

TEAM SVCE CHENNAI

CFastDx

EXPERIMENT PROTOCOL

SWISS-MODEL HOMOLOGY MODELING

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SWISS-MODEL HOMOLOGY MODELING PROTOCOL

STEPS

Prepare the Target Protein Sequence:

- Obtain the amino acid sequence of your target protein (the one you want to model). This can usually be retrieved from public databases like UniProt.
- Copy the protein sequence in FASTA format.

Access the Swiss-Model Portal:

- Visit the Swiss-Model website.

Submit the Protein Sequence:

- Select "Start Modelling" on the Swiss-Model homepage.
- Paste the FASTA sequence of your target protein into the input box.
- If you have a specific template in mind, you can manually specify a template protein (usually a PDB ID). If not, Swiss-Model will automatically search for templates.

Template Search:

- Swiss-Model will search for suitable templates based on sequence similarity to your target protein. These templates are proteins with known structures that closely resemble your target.

Review the list of potential templates. Choose the best one based on factors such as:

- Sequence identity (higher identity is preferable).
- Coverage (the extent to which the template covers your target sequence).
- Resolution of the structure (lower resolution numbers indicate better quality).

Model Building:

- Once the template is selected, the Swiss Model will align the target sequence to the template and generate a 3D model.
- The time taken for modeling depends on the complexity and length of the sequence.

Evaluate the Model:

- After the model is built, Swiss Model provides a summary with several important parameters:
- GMQE (Global Model Quality Estimation): A score between 0 and 1 indicates the model's reliability.
- QMEAN: A score that assesses the stereochemical quality of the model. This tool provides an in-depth assessment of your model, including Ramachandran plot analysis. After submitting the PDB file, the QMEAN tool will generate various quality metrics, including a Ramachandran plot. The plot will categorize residues into different regions:
 - **Allowed regions (favorable φ and ψ angles).**
 - **Disallowed regions (outliers).**
- You will see a graphical representation of the φ (phi) and ψ (psi) torsion angles of the protein's backbone.
- Evaluate these parameters to ensure the quality of the model.
- **Download the Model:**
 - You can download the model in PDB format for further analysis or visualization.
 - Swiss-Model also provides a detailed report, including information on the alignment, model quality, and any regions requiring further refinement.

Reference:

Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., & Schwede, T. (2018). SWISS-MODEL: Homology modeling of protein structures and complexes. Nucleic Acids Research, 46(W1), W296–W303. <https://doi.org/10.1093/nar/gky427>

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