



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.

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If you wish to choose PSIPRED

STEP 1 Select PSIPRED

We Require some inputs

Select a method to predict secondary structure. Clicking on names will redirect you to the server. Once there, copy and paste your protein sequence as instructed. To know more about these servers visit our reference section.

PSIPRED

CFSSP

NSPA

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.

Copy and paste prediction output

Click here

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.

- PSIPRED 4.0 (Predict Secondary Structure)
- MEMSAT-SVM (Membrane Helix Prediction)
- MetaPSICOV 2.0 (Structural Contact Prediction)
- GenTHREADER (Rapid Fold Recognition)
- pDomTHREADER (Protein Domain Fold Recognition)
- Domserf 2.1 (Automated Domain Homology Modelling)
- DISOPRED3 (Disopred Prediction)
- pGenTHREADER (Profile Based Fold Recognition)
- MEMPACK (TM Topology and Helix Packing)
- DomPred (Protein Domain Prediction)
- Bioserf 2.0 (Automated Homology Modelling)
- FFPred 3 (Eukaryotic Function Prediction)

Help...

Submission details

Protein Sequence

```
>1AKI:A|PDBID|CHAIN|SEQUENCE
KVFGRCELAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGGSTDYGILQINSRWWCNDGRTPGSRNLC
NIPCSALLSSDITASVNCACKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRLL
```

Help...

If you wish to test these services follow this link to retrieve [a test fasta sequence](#).

Job name

1AKI:A|PDBID|CHAIN|SEQUENCE

Paste protein sequence here

Email (optional)

Email (optional)

Reset

Submit

Submit

STEP 3 Download Horiz format output.

Name : 1AKI:A|PDBID|CHAIN|SEQUENCE

Copy Link: <http://bioinf.cs.ucl.ac.uk/psipred>

Sequence Plot

Show psipred Show memsat Show aatypes

1 K V F G R C E L A A A M K R H G L D N Y R G Y S L G N W V C A A K F E S N F N T Q A T N R N
51 T D Y G I L Q I N S R W W C N D G R T P G S R N L C N I P C S A L L S S D I T A S V N C A K
101 D G N G M N A W V A W R N R C K G T D V Q A W I R G C R L

Legend: Strand, Disordered, protein binding, Extracellular, Helix, Putative Domain Boundary, Re-entrant Helix, Coil, Membrane Interaction, Cytoplasmic, Disordered, Transmembrane Helix, Signal Peptide

Downloads

ZIP FILE
Get Zip file

JOB CONFIGURATION
Get Job Details

PSIPRED V4.0 DOWNLOADS
Horiz Format Output
SS2 Format Output

Segment Resubmission +

Download this

STEP 4 Open the downloaded file and copy the content.

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

Conf: 93151089999988941079886888877700563698566001799984168788073
Pred: CCCCCHHHHHHHHCCCCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCCEEEEECCC
AA: KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGDYGIQLQINS
    10      20      30      40      50      60

Conf: 021027999997654346768954479899999999999659983105999985179994
Pred: CHHCCCCCCCCCCCCCHHHHCCCCCHHHHHHHHHHHHHCCCCCHHHHHHHHHCCCCC
AA: RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCACKIVSDGNGMNAWAWNRNCKGTDV
    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.

PSIPRED CFSSP NSPA

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.

```
Conf: 93151089999988941079886888877700563698566001799984168788073
Pred: CCCCCHHHHHHHHCCCCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCCEEEEECCC
AA: KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGDYGIQLQINS
    10      20      30      40      50      60

Conf: 021027999997654346768954479899999999999659983105999985179994
Pred: CHHCCCCCCCCCCCCCHHHHCCCCCHHHHHHHHHHHHHCCCCCHHHHHHHHHCCCCC
AA: RWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCACKIVSDGNGMNAWAWNRNCKGTDV
    70      80      90      100     110     120

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

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 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.

```
Conf: 265169989
Pred: HHHHCCCCC
AA: QAWIRGRL
```

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.

```
CONNECT 601 724
CONNECT 630 513
CONNECT 724 601
CONNECT 889 238
CONNECT 981 48
MASTER 290 0 0 8 2 0 0 6 1079 1 8 10
END
```

Please suggest a name for this task

Using PSIPRED

Enter your username

username

New user? [Register here](#)

Submit →

Copy and paste coordinates here

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

We Require some inputs

Select a method to predict secondary structure. Clicking on names will redirect you to the server. Once there, copy and paste your protein sequence as instructed. To know more about these servers visit our reference section.



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.

Copy and paste prediction output

A red curved arrow originates from the 'CFSSP' button and points towards the text area below. The text 'Click here' is written in red cursive script next to the arrow.

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

This server predicts secondary structure of protein from the amino acid sequence. In this server, Chou & Fasman algorithm has been implemented.

— Enter the protein sequence (in fasta format) —

```
>1AKI:A|PDBID|CHAIN|SEQUENCE
KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGS TDYGILQINSRWWCNDGRTPGSRNLCN
IPCSALLSSDITASVNC AKKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRL
```

Paste protein sequence here

CLEAR

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 RMMCNDGRTP
80      90      100     110     120
GSRNLCNIPC SALLSSDITA SVNCAKKIVS DGNMGNAVVA WRNRCKGTDV QAWIRGCR L

```

Secondary Structure:

```

          *      *      *      *      *      *
Query 1  KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGSTDYGILQINSRMMCNDGRTP 70
Helix 1      HHHHHHHHHH          HHHHHHHHHH          HH          70
Sheet 1          EEEEEEE          EEEEEEE          EEEEEEE          70
Turns 1  T          T T T T T          T          TT          70
Struc 1  TCCCHHHHHHHHHCCCEEEEEEHHHHHHHHEEEEEETCCCTCEEEEEECTCCCCCTCCC 70

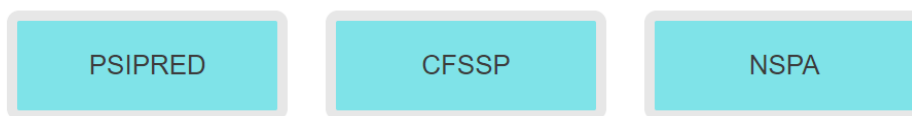
          *      *      *      *      *
Query 71  GSRNLCNIPCSALLSSDITASVNCAKKIVSDGNMGNAVVAWRNRCKGTDVQAWIRGCR L 129
Helix 71      HHHHHHHHHHHHHHHHH          HHHHHH          HH          129
Sheet 71      EEEE          EEEEEEE          129
Turns 71  T T          T          T T T          T          129
Struc 71  TCTCEEECCCCCHHTHHHHHHHHHHHHHTCTCHHHHHHCCTCCCEHEEEEECCCCC 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  GSRNLCNIPCSALLSSDITASVNCAKKIVSDGNMGNAVVAWRNRCKGTDVQAWIRGCR L 129
Helix 71      HHHHHHHHHHHHHHHHH          HHHHHH          HH          129
Sheet 71      EEEE          EEEEEEE          129
Turns 71  T T          T          T T T          T          129
Struc 71  TCTCEEECCCCCHHTHHHHHHHHHHHHHTCTCHHHHHHCCTCCCEHEEEEECCCCC 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.

```
Turns 1 T T T T T T T T 70
Struc 1 TCCCHHHHHHHHHCCCCCCCCCEEEEEHHHHHHHTHEEEEEETCCCTCTEEEEEECTCCCCCTTCCC 70
* * * * *
```

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.

```
HEADER HYDROLASE 19-MAY-97 1AKI
TITLE THE STRUCTURE OF THE ORTHORHOMBIC FORM OF HEN EGG-WHITE
TITLE 2 LYSOZYME AT 1.5 ANGSTROMS RESOLUTION
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: LYSOZYME;
COMPND 3 CHAIN: A;
COMPND 4 EC: 3.2.1.17
```

Copy and paste coordinates here

Please suggest a name for this task

Using CFSSP

Enter your username

username

New user? [Register 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.

We Require some inputs

Select a method to predict secondary structure. Clicking on names will redirect you to the server. Once there, copy and paste your protein sequence as instructed. To know more about these servers visit our reference section.



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Copy and paste prediction output

Click here

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

Choose methods :

- SOPM (Geourjon and Deleage, 1994) [Choose parameters](#)
- SOPMA (Geourjon and Deleage, 1995) [Choose parameters](#)
- HNN (Guermeur, 1997)
- MLRC on GOR4, SIMPA96 and SOPMA (Guermeur *et al.*, 1998)
When MLRC is checked GOR4, SOPMA and SIMPA96 predictions are not displayed.
- DPM (Deleage and Roux, 1987)
- DSC (King and Stenberg, 1996)
- GOR I (Garnier *et al.*, 1978) [Choose parameters](#)
- GOR III (Gibrat *et al.*, 1987)
- GOR IV (Garnier *et al.*, 1996)
- PHD (Rost *et al.*, 1994)
- PREDATOR (Argos *et al.*, 1996) [Choose parameters](#)
- SIMPA96 (Levin *et al.*, 1996)

Sequence name (optional) :

Paste a protein sequence below : [help](#)

```
KVFGRCELAAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRN
TDGSTDYGILQINSRWWCNDGRTPGSRNLCNIPCSALLSSDITASVNCA
KKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCRL
```

Output width :

Choose method(s)

Paste protein sequence here

STEP 3 Copy the alignment displayed on the resulting webpage.

Consensus prediction result for : Userxx0

View Consensus in: [AnTheProt (PC) , Download...] [HELP]

	10	20	30	40	50	60	70
Userxx0	KVFGRCELAAMKRHGLDNYRGYSLGNWVCAAKFESNFNTQATNRNTDGDSTDYGILQINSRWWCNDGRTP						
DSC	ccccchhhhhhhhhhhcc						
MLRC	ccccchhhhhhhhhhhcc						
PHD	ccccchhhhhhhhhhhccccccccchhhhhhhhhhhcc						
Sec. Cons.	ccccchhhhhhhhhhhcc						
	80	90	100	110	120		
Userxx0	GSRNLCNIPCSALLSSDITASVNCACKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCR						
DSC	ccccceehhhhhccccchhhhhhhhhhhcc						
MLRC	ccccccccccccchhhhchhhhhhhhhhhhhhhcc						
PHD	ccccccccceehhh						
Sec. Cons.	ccccccccceehhhhhchhh						

Sequence length : 129

Copy alignment

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Userxx0	GSRNLCNIPCSALLSSDITASVNCACKIVSDGNGMNAWVAWRNRCKGTDVQAWIRGCR
DSC	ccccceehhhhhccccchhh
MLRC	ccccccccccccchhhhchhh
PHD	ccccccccceehhh
Sec. Cons.	ccccccccceehhhhhchhh

Paste alignment

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Copy and paste atomic coordinates of 3D model

Paste alignment

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```
MLRC      cccccccccchhhchhhhhhhhhhhhhheccccceeeeeccccchhhhhcccc
PHD       cccccceehhhhhhhhhhhhhhhhhhhhhccccchhhhhhhhhccccchhhhhcccc
Sec.Cons. cccccceehhhchhhhhhhhhhhhhhhhhhhhhccccceeeee??ccccchhhhhcccc
```

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.

```
CONNECT 601 724
CONNECT 630 513
CONNECT 724 601
CONNECT 889 238
CONNECT 981 48
MASTER 290 0 0 8 2 0 0 6 1079 1 8 10
END
```

Copy and paste coordinates here

Please suggest a name for this task

Enter your username

New user? [Register here](#)

Submit →

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