ReadME

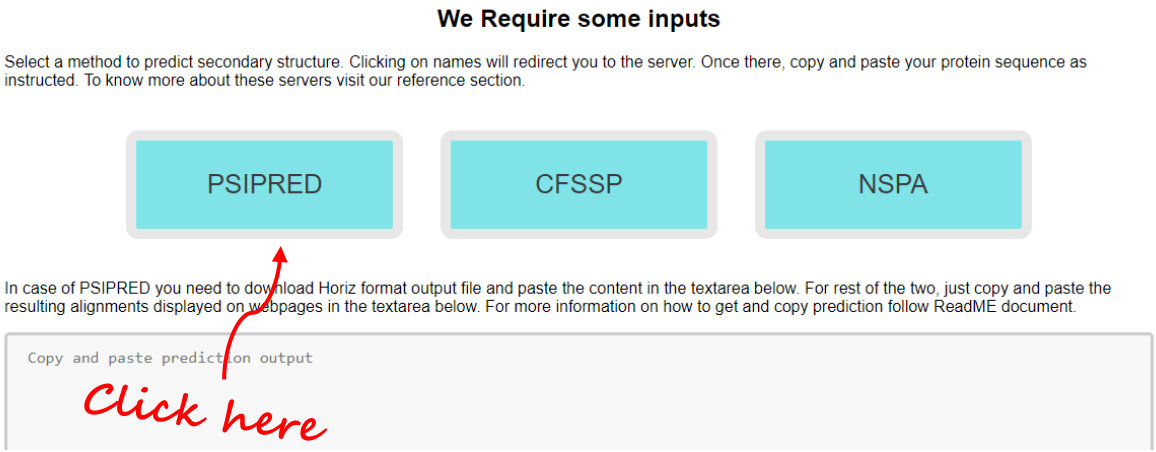
This ReadME documentation provides a guideline on how to perform a secondary structure comparison between predicted and assigned secondary structure elements in a protein using PreSSM. Follow the step by step instructions that are made easy to comprehend by pictorial representation.

PreSSM allows users to select any server from the given three choices to get secondary structure prediction for their protein.

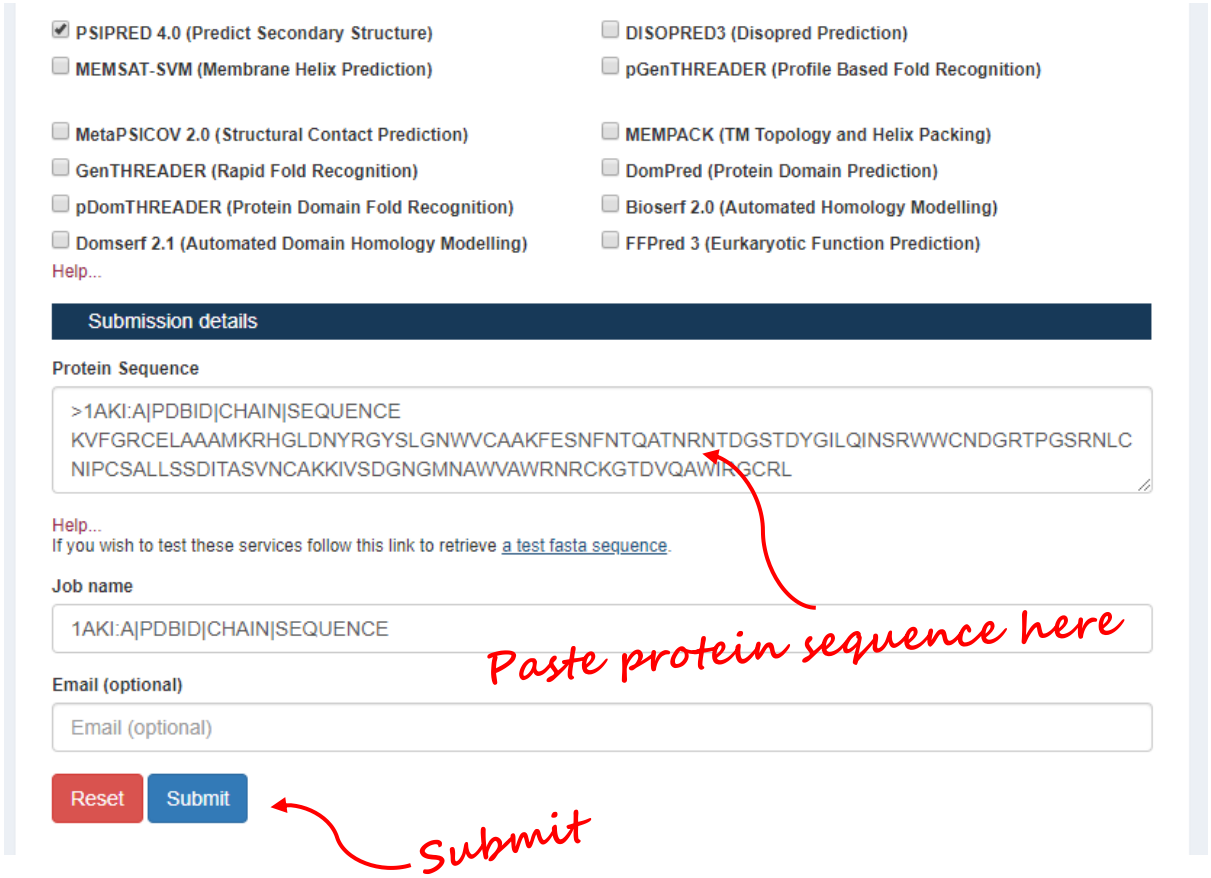
CONTENT

If you wish to choose PSIPRED

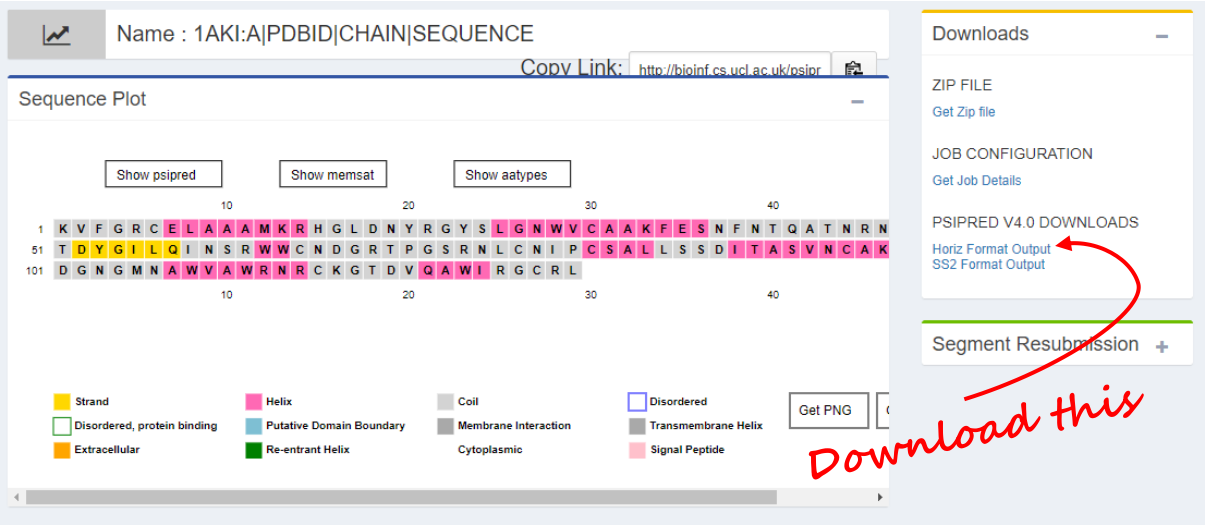
STEP 1 Select PSIPRED



STEP 2 Copy and paste your sequence in the text area and submit the sequence. PSIPRED 4.0 (Predict Secondary Structure) option is selected by default.



STEP 3 Download Horiz format output.

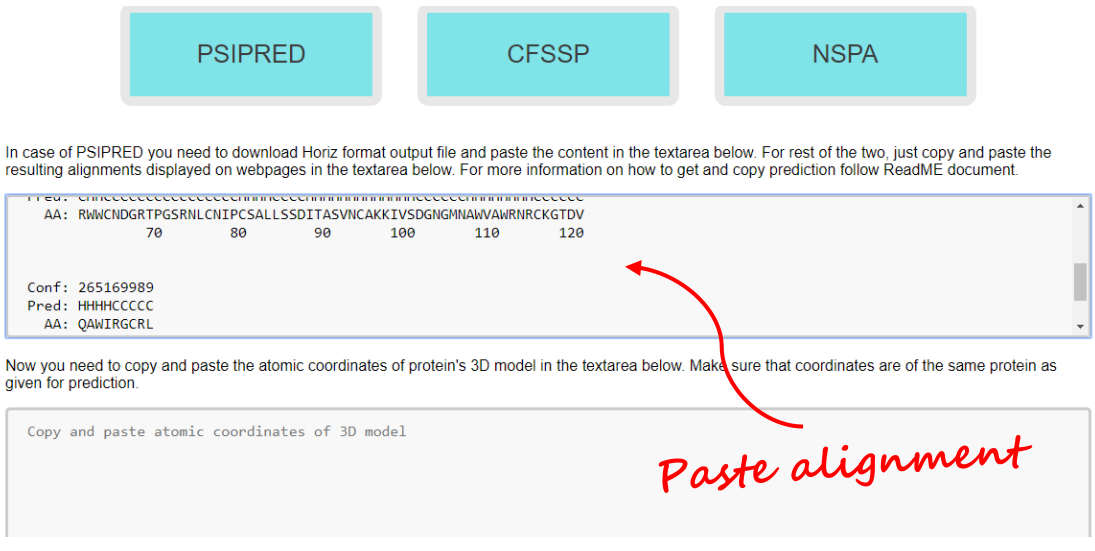


STEP 4 Open the downloaded file and copy the content.

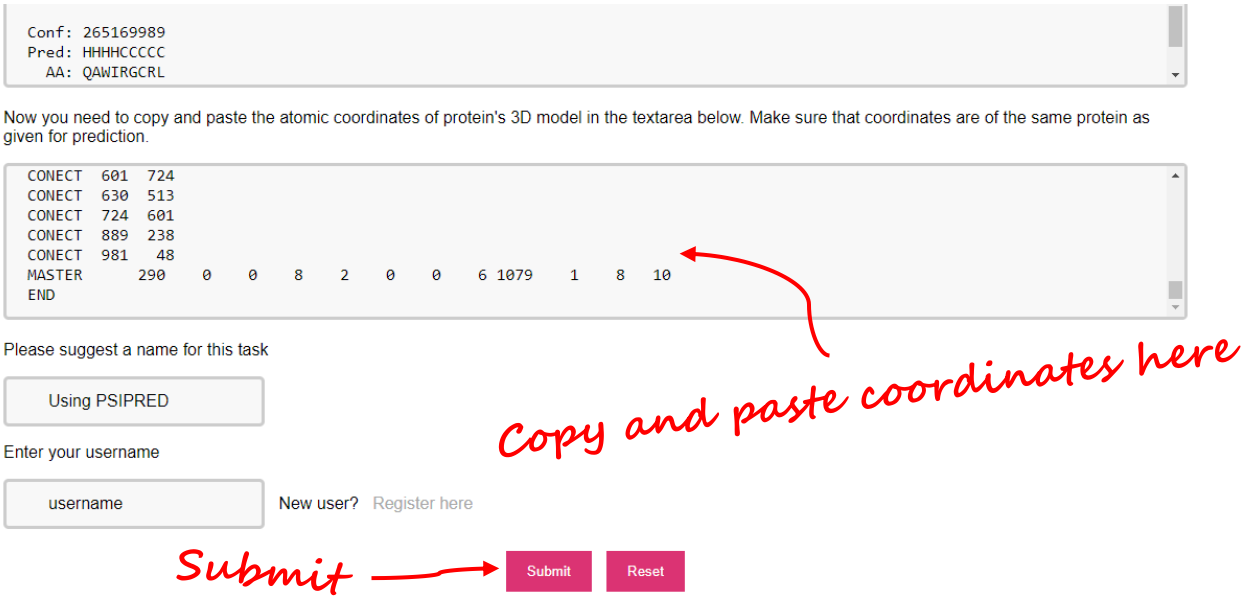
```
# PSIPRED HFORMAT (PSIPRED V4.0)

Conf: 9315108999999889410798868888777005636985660017999841687880 73
Pred: CCCCCCHHHHHHHHCCCCCCCCCCHHHHHHHHHHHHCCCCCCCCCCCCCCCEEEEEECCC
  AA: KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINS
              10        20        30        40        50        60

Conf: 0210279999976543467689544798999999999965998310599998517999 4
Pred: CHHCCCCCCCCCCCCCCCHHHHCCCCHHHHHHHHHHHHCCCCCCHHHHHHHCCCCCC
  AA: RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDV
              70        80        90       100       110       120

Conf: 265169989
Pred: HHHHCCCCC
  AA: QAWIRGCRL
```

Copy alignment

STEP 5 Go back to PreSSM and paste the alignment in the first text area.



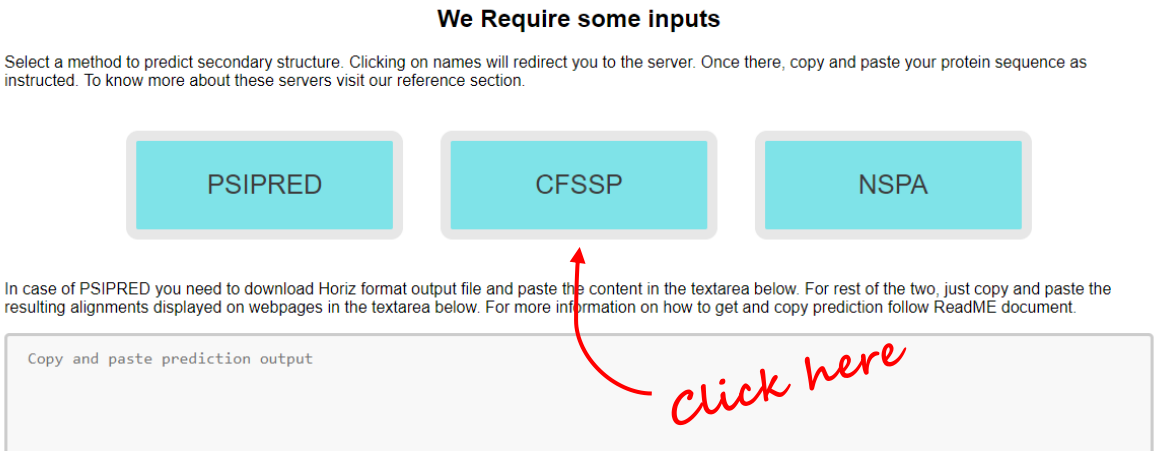
STEP 6 Now open your coordinate file (.pdb) in any text editor. Copy and paste the atomic coordinates in the second text area on PreSSM. Enter a task name of your choice and your username before submitting the information.



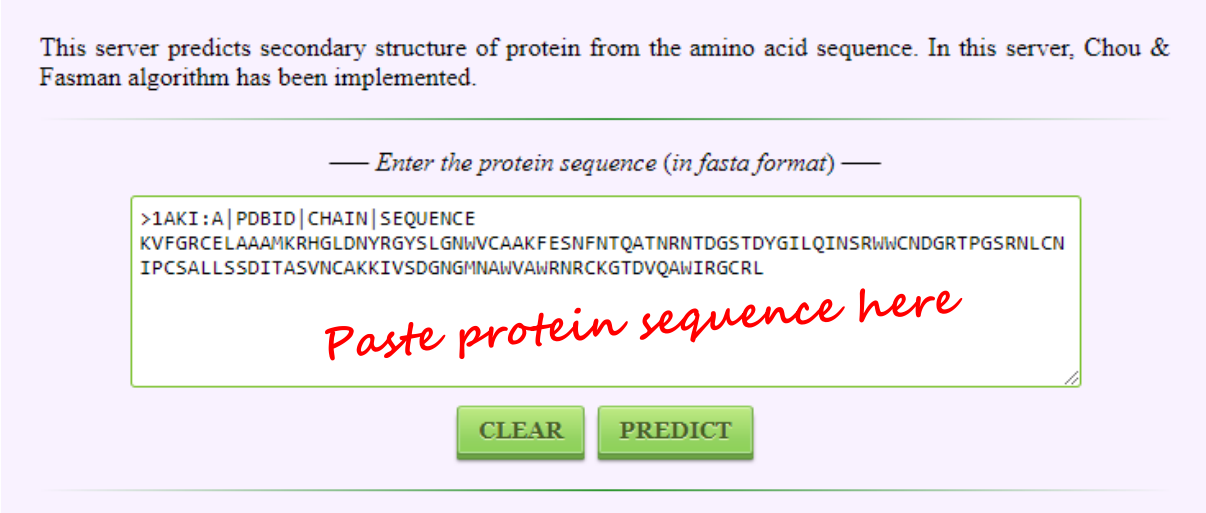
Upon submission a result webpage will be displayed with scores and alignment. Users can also download the results in text format.

If you wish to choose CFSSP

STEP 1 Select CFSSP



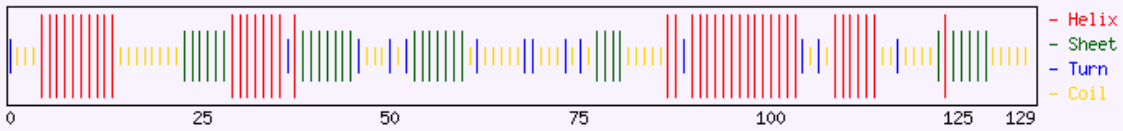
STEP 2 Copy and paste your sequence in the text area and submit the sequence by clicking PREDICT.



STEP 3 Copy the alignment displayed on the resulting webpage.

Target Sequence:

```
        10         20         30         40         50         60         70
KVFGRCELAA AMKRHGLDNY RGYSLGNWVC AAKFESNFNT QATNRNTDGS TDYGILQINS RWWCNDGRTP

        80         90        100        110        120
GSRNLCNIPC SALLSSDITA SVNCAKKIVS DGNGMNAWVA WRNRCKGTDV QAWIRGCRL
```



Secondary Structure:

```
                 *         *         *         *         *         *
Query 1   KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINSRWWCNDGRTP 70
Helix 1       HHHHHHHHHH             HHHHHHHHHH                 HH              70
Sheet 1                          EEEEEEE        EEEEEEE      EEEEEEEE            70
Turns 1   T                                   T   T    T   T T        T     TT    70
Struc 1   TCCCHHHHHHHHHHCCCCCCCCEEEEEEHHHHHHHTHEEEEEEETCCCTCTEEEEEEECTCCCCCTTCCC 70

                 *         *         *         *         *
Query 71  GSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRL 129
Helix 71              HHHHHHHHHHHHHHHHH    HHHHHH        HH           129
Sheet 71      EEEE                                     EEEEEEE       129
Turns 71  T T           T         T    T T         T                 129
Struc 71  TCTCEEEECCCCCHHTHHHHHHHHHHHHHHHTCTCHHHHHHCCTCCCCEHEEEECCCCC 129
```

Total Residues: H: 47 E: 33 T: 16
Percent: H: 36.4 E: 25.6 T: 12.4

Copy alignment

STEP 4 Go back to PreSSM and paste the alignment in the first text area.

In case of PSIPRED you need to download Horiz format output file and paste the content in the textarea below. For rest of the two, just copy and paste the resulting alignments displayed on webpages in the textarea below. For more information on how to get and copy prediction follow ReadME document.

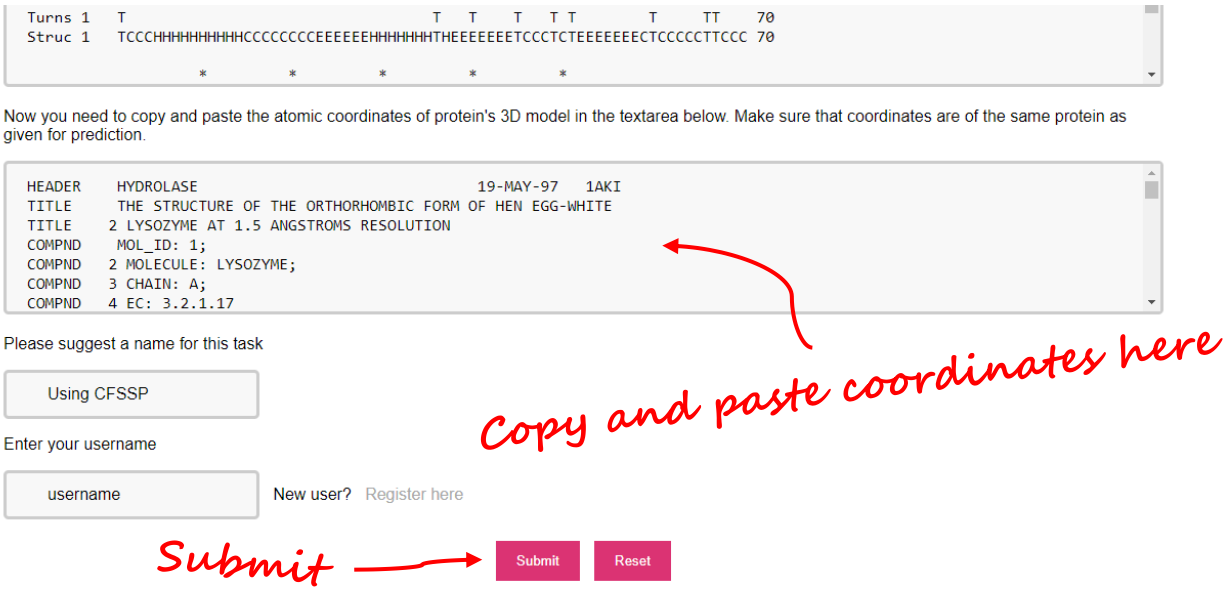
```
                 *         *         *         *         *
Query 71  GSRNLCNIPCSALLSSDITASVNCAKKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRL 129
Helix 71              HHHHHHHHHHHHHHHHH    HHHHHH        HH           129
Sheet 71      EEEE                                     EEEEEEE       129
Turns 71  T T           T         T    T T         T                 129
Struc 71  TCTCEEEECCCCCHHTHHHHHHHHHHHHHHHTCTCHHHHHHCCTCCCCEHEEEECCCCC 129
```

Now you need to copy and paste the atomic coordinates of protein's 3D model in the textarea below. Make sure that coordinates are of the same protein as given for prediction.

Copy and paste atomic coordinates of 3D model

Paste alignment

STEP 5 Now open your coordinate file (.pdb) in any text editor. Copy and paste the atomic coordinates in the second text area on PreSSM. Enter a task name of your choice and your username before submitting the information.



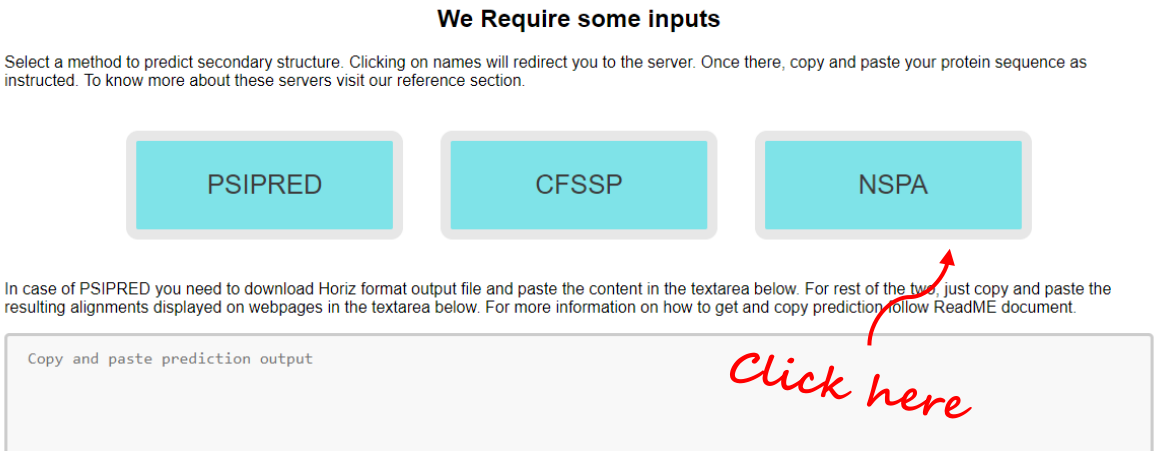
Copy and paste coordinates here

Submit

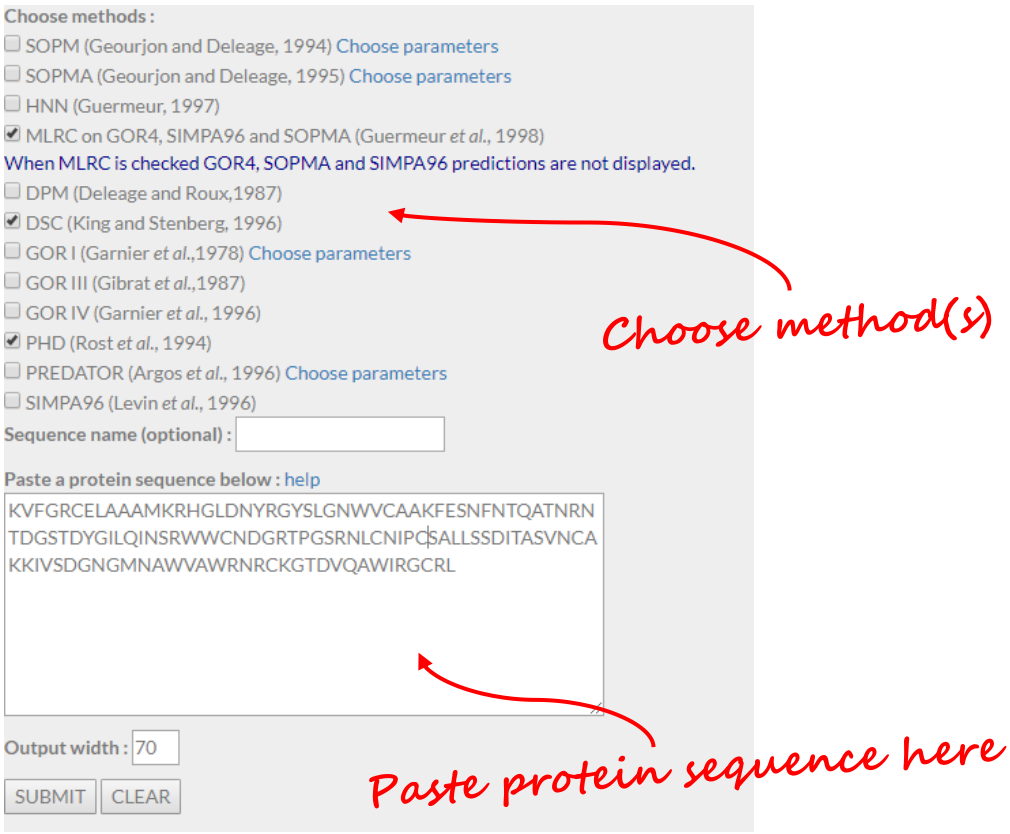
Upon submission a result webpage will be displayed with scores and alignment. Users can also download the results in text format.

If you wish to choose NSPA

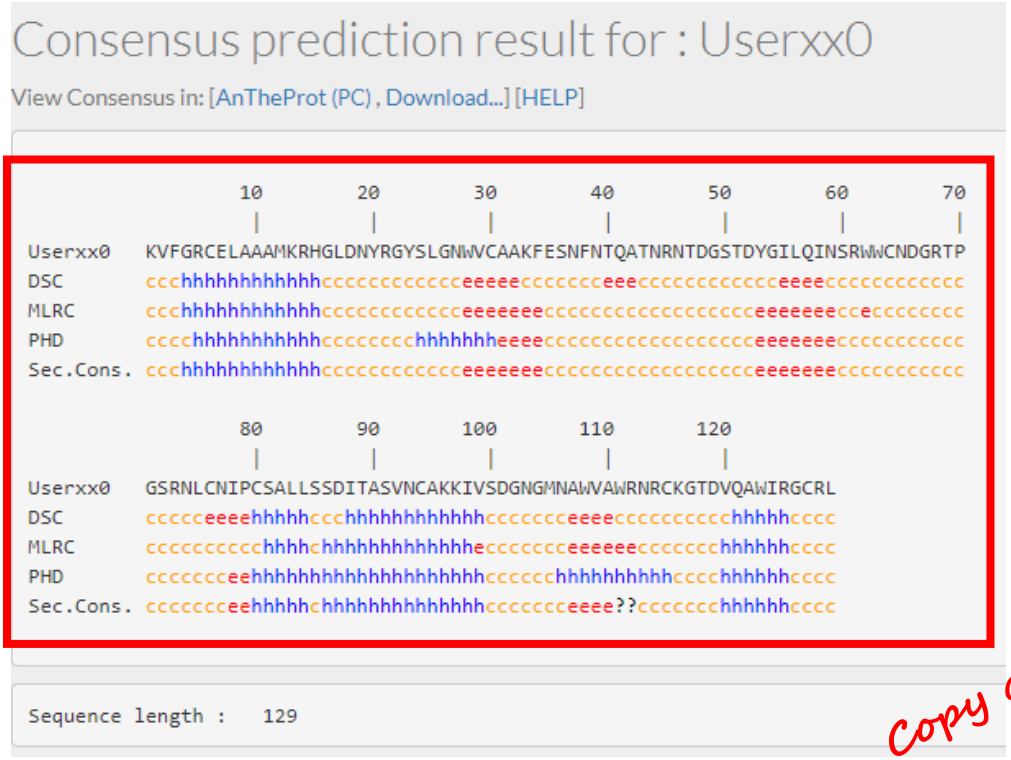
STEP 1 Select NSPA.



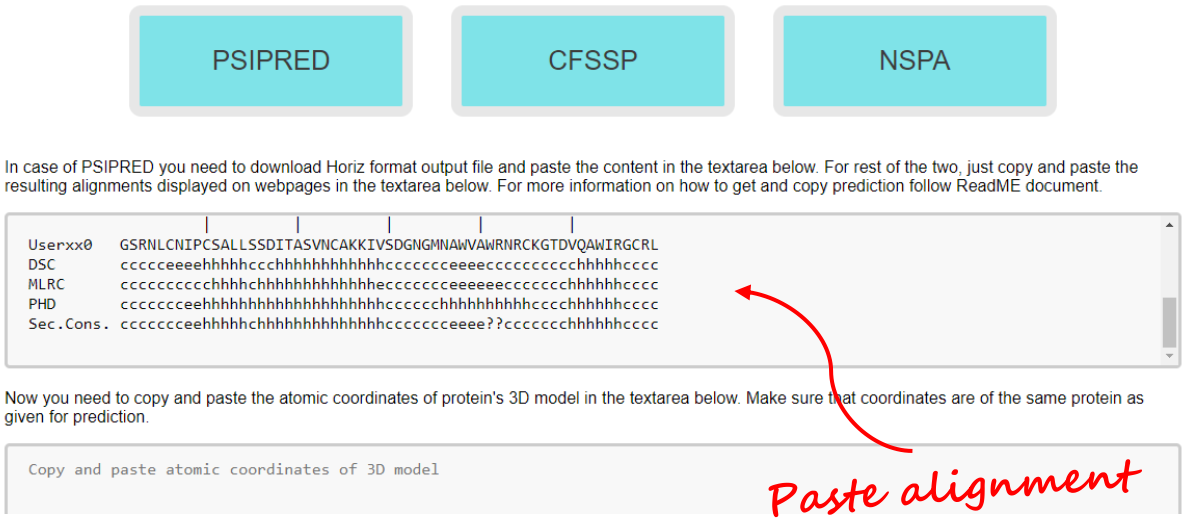
STEP 2 Choose methods (or single method) for predicting secondary structure. Copy paste your sequence in the text field and submit the information.



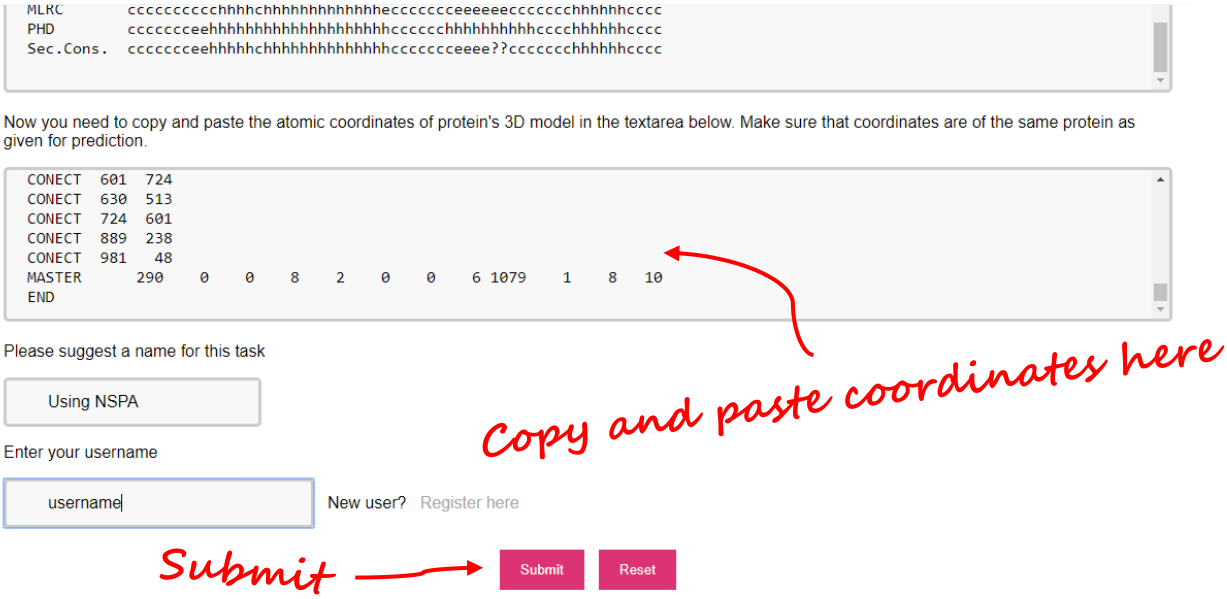
STEP 3 Copy the alignment displayed on the resulting webpage.



STEP 4 Go back to PreSSM and paste the alignment in the first text area.



STEP 5 Now open your coordinate file (.pdb) in any text editor. Copy and paste the atomic coordinates in the second text area on PreSSM. Enter a task name of your choice and your username before submitting the information.



Upon submission a result webpage will be displayed with scores and alignment. Users can also download the results in text format.