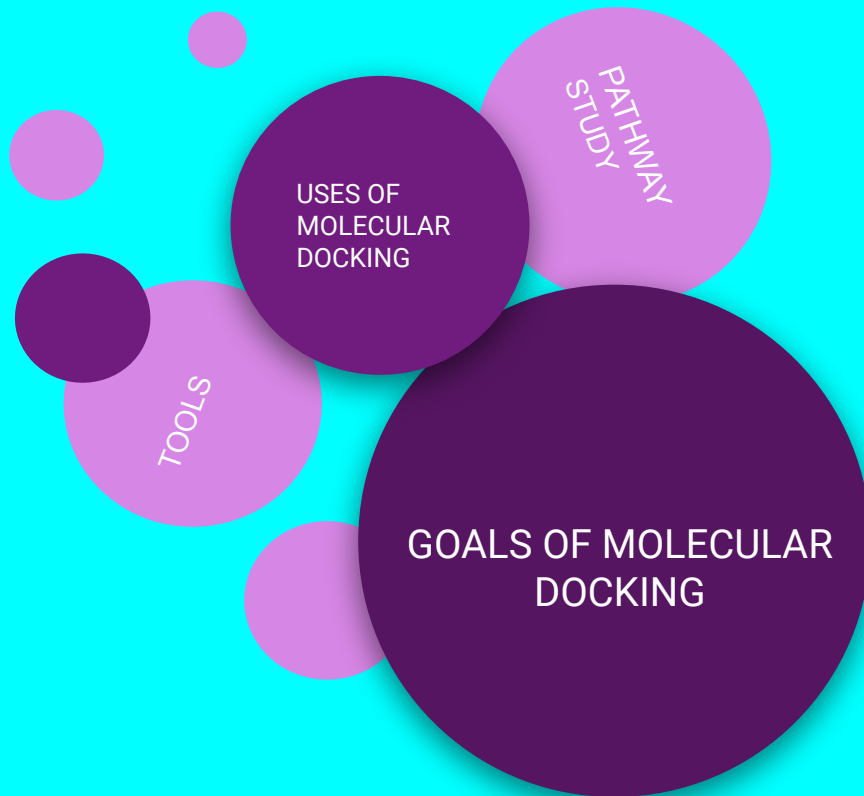


Preliminary study on Molecular Docking

- 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

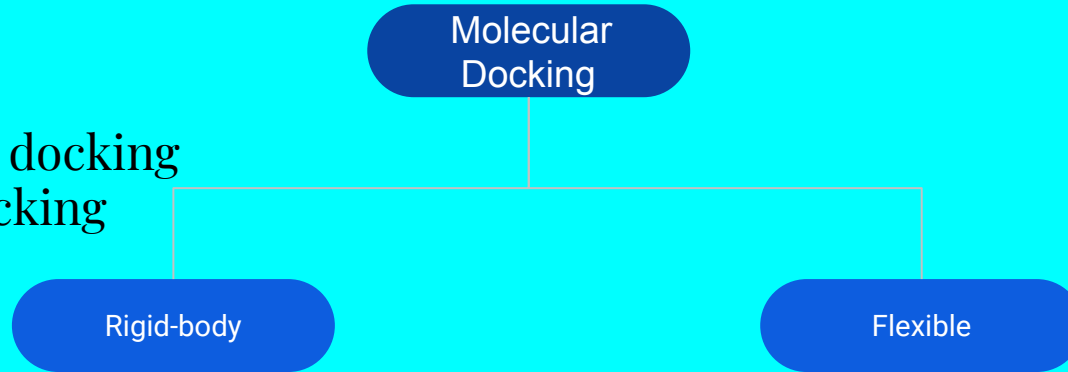
Low energy of complex: Stable system

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

1

PyMOL

PyMOL is an open source molecular visualization tool. It can produce high quality 3D images of small molecules and biological macromolecules such as proteins.

2

ZDOCK

ZDOCK is a protein docking program. It searches all possible binding modes between two proteins and evaluates each by an energy scoring function.

3

GRAMMX

GRAMMX is an protein surface representation tool to account for possible conformational change upon binding with rigid body docking approach.

Softwares and Tools

4

FRODOCK

FRODOCK represents the best element of the first 100 clusters created. It is an docking software where RMSD default value used in the clusterization is 5Å and scoring function is based on the interaction energy between two proteins.

5

CLUSPRO

CLUSPRO is widely used tool for protein-protein docking. Six different energy functions can be used depending on the type of proteins. Docking with each energy parameter set results in ten models defined by centres of highly populated clusters of low energy docked structures.

6

RCSB PDB

The Protein Data Bank is textual file format describing 3D structure of molecules held in Protein Data Bank.

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 NOX₄ , like NOX₁, GPVI, GPCR) Info: which can be used as antagonist to Kiwellin