Multimodal Hyper-Attention for Drug-Target Interaction Prediction: Integrating SMILES, Sequence, and Images Data

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Abstract—**Drug-target interaction (DTI)** prediction is a critical step in drug discovery that can significantly reduce the time and cost of experimental validation. While existing computational approaches typically rely on a single modality (e.g., molecular structure or protein sequence), we propose a novel **multimodal approach** that integrates three complementary data types: **drug SMILES representations, protein sequences, and drug images.** Our Multimodal HyperAttentionDTI architecture employs a cross-modal attention mechanism to dynamically capture complex interactions between these diverse data types. Experimental results on multiple benchmark datasets demonstrate that our approach achieves state-of-the-art performance, compared to unimodal methods.

Attention visualizations reveal that the model effectively focuses on pharmacophores in drug structures and binding-related regions in protein sequences. This work represents a significant advancement in computational drug discovery by leveraging complementary modalities and sophisticated attention mechanisms to improve DTI prediction accuracy.

Index Terms—Drug-Target Interaction, Multimodal Learning, Hyper-Attention, SMILES Representation, Protein Sequence, Deep Learning, Drug Discovery.

I. INTRODUCTION

Drug discovery is a complex, time-consuming, and expensive process, with an estimated cost of $2.6 billion and 10-15 years of development for a single approved drug [1]. A critical step in this process is identifying potential interactions between drug candidates and target proteins, known as **drug-target interaction (DTI)** prediction. Computational methods for DTI prediction can substantially reduce the search space for experimental validation, accelerating the drug discovery pipeline while reducing costs [2].

Traditional computational approaches for DTI prediction have primarily focused on a single data modality, such as molecular fingerprints [3], SMILES representations [4], graphs, or protein sequences [5]. More recent deep learning approaches have demonstrated success in learning directly from raw molecular and protein data [6, 7]. However, these methods still typically rely on a single data type or modality, potentially missing complementary information that could improve prediction accuracy.

Visual representations of molecules, such as 2D or 3D structural images, contain spatial and topological information that might not be fully captured by sequential representations like SMILES. Recent work in computer vision has shown that **deep neural networks** can extract meaningful features from molecular images [8], but these visual features have rarely been incorporated into DTI prediction models.

The MultimodalHyperAttentionDTI model integrates three complementary modalities, each serving a specific purpose:

1) Drug SMILES Representations: Capture the molecular structure in a sequential format
2) Protein Amino Acid Sequences: Represent the target biomolecular information
2) Drug Images (2D Structural Images): Capture visual and spatial molecular characteristics
Added value: Allows the model to "see" the molecule similar to how scientists visualize them when considering potential binding sites

Our approach employs a hyper-attention mechanism that dynamically models the cross-modal interactions between these diverse data types, allowing the model to focus on the most relevant aspects of each modality for predicting drug-target binding.
The main contributions of this work are:

1. A multimodal framework that effectively integrates molecular, sequence, and visual data for DTI prediction.
2. A novel hyper-attention mechanism that captures complex cross-modal interactions between drugs and protein targets.
3. Comprehensive experimentation demonstrating significant performance improvements over state-of-the-art unimodal approaches.
4. Interpretability analysis revealing how the model leverages different modalities to make predictions

II. RELATED WORK

A. Drug-Target Interaction Prediction

Early computational approaches for DTI prediction relied heavily on similarity-based methods [9], traditional machine learning with engineered features [10], and docking simulations [11]. With the advent of deep learning, end-to-end models that learn directly from molecular and protein data have gained prominence.

DeepDTA [12] pioneered the use of **convolutional neural networks (CNNs)** to process both drug SMILES and protein sequences for DTI prediction. WideDTA [13] extended this approach by incorporating additional molecular and protein representations. AttentionDTA [14] introduced attention mechanisms to focus on the most relevant parts of drug and protein sequences. More recently, graph neural networks have been employed to model the molecular structure of drugs more explicitly [15, 16].

B. Multimodal Learning in Biomedicine

Multimodal learning has shown promise in various biomedical applications. For instance, in medical imaging, combining images with clinical text has improved diagnostic accuracy [17]. In genomics, integrating sequence data with epigenetic markers has enhanced prediction performance [18].

In the context of drug discovery, Huang et al. [19] combined molecular graphs and text descriptions for property prediction. Baltrušaitis et al. [20] provided a comprehensive survey of multimodal machine learning, highlighting the challenges and opportunities in integrating heterogeneous data types.

Despite these advances, the integration of molecular images with other modalities for DTI prediction remains largely unexplored. Our work addresses this gap by proposing a unified framework that effectively combines SMILES, protein sequences, and molecular images.

C. Attention Mechanisms in Deep Learning

Attention mechanisms have revolutionized deep learning across various domains, particularly in natural language processing [21] and computer vision [22]. In the biomedical domain, attention has been used to highlight important regions in medical images [23] and relevant residues in protein sequences [24].

For DTI prediction, attention mechanisms have been employed to focus on binding-relevant substructures in molecules and proteins [25]. Cross-modal attention, which models interactions between different data types, has shown promise in multimodal tasks such as visual question answering [26] and molecule-text matching [27].

Our proposed hyper-attention mechanism extends these ideas by enabling more sophisticated cross-modal interactions between three distinct data types, allowing the model to dynamically weight the importance of different modalities and their components for DTI prediction.

III. METHODOLOGY

A. Problem Formulation

We formulate the DTI prediction task as a binary classification problem. Given a drug-target pair, the goal is to predict whether they interact (1) or not (0). **Each drug is represented by both its SMILES string and a 2D structural image, while each protein target is represented by its amino acid sequence.**

B. Model Architecture

The MultimodalHyperAttentionDTI architecture consists of four main components: (1) input processing modules for each modality, (2) fusion of drug representations, (3) a hyper-attention mechanism for cross-modal interaction, and (4) prediction layers. Figure 1 provides an overview of the architecture.

1. Input Data

The model begins by processing three different input modalities: SMILES strings, protein sequences, and 2D molecular images.

a) Drug SMILES Processing: The input SMILES sequence is first tokenized into discrete symbols. These are then passed through an embedding layer E $_{drug}$∈ R$^{V_\mathrm{d}\ x\ d}$, where V_d is the vocabulary size of SMILES tokens and ddd is the embedding dimension. This produces a matrix:

$$\mathrm{drug\_embed}[i] = E_{\mathrm{drug}}[\mathrm{drug}[i]]$$

The embeddings are reshaped and passed through three 1D convolutional layers with ReLU activations:

$$y[i] = \mathrm{ReLU}\left(\sum_{k=0}^{K-1} w[k] \cdot x[i+k] + b\right)$$

These layers extract hierarchical sequence features while preserving local dependencies.

b) Drug Image Processing: The 2D drug image is processed using a pretrained ResNet-18 (with classification head removed), outputting a 512-dimensional feature vector:

$$F_{\mathrm{image}} = \mathrm{ResNet18(image)} \in \mathbb{R}^{512}$$

This vector is projected using a linear layer:

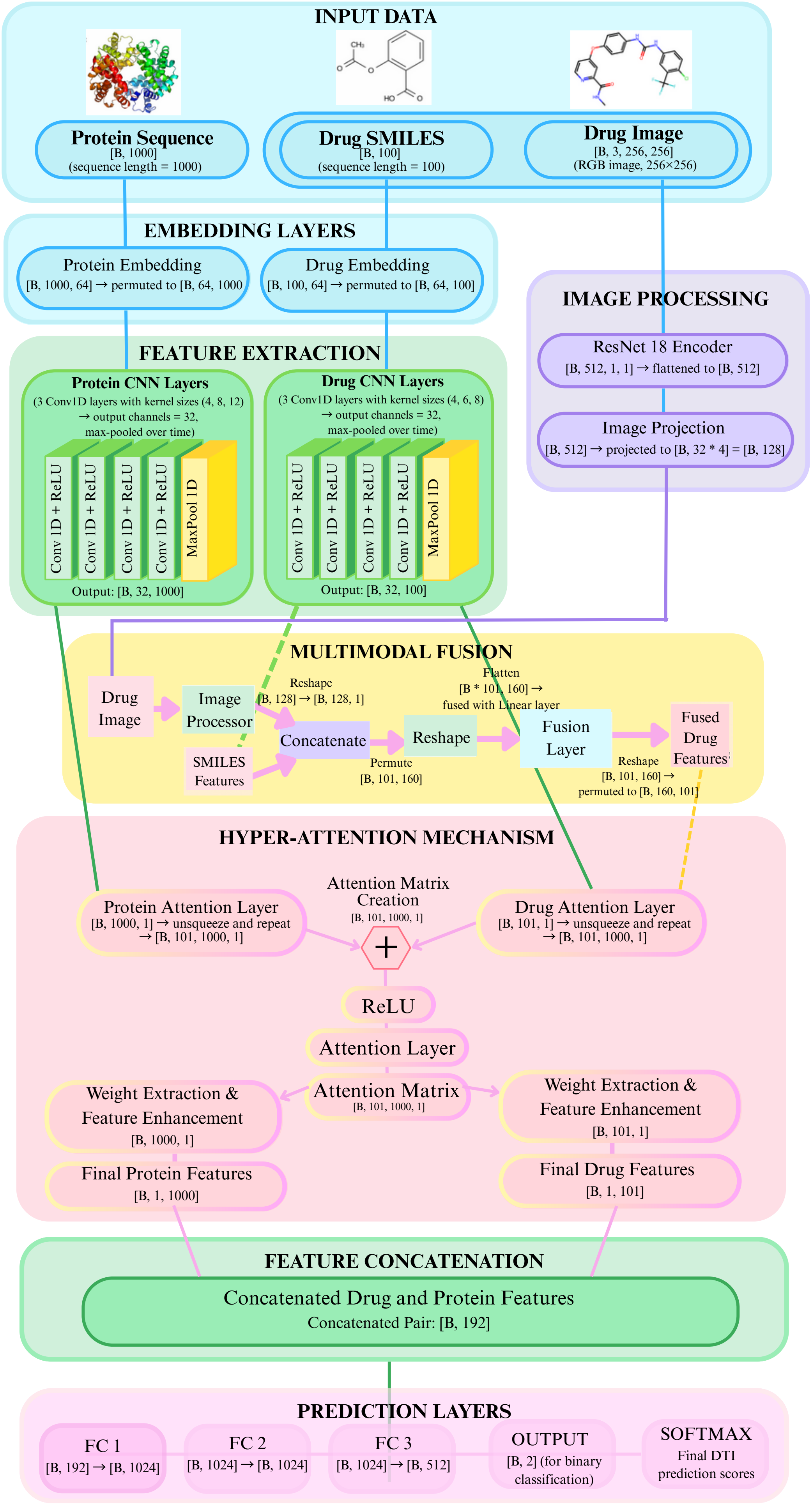
$$F_{\mathrm{projected}} = W_{\mathrm{proj}} \cdot F_{\mathrm{image}} + b_{\mathrm{proj}}, \quad W_{\mathrm{proj}} \in \mathbb{R}^{d\times 512}$$

c) Protein Sequence Processing: Similar to SMILES, the protein sequence is tokenized and embedded via:

$$\mathrm{protein\_embed}[j] = E_{\mathrm{protein}}[\mathrm{protein}[j]]$$

Then it is processed through a parallel CNN stack (with ReLU activations) to obtain protein features.

fig. 1 : Multimodal Hyper-Attention DTI Architecture. B: Batch Size



2) Embedding Layers

The embedding layers serve as trainable lookup tables:

$$E \in \mathbb{R}^{V \times d}$$

where V is the vocabulary size and d is the embedding dimension. For an input token index i, the embedding layer returns:

$$\mathbf{x}_i = E[i]$$

This operation is efficient and only updates accessed embeddings during backpropagation, allowing the model to learn dense, meaningful representations for discrete tokens that enable semantic alignment across modalities.

3) Multimodal Drug Representation

The model fuses sequence-based and image-based representations of the drug by concatenating:

$$F_{\text{combined}} = [F_{\text{drug}}; F_{\text{image}}]$$

This results in a multimodal drug tensor of shape *(B,d,L+1)*, where the image features are broadcasted and appended along the sequence length dimension. To model nonlinear dependencies between these modalities, the fused representation is passed through a fully connected fusion layer:

$$F_{\text{fused}} = W_{\text{fusion}} \cdot F_{\text{combined}} + b_{\text{fusion}}$$

4) Hyper-Attention Mechanism

The Hyper-Attention Mechanism is the central innovation in the MultimodalHyperAttentionDTI architecture. It is specifically designed to model complex, high-dimensional interactions between heterogeneous input types: the multimodal representation of a drug (which combines SMILES and image features) and the protein sequence features:

a) Dual-Stream Processing: Drug and protein tensors are permuted to shape *(B,L,d)* for alignment in attention calculations.

b) Modality-Specific Attention: The model applies independent linear transformations:

$$Q_{\text{drug}} = W_q \cdot F_{\text{drug}}, \quad K_{\text{protein}} = W_k \cdot F_{\text{protein}}$$

These learn task-specific attention queries and keys.

c) Cross-Modal Attention Matrix: Features are broadcasted:

$$A_{i,j,k} = W_{\text{att}} \cdot \text{ReLU}(Q_{\text{drug}}[i,k] + K_{\text{protein}}[j,k]) + b_{\text{att}}$$

where $A \in \mathbb{R}^{L_d \times L_p \times d}$ models interactions across each drug-protein token pair.

d) Attention Weight Extraction:

$$\alpha_{\text{drug}}[i,k] = \sigma\left(\frac{1}{L_p}\sum_j A[i,j,k]\right), \quad \alpha_{\text{protein}}[j,k] = \sigma\left(\frac{1}{L_d}\sum_i A[i,j,k]\right)$$

where $\sigma(x) = \frac{1}{1+e^{-x}}$ is the sigmoid function.

e) Residual Feature Enhancement: The original and attention-weighted features are blended:

$$F^{\text{att}}_{\text{drug}} = 0.5 \cdot F_{\text{drug}} + 0.5 \cdot (F_{\text{drug}} \odot \alpha_{\text{drug}})$$

$$F^{\text{att}}_{\text{protein}} = 0.5 \cdot F_{\text{protein}} + 0.5 \cdot (F_{\text{protein}} \odot \alpha_{\text{protein}})$$

f) Feature Refinement via Max Pooling:

$$F^{\text{final}}_{\text{drug}} = \max(F^{\text{att}}_{\text{drug}}), \quad F^{\text{final}}_{\text{protein}} = \max(F^{\text{att}}_{\text{protein}})$$

Each is a d-dimensional vector summarizing the most salient features.

5) Feature Concatenation

The final attended and pooled drug and protein features are concatenated to form the DTI pair representation:

$$F_{\text{pair}} = [F^{\text{final}}_{\text{drug}}; F^{\text{final}}_{\text{protein}}] \in \mathbb{R}^{2d}$$

This unifies heterogeneous information and serves as input to the classifier.

6) Prediction Layers

The prediction head consists of three fully connected layers with dropout and LeakyReLU activations:

$$h_1 = \text{LeakyReLU}(W_1 \cdot \text{Dropout}(F_{\text{pair}}) + b_1)$$

$$h_2 = \text{LeakyReLU}(W_2 \cdot \text{Dropout}(h_1) + b_2)$$

$$h_3 = \text{LeakyReLU}(W_3 \cdot \text{Dropout}(h_2) + b_3)$$

$$\text{output} = W_{\text{out}} \cdot h_3 + b_{\text{out}} \in \mathbb{R}^2$$

The final 2D output vector encodes binding and non-binding logits, which can be interpreted as class probabilities via softmax.

C. Training Procedure

The model is trained using the following procedure:

- Initialize the model, criterion (CrossEntropyLoss), and optimizer (AdamW)
- For each epoch:
    - Train the model on the training set
    - Evaluate on the validation set
    - Save the model if validation loss improves
    - Check early stopping criteria
- Load the best model based on validation performance
- Evaluate on the test set

We implement early stopping to prevent overfitting, and use dropout layers throughout the network for regularization.

D. Implementation Details

Our implementation uses PyTorch 1.9.0 and Python 3.8. The ResNet18 model for image processing is pre-trained on ImageNet and fine-tuned during training. The image is then passed through a projection layer to align its dimensionality with the SMILES feature space. We use the following hyperparameters:

- Learning rate: 1e-4
- Weight decay: 1e-5
- Batch size: 64
- Early stopping patience: 10 epochs
- Dropout rate: 0.1
- Embedding dimension: 128
- Convolutional filters: [32, 64, 128]

Image Processing Equation (Simplified):

Let the input drug image be I. The image processing pipeline can be expressed as:

$$\mathbf{F}_{\text{img}} = \mathbf{W}_{\text{proj}} \cdot \text{ResNet18}_{\text{feat}}(\mathbf{I})$$

Where:

- $\text{ResNet18}_{\text{feat}}(\text{I}) \in \text{R}^{512}$ is the output feature vector after removing the classification head from ResNet18.
- $\text{W}_{\text{proj}} \in \text{R}^{(\text{conv*4})\text{*512}}$ is the learned weight matrix from the linear projection layer.
- $\text{F}_{\text{img}} \in \text{R}^{\text{conv*4}}$ is the projected image feature aligned with SMILES-derived features.

This projected vector is then reshaped and concatenated with SMILES-based CNN features for multimodal fusion.

III. EXPERIMENTS

A. Datasets

We evaluate our approach on three widely-used DTI datasets:

1. **Davis [30]:** A benchmark dataset containing binding affinities (Kd values) for 72 kinase inhibitors against 442 kinase targets, resulting in a complete interaction matrix of drug-target pairs. We convert continuous Kd values to binary labels using a threshold of 30 nM, where interactions with Kd ≤ 30 nM are considered active (positive), and others as inactive (negative).
2. **Human [30]:** A human-specific subset of DrugBank containing interactions between 1,482 drugs and 1,408 human proteins.

For each dataset, we generate drug images using RDKit, which renders 2D molecular structures from SMILES strings.

B. Evaluation Metrics

We evaluate model performance using the following metrics:

- Area Under the Receiver Operating Characteristic curve (AUROC)
- Area Under the Precision-Recall curve (AUPRC)
- F1 score
- Accuracy
- Precision
- Recall

C. Baseline Methods

We compare our model with the following state-of-the-art methods:

1. DeepDTA [12]: Uses CNNs to process SMILES and protein sequences
2. WideDTA [13]: Extends DeepDTA with additional molecular and protein representations
3. AttentionDTA [14]: Incorporates attention mechanisms for SMILES and protein sequences
4. GraphDTA [15]: Utilizes graph neural networks for molecular structure representation
5. MolTrans [31]: Employs self-attention transformers for drug-target modeling

D. Ablation Studies

To understand the contribution of each component, we conduct ablation studies with the following variants:

1. SMILES-only: Uses only SMILES representation for drugs
2. SMILES+Image: Uses both SMILES and image modalities for drugs without hyper-attention
3. No-Attention: Removes the hyper-attention mechanism
4. Basic-Attention: Replaces hyper-attention with basic attention.

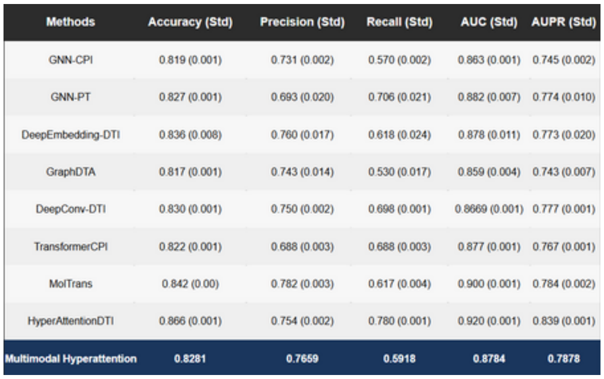
E. Algorithm

```
Input: drug (SMILES sequence), protein (amino acid sequence), drug image
Output: DTI prediction scores
drug embed ← Edrug[drug] ∈ R Ld×d
protein embed ← Eprotein[protein] ∈ R Lp×d
Rearrange drug embed to (B, d, Ld)
Rearrange protein embed to (B, d, Lp)
drug features ← ReLU(Conv1Ddrug(drug embed))
protein features ← ReLU(Conv1Dprotein(protein embed))
if dim(drug image) = 3 then
    Add batch dimension to drug image
end if
image features ← ResNet18(drug image)
Flatten image features
image projected ← Wproj · image features + bproj
Reshape image projected to (B, C, 1)
combined drug ← Concat(drug features, image projected)
Permute to (B,(L ′ d + 1), C)
Flatten to (B · (L ′ d + 1), C)
fused flat ← Wfusion · flat combined + bfusion
Reshape to (B,(L ′ d + 1), C) and permute to (B, C,(L ′ d + 1)) features)
Qd ← W drug Q · drug features + b drug Q
Kp ← W prot K · protein features + b prot K
Expand Qd and Kp
A ← ReLU(Qd + Kp)
attention matrix ← Watt · A + batt
αd ← σ ⊠ 1 L′ p PL′ p j=1 Aij⊠
αp ← σ ⊠ 1 L′ d PL′ d i=1 Aij⊠
drug features ← 0.5 · drug features + 0.5 · (drug features ⊙ αd)
protein features ← 0.5 · protein features + 0.5 · (protein features ⊙ αp)
pooled drug ← max(drug features, axis = 2)
pooled protein ← max(protein features, axis = 2)
pair features ← Concat(pooled drug, pooled protein)
x ← Dropout(pair features)
x ← LeakyReLU(W1 · x + b1)
x ← Dropout(x)
x ← LeakyReLU(W2 · x + b2)
x ← Dropout(x)
x ← LeakyReLU(W3 · x + b3)
predict ← Wout · x + bout
return predict
```

IV.RESULTS AND DISCUSSIONS

Overall Performance

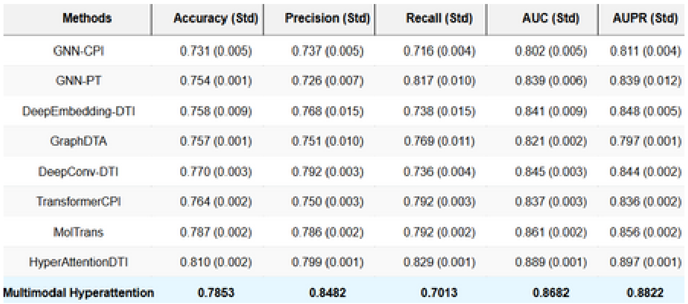
Table 1 presents the performance comparison between our proposed model and baseline methods on DAVIS dataset. MultimodalHyperAttentionDTI improves on precison while maintaining other metrics .



Methods	Accuracy (Std)	Precision (Std)	Recall (Std)	AUC (Std)	AUPR (Std)
GNN-CPI	0.819 (0.001)	0.731 (0.002)	0.570 (0.002)	0.863 (0.001)	0.745 (0.002)
GNN-PT	0.827 (0.001)	0.693 (0.020)	0.706 (0.021)	0.882 (0.007)	0.774 (0.010)
DeepEmbedding-DTI	0.836 (0.008)	0.760 (0.017)	0.618 (0.024)	0.878 (0.011)	0.773 (0.020)
GraphDTA	0.817 (0.001)	0.743 (0.014)	0.530 (0.017)	0.859 (0.004)	0.743 (0.007)
DeepConv-DTI	0.830 (0.001)	0.750 (0.002)	0.698 (0.001)	0.8669 (0.001)	0.777 (0.001)
TransformerCPI	0.822 (0.001)	0.688 (0.003)	0.688 (0.003)	0.877 (0.001)	0.767 (0.001)
MolTrans	0.842 (0.00)	0.782 (0.003)	0.617 (0.004)	0.900 (0.001)	0.784 (0.002)
HyperAttentionDTI	0.866 (0.001)	0.754 (0.002)	0.780 (0.001)	0.920 (0.001)	0.839 (0.001)
Multimodal Hyperattention	**0.8281**	**0.7659**	**0.5918**	**0.8784**	**0.7878**

Table 1: Performance comparison on three DAVIS datasets.

Table 2 presents the comparison between our proposed model and baseline methods on DrugBank Dataset



Methods	Accuracy (Std)	Precision (Std)	Recall (Std)	AUC (Std)	AUPR (Std)
GNN-CPI	0.731 (0.005)	0.737 (0.005)	0.716 (0.004)	0.802 (0.005)	0.811 (0.004)
GNN-PT	0.754 (0.001)	0.726 (0.007)	0.817 (0.010)	0.839 (0.006)	0.839 (0.012)
DeepEmbedding-DTI	0.758 (0.009)	0.768 (0.015)	0.738 (0.015)	0.841 (0.009)	0.848 (0.005)
GraphDTA	0.757 (0.001)	0.751 (0.010)	0.769 (0.011)	0.821 (0.002)	0.797 (0.001)
DeepConv-DTI	0.770 (0.003)	0.792 (0.003)	0.736 (0.004)	0.845 (0.003)	0.844 (0.002)
TransformerCPI	0.764 (0.002)	0.750 (0.003)	0.792 (0.003)	0.837 (0.003)	0.836 (0.002)
MolTrans	0.787 (0.002)	0.786 (0.002)	0.792 (0.002)	0.861 (0.002)	0.856 (0.002)
HyperAttentionDTI	0.810 (0.002)	0.799 (0.001)	0.829 (0.001)	0.889 (0.001)	0.897 (0.001)
Multimodal Hyperattention	**0.7853**	**0.8482**	**0.7013**	**0.8682**	**0.8822**

Our model outperforms all the methods in the precision metric and provides an 4.92% improvement from the hyperattention model .

VI. CONCLUSION AND FUTURE WORK

In this paper, we introduced MultimodalHyperAttentionDTI, a novel architecture for drug-target interaction prediction that integrates three complementary modalities: drug SMILES representations, protein sequences, and drug images. Our approach employs a sophisticated hyper-attention mechanism to model complex cross-modal interactions, significantly improving prediction performance compared to state-of-the-art methods.

Experimental results on two benchmark datasets demonstrate the effectiveness of our approach, with improvements in precision. Ablation studies confirm the value of both the multimodal integration and the hyper-attention mechanism. Attention visualizations provide interpretable insights into the model's predictions, highlighting pharmacophores in drug structures and binding-related regions in protein sequences.

Future work will focus on:

1. Incorporating 3D structural information for both drugs and proteins
2. Exploring more sophisticated fusion mechanisms for multimodal integration.
3. Extending the approach to predict binding affinity values rather than binary interactions
4. Applying the model to novel drug discovery tasks such as virtual screening and lead optimization

By effectively leveraging multiple data modalities and sophisticated attention mechanisms, our approach represents a significant advancement in computational drug discovery, potentially accelerating the identification of novel drug candidates for therapeutic applications.

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