

## Lecture 8. Protein Modeling And De Novo Design

- Download course materials  
<https://mulan.swmed.edu/lecture8.tar.gz>

*To unpack the tar.gz ball, run the following command:*

*`tar xvfz lecture8.tar.gz`*

*A new directory, lecture8 will be created*

- Read the papers in the “Reading” subdirectory and the book chapters of “Molecular Modelling: Principles and Applications (2nd Edition)” entitled “10 Protein structure prediction, sequence analysis and protein folding”
- Perform protein modeling for Dishevelled PDZ domain
  1. Download a crystal structure and sequence file of “A Dvl2 PDZ Domain in Complex with the C1 Inhibitory Peptide” (PDB Code 3CBX).
  2. Download PSD95 PDZ domain (PDB Code 1BE9) as the template to generate a homology model for the Dvl2 PDZ sequence.
  3. Sequence alignment with Promals3D  
(<http://prodata.swmed.edu/promals3d/promals3d.php>)
  4. Use modeller to generate a homology model (exemplary input and command files are in /home/mmms/project4/modeler)
  5. Evaluate the homology model and 3CBX using procheck, then compare the homology model to the crystal structure.