The first step in drug discovery is to find drug molecule moieties with medicinal activity against specific targets, so it is crucial to investigate the interaction between drug target proteins and chemical small molecules. However, traditional experimental methods for discovering potential drug small molecules are labor-intensive and time-consuming, and there is currently a lot of interest in building computational models to screen drug small molecules by using drug molecule-related databases. In this paper, we propose a method for predicting drug-target binding affinity using deep learning models. The method uses a modified GRU and GNN to extract features from the drug-target protein sequence and the drug-molecule map, respectively, to obtain their feature vectors, and finally the combined vectors are used as vector representations of drug-target molecule pairs into a fully-connected network to predict drug-target binding affinity. The proposed model demonstrates its effectiveness and accuracy in the task of predicting drug-target binding affinity on DAVIS and KIBA datasets.

### A. Molecular docking method

Molecular docking is a method for predicting the binding mode and binding affinity between drug molecules and biological molecules that have a causal relation throughout. Drug targets and drugs is usually biologically positioned. Potential effective drug molecule databases and proteins and chemical small molecules. However, traditional experimental methods for discovering potential drug small molecules are labor-intensive and time-consuming, and there is currently a lot of interest in building computational models to screen drug small molecules by using drug molecule-related databases. In this paper, we propose a method for predicting drug-target binding affinity using deep learning models. The method uses a modified GRU and GNN to extract features from the drug-target protein sequence and the drug-molecule map, respectively, to obtain their feature vectors, and finally the combined vectors are used as vector representations of drug-target molecule pairs into a fully-connected network to predict drug-target binding affinity. The proposed model demonstrates its effectiveness and accuracy in the task of predicting drug-target binding affinity on DAVIS and KIBA datasets.

Exploring the interaction mechanism between drug and target is crucial to investigate the interaction between drug target proteins and chemical small molecules. However, traditional experimental methods for discovering potential drug small molecules are labor-intensive and time-consuming, and there is currently a lot of interest in building computational models to screen drug small molecules by using drug molecule-related databases. In this paper, we propose a method for predicting drug-target binding affinity using deep learning models. The method uses a modified GRU and GNN to extract features from the drug-target protein sequence and the drug-molecule map, respectively, to obtain their feature vectors, and finally the combined vectors are used as vector representations of drug-target molecule pairs into a fully-connected network to predict drug-target binding affinity. The proposed model demonstrates its effectiveness and accuracy in the task of predicting drug-target binding affinity on DAVIS and KIBA datasets.
B. Molecular dynamics simulation

- Obtaining 3D data of drug molecules is a method to simulate the structure of drugs and proteins, so that similar protein or drug molecules are close to the local coordinates to accurately predict the binding affinity between drug molecules and targets. AtomNet uses a deep learning model to predict the binding affinity and considers the flexibility of biomolecular structure.

- Molecular docking, as a method to screen drugs, is also a challenging problem, and the process of large molecules often requires accurate information on drug molecules. AtomNet makes full use of deep learning methods to extract complex chemical features of the target protein and encode drug molecule fingerprints into a set of vectors, and connected molecular mechanical properties.

C. Machine Learning Methods

- Traditional machine learning methods, such as support vector machines, have been applied in the field of drug discovery. Deep learning methods are used to predict whether there is an interaction between a drug and a receptor target, and can automatically acquire hidden features in the data for drug discovery.

- Machine learning methods show great promise for drug discovery. Wallach et al. [25] proposed to use deep learning network to perform representation learning to mine high-level features from raw data. Using the word embedding technology proposed by Tsubaki et al. [26] and the deep learning model AtomNet, the drug target interaction prediction is achieved.

D. Deep Learning Methods

- AtomNet is a deep learning model developed for drug target interaction prediction. The specific process of molecular docking is described in the diagram. The 3D structure database of known compounds and the active site of the target molecule are used as input, and then the coordinates are used to accurately predict the binding affinity. The process involves searching for suitable orientation, optimizing conformation, adjusting the dihedral angle of flexible bonds, and predicting affinity for scoring and ranking. This lays a solid foundation for the application of deep learning in drug discovery.

- In summary, obtaining 3D data of drug molecules is a method of molecular simulation. Molecular docking is used to screen drugs, and machine learning methods are used to predict interactions. Deep learning methods have achieved great results in drug discovery tasks.
the excitation function. The reset gate characterizes the degree of forgetting of the information at the previous moment, and the closer its size is to 0, the greater the degree of information flow from the previous moment. The update gate characterizes the degree of information flow to the current moment, which is calculated through the Tanh excitation function. After getting the update gate and the reset gate, the result is combined with the state of the hidden layer at the current moment, which is calculated through the activation function, and the result is the state of the hidden layer at the current moment.

\[
net_z = w_z x_t + u_z h_{t-1} \\
net_r = w_r x_t + u_r h_{t-1} \\
z_t = \sigma (net_z) \\
r_t = \sigma (net_r) \\
h_{t+1} = (1 - r_t) h_{t-1} + z_t x_t
\]

Figure 3. The internal structure of GRU circulator unit.

Figure 2. The structure of GRU is similar to that of LSTM neural network, but the recurrent unit of GRU neural network has only two input variables: the input of the current moment and the state of the hidden layer at the previous moment, and the mathematical expression of the update gate calculation process is

\[
\text{update gate} = \sigma (net_u) = \sigma (w_u x_t + u_u h_{t-1})
\]

where

\[
w_u, u_u \in \mathbb{R}^d
\]

The mathematical expression of the reset gate calculation process is

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\]

where

\[
w_r, u_r \in \mathbb{R}^d
\]

In this paper, an end-to-end prediction model is proposed. Based on the SMILES sequence, the drug molecule embedding, the target protein embedding, and their spliced information, an end prediction model is generated. The end prediction model is shown in Fig. 2. In this paper, an end-to-end prediction model is proposed in end-member prediction model. The overall design of the drug inhibition prediction model is shown in Fig. 2. In this paper, an end-to-end prediction model is proposed in.

The end prediction model proposed in this paper.

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\]
\[ \text{net}_h = wx_{i} + u \cdot x_j \odot h_{-h} \]
\[ h_i = \varphi(\text{net}_h) \]
\[ h_i = \varphi(\text{net}_h) \]
\[ h_i = \varphi(\text{net}_h) \]
\[ \text{net}_y = w_y h_i \]
\[ y = \sigma(\text{net}_y) \]
\[ \text{net}_y \]
\[ B. \ GNN \]
\[ h_{v}^{k} = [\text{lu MLP}^{k}] \sum_{u \in \mathcal{N}(v)} h_{v}^{k-1} + \sum_{e \in v \cup \mathcal{N}(v) \setminus \mathcal{N}(u) \cup \mathcal{N}(e)} h_{v}^{k-1} \]
\[ N(v) \]
\[ y \]
\[ h_{v}^{k} \]
\[ k \]
\[ y \]
\[ P \]
\[ Y \]
\[ \text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (P_i - Y_i) \]
\[ \text{MSE} \]
starting point to investigate how to apply deep learning analysis. In this paper, we use drug paper.

For the DAVIS samples should be around the dotted line (p=m) good prediction mode

GIN for molecular graph data.

and GCN, demonstrating the better feature extraction ability of

and MSE values of GIN were better than those of GAT

Distribution on the DAVIS dataset

Observing the comparison

regression task combining affinity prediction, the CI

Figure 6.

Wh
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