

I. Protein Complexes

- Two or more proteins interact and form larger machines, i.e. complexes.
- Involved in most of the biological processes
- Very important for many problems such as drug design, protein engineering, anti-body generation, etc.



2. Rigid Body Docking

Rigid Docking: Given the structures of the individual proteins, predict 3D structures of protein-protein complexes. Proteins are treated as rigid bodies (no assumed flexibility).

Traditional Docking Methods:

- Heavy candidate sampling + ranking + fine-tuning
- Very time consuming



Our goal: direct prediction of the protein complex.

Research questions:

- Which geometrical and physical constraints for protein-protein docking to consider for DL models ?
- How to inject them in DL models ?

