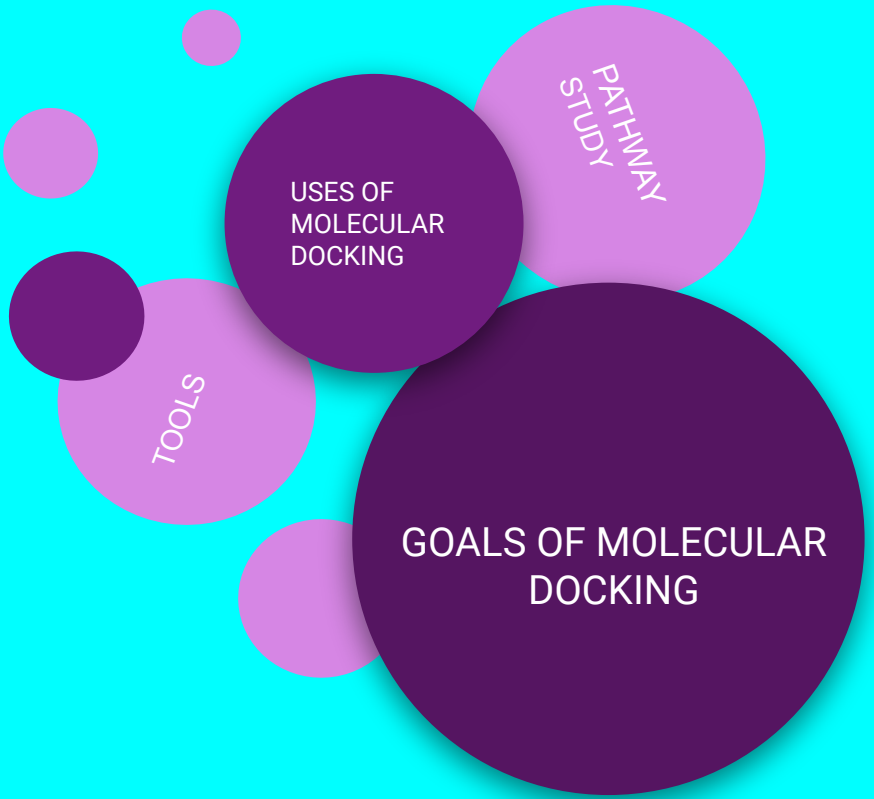
Preliminary study on Molecular Docking

- By Smruti and Taniya

Topics Covered



Terms Included

Binding Affinity: Definition

Receptor: Definition

Ligand: Definition

Docking: Definition

Binding mode: Definition

Scoring: Definition

Pose: Definition

Interface residues

Docking Assessment: Definition

Signal produced: Types

Best Fit: Lock and Key type

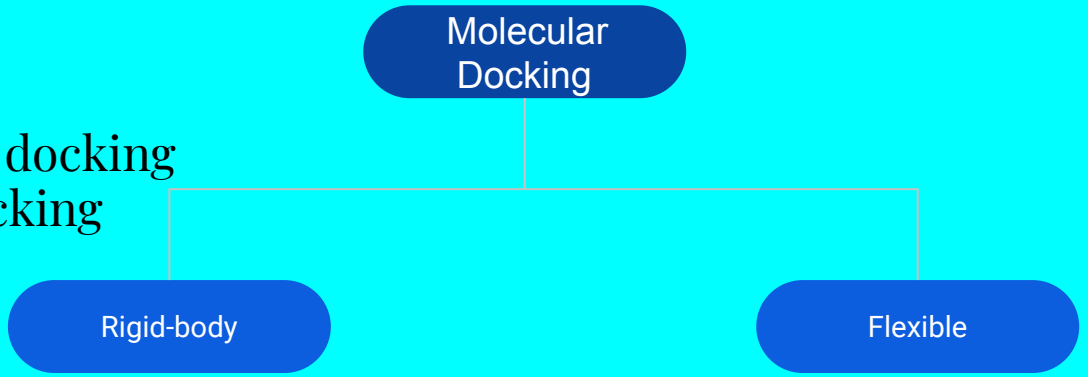
Low energy of complex: Stable system

Ranking: Definition

Types of docking and Energy involved

Docking types :-

1. Rigid-body docking
2. Flexible docking

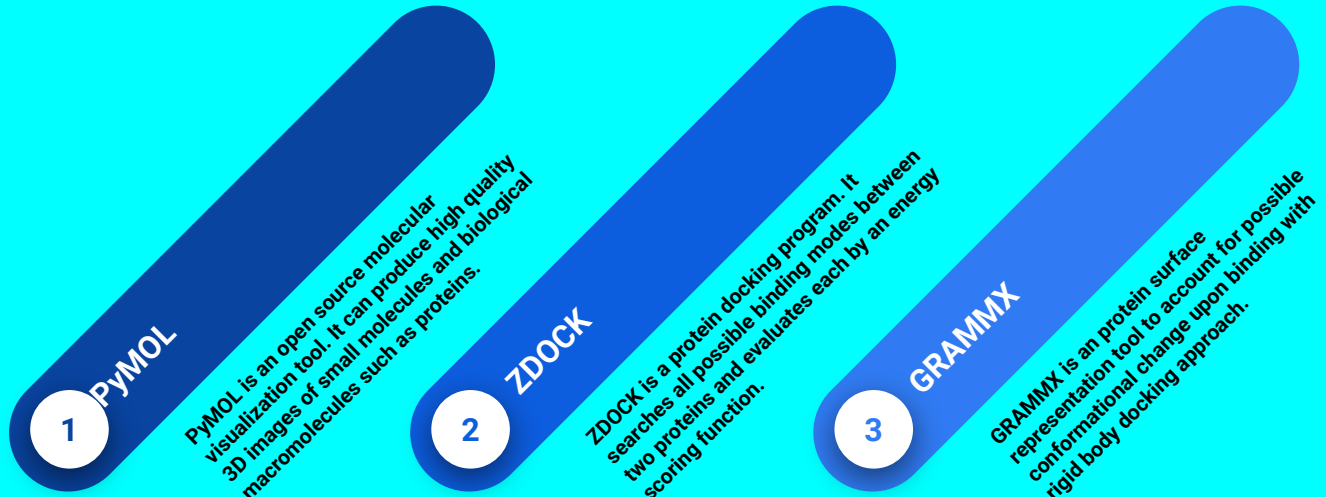


Energy :-

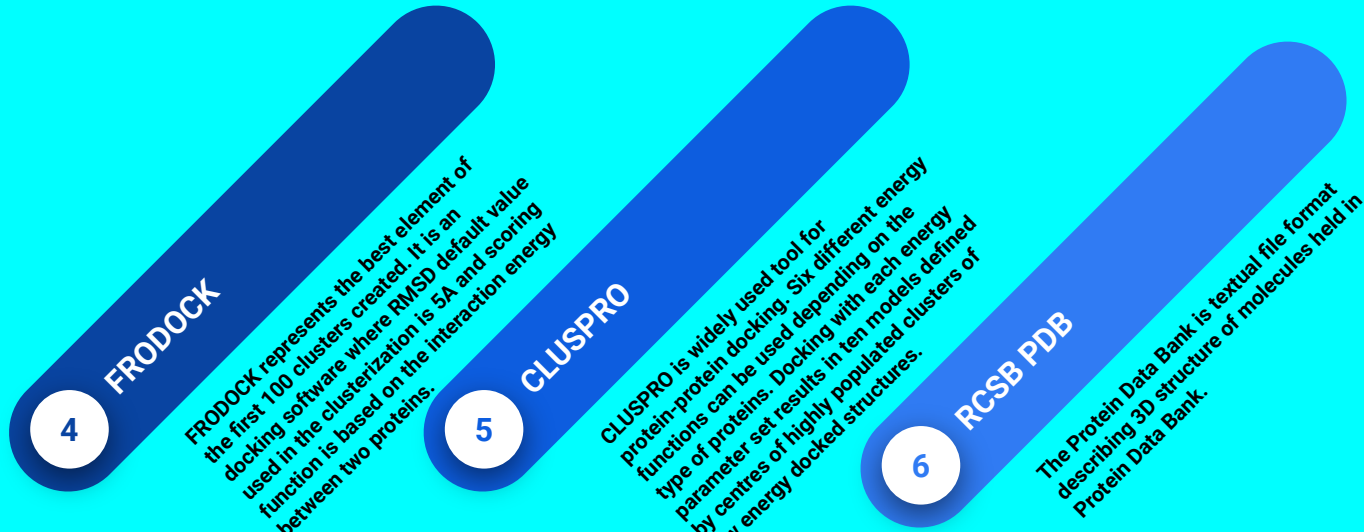
Gibbs Free energy

RMSD Value- Root Mean Square Deviation Value

Softwares and Tools



Softwares and Tools



Project work

- Project Idea
- Expected outcome
- Hypothesis
- All protein's pathways
- All the terms which are being included in NOX4-KIWELLIN Pathway hypothesis
- Other protein's (Excluding NOX 4 , like NOX1,GPVI,GPCR)Info: which can be used as antagonist to Kiwellin