

Secondary and Tertiary Structure prediction of protein / Nucleotides.

Aim:- To predict the secondary & tertiary structure of protein using relevant software tools.

Introduction:-

Some of the important secondary & tertiary structure prediction tools available at expasy.org

ALADIR:- An algorithm to predict the helical contents of peptides.

APSSP:- Advanced protein secondary structure prediction server.

CRSSP:- Char and amp : Fasman secondary structure prediction server.

HNN:- Hierarchical Neural Network method (Guernsey, 1997).

EXOR:- Exorner at 1996.

HTMSRAP:- Helical Transmembrane segment rotational angle prediction

Jpred:- A consensus method for the protein secondary structure at university of Dundee.

PSI pred:- Various protein structure prediction method at bloomslawry center for bioinformatics.

SOPMA:- Pourjan and Delage, 1995.

→ The PSI pred protein structure prediction server aggregates several of our structure sequence, perform the prediction of their choice and receive the results of the prediction via e-mail. You may

- detect one of three prediction methods, to apply to your sequences.

PSI pred:- A highly accurate method for the protein secondary structure prediction.

MEMSAT and MEMSAT-SVM:- widely used transmembrane topology prediction method and one of QENTHREADAR.

PQENTHREADAR, and PDOMTHREADAR - sequence profile based fold recognition methods.

* Query :- Fibrinogen

* URL:- Jpred → compbio.dundee.ac.uk/jpred/ (Secondary structure prediction)

AlphaFold:- <https://alphafold.ebi.ac.uk/>

Procedure:-

i) Jpred

#1) Log on to NCBI and retrieve a protein sequence in FASTA format.

#2) Log on to compbio.dundee.ac.uk/jpred/

#3) paste the retrieved protein sequences.

#4) Click on make prediction button.

#5) Hits of the given query with respect to is obtained Click on Continue option.

#6) Result will be displayed.

- * In this annotation indicates that Trnet jury was involved to rationalize significantly different primary prediction.
- * (-) - other type of secondary structure.
- * Trnet.conf -> the confidence estimate for prediction. Lipus 14&18 coded prediction sequence. These are binary prediction for each location.

↳ Alpha fold:-

- * If AI system predicts protein 3D structure from it the tool contains 200 million entries with broad coverage of uniprot & pdb the alpha fold is able to produce highly accurate side chain when backbone is accurate, considerably improves over template even when strong template are available.
- The pLDDT measure of confidence is obtained on a scale of 0-100 it is a measure of per residue estimate of its confidence.

P-10

C-10

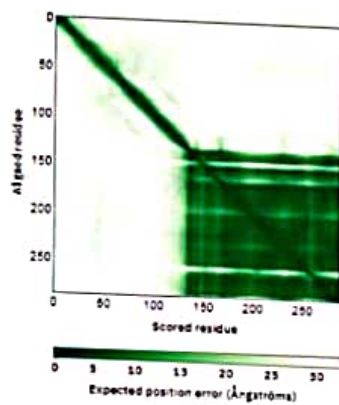
V-10

R-15

 45

22/1/24

Predicted aligned error (PAE)



Click and drag a box on the PAE viewer to select regions of the structure and highlight them on the 3D viewer.

PAE data is useful for assessing inter-domain accuracy – go to Help section below for more information.

Jpred 4

Incorporating Jnet

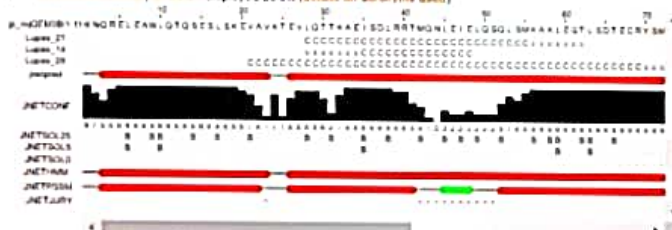
A Protein Secondary Structure Prediction Server

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Results

After much trouble and strife, Bob the scheduling penguin has retrieved your results! Rejoice. For your pleasure the following viewing options are available. You may bookmark this page for future reference although data is not kept on the server for more than two days.

- View results summary in SVG - displayed below (details on acronyms used)



- View full results in HTML
- View simple results in HTML
- View results in PDF
- View results in Jalview (Link to a separate page with the Jalview Java Desktop application)
- View everything in a results directory (details on data each file contains are available through README file)
- Get all files in TAR.GZ archive