

Protein Model Portal and SWISS-MODEL Workspace:

Giving The Proteome A Third Dimension

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Summary

Protein structure modeling is widely used in the life science community to build models for proteins, for which no experimental structures are available. The Protein Model Portal (PMP, <http://www.proteinmodelportal.org>) contains more than 21 million models for more than 5.1 million distinct UniProt sequences provided by various partner sites, such as the Center for Structures of Membrane Proteins (CSMP), GPCRDB, MODBASE, Midwest Center for Structural Genomics (MCSG), the New York Structural Genomics Research Consortium (NYSGR), the Northeast Structural Genomics (NESG) consortium and SWISS-MODEL Repository. PMP presents models in a uniform interface allowing the user to easily navigate between experimental structures and computational models. For more detailed information on specific structures or models, PMP links back to the partner websites. PMP provides access to the interactive modelling services featuring fully automated pipelines by HHPred, IntFOLD2-TS, ITasser, ModWeb, M4T, Phyre2, RaptorX and SWISSMODEL. As the accuracy of a model determines its suitability for specific applications, each model on PMP has an estimated quality attached, and can additionally be submitted to several state-of-the-art model quality estimation servers (ModFOLD, ModEVAL and QMEAN).

In the second part of the tutorial, we will present interactive protein structure homology modelling using the latest release of SWISS-MODEL Workspace. The new web site allows users to interactively search for templates, cluster them by sequence similarity, structurally compare alternative templates and select the ones to be used for model building. In cases where multiple alternative template structures are available for a protein of interest, a user-guided template selection step allows building models in different states. The SWISS-MODEL Template Library acts as a base to this service, providing annotation of quaternary structure and essential ligands and co-factors to allow for building of complete structural models, including their oligomeric structure. The SWISS-MODEL pipeline makes extensive use of model quality estimation for selection of the most suitable templates and provides estimates of the expected accuracy of the resulting models. The accuracy of the models generated by SWISS-MODEL is continuously evaluated by the Continuous Automated Model Evaluation (CAMEO) system. SWISS-MODEL is available at <http://swissmodel.expasy.org>.

Questions are welcome at the end of each part.