

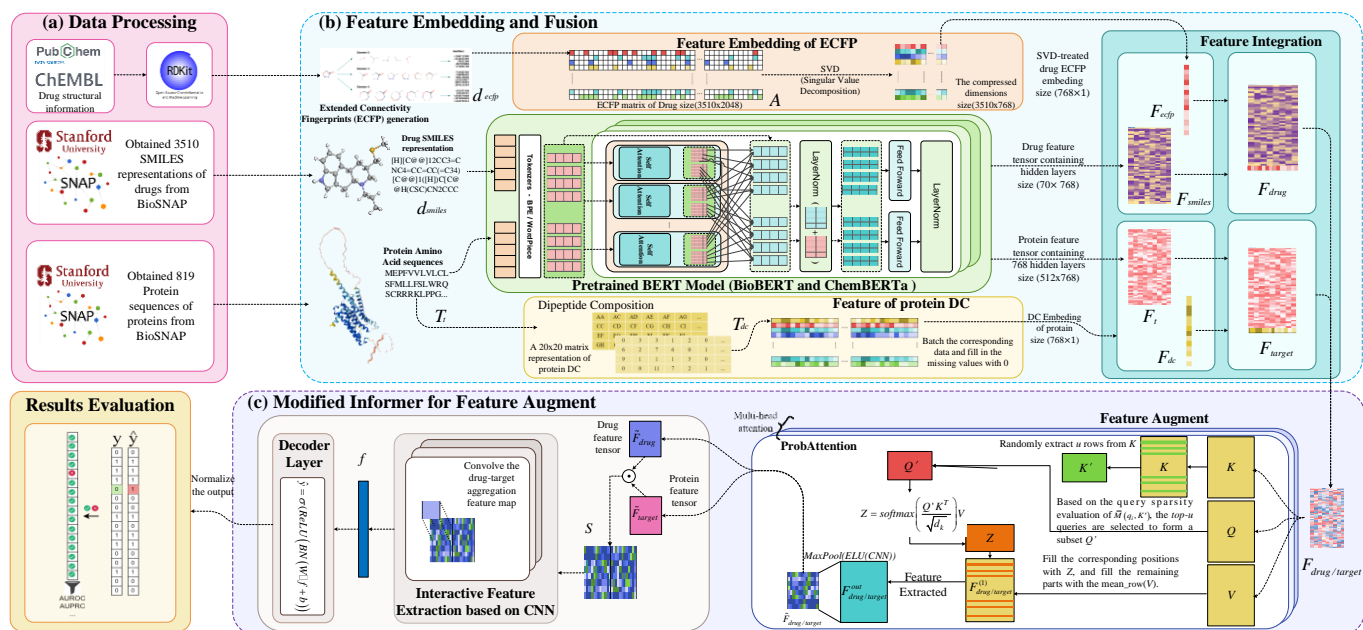
DTIBFAI: Drug-target Interaction Prediction Based on BERT and Feature Augment of Informer

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Problems & Ideas

- Problems of conventional Transformer-based DTI approaches:
 - Transformer-based self-attention mechanisms often fail to capture fine-grained drug-target interactions.
 - Single-mode feature representations limit the ability to fully characterize DTI.
- Ideas: A new method (DTIBFAI) uses BERT and Informer models to predict DTI by considering multiple feature representations of both drugs and targets.

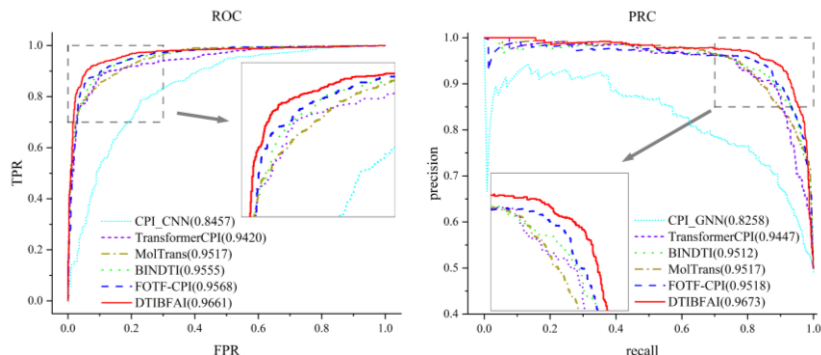


Flowchart of DTIBFAI. (a) The data processing; (b) Feature embedding and feature fusion; (c) The application of the modified Informer model for feature augment, along with the CNN-based method for predicting DTI.

Main Contributions

- Contributions:

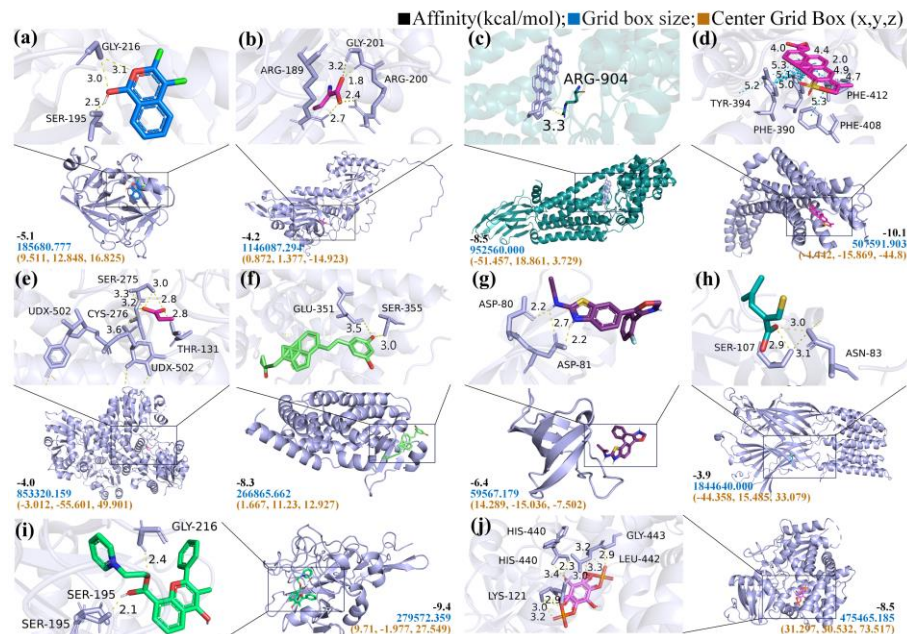
- A novel feature fusion strategy combining BioBERT and ChemBERTa embeddings with molecular fingerprints and dipeptide composition to enhance drug and protein representations.
- A modified Informer model for DTI prediction, using self-attention mechanisms to augment feature.
- Validation through simulation of high-confidence novel DTIs, demonstrating the model's potential to identify previously unknown DTIs.



The ROC and PRC curves for the comparison experiments

Comparison of Training Efficiency

Methods	Time/ Epoch	GPU Usage on Training/Batch	GPU Usage on Validation/Batch
Informer→ Transformer	176.06s	10095.01MB	5161.33MB
DTIBFAI	132.27s	1132.26MB	335.62MB



Molecular docking situations of the predicted 10 new drug-target pairs