**Molecular Dynamics Simulation Projects**

**Estimation of binding energy for Protein interactions**

Tumor Antigen P53 interaction with Tumor Suppressor with P53 binding Protein

Part 1: Download the PDB file for the complex.

   Go to [http://www.rcsb.org](http://www.rcsb.org/)

   Search for 1KZY i.e.  PDB code == 1KZY

    Then download

Prepare the pdb file, you need chains A to D as well as the ions (if present)

Chains A+B represents P53

Chains C+D represents the Tumor Suppressor component (53BP1 BRCT)

Solvation: Add solvent to the system (soak the protein in a box of water) and add ions to neutralize the system

Use energy minimization followed by MD simulations to estimate the equilibrium total energy of the complex (A, B, C, D)

Part 2:

Preparation of P53 and simulation

Prepare separate pdb file containing just only chains A and B and the ions ( if present)

Solvation: Add solvent to the system (soak the protein in a box of water) and add ions to neutralize the system

Use energy minimization followed by MD simulations to estimate the equilibrium total energy of P53 Antigen i.e. chains (A, B)

Part 3:

Preparation of Tumor suppressor P53-binding protein1 (53BP1) and simulation

Prepare separate pdb file containing just only chains C and D

Solvation: Add solvent to the system (soak the protein in a box of water) and add ions to neutralize the system

Use energy minimization followed by MD simulations to estimate the equilibrium total energy of 53BP1 BRCT chains (C, D)

Finally: Compute the binding energy

Compute the binding energy (BE)

BE =Energy for (P53) + Energy for (53PB1) -    Energy for complex (53BP1 - P53)