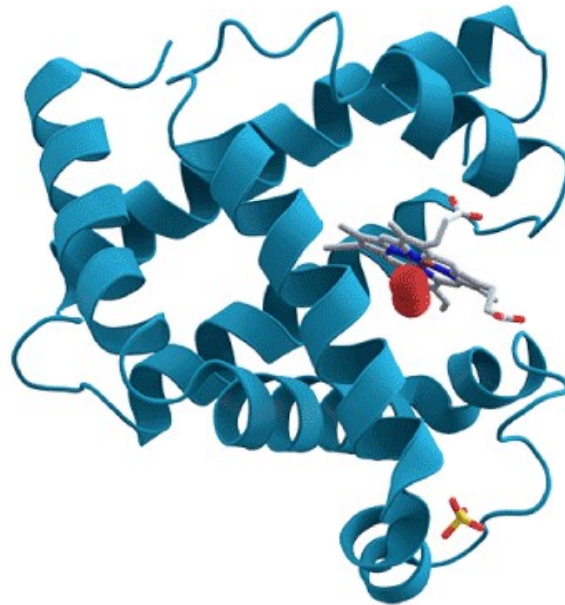
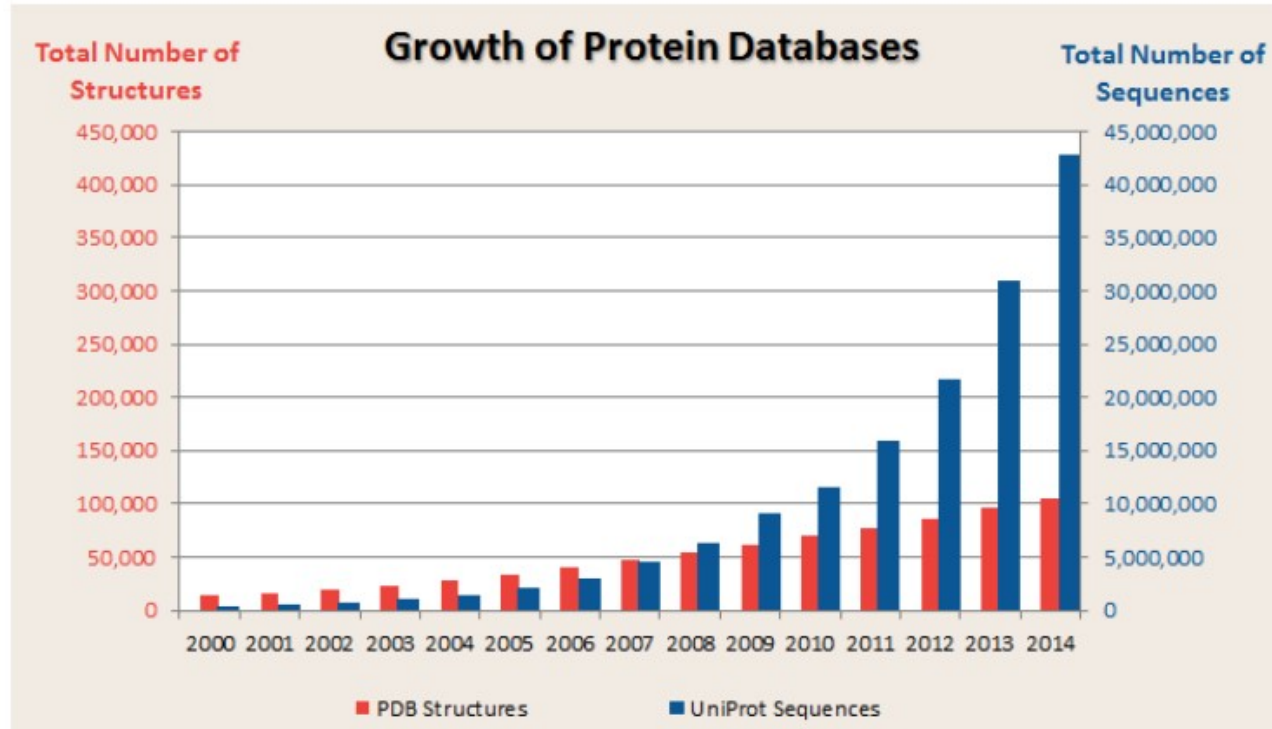


Homology Modelling



WHAT IS THE NEED OF COMPUTATIONAL PREDICTION OF PROTEIN STRUCTURE

- It is because the number of protein structures solved so far are fewer than the number of genes known.
- The rate of discovery of new proteins far outweighs our ability to functionally characterize them



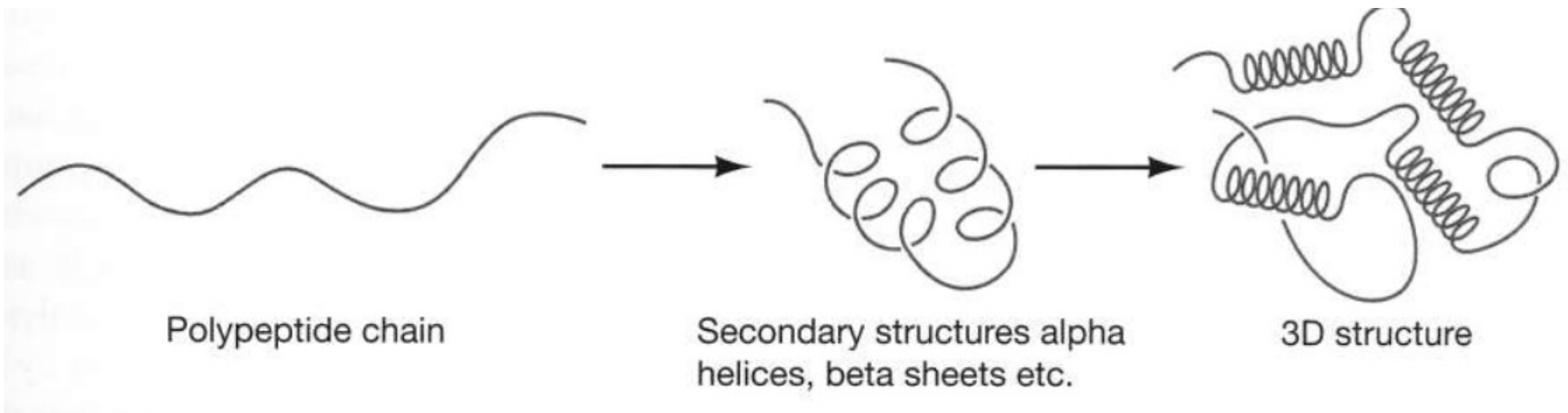
WHAT IS THE NEED OF COMPUTATIONAL PREDICTION OF PROTEIN STRUCTURE

- Structures of membrane proteins, ion channels, transporters can be large and difficult to crystallize....
- Hence scientists opt for computational prediction of protein structures

Computational methods for protein structure prediction

- There are mainly three methods of computational protein structure prediction such as....
- Homology or comparative modelling
- Fold recognition or otherwise also called Threading
- *Ab initio* methods

Protein structure

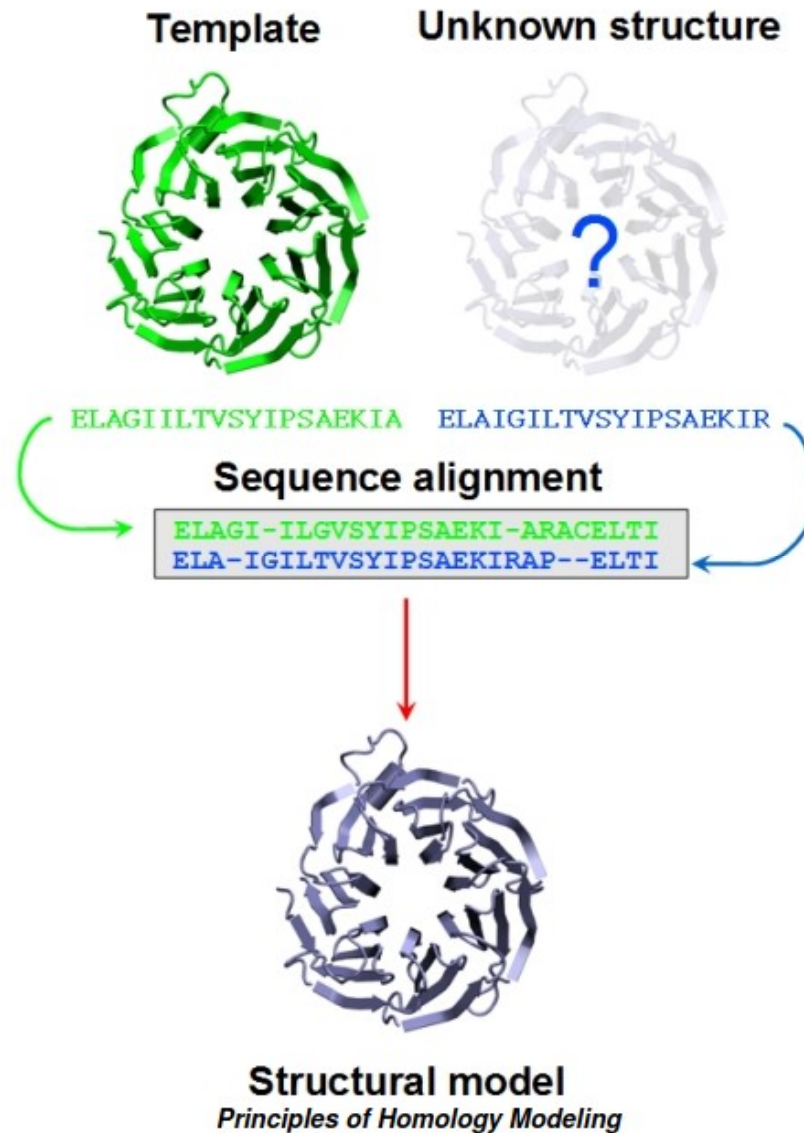


- Folding of a protein from a linear chain of amino acids to a three dimensional structures involves in amino acids interaction.

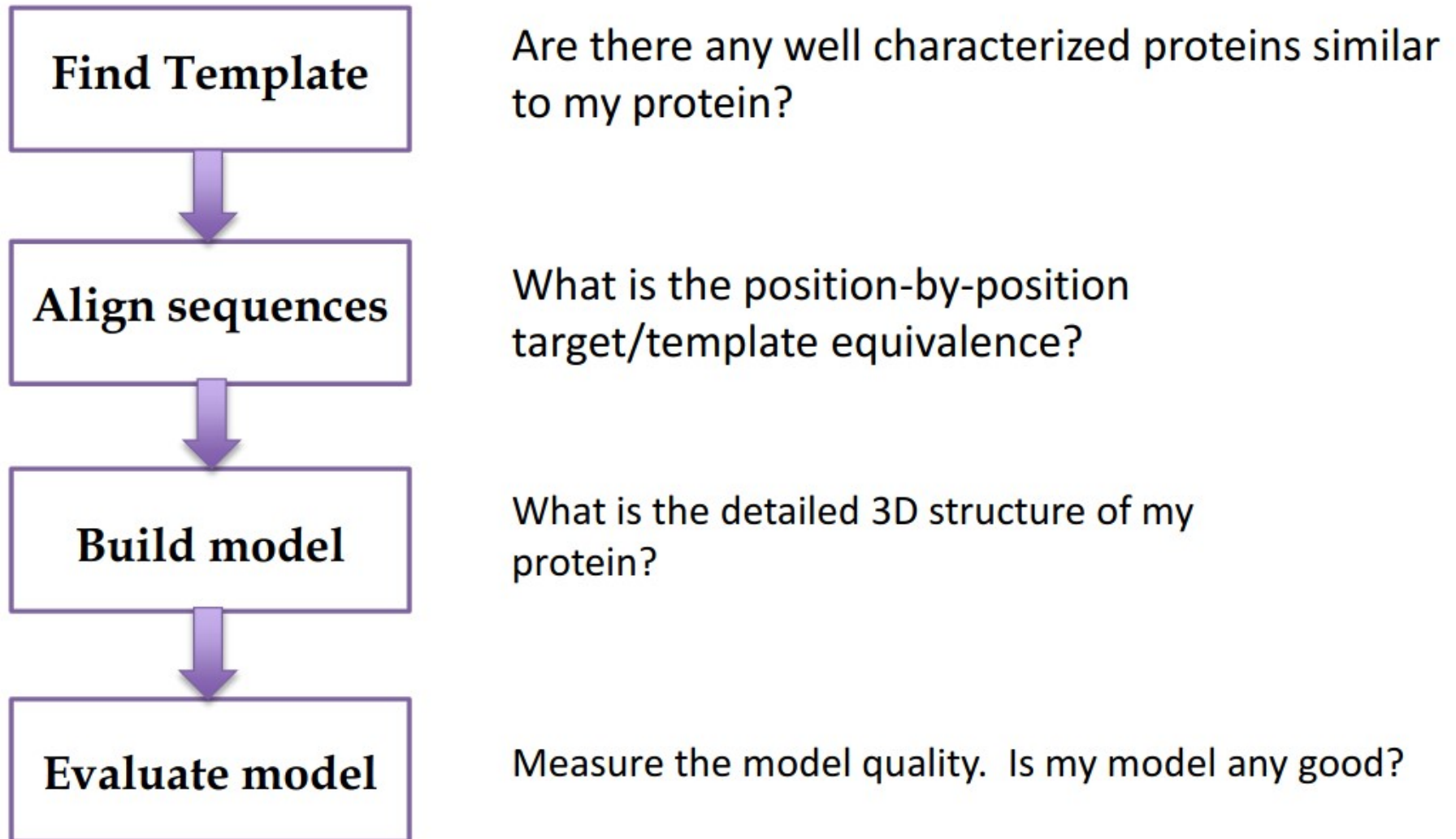
What is Homology modelling

- Homology modeling uses homologous sequences with known 3D structures for the prediction of the structure of a target sequence.
- Proteins sharing a significant similarity of sequence can be expected to share also a significant similarity of structure
- Protein tertiary structure is better conserved than amino acid sequence

Scheme of Homology modelling



Homology modelling



Homology modelling software

Databases

- ModBase
- Genomic Threading Database

Proprietary

- Orchestrar (*Tripos*)
- Composer (*Tripos*)
- Modeller (*Accelrys*)
- Prime (*Schrödinger*)
- MOE (*Chemical Computing Group*)
- ICM (*MolSoft*)

Free or Open-Source

- MolIDE
- DeepView
- Mint
- Permol
- WhatIf
- Rosetta

Web Servers (sequence-based)

- PredictProtein
- **SWISS-MODEL**
- **(PS)2**
- CPHmodels 2.0
- 3D-JIGSAW
- ESyPred3D
- PROTEUS2
- HOMODELLER

Web Servers (sequence, secondary structure, other criteria)

- PHYRE
- LOOPP
- LOMETS → I-TASSER
- MUSTER

