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Winmostar tutorial

Gromacs

Protein

V8.007

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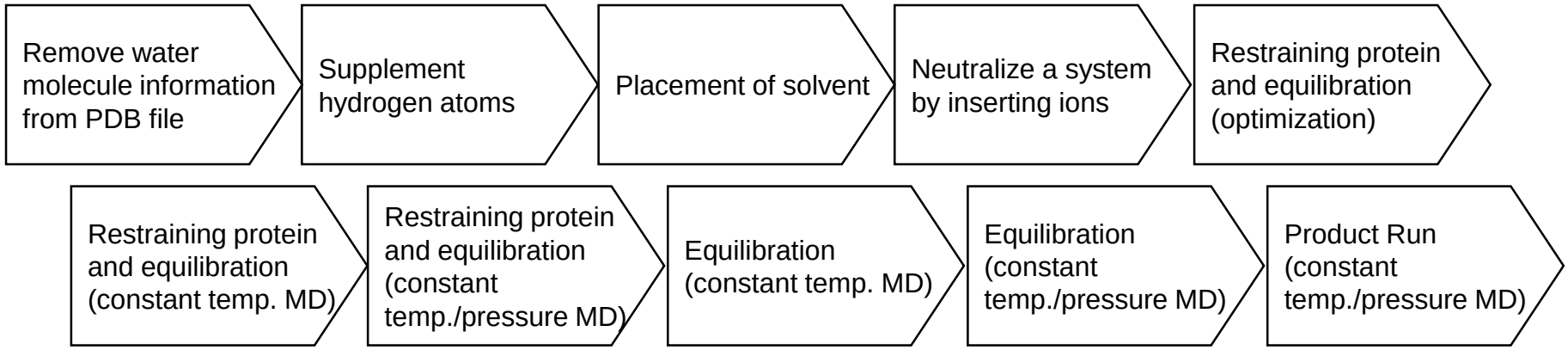
Summary

- In this tutorial, we will use Gromacs to execute calculations on a PDB file of Hen Egg-White (HEW) Lysozyme.



Notes:

- It is necessary to remove crystal water data contained in the XRD of PDB and supplement hydrogen which is not initially included.
- Size of systems (number of solvents) will affect behavior of proteins.
- The number of steps required for equilibration depends on the type of molecule and initial density varies and may be different from this example.
- The method for interaction calculations and/or the force field also affect simulation results.

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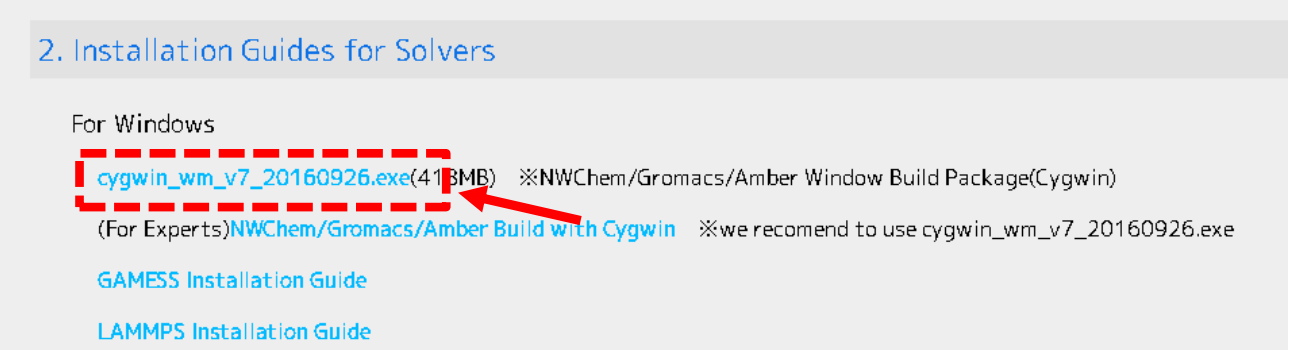
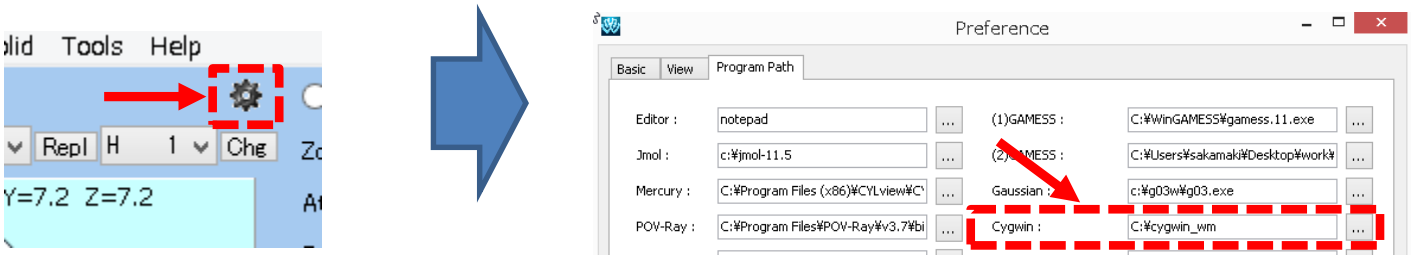
Configuration

You must set up Cygwin to use Gromacs on Winmostar.

- Obtain the installer for Cygwin, which contains the all programs needed by Winmostar, at https://winmostar.com/en/manual_en.html.



- When you change the installation path for Cygwin from the default one, specify it on the preference panel.



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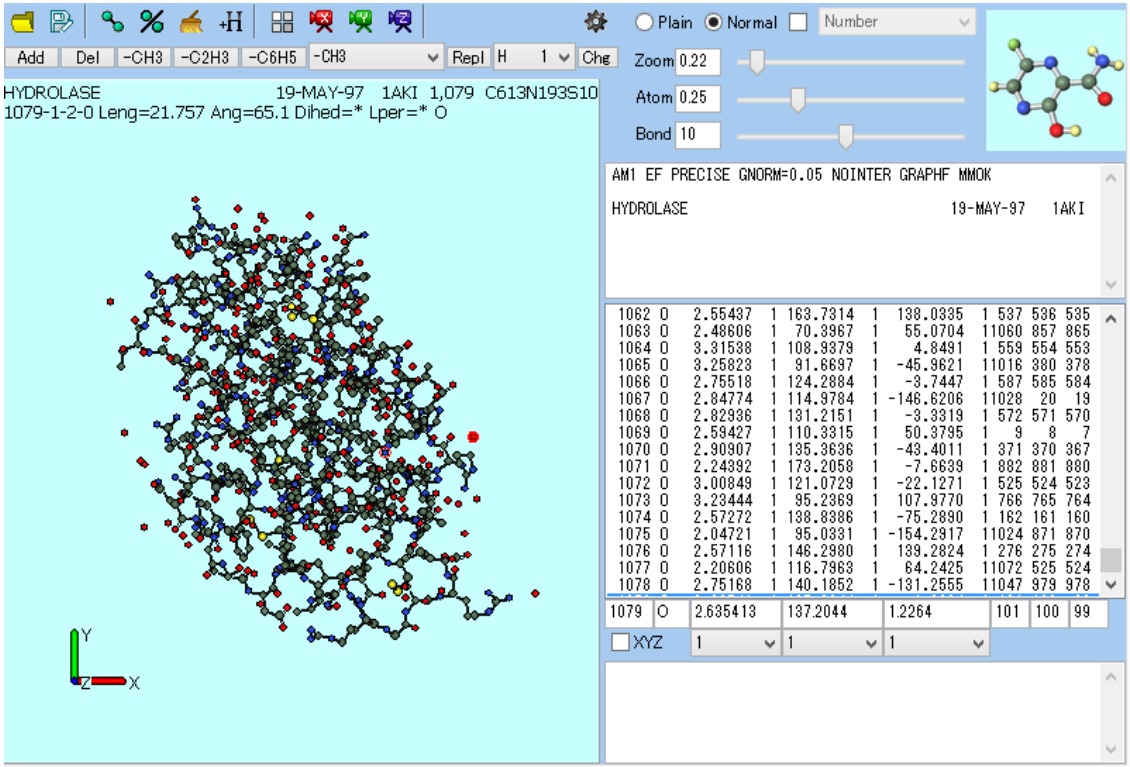
I. Build a simulation cell

1. Click **File** | **Open**.
2. Open **1AKI.pdb** in sample directory.
   （default: C:¥winmos8¥samples¥1AKI.pdb）



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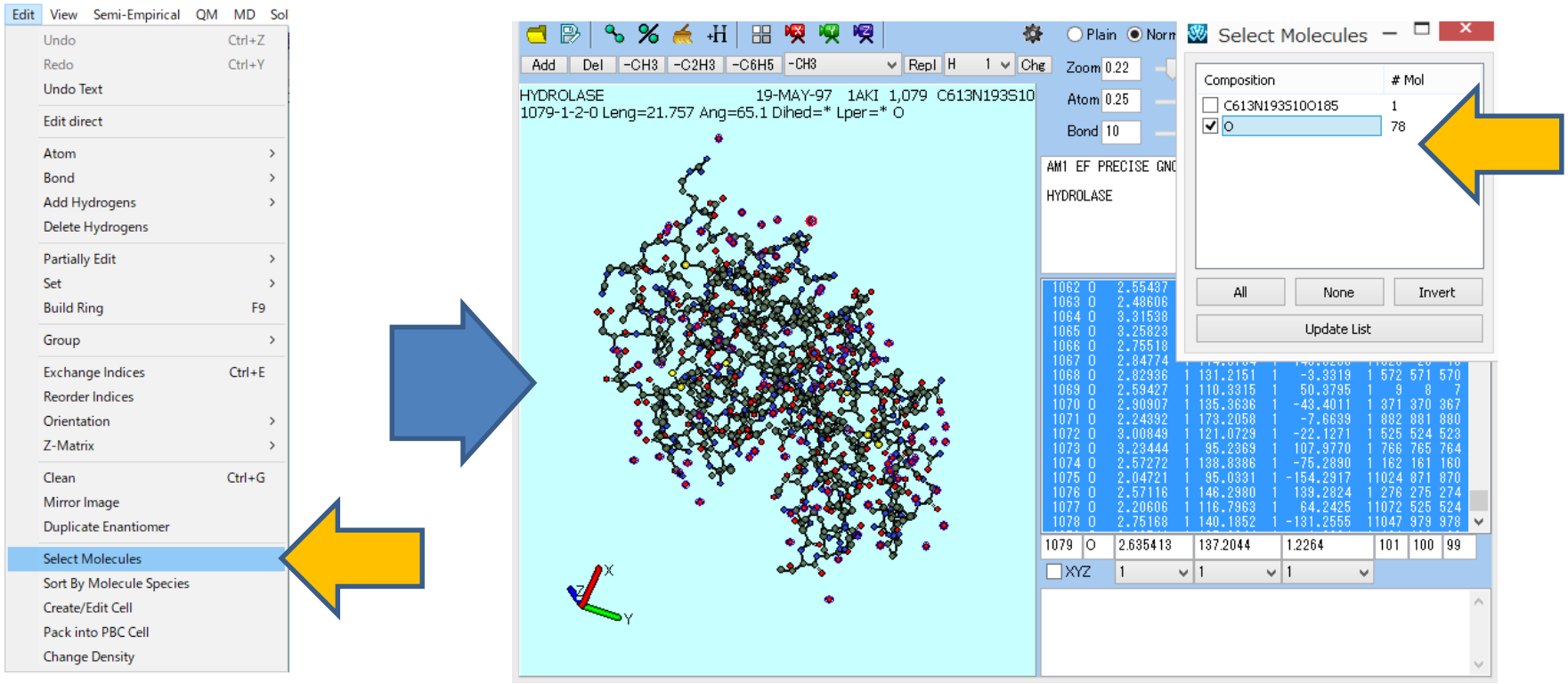
I. Build a simulation cell

1. Click **Edit | Select Molecules**.
2. On **Select Molecules** window, check “**O 78.**” This will add blue circles around oxygen atoms of crystallization water as shown below (i.e. partial selection).



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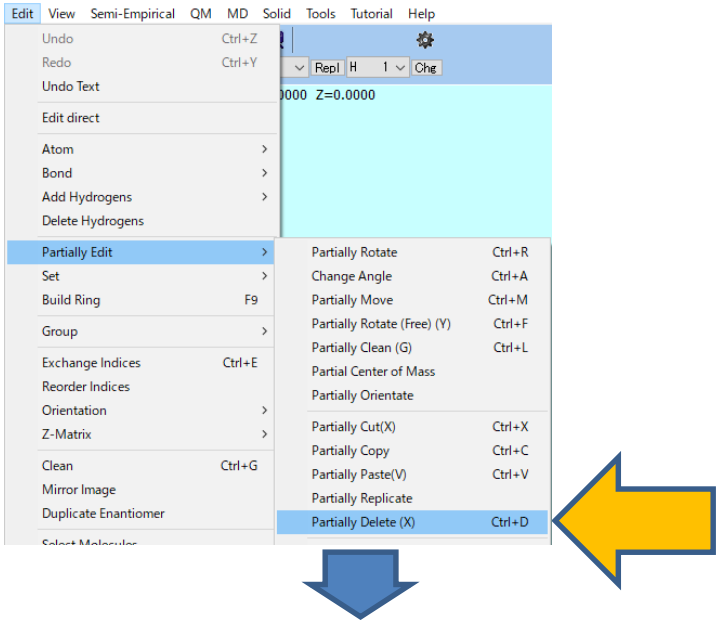
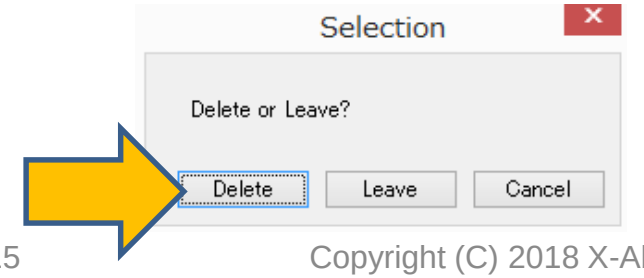
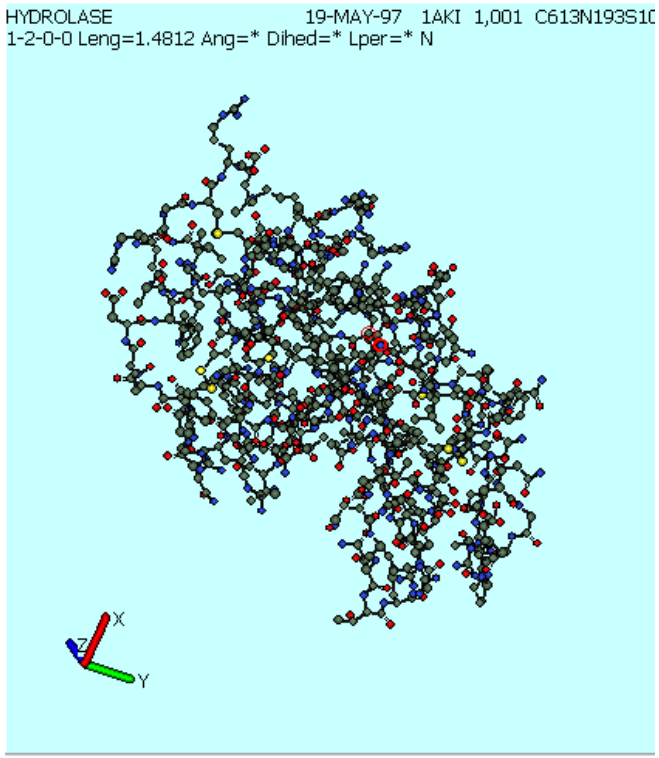
I. Build a simulation cell

1. After ensuring that oxygen atoms have been selected in the crystallization water, click **Edit** | **Partial Edit** | **Partial Delete**.
2. Click **Delete** on **Selection** to delete crystallization waters.







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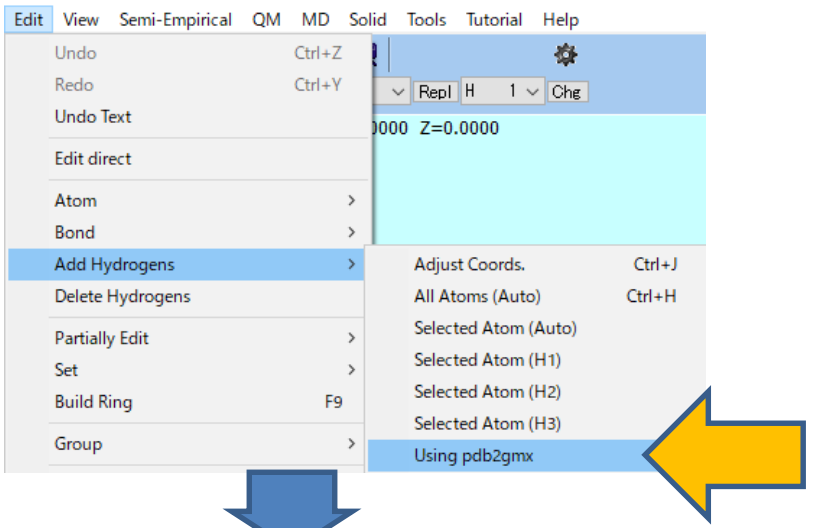
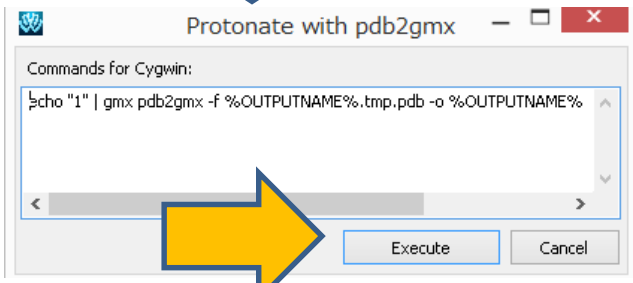
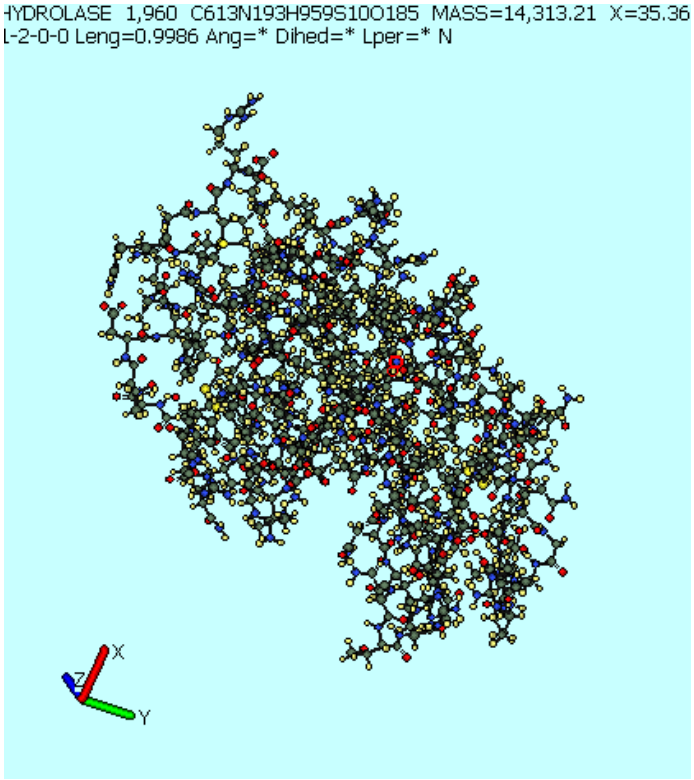
I. Build a simulation cell

1. Click **Edit** | **Add hydrogens** | **Using pdb2gmx**.
2. In the **Protonate with pdb2gmx** window, click **Execute**. This will add hydrogen atoms to the protein. This process is sometimes required even when the pdb file has hydrogens data.







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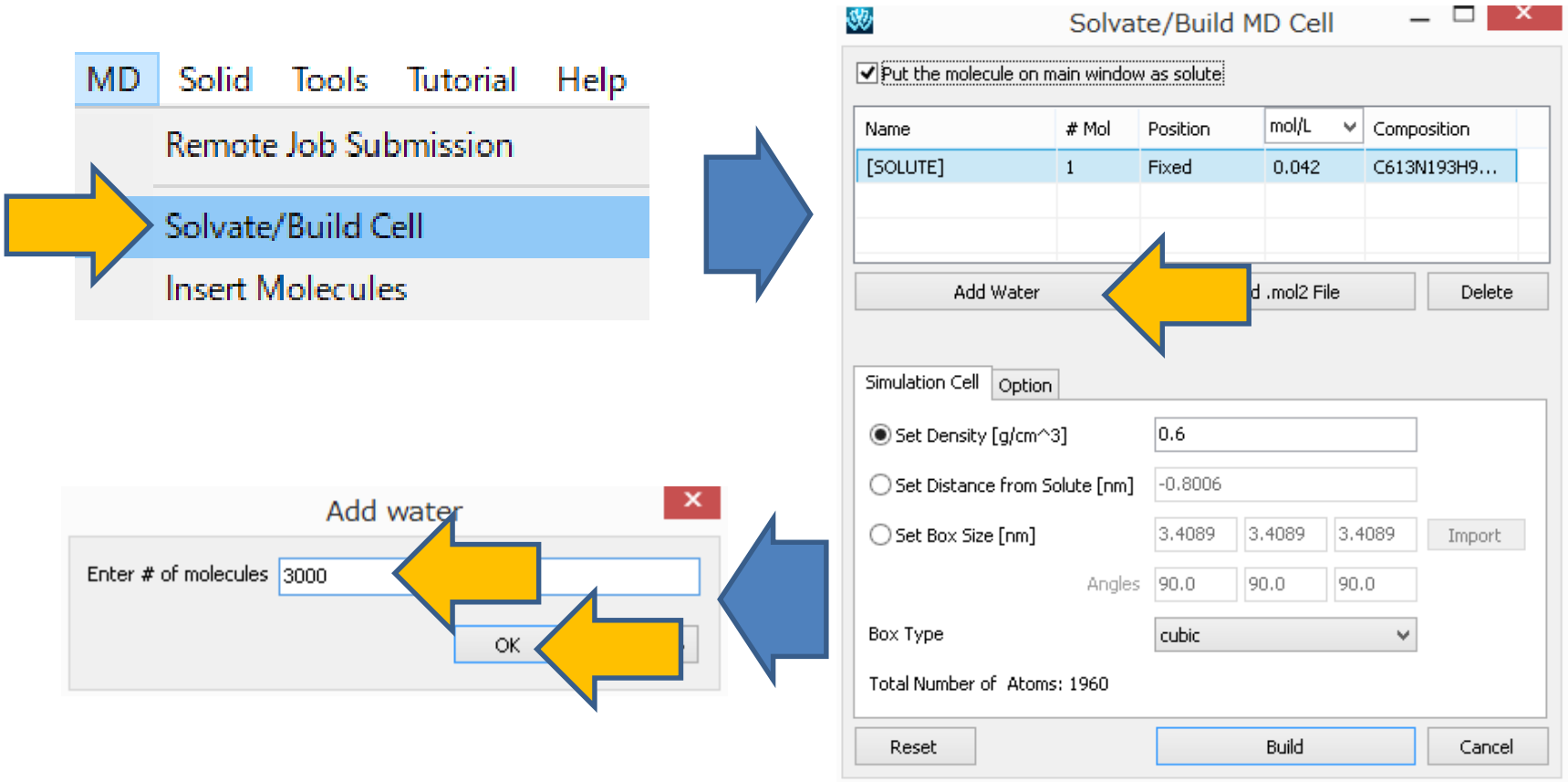
I. Build a simulation cell

1. Click **MD** | **Solvate/Build Cell**
2. Click **Add Water**, then set **Enter # of molecules** to **3000**, click **OK**.



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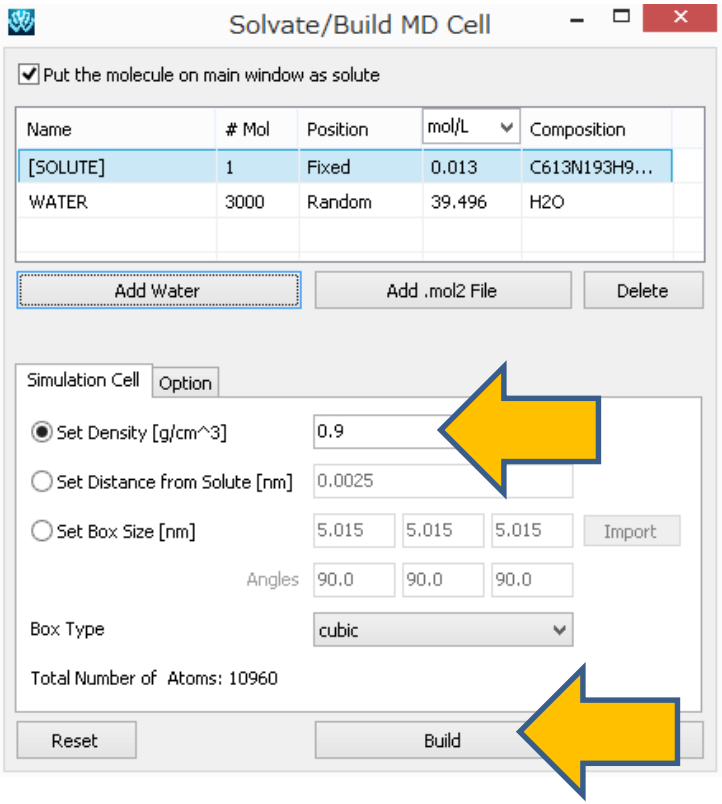
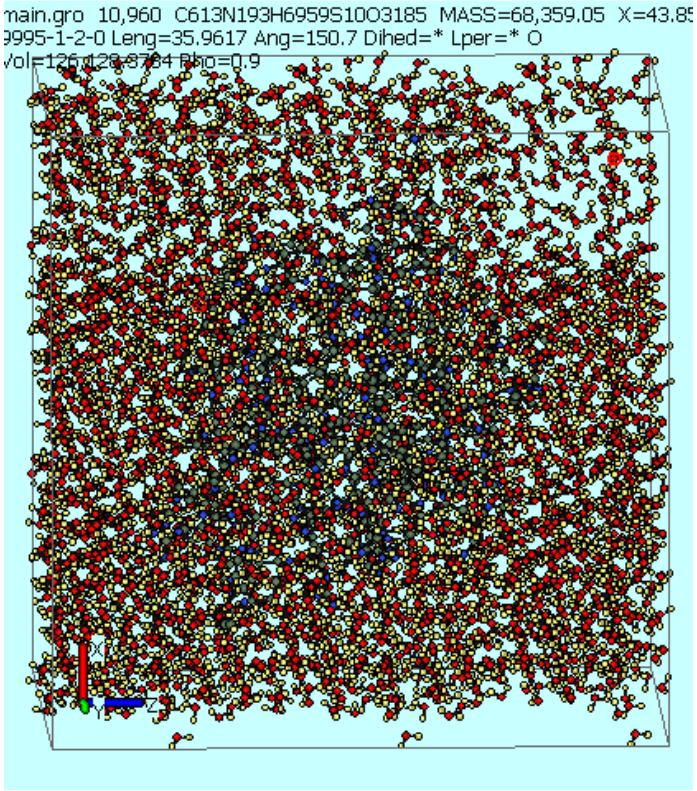
I. Build a simulation cell

Set **Set Density** to **0.9**, click **Build** to build the simulation cell with water molecules.





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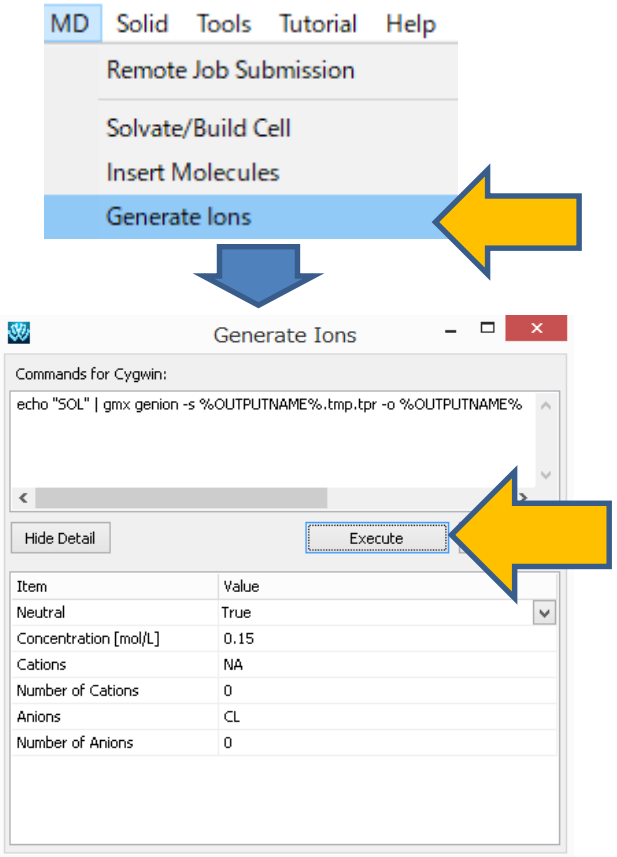
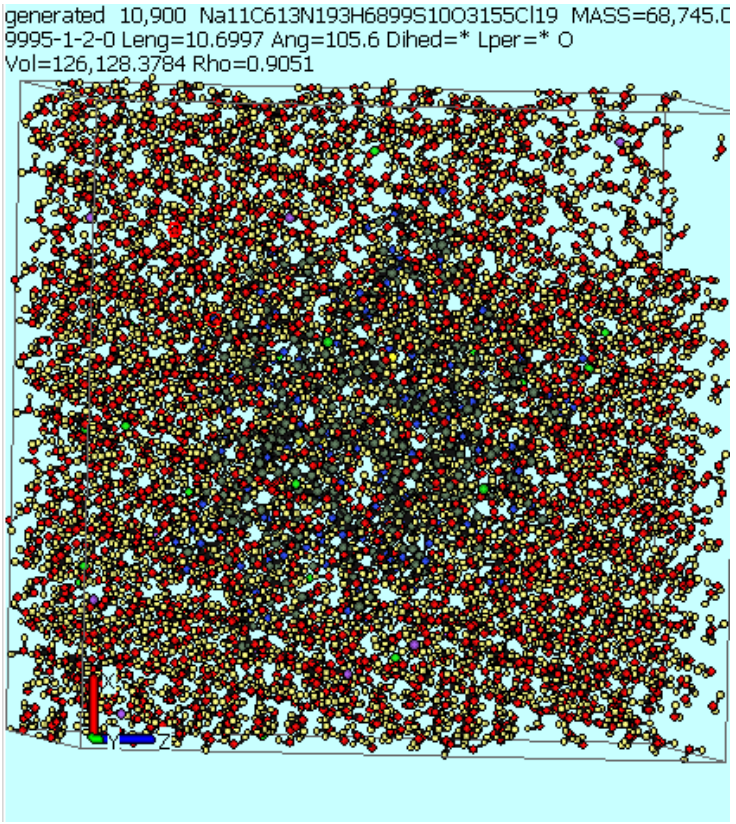
I. Build a simulation cell

1. Click **MD** | **Generate Ions**.
2. On **Generate Ions** window, click **Execute.** Ions will be arranged and the system will neutralize.





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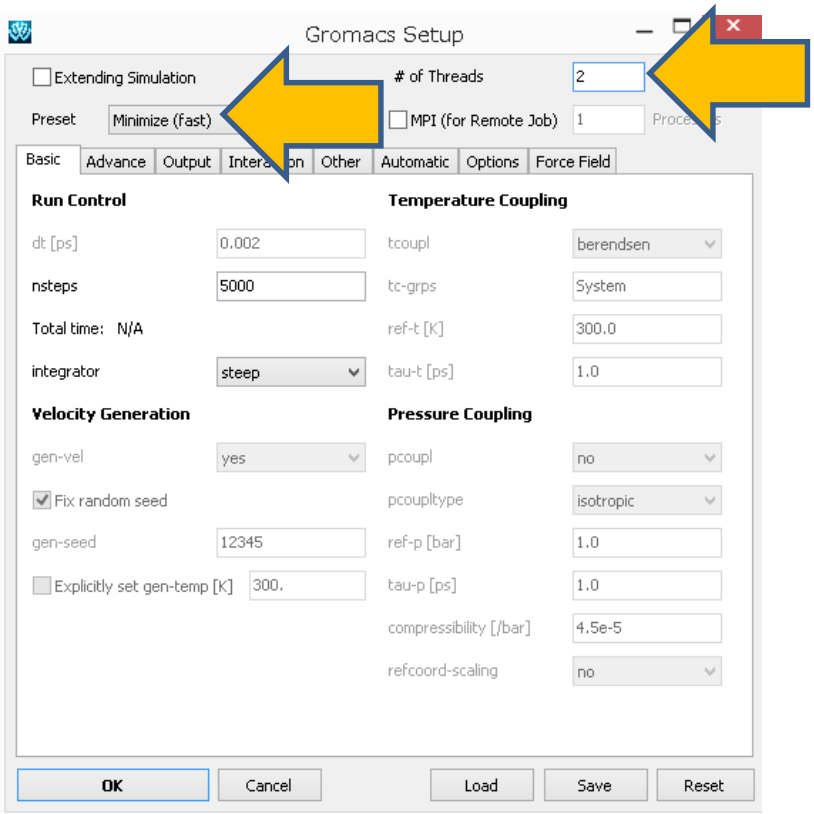
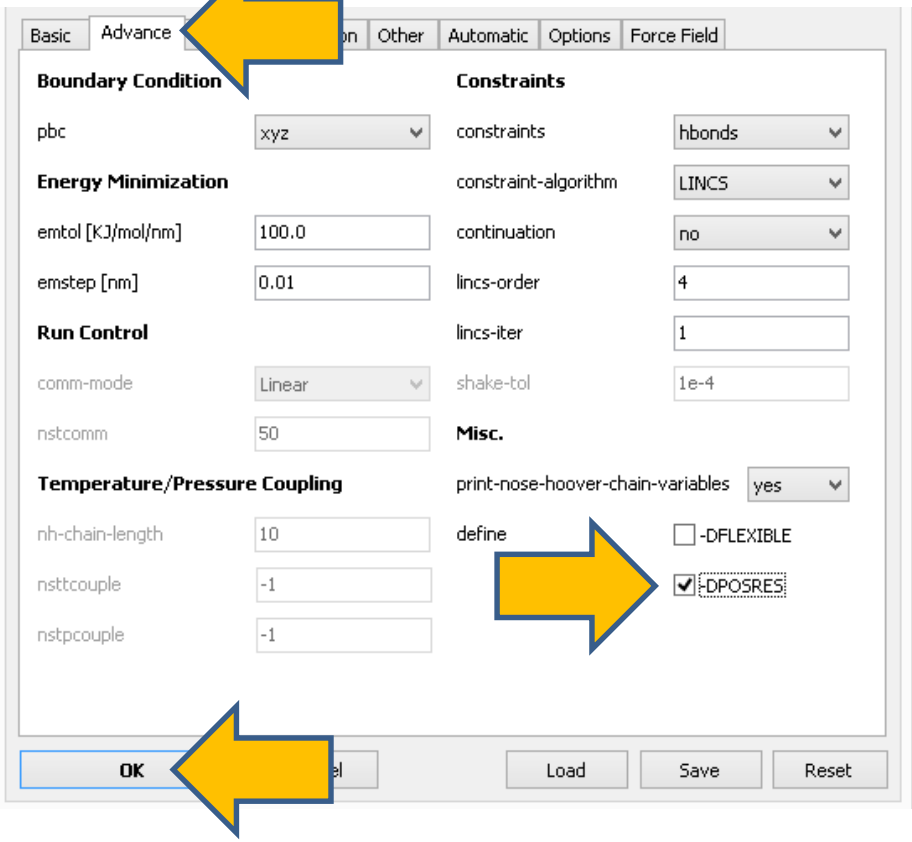
II. Execute simulations

1. Equilibration (Energy minimization with restraint)

1. Click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **Minimize (fast)**, **# of Threads** to a parallel number.
3. On **Advance** tab, check **-DPOSRES**, then click **OK**.





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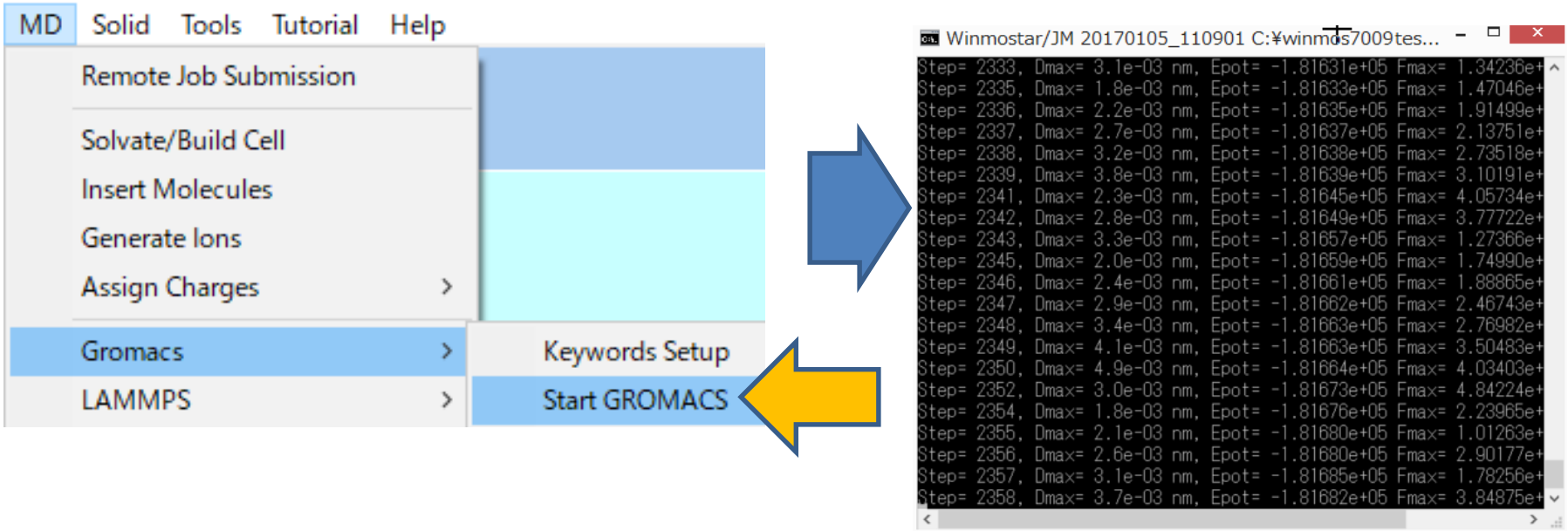
II. Execute simulations

1. Equilibration (Energy minimization with restraint)

1. Click **MD** | **Gromacs** | **Start Gromacs**.
2. Save coordinate file as “**1AKI.gro”**, topology file as “**1AKI.top**”. This will launch **Winmostar JM** and start calculation on Cygwin.



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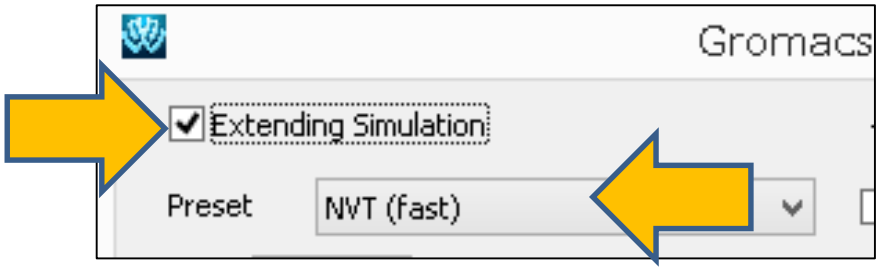
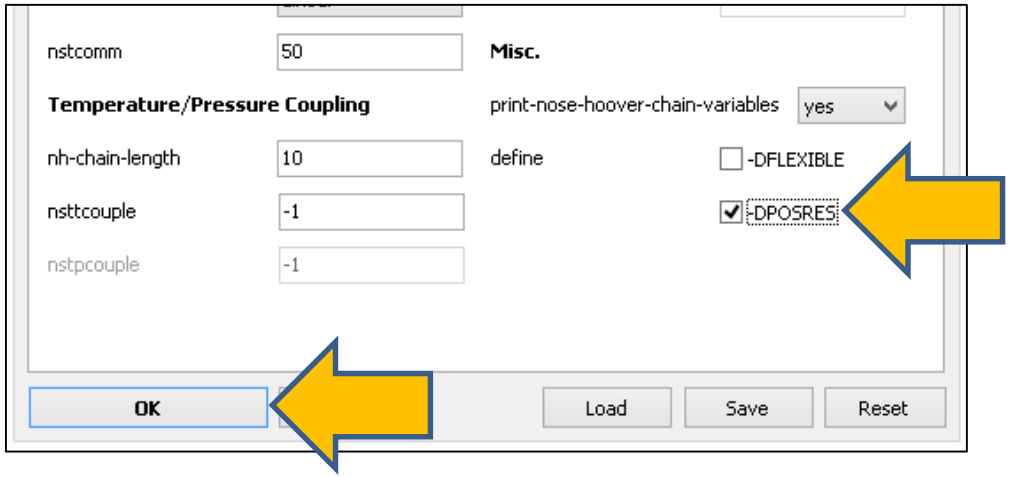
II. Execute simulations

1. Equilibration (*NVT* with restraint)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NVT (fast)**, check **Extending Simulation**.
3. On **Advance** tab, check **–DPOSRES**, then click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.





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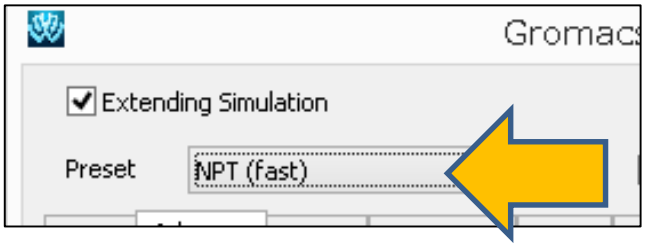
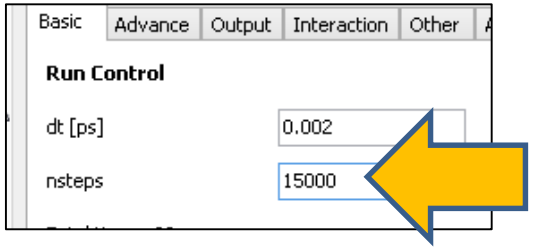
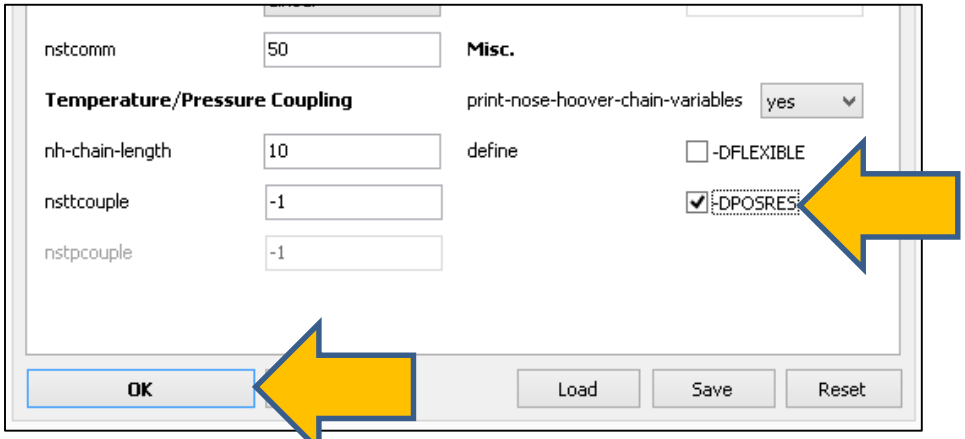
II. Execute simulations

1. Equilibration (*NPT* with restraint)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NPT (fast)**.
3. On **Basic** tab, set **nsteps** to **15000**.
4. On **Advance** tab, check **–DPOSRES**, then click **OK**.
5. Click **MD** | **Gromacs** | **Start Gromacs**.







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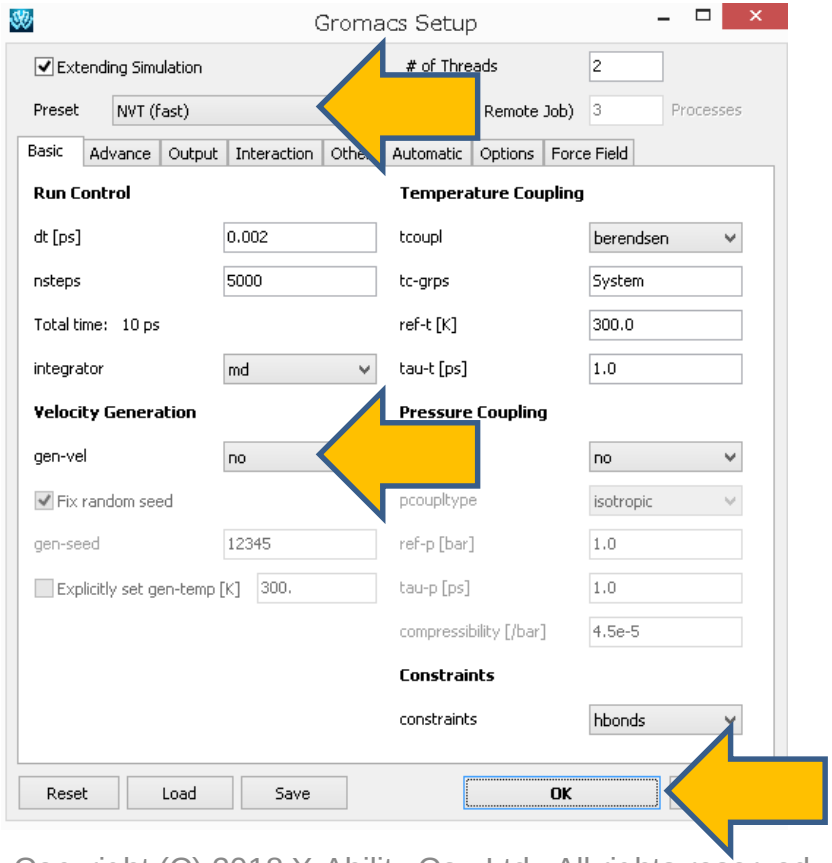
II. Execute simulations

1. Equilibration (*NVT*)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NVT (fast)**, set **gen-vel** to **no**, then click **OK**.
3. Click **MD** | **Gromacs** | **Start Gromacs**. Calculation will start without any restraints.

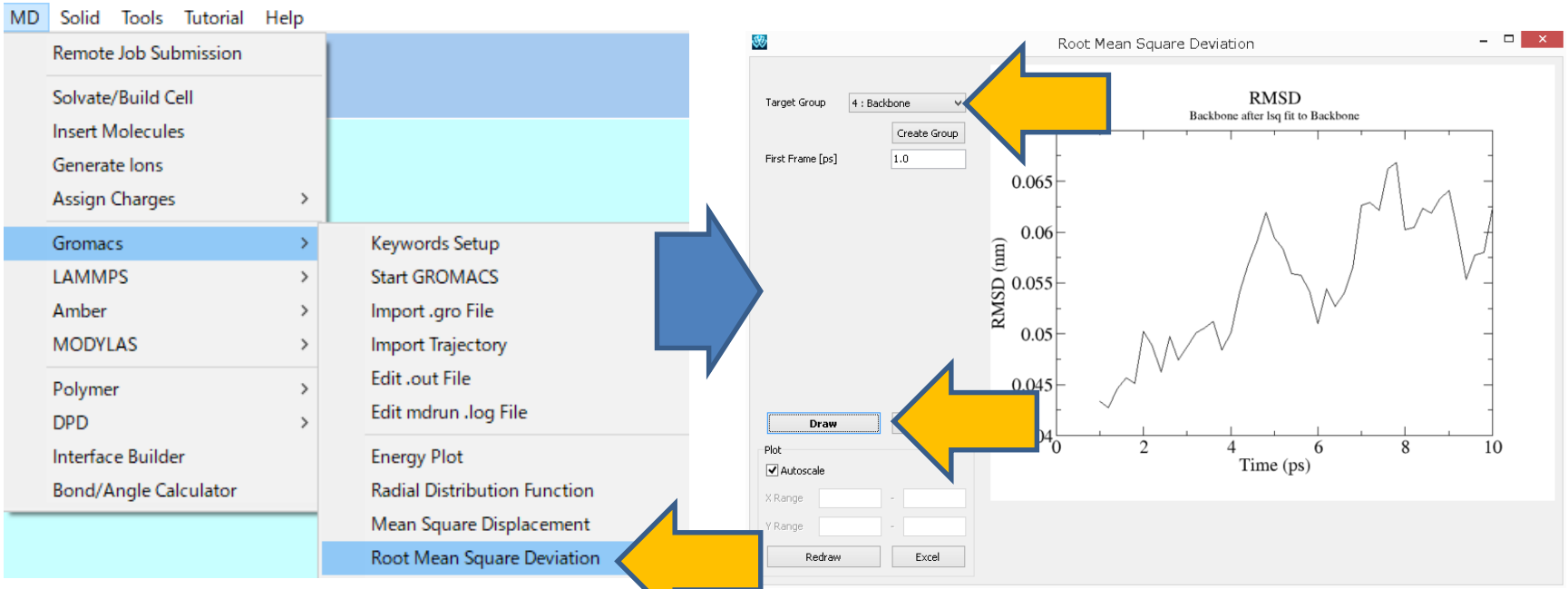


II. Execute simulations

1. Equilibration (RMSD)

We've executed the calculation without restraints to the protein. So let us check the time changes of RMSD. This process should be carried out as necessary.

1. After the calculation, click **MD** | **Gromacs** | **RMSD**.
2. Open the default files. Repeat three times.
3. Set **Target Group** to **Backbone**, then click **Draw** to get the time changes of RMSD.
   The radius of gyration can be obtained in the same way.



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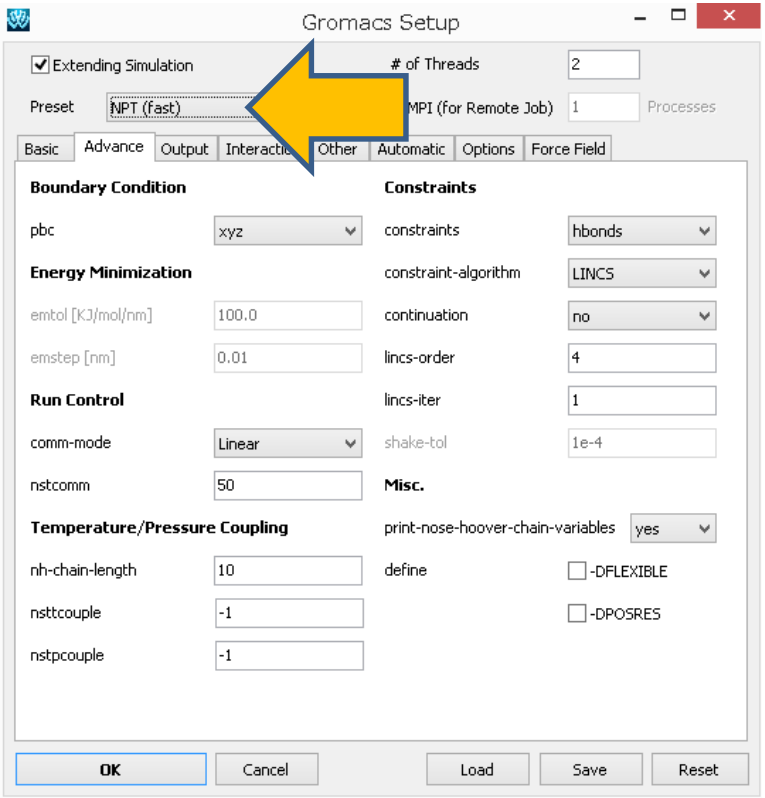
II. Execute simulations

1. Equilibration (*NPT*)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NPT (fast)**, then click **OK**.
3. Click **MD** | **Gromacs** | **Start Gromacs**.



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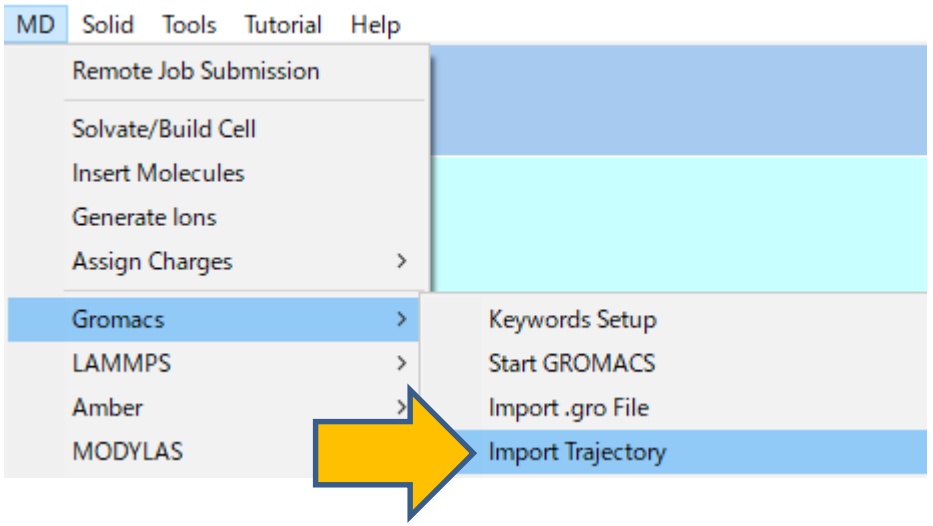
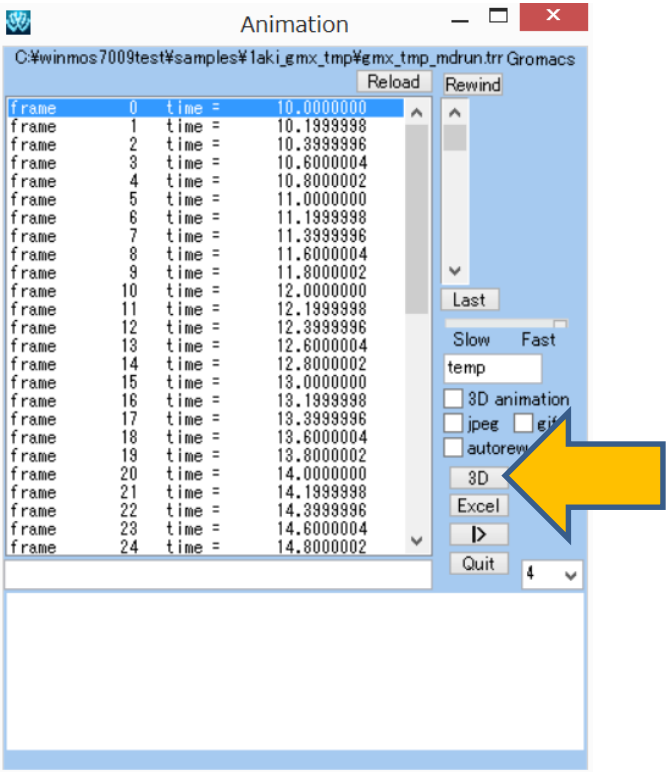
III. Product Run & Animation

1. After the calculation, click **MD** | **Gromacs** | **Start Gromacs**.
   (The same condition as the last calculation for equilibration.)
2. After the product run, click **MD** | **Gromacs** | **Import Trajectory**.
   Open the default files.
3. On **Animation** window, click **3D**.





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III. Product Run & Animation

1. On **Winmostar 3D**, click **View** | **Preferences**.
2. Check **Mol. Weight** to change the view preferences to each atom.
3. Click **|>** (play button) in the upper-left box to start the animation.