Molecular Dynamics Simulation Projects

Project 2:

Bcl-xL in complex with BIM BH3 domain

Part 1: Download the PDB file for the complex.

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

   Search for 4QVF i.e.  PDB code ==  4QVF

    Then download

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

Chains A  represents Bcl-2-like protein 1

Chains B  represents BIM BH3 DOMAIN or Peptide from Bcl-2-like protein 11

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)

Part 2:

Preparation of Bcl-2 and simulation

Prepare separate  pdb file containing just only chains A  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 Bcl-2  i.e.. chains(A)

Part 3:

Preparation of BIM BH3 DOMAIN and simulation

Prepare separate pdb file containing just only chains B

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 BIM BH3 DOMAIN chains (B)

Compute the binding energy (BE)

BE = Energy for (BCL-2) + Energy for (BIM-BH3)  -    Energy for complex (BCL-2-BIM-BH3)

You have an account on the following server to your homework

172.23.39.9

username= dseibert2

Password = dPSID$1312637

You would need to follow the example script in section 5 of the OpenMM user guide (link below) to build the model of the protein or protein components you need to work on. You start by cleaning up the

PDB file  you downloaded from the PDB databank  ([www.rcsb.org](http://www.rcsb.org/)) using a file editor, for example  nano, vi, or edit,  before you start the python scripts.

<http://docs.openmm.org/7.1.0/userguide/application.html#model-building-and-editing>

Report

* Abstract: Half page description of an application that you plan on implementing. (This is an "elevator" pitch with purpose and features of the project.)
* Mathematical statement of the problem
* Discretized version of the equations
* Description of the numerical method (pseudo code included)
* Technical specifications of the computer used
* Results (include graphs and comments)
  + Specifications of parameters used in simulations
  + Evaluate the effect of number of points used for discretization
  + Comparison of results with expected theoretical behavior
* Commit your report to your git repository