Analysis of molecular dynamic simulations

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Packages

- There are different packages to perform MD simulations, such as, CHARMM, NAMD, GROMACS, OPENMM and etc.
- Here we use Gromacs for performing our simulations and part of generated data analysis.

Gromacs Installaion

- The documantation for the Gromacs installation can be seen here:

  Installation guide

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Command line

- To perform analysis you need to know about available command-line in Gromacs.

- You can check different command-line here:

  cmdline

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Minimization

- Before we observe dynamic we have to be sure that the system is in an appropriate geometry without clashes. The system would get relaxed during energy minimization process.
- Task1: Check the potential energy for your system. (Hint: Energy)
- You can plot the result using Xmgrace.

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Equilibration

- The system may collapse if we remove the restrain once. After we lead the system to the certain temperature, we will implement preussre to the system to observe proper density.
- Task2: Check the temperature, pressure and density progression. (Hint: Energy)

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RMSD

- Root mean square deviation (RMSD) can be computed to compare two or more structures.

- Each structure from a trajectory is compared to a reference structure. The reference structure can be from the crystal structure or minmized crystal structure.

- Task3: Compute RMSD of the 3sn6 structure. What you can learn from it? rms

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RMSF

- Root mean square fluctuation (RMSF) can be computed to investigate atomic positions in the trajectory.

- Task4: Compute rmsf for individual residues, what you can learn from it? (Hint: rmsf)

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SASA

- Solvent accessibility surface areas (SASA) is the surface area of a biomolecule that is accessible to a solvent.

- Task5: Calculate SASA of your ligand (P0G) as the function of time.

Eisenhaber F, Lijnzaad P, Argos P, Sander C, & Scharf M (1995) J. Comput. Chem. 16, 273-284