Installing and running B^3P^2Augur

Installation

Prior to installing and running B^3P^2Augur, 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 B^3P^2Augur, go to the installation folder of B^3P^2Augur and enter the following content into Command Prompt:

python B3P2Augur.py

Once B^3P^2Augur has started, the interface will show as demonstrated in Figure 1.

The input format of B^3P^2Augur

The input of B^3P^2Augur 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.

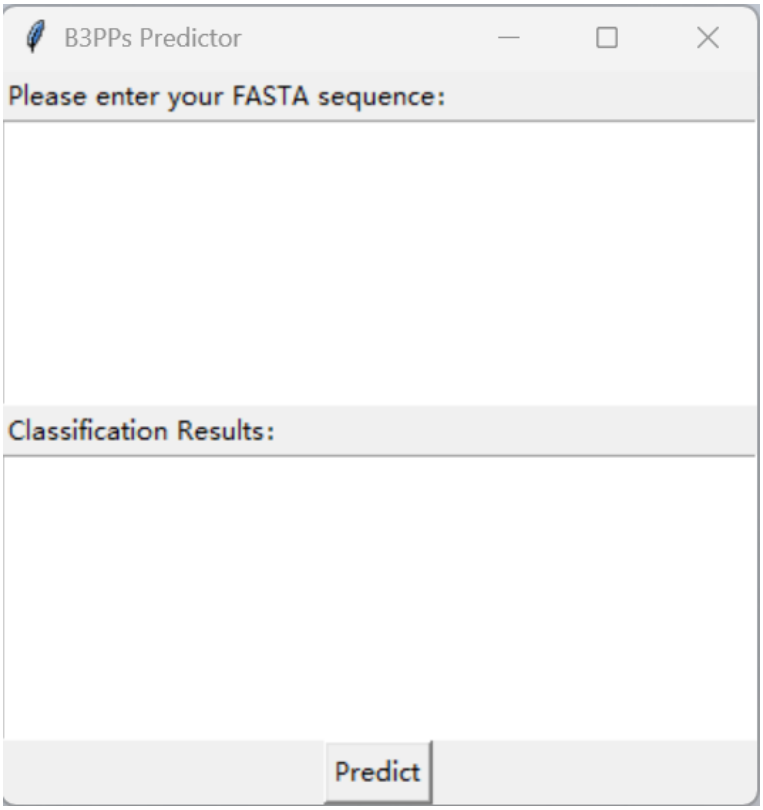

Figure 1 The main interface of B^3P^2Augur

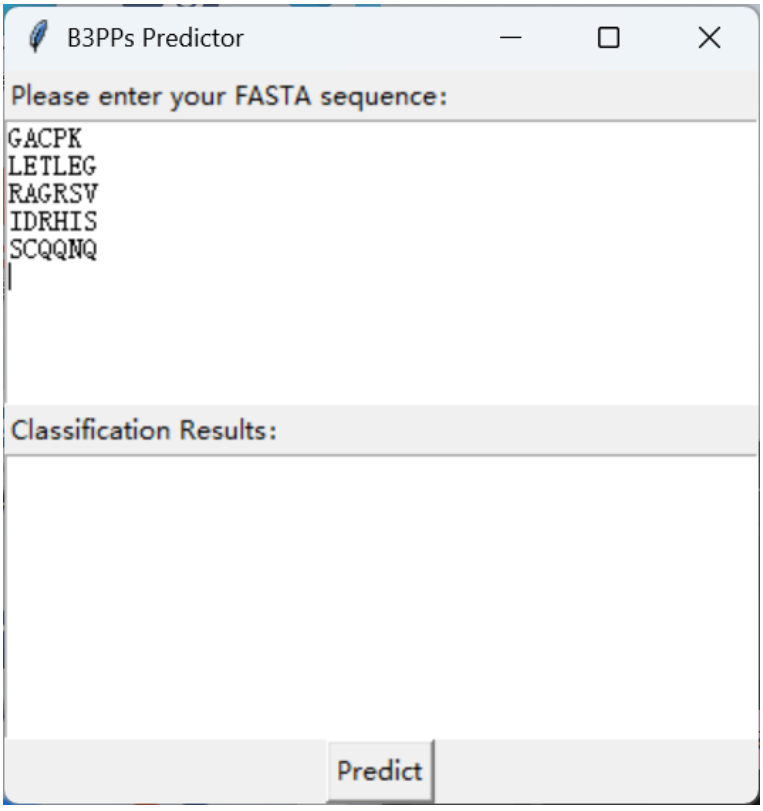

Figure 2 The example input for B^3P^2Augur

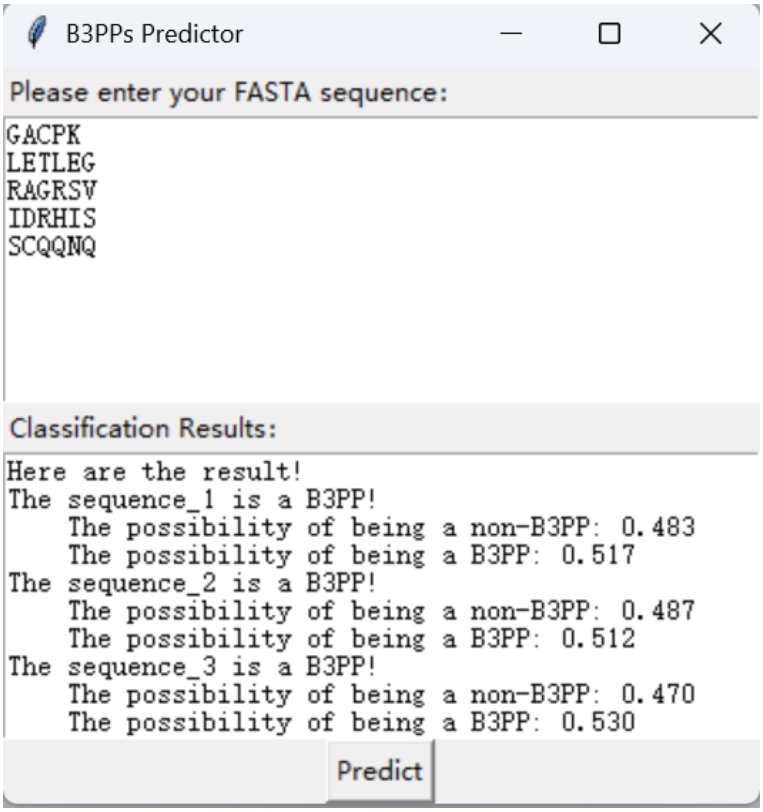

Figure 3 The output of B^3P^2Augur