

Installing and running B³P²Augur

Installation

Prior to installing and running B³P²Augur, all the dependencies should be installed in the Python environment, including numpy, pandas, scikit-learn, math, scipy, collections, torch, lightgbm, xgboost, matplotlib (3.1.1), joblib, random, and time. For convenience, we strongly recommend users install the Anaconda Python environment in their local computers, which can be freely downloaded from <https://www.anaconda.com/>. The detailed steps of installing these dependencies are provided as follows:

Step 1. Download and install the anaconda platform:

Download from: <https://www.anaconda.com/products/individual>

Step 2. Install PyTorch:

Please refer to <https://pytorch.org/get-started/locally/> for PyTorch installation.

Step 3. Install dependent packages

```
pip install lightgbm
pip install pandas
pip install joblib
pip install scikit-learn
pip install numpy
pip install scipy
```

Running

To run B³P²Augur, go to the installation folder of B³P²Augur and enter the following content into Command Prompt:

```
python B3P2Augur.py
```

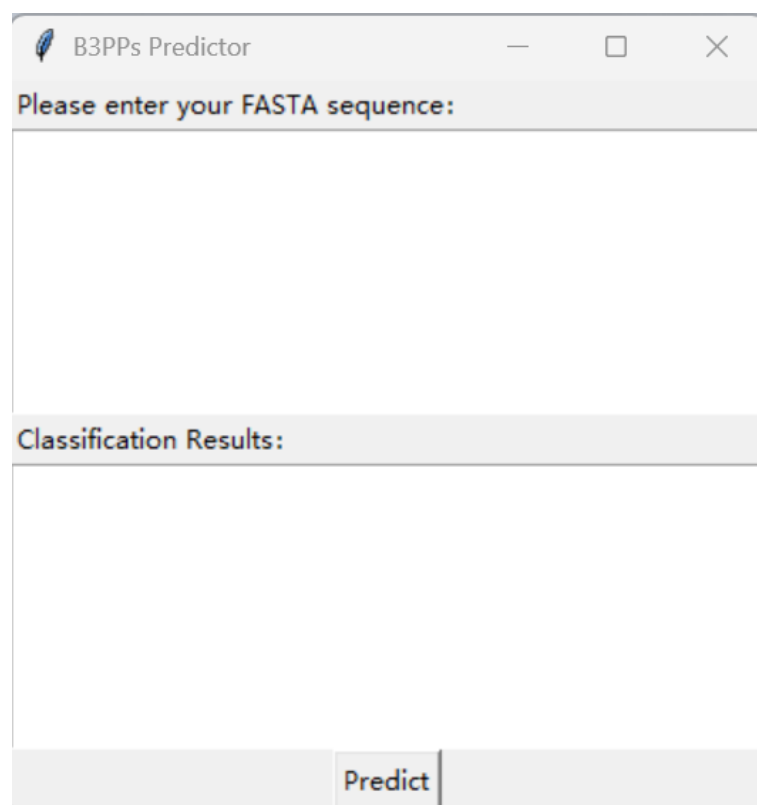
Once B³P²Augur has started, the interface will show as demonstrated in Figure 1.

The input format of B³P²Augur

The input of B³P²Augur is a set of protein sequences in FASTA format, as shown in Figure 2.

Prediction

Upon completing the input of the protein sequence to be tested, clicking the "Predict" button will yield the prediction results, as shown in Figure 3.



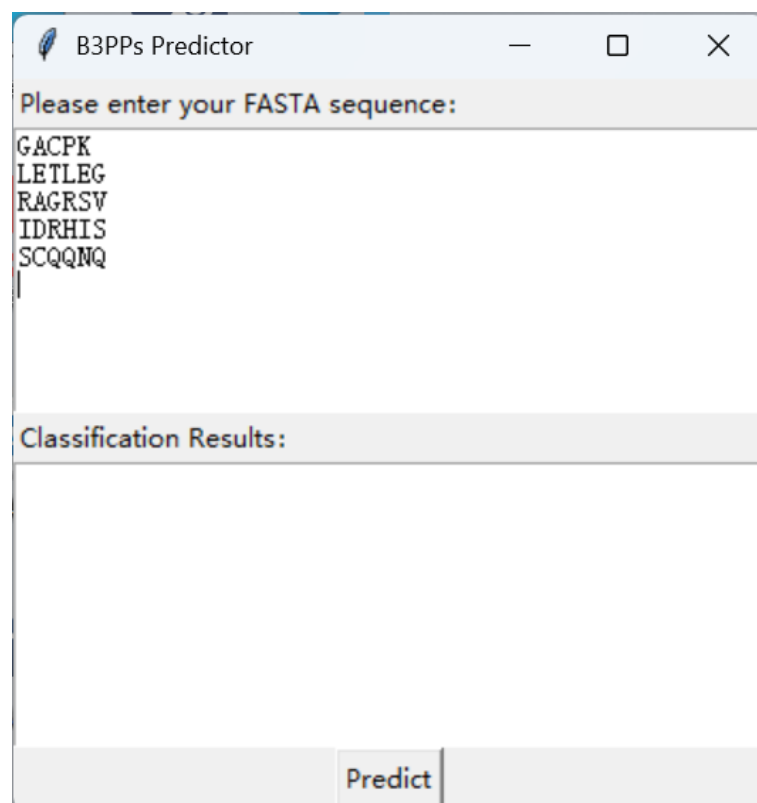
B3PPs Predictor

Please enter your FASTA sequence:

Classification Results:

Predict

Figure 1 The main interface of B³P²Augur



B3PPs Predictor

Please enter your FASTA sequence:

GACPK
LETLEG
RAGRSV
IDRHS
SCQQNQ
|

Classification Results:

Predict

Figure 2 The example input for B³P²Augur

B3PPs Predictor

Please enter your FASTA sequence:

GACPK
LETLEG
RAGRSV
IDRHIS
SCQQNQ

Classification Results:

Here are the result!

The sequence_1 is a B3PP!
The possibility of being a non-B3PP: 0.483
The possibility of being a B3PP: 0.517

The sequence_2 is a B3PP!
The possibility of being a non-B3PP: 0.487
The possibility of being a B3PP: 0.512

The sequence_3 is a B3PP!
The possibility of being a non-B3PP: 0.470
The possibility of being a B3PP: 0.530

Predict

Figure 3 The output of B³P²Augur