

Installing and running Augur

Installation

Prior to installing and running Augur, 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 Augur, go to the installation folder of Augur and enter the following content into Command Prompt:

```
python Augur.py
```

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

The input format of Augur

The input of Augur 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.

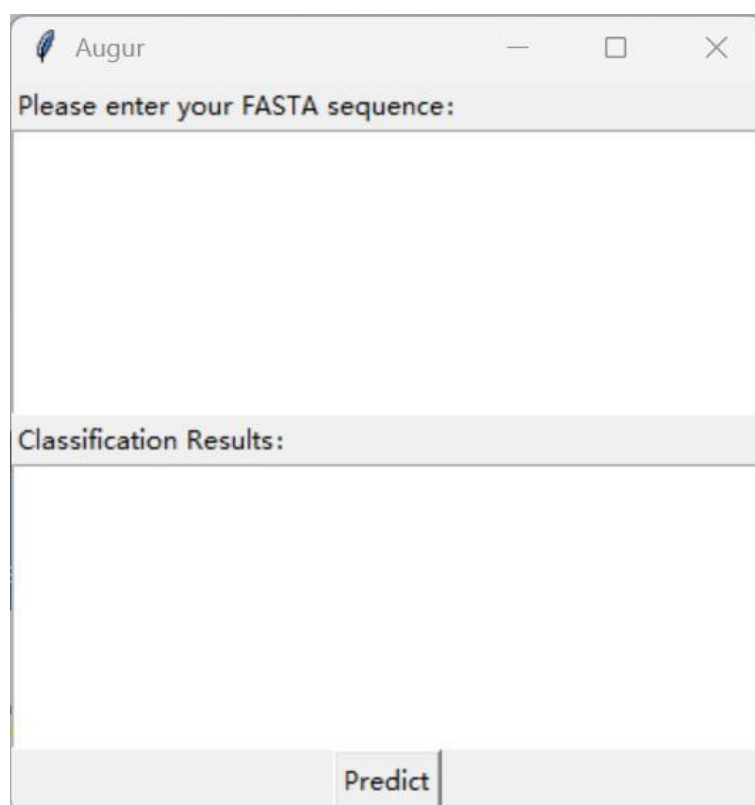


Figure 1 The main interface of Augur

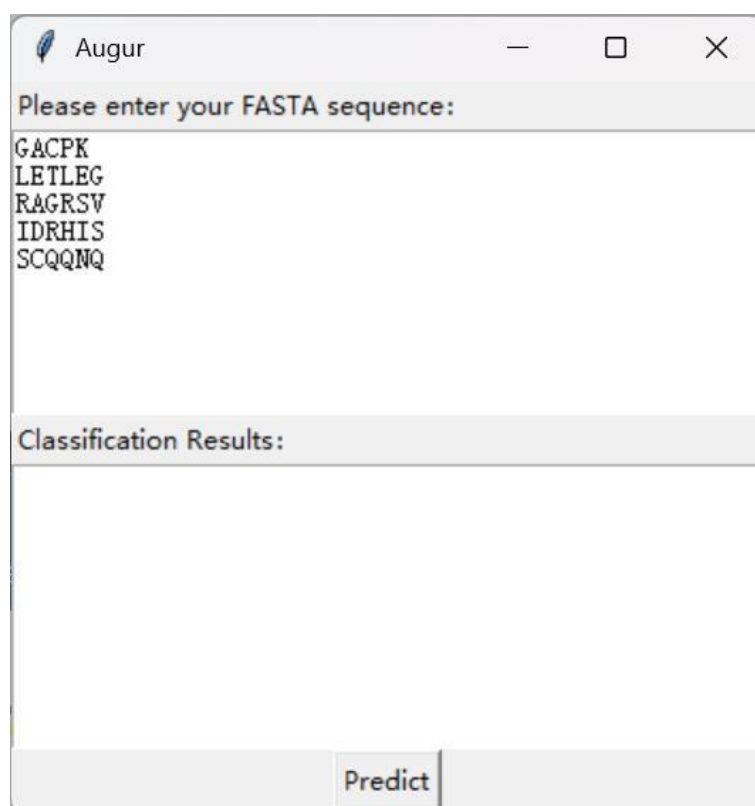


Figure 2 The example input for Augur

Augur

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 Augur