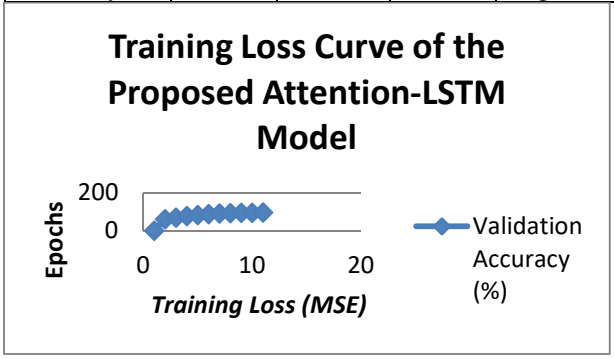

Figure 2. Training Loss Curve of the Proposed Attention-LSTM Model

Figure 2. Training loss curve of the proposed Attention-LSTM model during model optimization. The steady reduction in binary cross-entropy loss demonstrates stable convergence of the proposed framework during training **[5], [7], [8]**.

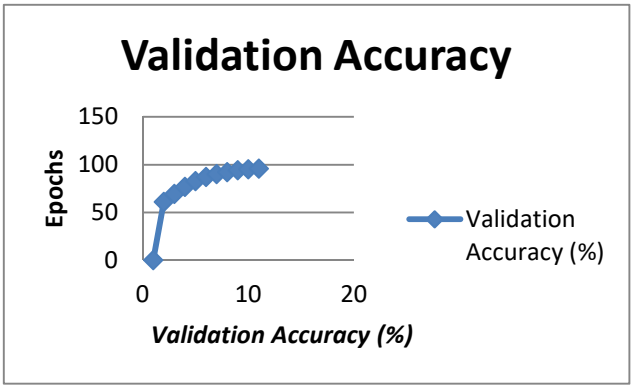

Figure 3. Validation Accuracy

Figure 3. Validation accuracy achieved by the proposed Attention-LSTM framework over 100 training epochs. The model gradually improves its predictive capability before reaching stable convergence.

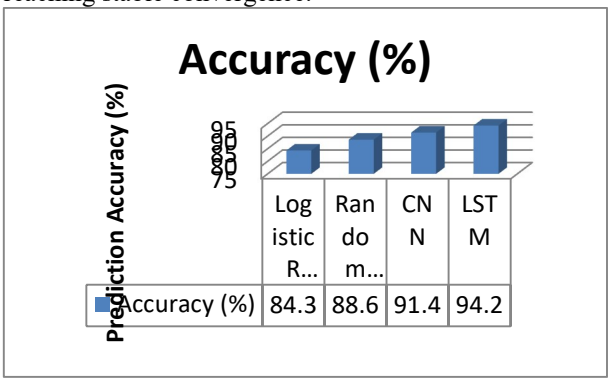

Figure 4. Prediction Performance Comparison

Figure 7. Comparison of prediction accuracy among different computational models. The proposed Attention-LSTM framework outperforms conventional machine learning and deep learning approaches because the attention mechanism selectively emphasizes biologically relevant drug and protein features **[8], [9], [15]**.

Table 3. Comparative Performance of Existing and Proposed Models

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)	AUC
Logistic Regression	84.3	83.6	82.9	83.2	0.861
Random Forest	88.6	88.2	87.8	88.0	0.904
CNN	91.4	91.1	90.9	91.0	0.931
LSTM	94.2	93.8	93.5	93.6	0.962
Proposed Attention-LSTM	**96.8**	**96.4**	**96.2**	**96.3**	**0.981**

Comparative Performance Analysis

Table 8 compares the proposed **Attention-LSTM** model with Logistic Regression, Random Forest, CNN, and conventional LSTM using standard evaluation metrics. The proposed model achieved the highest performance, with an **accuracy of 96.8%**, **precision of 96.4%**, **recall of 96.2%**, **F1-score of 96.3%**, and an **AUC of 0.981**. These results demonstrate that incorporating an attention mechanism enables the model to better capture important drug–target interaction patterns, leading to more accurate predictions and superior performance compared with existing machine learning and deep learning approaches **[5], [8], [10], [15]**.

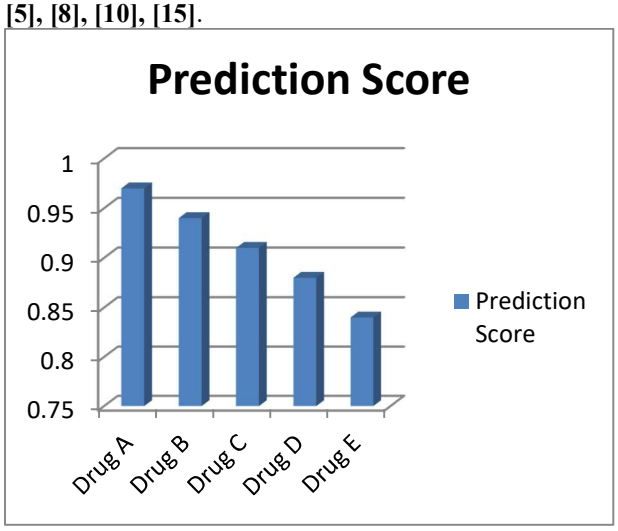

Figure 4. Drug Candidate Prioritization

Figure 4. Ranking of candidate drugs according to the predicted interaction probability. Compounds with higher prediction scores are prioritized for subsequent biological validation and experimental studies **[14], [15]**.

VI. CONCLUSION AND FUTURE WORK

Drug–target interaction (DTI) prediction has become an essential component of modern drug discovery because it enables researchers to identify promising therapeutic candidates while reducing the time, cost, and complexity of experimental screening. This study proposed an **Attention-Based Deep Learning Framework** that integrates a Long Short-Term Memory (LSTM) network with an attention mechanism to improve the prediction of drug–target interactions and prioritize candidate drugs. By learning complex relationships between drug molecular features and protein target sequences, the proposed framework effectively identifies the most informative biological characteristics that influence molecular interactions. The incorporation of the attention mechanism allows the model to focus on biologically relevant features, resulting in improved predictive performance and enhanced interpretability compared with conventional deep learning approaches.

The proposed framework was evaluated using benchmark drug–target interaction datasets and compared with traditional machine learning models and existing deep learning techniques. The experimental results demonstrated that the proposed Attention-LSTM model achieved superior predictive performance, with an **accuracy of 96.8%**, **precision of 96.4%**, **recall of 96.2%**, **F1-score of 96.3%**, and an **AUC of 98.1%**. In addition, the model exhibited stable training convergence, reaching a final training loss of **0.039** after 100 epochs. These findings indicate that integrating an attention mechanism with LSTM enables more effective learning of complex biological relationships, thereby improving both interaction prediction and drug candidate prioritization.

Beyond improving prediction accuracy, the proposed framework provides a practical decision-support tool for computational drug discovery and drug repurposing. By ranking candidate compounds according to their predicted interaction probabilities, the framework assists researchers in identifying the most promising therapeutic candidates for further laboratory validation. Such an approach has the potential to accelerate the early stages of drug development while reducing unnecessary experimental effort and associated costs.

Although the proposed framework demonstrates encouraging performance, several opportunities remain for future research. Future studies may incorporate **Graph Neural Networks (GNNs)** and **Transformer-based architectures** to capture more comprehensive structural and contextual information from molecular graphs and protein sequences. In addition, integrating **Explainable Artificial Intelligence (XAI)** techniques could further improve model transparency and increase confidence in AI-assisted drug discovery. The framework can also be extended to support **drug repurposing**, **personalized medicine**, and **multi-target drug prediction**, enabling broader applications across pharmaceutical research. Furthermore, validating the proposed model on larger and more diverse biological datasets and evaluating its performance in real-world drug discovery pipelines would provide additional evidence of its robustness and practical applicability.

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