# CHM579 LAB 3B(II): MOLECULAR DYNAMICS OF LYSOZYME IN WATER

The goal of this lab is to simulate a protein, called lysozyme, in a box of water with ions using the GROMACS program package.

**Lab Procedure:**

The first part of this procedure will give you some important notes on the use of GROMACS on Scholar. On the second part you will carry out your Molecular Dynamics simulation using GROMACS.

**Step 1:**

**IMPORTANT:** Since parameters of GROMACS programs depend on version of the package (GROMACS version 5.0 is installed on the Scholar cluster), please follow the the tutorial by Justin Lemkul that corresponds to 5.x version:

**I.** Before running any GROMACS command, set up the program environment by issuing the following command:

**To load the GROMACS module:** `module load gromacs`

**II.** You will need to generate a topology file using a special script called `pdb2gmx`:

**To generate a topology for lysozyme using pdb2gmx:** `pdb2gmx -f 1AKI.pdb -o 1AKI_processed.gro -water spce`

And then select the Force Field: 15`: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)`

**III.** You will also need to add ions in your simulation box using the genion script:

**To add ions using:** `genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname NA+ -nname CL- -nn 8`

Pay attention to capital letters and + and - signs in names of sodium and chloride ions: `NA+` and `CL-`

**IV.** To run the most time consuming energy minimization and molecular dynamics simulations jobs (e.g. `mdrun -v -deffnm em`, `mdrun -deffnm nvt`, `mdrun -deffnm npt`, and `mdrun -deffnm md_0_1`) you have to use the PBS submission scripts provided instead of direct call of `mdrun` tool.

For example: when running the energy minimization, take the following steps:
First, copy the `em.csh` and `emsub.csh` scripts from the Scholar location and make the scripts executable:

To copy the folder for this assignment in your 'CHM579' folder you created on Scholar:

```
cd CHM579
cp –a /scratch/carter/g/gchopra/class/CHM579/lab3b_2 .
```

To convert a file into an executable: **`chmod +x emsub.csh`**

Then submit energy minimization job to PBS by executing the file:

**To run the program:** `./emsub.csh`

Similarly use `nvt.csh` and `nvtsub.csh` for NVT equilibration; `npt.csh` and `nptsub.csh` for NPT equilibration; `md_0_1.csh` and `md_0_1sub.csh` for MD run.

**V.** The `.xvg` files obtained from `g_energy` tool can inspected using Grace.

**To load the Grace module:** `module load xmgrace`

***WARNING:*** The following instructions will only work if you are connected to Scholar through a terminal that supports X11. SecureCRT or Cygwin-X are recommended. For example, you could launch Xming and then SecureCRT with enabled X11 support.

**To plot the energy.xvg file using grace on Scholar:** `xmgrace energy.xvg`

**IMPORTANT**: If you get a message saying:

```
Can't open display
Failed initializing GUI, exiting
```

It means your terminal does not support X11.

The `.xvg` files obtained from `g_energy` tool can also be visualized using Microsoft Excel program on your local Windows computer. In the `.xvg` file delete all lines starting with symbols # and @, then open `.xvg` file with Microsoft Excel using *delimiters space* mode.

**Step 2: YOUR TURN**

Follow the instructions in GROMACS Tutorial "Lysozyme in Water" by Justin Lemkul:
http://www.bevanlab.biochem.vt.edu/Pages/Personal/justin/gmx-tutorials/lysozyme/index.html

**(A)** Summarize the results obtained for lysozyme in water:

**1.** Visualize protein geometry using VMD program.

**2.** Plot potential energy vs. energy minimization (EM) step.

**3.** Plot temperature vs. time for NVT equilibration.

**4.** Plot pressure vs. time for NPT equilibration.

**(B)** Analyze the resulting MD trajectory:

**5.** Plot Backbone RMSD vs. time

**6.** Plot the radius of gyration for lysozyme vs. time

**(C)** Analysis:

**7.** What conclusions can you draw about compactness of protein lysozyme in water based on analysis of the obtained MD trajectory?