

1st MedILS Summer School
Structure and Evolution: from Bench to Terminal

Homology Modeling

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Structure Prediction

« *The 3D structures of proteins in a family are more conserved than their sequences* »

Homology Modeling is based on the reasonable assumption that two homologous proteins will share very similar structures.

Protein Threading scans the amino acid sequence of an unknown structure against a database of solved structures. In each case, a scoring function is used to assess the compatibility of the sequence to the structure, thus yielding possible three-dimensional models.

ab-initio protein modeling methods seek to build three-dimensional protein models "from scratch", i.e., based on physical principles rather than (directly) on previously solved structures.

The 4 steps of Homology Modeling

Tools:

- Blast
- Clustalw
- Modeler
- Evaluations Methods as ProsaII, Eval3D ...

