DeepPurpose: a Deep Learning Based Drug Repurposing Toolkit

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ABSTRACT

We present DeepPurpose, a deep learning toolkit for simple and efficient drug repurposing. With a few lines of code, DeepPurpose generates drug candidates based on aggregating five pretrained state-of-the-art models while offering flexibility for users to train their own models with 15 drug/target encodings and 50+ novel architectures. We demonstrated DeepPurpose using case studies, including repurposing for COVID-19 where promising candidates under trials are ranked high in our results.

Drug repurposing is about investigating existing drugs for new therapeutic purposes which can potentially speed up drug development. With a large number of existing drugs, it is important to quickly and accurately identify promising candidates for new indications. Especially in facing COVID-19 pandemic today, drug repurposing become particularly relevant as a potentially much faster way to discover effective and safe drugs for treating COVID-19.

Deep learning has recently demonstrated its superior performance than classic methods to assist computational drug discovery, thanks to its expressive power in extracting, processing and extrapolating patterns in molecular data. For example, an existing study shows with deep learning we can quickly generate a drug candidate to act against untreatable strain of bacteria.

We introduce a deep learning toolkit for drug repurposing called DeepPurpose. There are many deep learning models designed for drug target interaction prediction, which can be extended to drug repurposing. However, to acquire the results for drug repurposing and test their validity require substantial code development skills and biochemical domain knowledge, which are hard to acquire both. For example, the existing tools are designed for computer scientists and hard to use by domain researchers with limited machine learning and coding experience. Furthermore, each individual open-sourced tool was designed and coded differently, which prevents easy integration of the diverse methods or model ensembles.

In this work, we aim to break the technical barrier by introducing DeepPurpose, a powerful and easy-to-use Python toolkit that can recommend the top binding drug candidates. With only one line of code that specifies the target amino acid sequences and the drug candidates, DeepPurpose loads and processes input molecular data, feeds them into multiple deep learning models pretrained on the large BindingDB datasets with different encoding schemes, aggregates the prediction results, and generates a descriptive ranked list of drug candidates with top binding scores. Then biomedical researchers can inspect this short list for further wet-lab validation. The ensemble of many models allow DeepPurpose to use different encoding algorithms (i.e., input representations), which broaden the search horizons and catches drugs that were missed by existing works due to the bias from only using one particular encoding model. DeepPurpose also allows users to input customized drug-target training data for specific target protein to train a new model from scratch.

DeepPurpose is a python package with a Jupyter Notebook interface. It can run locally to ease the concern of processing proprietary drug data. It can also run on the cloud which alleviate the computational resource burdens faced by some users. DeepPurpose uses the most accessible input format: SMILES string for drugs and amino acid sequence for target. The output of DeepPurpose is a score that measures the binding activity of the input drug target pair.

In addition to the aforementioned design for helping domain scientists, DeepPurpose also offers a flexible framework for computer scientists to innovate new models for repurposing. Particularly, DeepPurpose includes multiple molecular encodings, varying from deep neural networks on classic computational biology and cheminformatics descriptors, to convolutional neural network, convolutional recurrent neural network (CNN-RNN), Transformer encoders and Message-Passing Neural Network. In total, by combining 7 encodings for proteins and 8 encodings for drugs, DeepPurpose offer 50+ models. To the best of our knowledge, majority of the encodings and models are novel for drug repurposing. Besides the functionality, DeepPurpose is
simple to use. With less than 10 lines of codes, DeepPurpose downloads, prepossesses the training data, trains the model with multiple encodings, and evaluates various performance metrics on the test set. We also provide 10+ pretrained models trained on large benchmark datasets that are ready to use.

Next we provide four case studies of DeepPurpose through the lens of (1) a biomedical student aiming to do drug repurposing using only the new target amino acid sequence; (2) a biomedical researcher who wants to do virtual screening for a list of drug-target pairs; (3) a biomedical researcher who wants to obtain drug candidates from a proprietary drug library for a special target that has available high throughput screening assay data and (4) a machine learning researcher aiming to develop new methods in drug repurposing.

The first case considers drug repurposing for COVID-19. Suppose a biomedical student want to identify which existing antiviral drugs can be repurposed to target SARS-CoV2 3CL Protease (3CLPro), which is related to virus replication. With only one line of code (A, Figure. 2), DeepPurpose aggregate multiple pretrained models and outputs top-ranked antiviral drug candidates. We present the results in Figure 2. Out of the 81 antiviral drugs in the library, DeepPurpose recommend 13 potentially active drugs that have Kd values within 500^7 units. We conduct literature search for the 13 drugs and find that Ritonavir, Darunavir, Lopinavir are three of few drug candidates that are currently undergo clinical trials for SARS-CoV2-3CLPro^8–10. The top recommending drug Sofosbuvir is an anti-HCV protein inhibitors and is currently undergo many in-vitro investigations for its potential usage for COVID19^11. Some other molecular docking studies also reported potential efficacy of Simeprevir^12 and Amantadine^13. Overall, 6 recommendations out of 13 have promising evidence based on literature or clinical trials, which confirms the potential of DeepPurpose for suggesting high-quality repurposing candidates.

The second case is about screening a list of drug-target pairs. After inputting the drug target sequence information, DeepPurpose generates a ranked list of drug-target pairs based on its binding affinity output from the pretrained models. To evaluate the predictive efficacy, we report the test set predictive performance for the drug target binding affinity prediction for each pretrained model, which is trained on BindingDB dataset with Kd values (Table 1. Figure. 2) using 7:1:2 train:validation:test split. We see all five models achieve high performance on all the metrics in the test set. Since in many cases the users may use drug-target pairs that are different from the training dataset, to test model’s generalizability, we test on the DAVIS dataset^14, which has zero overlap with the pretrained BindingDB dataset. We then sample 1,000 unseen drug-target pairs from DAVIS and feed them into the pretrained models. We find the predicted Kd values of DeepPurpose is highly correlated with the true values with pearson correlation 0.7789, indicating the reliable predictions from DeepPurpose, even on new data (B, Figure. 2).

The third case illustrates the flexibility of DeepPurpose for more customized biomedical use case. We still consider the 3CL Protease for repurposing for COVID-19, but in this case, a biomedical scientist wants to train a deep learning model from past bioassay data such as high throughput screening (HTS) assay on SARS-CoV 3CL Protease^15, which conserves 96% of gene with SARS-CoV-2. This is potentially a better training dataset than the general BindingDB dataset for COVID-19. Specifically, DeepPurpose takes the customized training dataset as input. DeepPurpose then trains multiple deep learning models using this assay data to score drug candidates from the antiviral library or any proprietary data (C, Figure. 2). This resulting candidate list has support from literature. We find most of them are protein synthesis inhibitors, which is consistent with the general 3CLPro inhibition mechanism. Specifically, in addition to the Ritonavir, it surprisingly outputs Remdesivir with high confidence, which is a star candidate for COVID19 by blocking the RNA polymerase and has shown initial clinical effects^16. There are also initial literature evidence or clinical trials for Tipranavir^17, Methisazone^18, Baloxavir^19, Indinavir^8 to tackle COVID-19. Since this bioassay has a binary label, DeepPurpose automatically switches from regression for binding affinity to binary classification by using different loss functions.

The fourth case is about developing new methods for drug-target interaction prediction. The researcher can benefit from DeepPurpose in the following way. First, DeepPurpose provides benchmark dataset loaders that obviates extensive searching and preprocessing. It supports various input data including drug-target pairs, one target, and accommodates both drug target binding affinity prediction and drug target interaction prediction. Second, DeepPurpose supports various settings such as cold target, cold drug setup to test the robustness of the model. Third, DeepPurpose provides 50+ novel model architectures, which can be trained, and evaluated on user data using less than 10 lines of codes. We reproduce the state of the art methods DeepDTA^2 using our CNN+CNN encodings, and report the results on two benchmark dataset DAVIS^14 and KIBA^20 in (D, Figure. 2), along with other encodings. This confirms DeepPurpose’s usability and generalizability.

Through these case studies, we demonstrate DeepPurpose’s functionality and easy usage for drug repurposing and screening for both biomedical scientists and machine learning researchers. We hope DeepPurpose can increase the accessibility of deep learning tools for drug repurposing and create valuable insights that can benefit the patients. We also call for domain and method researchers to contribute to this open-sourced project^1.

https://github.com/kexinhuang12345/DeepPurpose
**Figure 1.** DeepPurpose method illustration. DeepPurpose takes the accessible drug’s SMILES string and target’s amino acid sequence and encode them through one of the selected 15+ encoder model. Then, the latent representations are concatenated and fed into a decoder to classify. The model is trained end-to-end and the training process, along with the test set performance is automatically-generated and reported. For drug repurposing & virtual screening, given a drug library and a new target of interest or new drug-target pairs of interest, DeepPurpose feeds them into five pretrained models and the predictions are aggregated and ranked to generate a drug-target list. This list can then be used for wet-lab validation. This entire process can be done using one line of code in DeepPurpose.
**A. Case Study I: Drug Repurposing for 3CLPro**

- Literature Evidence
  - Supported by other literature evidence
  - Undertake Clinical Trial for COVID-19

**C. Case Study III: Drug Repurposing with Customized Data**

- Literature Evidence
  - Supported by other literature evidence
  - Undertake Clinical Trial for COVID-19

**D. Case Study IV: Reproducing DAVIS & Model Performance**

- Literature Evidence
- Literature Evidence
- Literature Evidence
- Undertake Clinical Trial for COVID-19

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**Figure 2.** Case study illustration. A. Using one line of code, DeepPurpose generates a drug candidate list for SARS-CoV2-3CLPro target, aggregated from five pretrained model. B. With one line of code, DeepPurpose can obtain a list of drug-target pairs’ predicted binding score. The figure showcases that DeepPurpose pretrained model is able to generalize to unseen drug-target pairs and the table shows that DeepPurpose has strong predictive performance on test set. C. Still using one line of code, DeepPurpose is able to take in customized training data, such as AID1706 bioassay data in this case and train five new models to generate a drug candidate list. The ROC-AUC and PR-AUC curves are automatically generated and they compare different training model’s predictive performance. D. For method researchers, DeepPurpose provides a flexible framework to try on different encodings for drug and proteins, using less than 10 lines of code. It is able to reproduce the state-of-the-art DeepDTA’s performance on two benchmark datasets. Table 2 & 3 report the predictive performance using various encodings and we see DeepPurpose has competitive predictive performance.
Methods

Model Overview. DeepPurpose approaches drug repurposing task via predicting drug target binding. This is due to most bioactive small molecules mediate their effects by interacting with proteins. If we can accurately identify potential off-target proteins or novel drug target interactions, then we will able to repurpose existing drugs with new therapeutic indications. DeepPurpose uses an encoder-decoder framework for drug target binding prediction. The input of DeepPurpose is a drug SMILES string and target amino acid sequence pair. The output of DeepPurpose is a score that measures the binding activity of the input drug target pair. The power of deep learning models comes from its ability to create predictive feature vectors also called *embeddings*. In particular, DeepPurpose encodes both input drug and target through various deep learning encoders to obtain their deep embeddings, then concatenates and feed them into a decoder, which is another deep neural network that aims to classify whether the input drug and target protein bind.

Encoders. DeepPurpose provides 8 drug encoders and 7 target encoders with numerous variants, ranging from classic chemical informatics fingerprints to various deep neural networks. DeepPurpose feed two latent vectors generated from drug and target encoders into the decoder to produce the final prediction score. With such a pipeline design, switching encoders is very simple in DeepPurpose. By configuring a different encoder name DeepPurpose will automatically switch to the required encoder model and connect them with the decoder for prediction.

Drug Encoders. The input drug is represented by SMILES strings corresponding to molecule graphs (Figure. 3).

1. **Morgan Fingerprint**\(^2\) is a 1024-length bits vector that encodes circular radius-2 substructures. A multi-layer perceptron is then applied on the binary fingerprint vector.

2. **Pubchem**\(^2\) is a 881-length bits vector, where each bit corresponds to a hand-crafted important substructures. A multi-layer perceptron is then applied on top of the vector.

3. **Daylight**\(^2\) is a 2048-length vector that encodes path-based substructures. A multi-layer perceptron is then applied on top of the vector.

4. **RDKit-2D**\(^3\) is a 200-length vector that describes global pharmacophore descriptor. It is normalized to make the range of the features in the same scale using cumulative density function fit given a sample of the molecules.

5. **CNN**\(^23\) is a multi-layer 1D convolutional neural network. The SMILES characters are first encoded with an embedding layer and then fed into the CNN convolutions. A global max pooling layer is then attached and a latent vector describe the drug is generated.

6. **CNN+RNN**\(^24,25\) attaches a bidirectional recurrent neural network (GRU or LSTM) on top of the 1D CNN output to leverage the more global temporal dimension of drug. The input is also the SMILES character embedding.

7. **Transformer**\(^26\) uses a self-attention based transformer encoder that operates on the sub-structure partition fingerprint\(^27\).

8. **MPNN**\(^28\) is a message-passing graph neural network that operate on the drug molecular graph. It transmits latent information among the atoms and edges, where the input features incorporate atom/edge level chemical descriptors and the connection message. After obtaining embedding vector for each atom and edge, a readout function (mean/sum) is used to obtain a (molecular) graph-level embedding vector.

Target Encoders. The input targets are proteins represented as sequences of 20 different kinds of amino acids (Figure. 3).

1. **AAC**\(^29\) is a 8,420-length vector where each position corresponds to an amino acid k-mers and k is up to 3.

2. **PseAAC**\(^30\) includes the protein hydrophobicity and hydrophilicity patterns information in addition to the composition.

3. **Conjoint Triad**\(^31\) uses the continuous three amino acids frequency distribution from a hand-crafted 7-letter alphabet.

4. **Quasi Sequence**\(^32\) takes account for the sequence order effect using a set of sequence-order-coupling numbers.

5. **CNN**\(^23\) is a multi-layer 1D convolutional neural network. The target amino acid is decomposed to each individual character and is encoded with an embedding layer and then fed into the CNN convolutions. It follows a global max pooling layer.

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2Daylight chemical information systems: https://www.daylight.com/
3https://github.com/bp-kelley/descriptastorus
Ritonavir: \[
\text{CC(C)C1=NC(=CS1)CN(C)C(=O)NC(C(C)C)C(=O)NC(CC2=CC=CC=C2)CC(C(CC3=CC=CC=C3)NC(=O)OCC4=CN=CS4)O}
\]

SARS-CoV2-3CL Protease: \[
\text{SGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDVVYCPRHVICTSEDMLNPNYEDLLIRKSNHNFLVQA}
\]
\[
\text{GNVQLRVIGHSDMCYELRKLVTAPIKTKYFVQRDPQGSVSYACNYSGSVGVMHNDVDCSFCSYMHH}
\]
\[
\text{MEIPTGVHAGTILEGMNGPVYQRQDAEADTTTIVNLAWVAAINGDWRRTNRTTTLNDFNILAMKYNEPITGQHVLGLPSAQG}
\]
\[
\text{IVLDMCASKELLGOMNGRTILGSALEDEFTPFDVRQCSGVFQ}
\]

Figure 3. Examples of input representation. Drug is represented as SMILES string and target is represented as amino acid sequence. The length distribution of the input are provided.

6. **CNN+RNN**\(^{24, 25}\) attaches a bidirectional recurrent neural network (GRU or LSTM) on top of the 1D CNN output to leverage the sequence order information.

7. **Transformer**\(^{26}\) uses a self-attention based transformer encoder that operates on the sub-structure partition fingerprint\(^{27}\) of proteins. Since transformer’s computation time and memory is quadratic on the input size, it is computational infeasible to treat each amino acid symbol as a token. The partition fingerprint decomposes amino acid sequence into protein substructures of moderate sized such as motifs and then each of the partition is considered as a token and fed into the model.

**Decoder, Loss and Inference.** After DeepPurpose obtains latent drug and protein embedding, both are fed into a multi-layer perceptron decoder. There are two classes of tasks/datasets in drug target interaction prediction. One’s label is binding score such as Kd, IC50, and they are continuous values while the other one’s label is binary, whether or not they can bind. DeepPurpose is able to automatically detect whether the task is regression for continuous label or classification for binary label by counting the number of unique labels in the data. For binding affinity score prediction, it uses mean squared error (MSE) loss (Eq. 1). For binary interaction prediction, it uses binary cross entropy (BCE) loss (Eq. 2).

\[
\mathcal{L}_{\text{MSE}} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2
\]

\[
\mathcal{L}_{\text{BCE}} = \frac{1}{n} \sum_{i=1}^{n} y_i \log (\hat{y}_i) + (1 - y_i) \log (1 - \hat{y}_i),
\]

where \(y_i\) is the true label and \(\hat{y}_i\) is the predicted label for \(i\)-th drug-target pair. For evaluation metrics, we use MSE, Concordance Index, and Pearson Correlation for continuous regression and Receiver Operating Characteristics-Area Under the Curve (ROC-AUC), Precision Recall-Area Under the Curve (PR-AUC) and F1 score at threshold 0.5 for binary classification.

During inference, given new targets or new drugs, the model prediction is used as the predicted binding score/interaction probability.

**Pretrained Models and Prediction Aggregation.** Many deep learning models require significant computational resources to achieve desired performance. DeepPurpose also includes numerous pretrained models on a large public dataset BindingDB and also models to reproduce previous works. This could significantly reduce the time and resource for users since they do not need to train the model from scratch. Using pretrained model is also desirable for a new target with low amount of training data since applying transfer learning could transfer existing knowledge learnt from a large model, thus reduce the amount of data to learn\(^{33}\). Instead of using one model for prediction as in most of the previous works, since DeepPurpose integrates numerous encodings in one framework, it can easily leverage the ensembling effect and use several models aggregation result for repurposing and virtual screening. This is valuable especially because different encodings look at different signals from drug/target. One model could potentially miss a very important drug candidate. By aggregating predicted binding scores/interaction probability from five models, we greatly reduce the likelihood of this scenario. We have three modes of aggregation: mean, max, and the average of mean and max. Mean is an overall performance measure across models but as some encodings may include signals that other
encodings cannot, the max is favorable. Hence, to leverage both advantages, we also include an aggregation scheme to take the average of mean and max. For the one-line default mode for biomedical scientists, we use the latter option.

DeepPurpose provides five pretrained models as the starting point such that users can apply those model directly or finetune the model parameters on new training data. The pretrained models are listed below:

**m1**: CNN for drug and CNN for proteins;

**m2**: MPNN for drug and CNN for proteins;

**m3**: Daylight for drugs and AAC for proteins;

**m4**: Morgan fingerprint for drugs and AAC for proteins;

**m5**: Morgan fingerprint for drugs and CNN for proteins.

The above pretrained model architectures are selected based on the following principles.

- The pretrained models should have literature support, i.e., GraphDTA\(^5\) (Graph Neural Network+CNN) for m2 and DeepDTA\(^2\) (CNN+CNN) for m1;
- The models should include classic informatics encoding since they sometimes contain more global information that deep learning based methods may miss\(^6\) (Morgan+AAC, Daylight+AAC) as m3 and m4;
- A hybrid model between deep learning based method and classic encodings (Morgan+CNN) as m5. We omit transformers and CNN-RNN based methods due to the consideration that pretrained models need to be relatively lightweight for deployment.

**Additional Functionalities.** DeepPurpose provides several additional functions that can aid users in drug repurposing and virtual screening. First, DeepPurpose provides many types of data: public large binding affinity dataset such as BindingDB, KIBA, DAVIS; bioassay data such as AID1706 for SARS-CoV 3CL Protease; repurposing library such as Broad Repurposing Hub, antiviral drugs; target proteins such as SARS-CoV2 3CL Protease, Helicase, endoRNAse and etc. This can save users valuable time since the data sources are scattered and information to process the raw data is limited online. With one line of code, DeepPurpose downloads and preprocesses the dataset to downstream models’ compatible input. We also provide data loading functions from users’ txt files. Second, binding affinity score such as Kd, IC50 are recorded in nM unit. However, the label distribution is very skewed. Hence, DeepPurpose also provides a convert unit function that can transform label unit to log-scale for easy regression and also convert back when doing repurposing and virtual screening. Third, some classic encodings require some preprocessing time. DeepPurpose provides a reference time to help user estimate the computing hours.

**Software.** DeepPurpose uses Python\(^34\) as the programming language. The deep learning framework uses PyTorch\(^15\). It also depends on Pandas\(^36\) for data processing, Numpy\(^37\) for numerical computing, scikit-learn\(^38\) for evaluation metrics calculation, PyBioMed\(^39\) for classic fingerprints encoding, matplotlib\(^40\) for visualization. DeepPurpose is available at https://github.com/kexinhuang12345/DeepPurpose with installation instruction and demonstrations.

**Case Study Implementation.** The main section provided four cases. Here are the overview of the case study implementation using DeepPurpose.

**Case Study I. Antiviral Drug Repurposing for SARS-CoV2-3CLPro using one line of code.**

Here the target is 3CLPro for SARS-CoV2. We want to obtain a ranked list of drugs from the antiviral drug library for repurposing for COVID-19. Using the dataset loader from our library, the result can be generated via:

```python
>>> from DeepPurpose import oneliner
>>> from DeepPurpose.dataset import *
>>> oneliner.repurpose(*read_file_target_sequence('target.txt'), \
                      *read_file_repurposing_library('repurpose.txt'))
```

The user defined input txt files are read and input to the oneliner. A ranked list of drugs from antiviral drug library is generated, along with its predicted Kd binding scores from five pretrained model’s aggregation.

**Case Study II. Virtual Screening for Unseen Drug-Target Pairs**

For virtual screening, we can still use the one-line mode. The input is an array of SMILES strings and an array of target amino acid sequence where the two arrays are paired. A ranked list based on the predicted binding score is returned using the five pretrained models.
Case Study III. Antiviral Drug Repurposing for SARS-CoV 3CLPro using Customized Training Dataset.

In the third case study, we want to repurpose for SARS-CoV 3CL Protease using the SARS-CoV AID1706 bioassay training data and repurpose using the antiviral drug library. This can be done using:

```python
>>> from DeepPurpose import oneliner
>>> from DeepPurpose.dataset import *

>>> oneliner.virtual_screening([['MKK...LIDL', ...], ['CC1=C...C4)N', ...]])
```

The data is loaded from three txt files. The training data split method is set to 'HTS' (High Throughput Screening) mode for one target processing, other split method includes random split, cold drug/target split. In this example, we train from scratch, hence, we set the 'pretrained' variable to 'False'. The training:validation:testing split is set to be 8:1:1 using the frac parameter. Under the hood, DeepPurpose first loads five models' configuration files and trains them using AID1706 bioassay data. Then, it feeds the drug repurposing data along with the 3CL target into the trained model and outputs an aggregated predicted probability and based on that, a ranked list of drug candidates.

Case Study IV. Reproducing DeepDTA.

Suppose we want to reproduce the DeepDTA paper using DAVIS dataset from scratch. Here are the steps:

1. Use the DeepPurpose.dataset to load DAVIS data:

```python
>>> from DeepPurpose import models
>>> from DeepPurpose.utils import *
>>> from DeepPurpose.dataset import *

>>> X_drug, X_target, y = load_process_DAVIS(SAVE_PATH, binary=False)
```

2. Select DeepDTA encodings, which is CNN for both drug and target:

```python
>>> drug_encoding, target_encoding = 'CNN', 'CNN'
```

3. Process the data to be model-ready:

```python
>>> train, val, test = data_process(X_drug, X_target, y, drug_encoding, 
                                 target_encoding, split_method='random', 
                                 frac=[0.7,0.1,0.2], random_seed = 1)
```

4. Generate customized model configurations. Users can adjust model parameters, training hyperparameters and etc in this function. We use DeepDTA's configurations:

```python
>>> config = generate_config(drug_encoding, target_encoding, 
                           cls_hidden_dims = [1024,1024,512], 
                           train_epoch = 100, LR = 0.001, batch_size = 256, 
                           cnn_drug_filters = [32,64,96], 
                           cnn_drug_kernels = [4,8,12], 
                           cnn_target_filters = [32,64,96], 
                           cnn_target_kernels = [4,8,12])
```
5. Initialize the model:

```python
>>> model = models.model_initialize(**config)
```

6. Train the model. DeepPurpose will print the training process and save the testing metrics and figures in the result folder:

```python
>>> model.train(train, val, test)
```

Note that the steps 2-6 is for training from scratch. To directly use DeepDTA, we also offer the pretraining model:

```python
>>> models.model_pretrained(model = 'DeepDTA')
```

Various other pretraining models are also included for easy usage.

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**Author Contributions**

K.H., C.X., and J.S conceived the DeepPurpose project. K.H. and T.F. designed, implemented, analyzed, and documented DeepPurpose. J.S. supervised the project. K.H., T.F, C.X., L.G., J.S. wrote the manuscript.

**Competing interests**

The authors declare no competing interests.
**Code and Data Availability**

Codes to reproduce all case studies are provided in the github repository: [https://github.com/kexinhuang12345/DeepPurpose](https://github.com/kexinhuang12345/DeepPurpose). The datasets used in this work can be loaded via the DeepPurpose.dataset loader.