


SWISS-MODEL

Modelling
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Start a New Modelling Project

Target
Sequence(s):
(Format must be FASTA, GenBank, plain string, or a valid UniProtKB AC)

Target: 75
Target: 158
Target: 225
Target: 389

Add Hetero Target
Reset

Project Title:
Email:

Search For Templates

Build Model

Supported Inputs

Sequence(s)
Target-Template Alignment
User Template
DeepView Project

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Result:-

- * In model details it displays the 3D Structure of model & target template sequence alignment as well as your quadrants.
- * Model quadrants available at deep view projects & PDB formats.
- * By default the final model is presented in colour is based on Qmean model quality. Alignment State & as well as bound Legend value was provided.

Model evaluation:-

QMQE [Global model Quality estimate] is quality estimate & for given query it was found to be 0.56

- * The value should be 0 & 1

QMEAN Disco Global

Is the average per residue & represents the RMSD between QMEAN DI & IDTI

* QMEAN - Z score:-

It is based on 4 Statistical score & mean score & linear combination.

Z score around 0.01 \rightarrow native like structure.

\rightarrow Qmean Z score below -4.0 indicates the model with low quality.

\rightarrow Structure assignment was done & the structure compared with 2D Ramachandran plot to identify helix & sheet position.

Experiment 1
⑨ Now click on search for template, option provided (Never select the option "build model directly)". This step helps in your Query Sequence being searched for template.

⑩ This step will find the most suitable template based on sequence alignment using parameters the database consist of already predicted & verified structure.

⑪ This step presents the result by finding specific sequence whose similarity Query is at least 30-40% or more. Here coverage identity & on maximum query coverage identity & QMDF parameters & click on build model.

[Optional: You can select max than 1 template.

⑫ The result with built structure will be displayed. The structure can be visualized in different forms.

⑬ In the displayed result, Check the QMDF value, it should be close to 1, & Qmean Zscore, Comparison graph should show the model on template structure.

⑭ These parameters decide if the structure is eligible to use in docking studies.

⑮ ~~Do~~ the modelling if the above parameters are not satisfied.

⑯ Further validation can be done using same tool.

URL:- ① <https://www.uniprot.org>
② <https://swissmodel.expasy.org>

Query:- Serotonin, dopamine, ILK, TNF,
dopamine receptor D1 ✓

Procedure:-

- ① Log on to uniprot using the URL <https://www.uniprot.org>.
- ② Type the Query + search for it result will be displayed in table format.
- ③ Select the appropriate sequence based organism method of length of the protein.
- ④ Result for the selected Query will be displayed containing all biological information, go to sequence section & copy the sequences.
- ⑤ Log on to Swiss model using URL <https://swissmodel.expasy.org> & Click on Start model
- ⑥ Paste the sequence copied from uniprot databases in the target sequence box provided. If the sequence is shown in different colours, it indicates that the sequence is correctly compatible & eligible for structure predictions.
- ⑦ Type the name in the project title option provided.
- ⑧ In the "Supported Inputs" option present on right side of the page. Select the appropriate parameters & Choose the target option you wish to use for modeling.

Comparative modelling of homologous sequences & Validation of modelled structure

Aim:-

To carryout homology modelling for 3° protein structure prediction using SWISS model.