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Homology modeling with trRosetta

Chris Berndsen[1]

[1]James Madison University

In Development Share

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Berndsen Lab

Chris Berndsen
James Madison University

ABSTRACT

Protocol for homology modeling using trRosetta written for students in Biochemistry I at James Madison University.

DOI

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PROTOCOL CITATION

Chris Berndsen 2021. Homology modeling with trRosetta. **protocols.io** https://dx.doi.org/10.17504/protocols.io.bw9nph5e

MANUSCRIPT CITATION please remember to cite the following publication along with this protocol

J Yang, I Anishchenko, H Park, Z Peng, S Ovchinnikov, D Baker, Improved protein structure prediction using predicted interresidue orientations, PNAS, 117: 1496-1503 (2020)

KEYWORDS

null, homology modeling, trRosetta, protein, prediction

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52238

MATERIALS TEXT

Internet access
trRosetta server

BEFORE STARTING

Have a sequence in FASTA format.

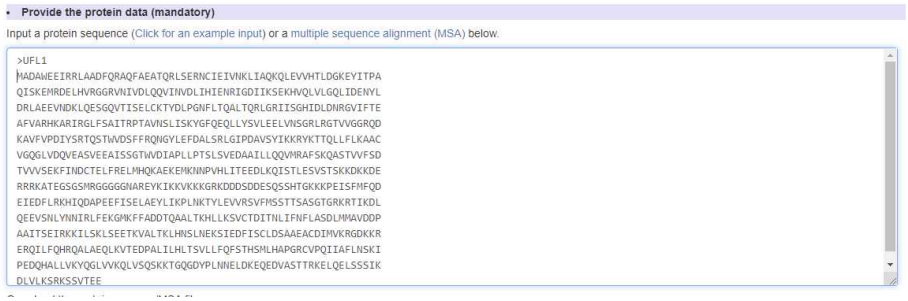
Ex.
>protein_seq

MASDTERFFGGYP...

Setting up modeling

1 Navigate to the trRosetta homepage.

2 Input your sequence in FASTA format.
The first list should start with > as shown in the example below.



Sequence format for trRosetta

3 Enter your email address and give a target name.

> It is always a good idea to include target name or identifier in case you have multiple sequences that you are predicting.

4 Adjust any options that you want and record these changes as a note on this step.

5 Press submit and wait for the job finish email. Typically takes 2 to 24 hours to get a result.

Modeling results

6 When your receive the job finished email, navigate to the results link.

> Help guide for trRosetta: https://yanglab.nankai.edu.cn/trRosetta/help/

7 The top model will be shown in a window like below with an estimated TM score.

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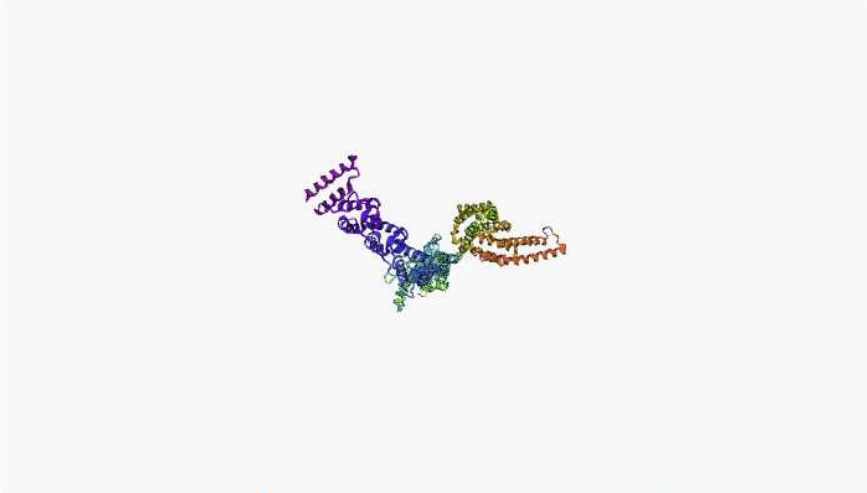
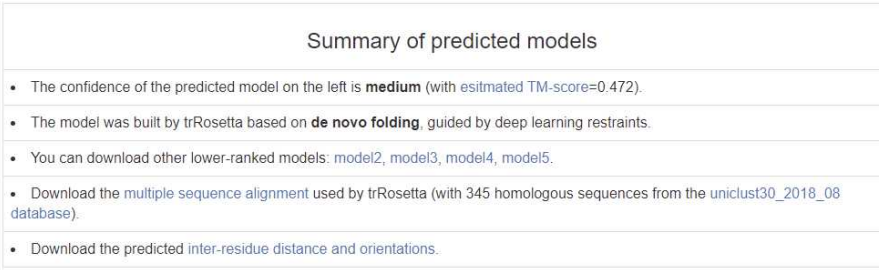


Download Model 1 (colored by rainbow from N to C terminus)
Estimated TM-score: 0.472

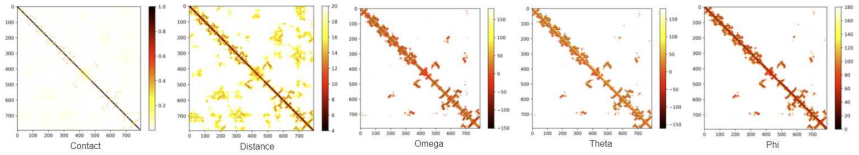
The TM-score is a template model score and measures the similarity between two proteins. 0 is no match, while 1 is a good match. Models with scores >0.5 are likely to be reliable.

8 The summary indicates how the model was built during the modeling along with links to the data that was used during modeling and the 4 "next best" models.



Summary of modeling. Blue text indicates links to data.

9 The predicted 2D information shows the predicted long range interactions within the structure along with information on the dihedral angles.



2-D prediction heatmaps

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This information is good for quickly identifying interesting inter-domain interactions or potential sites of regulation.

10 The predicted 1-D information shows the secondary structure prediction and predicted regions of disorder.

Secondary structure prediction

Saving data

11 At the top of the window you can download the entire file in .tar.bz2 format. To open this file it must be decompressed.

Alternatively, you can download the relevant models and data individually from the summary table.

Save files as

[date]_[proteinname]_[teamname]_trRosetta

Replace [proteiname] with the target protein name, [teamname] with your name or your team's name, [date] with the date.

Ex.: 20210810_UFL1_Berndsen_trRosetta

12 Indicate WHERE you saved the file as a note on this step.

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