FIRM-AVP User's Guide

(Version 1.0)

FIRM-AVP is a standalone software package developed to predict antiviral peptide sequences. It is written mainly in python3 though some modules are implemented in R and called from the main python script.

To install and use MLAVP:

- Download all from Github link- https://github.com/abu034004/FIRMAVP and save it in a directory.
- You will need to install "Jupyter Notebooks" if you want to use the notebook version of this program. For installation, visit the link: https://www.anaconda.com/download/ and install anaconda for python 3. To install it from a terminal window, please visit the link: https://jupyter.org/install .
- Edit the fasta file "input_seq.fasta" to include sequences you want to test. Note that there are some default example test sequences in this file, and you can also use example test sequences available in the folder "test examples".
- Next, use the 'cd' command to go to the directory where the "FIRMAVP" has been saved and then type the command "jupyter notebook".

After a couple of seconds, a new page for Jupyter Notebook will appear in your default browser. Click on FIRMAVP.ipynb. FIRMAVP will open up in a new browser window or tab. A screenshot is shown below.

Before running the notebook, please install the rpy2 package using the command "conda install -c r rpy2" from the command prompt. Also, please install the tzlocal package using command "conda install -c conda-forge tzlocal" if needed. For details, please visit https://anaconda.org/r/rpy2 and https://anaconda.org/conda-forge/tzlocal for the rpy2 and tzlocal packages, respectively. If your system cannot locate the e1071 package, please install the e1071 package using the command "conda install -c r r-e1071". For details, please visit https://anaconda.org/r/r-e1071 for the e1071 packages. All of the remaining packages should come with Jupyter Notebook by default. In the worst case, if any package is missing, please use the 'conda install' command to install the required packages. Alternatively, users can use the 'pip install' command to install the necessary packages rather than using the 'conda install' command.

Next, click inside a code cell and then click on the "Run" button.

If you want to stop running the notebook, please click on "Interrupt the kernel" (i.e., the stop button). If an error occurs, you can restart the kernel. Click on the "restart the kernel" button.

After starting the notebook or script, a GUI should appear as in the following screenshot.
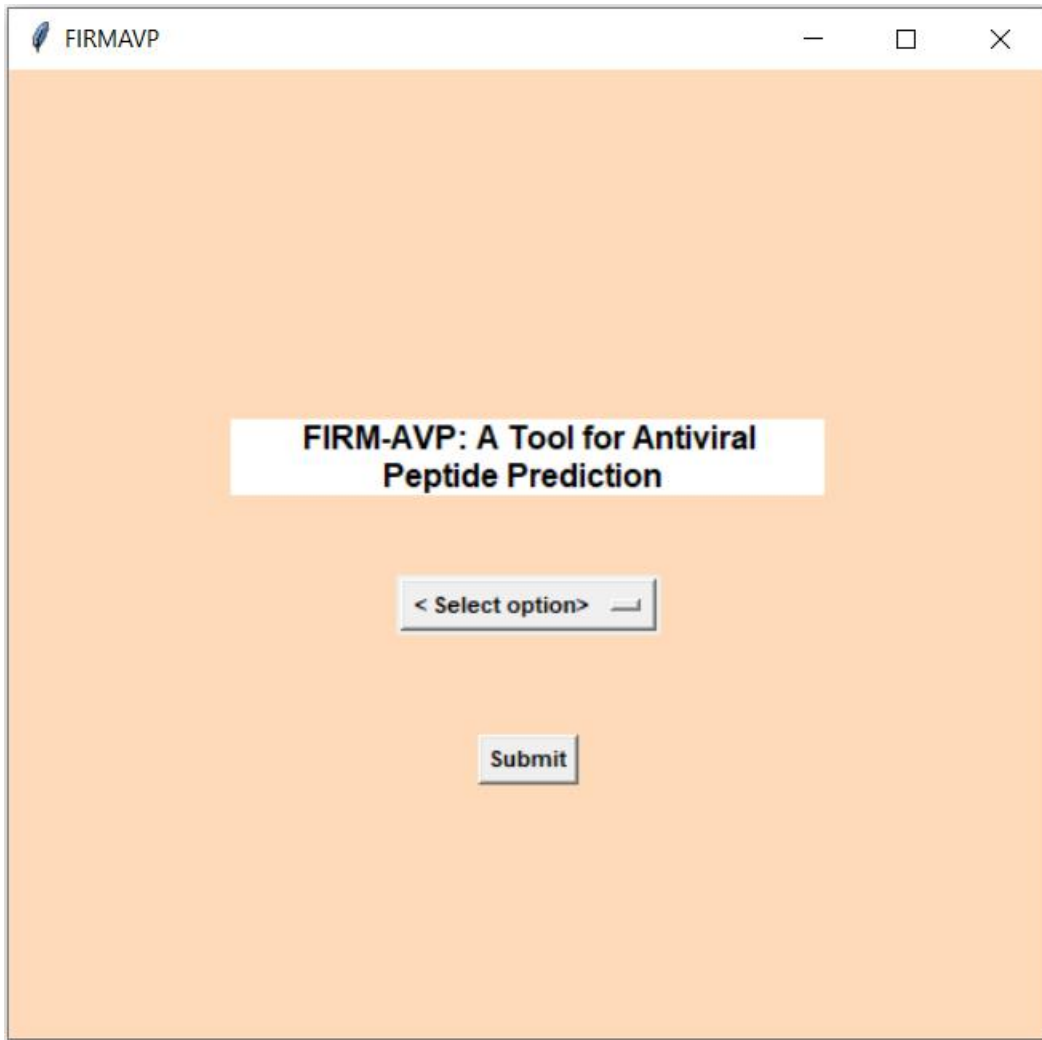
Please click on the option menu to see all options available in the tool as shown in the following screenshot.
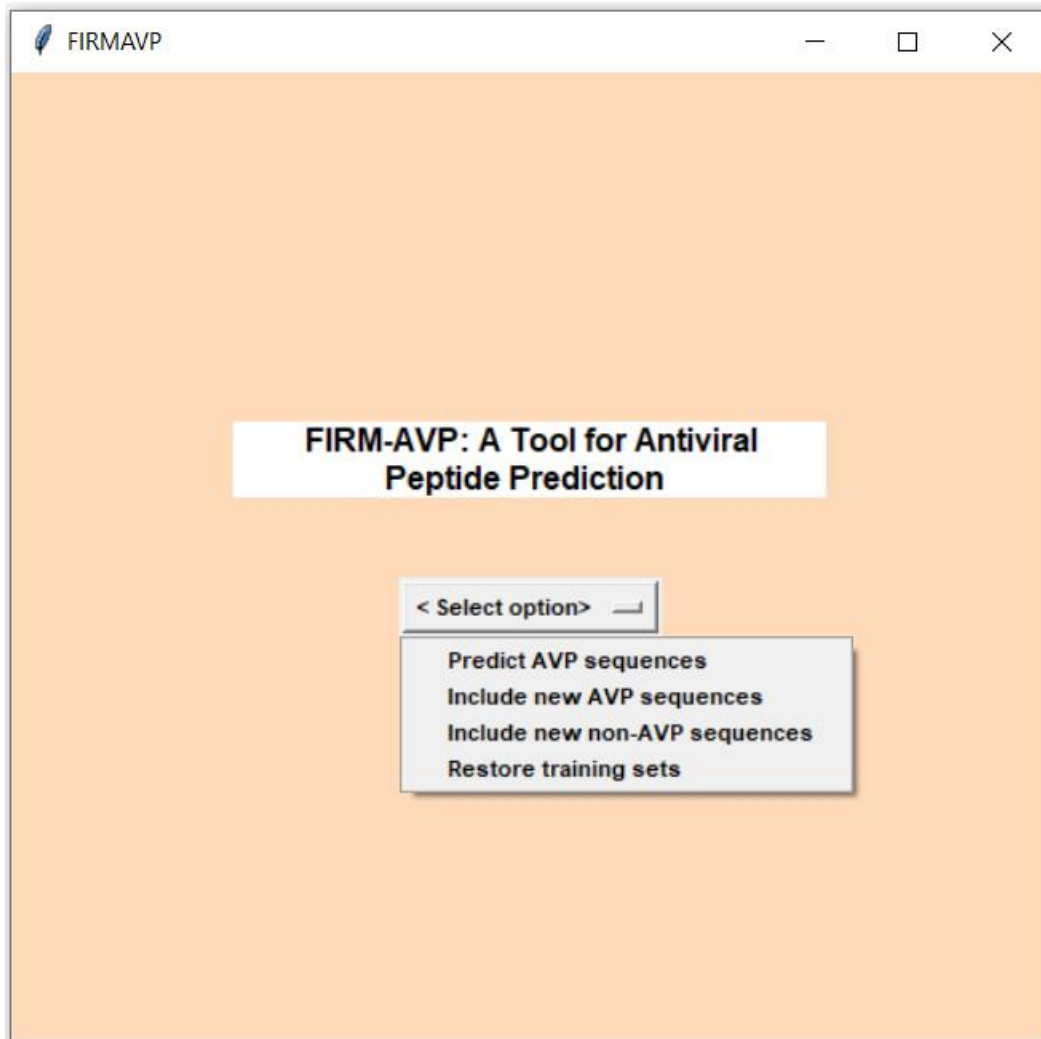
A brief description of the options is given below.

(a) **Predict AVP sequences**: This option is for predicting antiviral peptide sequences from the input fasta sequences in the default "input_seq.fasta" file.

(b) **Include new AVP sequences:** These options are given for a user who wants to include new known AVP sequences to the original training data that comes with this tool. Again the sequences that a user wants to add need to be placed in the "input_seq.fasta" file.

(c) **Include new non-AVP sequences:** These options are given for a user who wants to include new known non-AVP sequences to the training data that comes with this tool. Again the sequences that a user wants to add need to be placed in the "input_seq.fasta" file.

(d) **Restore training sets:** This option allows a user to reset all training datasets back to the original versions that came with this tool.

After successful execution, the tool will show a message- "The operation is successful!" and the predicted output will be available in the "predicted_AVP_sequences.fasta" file located in the folder where you saved "FIRMAVP".

If you find our tool useful, please cite the following paper.

Citations:

1. Chowdhury, A.S., Kehn-Hall K., Bishop B., Webb-Robertson, B.M., Submitted. Improved Antiviral Peptide Prediction via Effective Feature Selection. Scientific Reports.