X-Ability
クロスアビリティ

# Winmostar tutorial

## Gromacs

## Protein

V7.025

X-Ability Co,. Ltd.

question@winmostar.com

2017/8/8

X-Ability
クロスアビリティ

# Contents

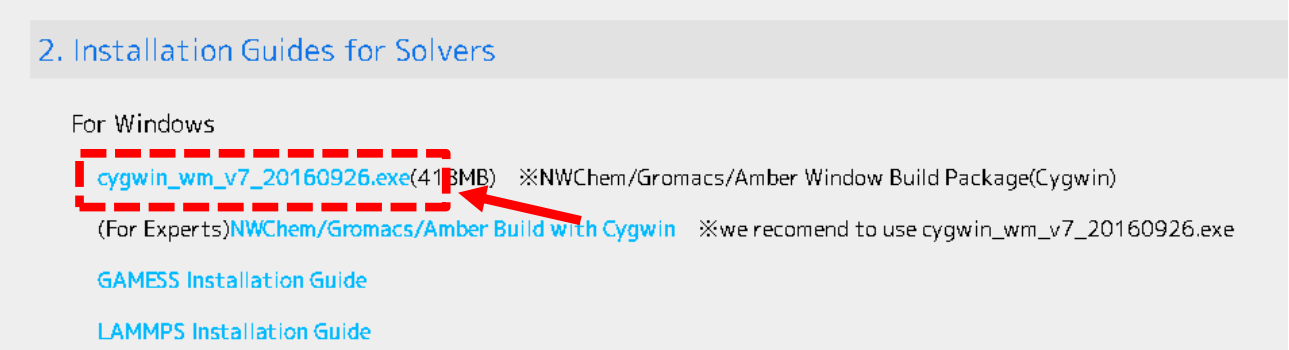
I. Build a simulation cell
II. Execute simulations
III. Animation

X-Ability
クロスアビリティ

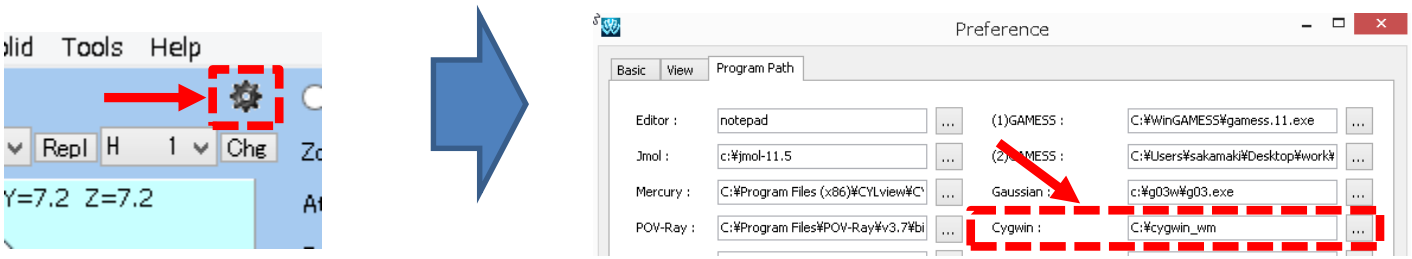
# Configure

**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.



X-Ability
クロスアビリティ

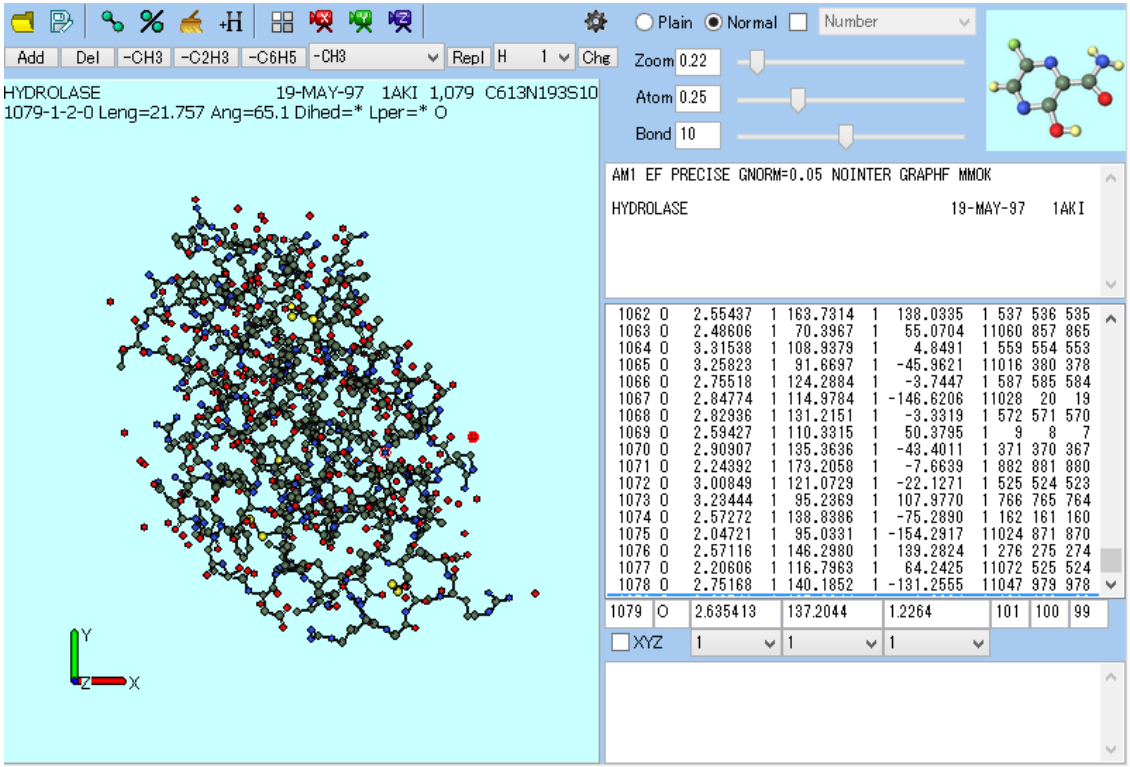
# Note

- The simulation steps required are dependent on molecular species and initial density.
- Setting longer simulation times is ideal to obtain accurate and reproducible results.
- The method for interaction calculations and/or the force field also affect simulation results.
- For purposes of this tutorial, size of systems (number of solvents) are set to radically low numbers to reduce calculation duration.

X-Ability
クロスアビリティ

# I. Build a simulation cell

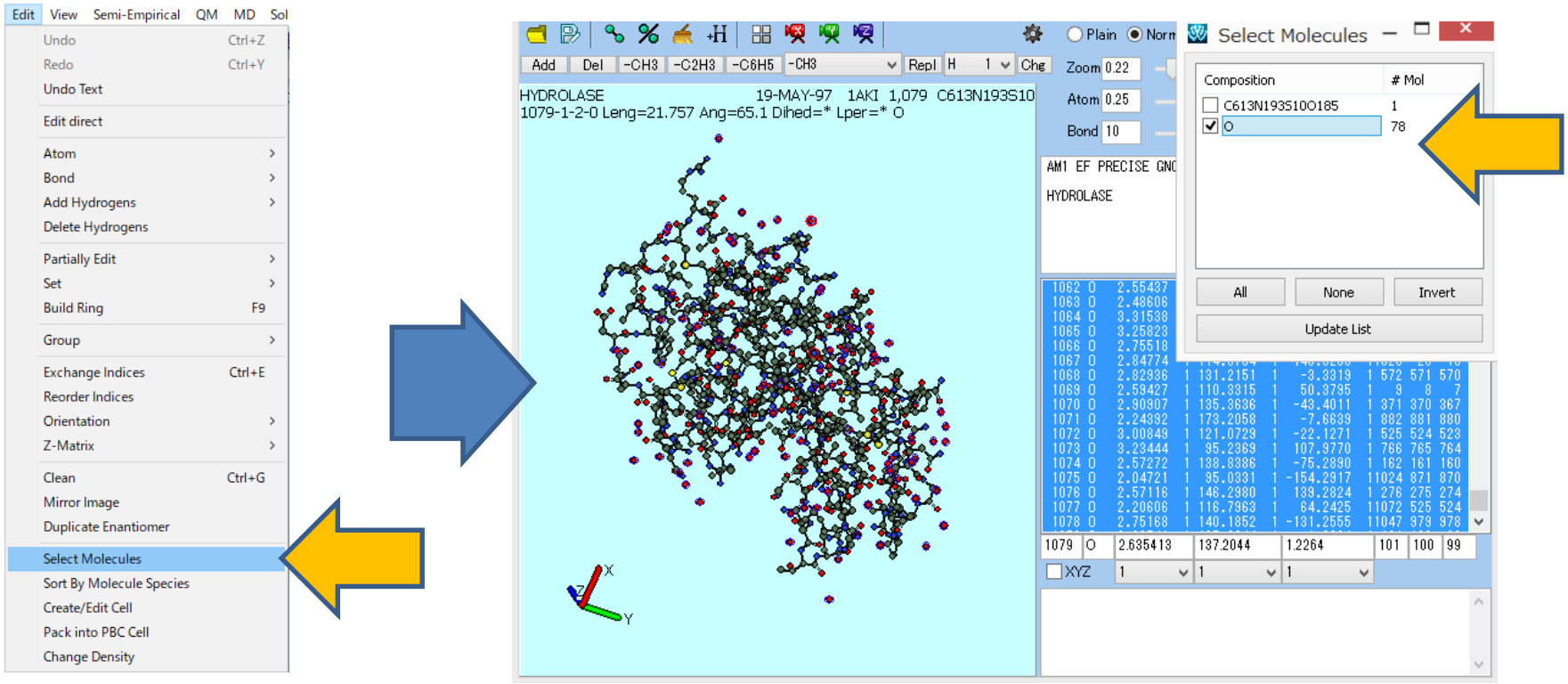
1. Click **File** | **Open**.
2. Open **1AKI.pdb** in sample directory.
   （default: C:¥winmos7¥samples¥1AKI.pdb）



X-Ability
クロスアビリティ

# I. Build a simulation cell

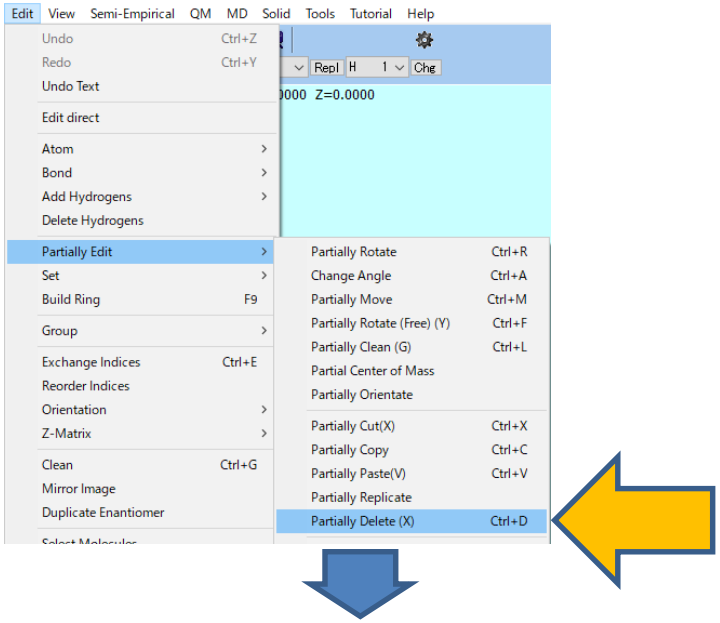
1. Click **Edit | Select Molecules**.
2. On **Select Molecules** window, check “**O 78.**” This will add blue circles around oxygen atoms of crystallization water as shown below (i.e. partial selection).

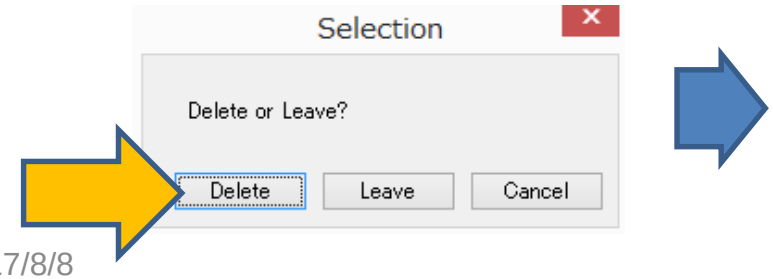


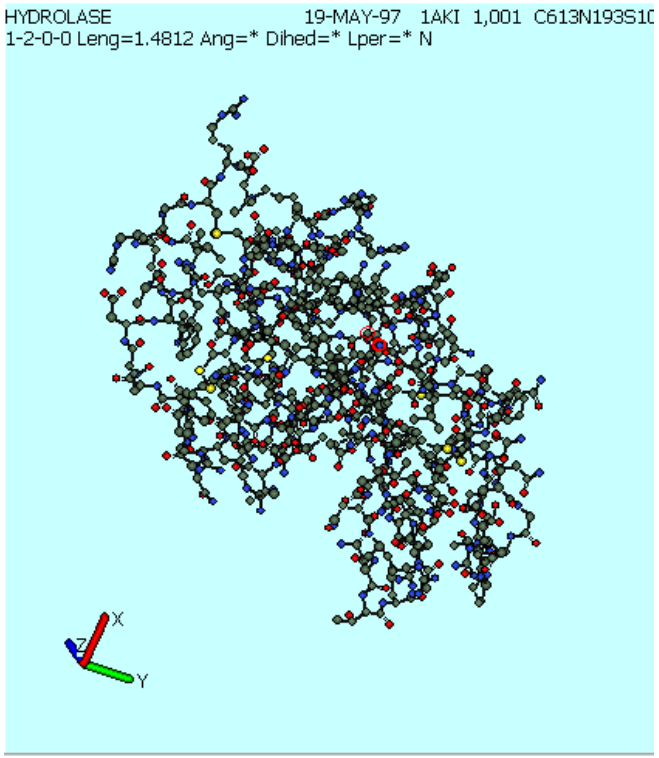
X-Ability
クロスアビリティ

# 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.



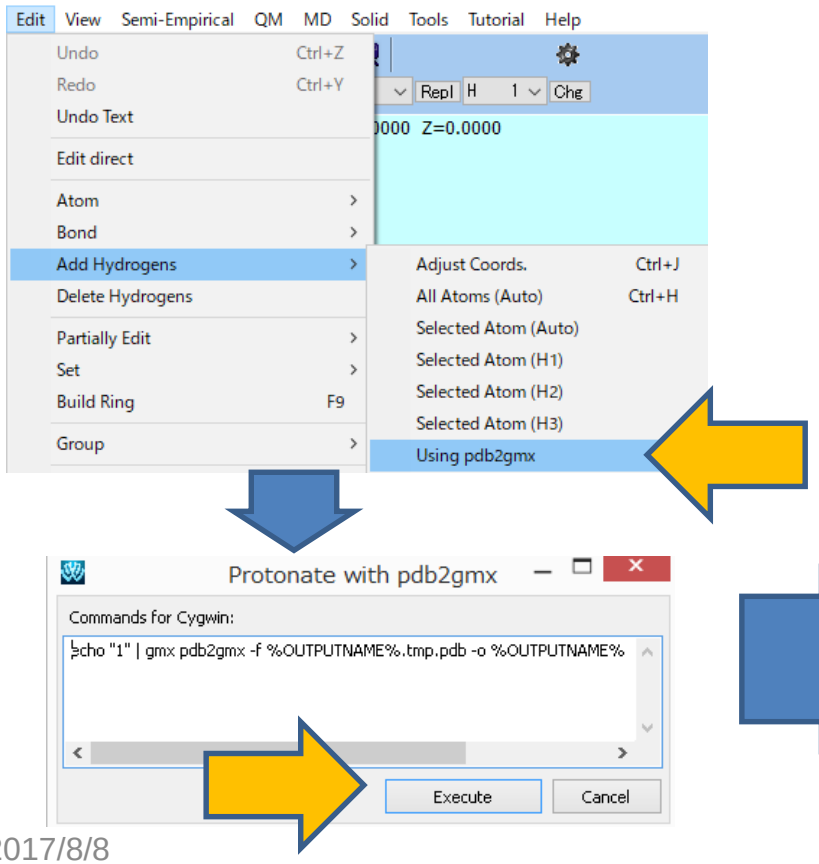



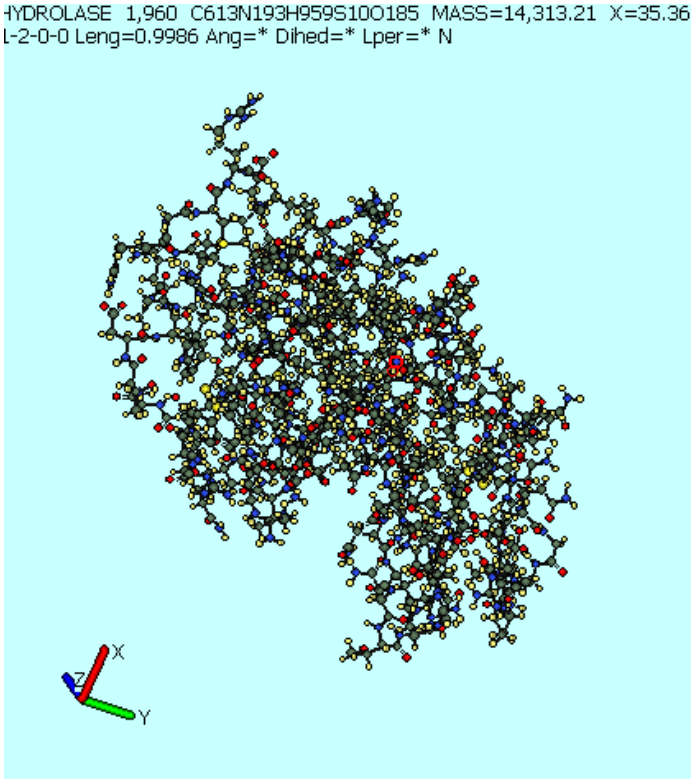



X-Ability
クロスアビリティ

# 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.

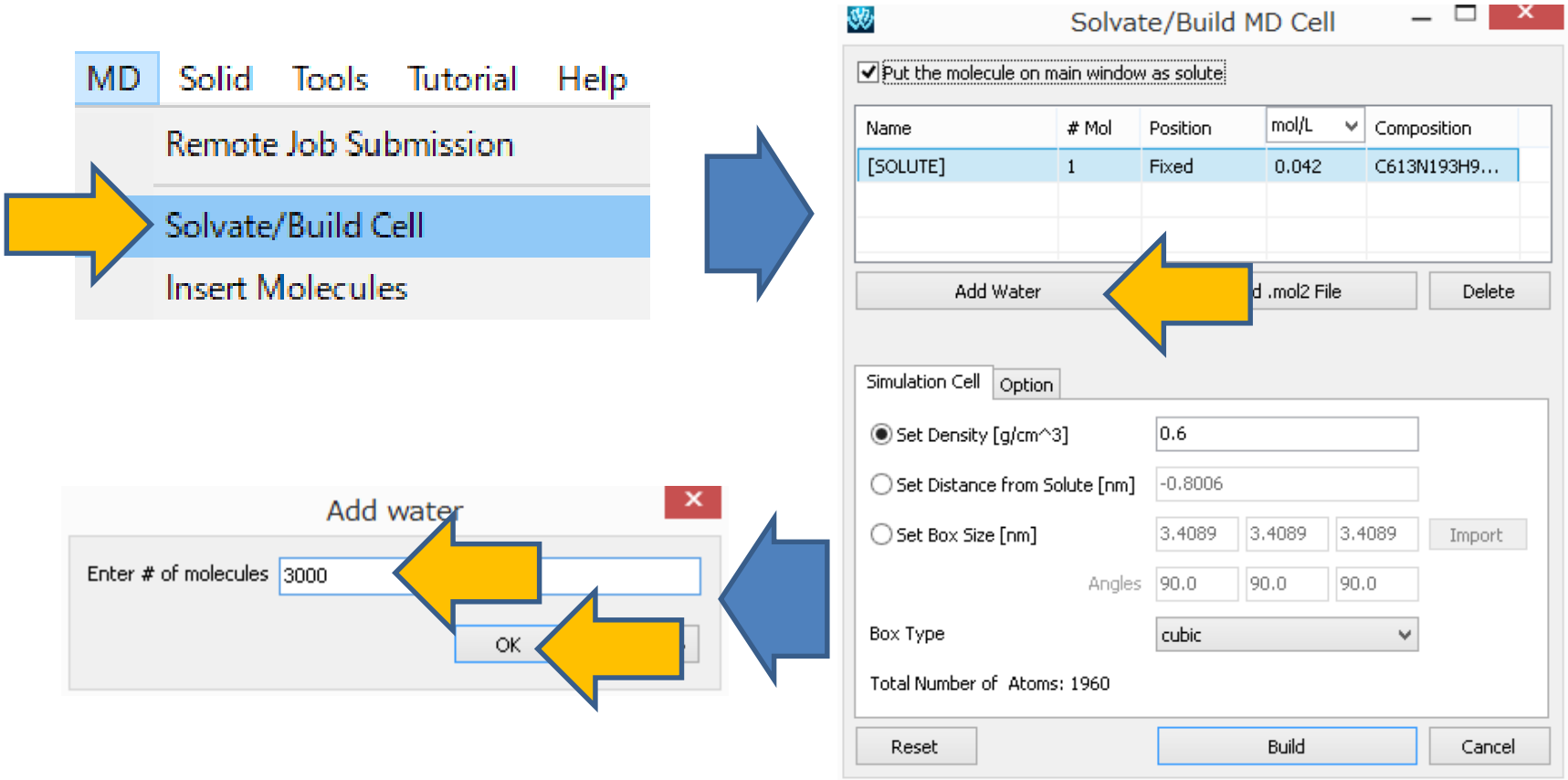


X-Ability
クロスアビリティ

# I. Build a simulation cell

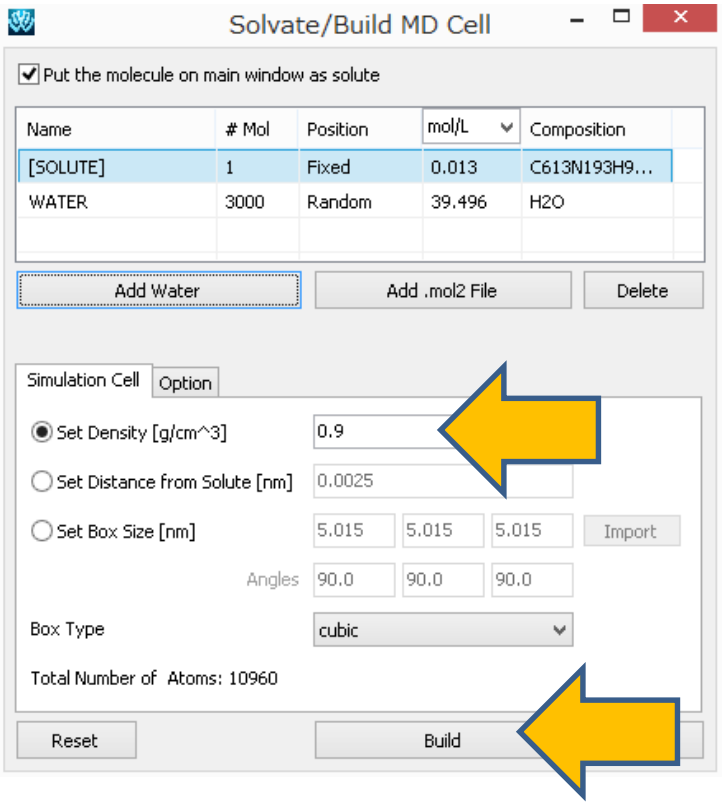
1. Click **MD** | **Solvate/Build Cell**
2. Click **Add Water**, then set **Enter # of molecules** to **3000**, click **OK**.

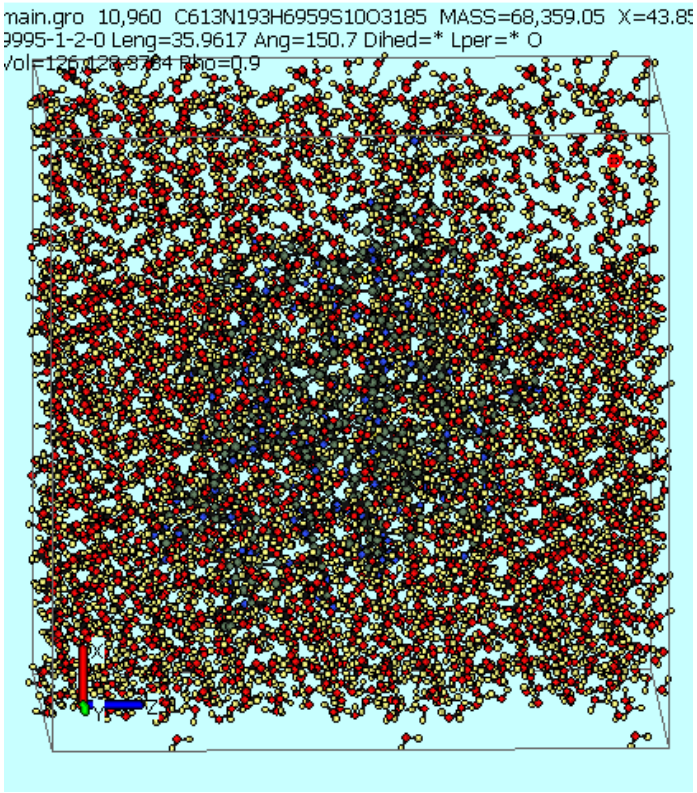


X-Ability
クロスアビリティ

# I. Build a simulation cell

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

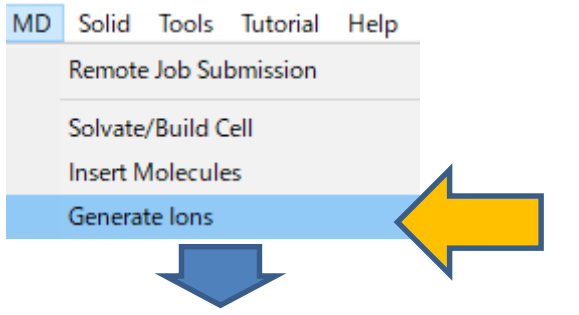


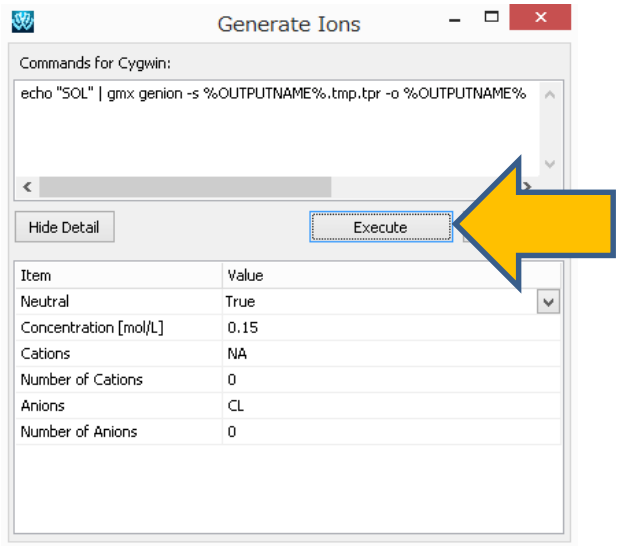



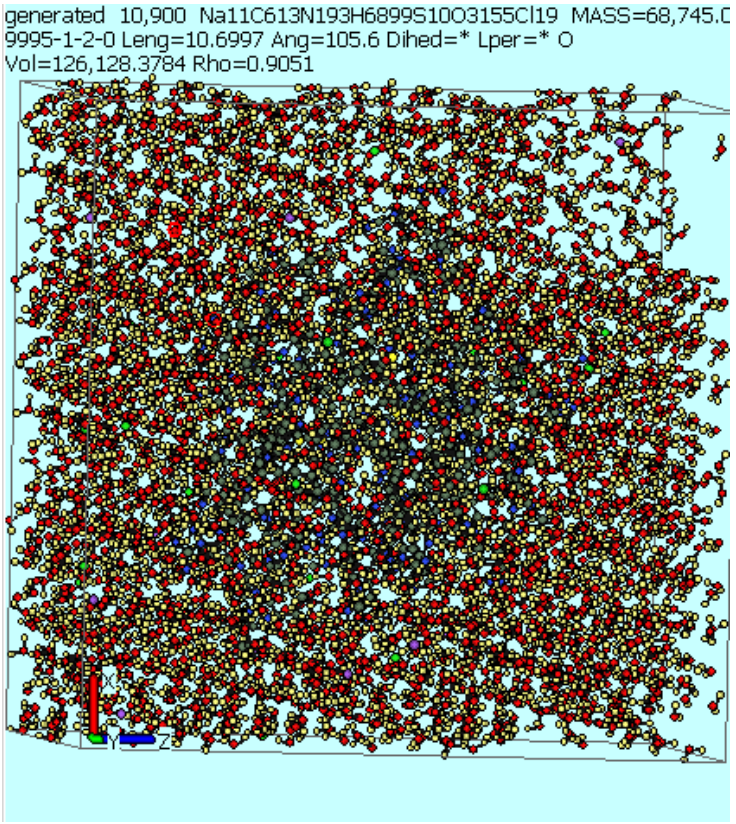
X-Ability
クロスアビリティ

# 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.



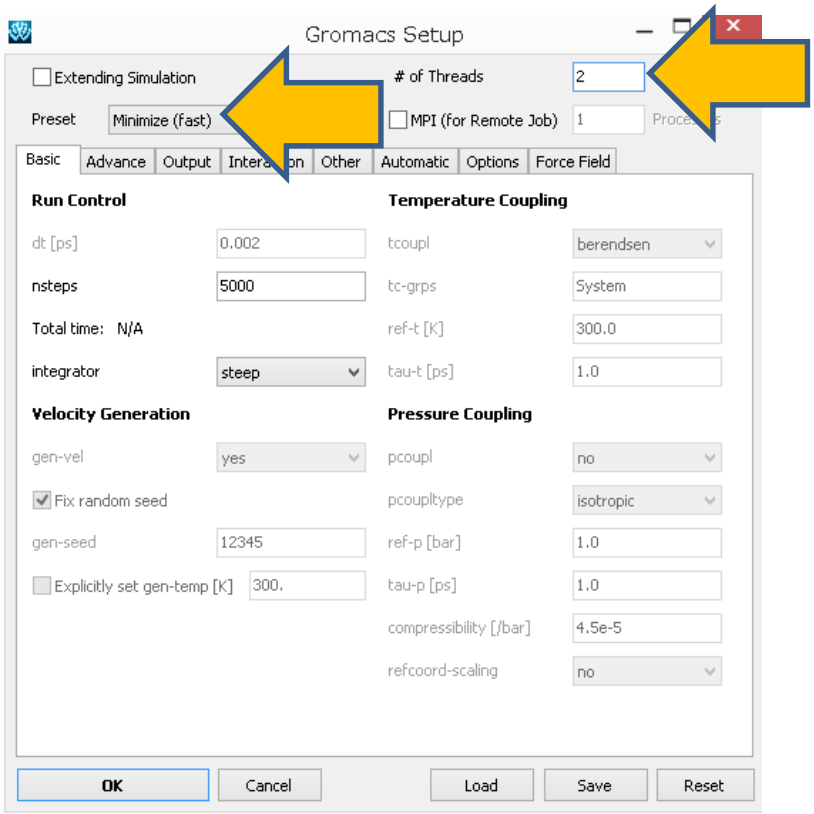



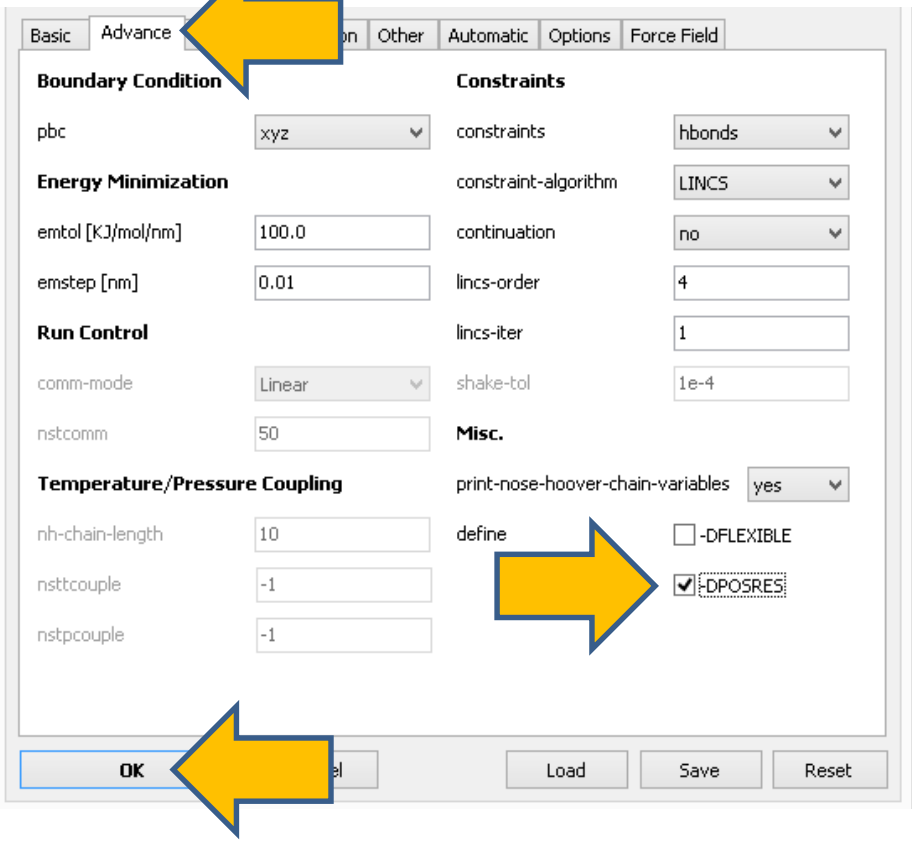
X-Ability クロスアビリティ

# 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**.



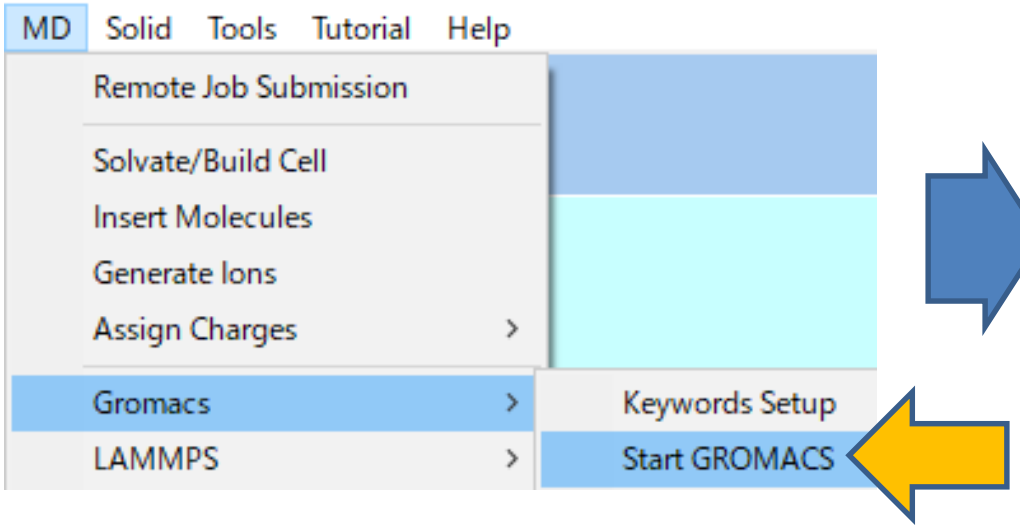



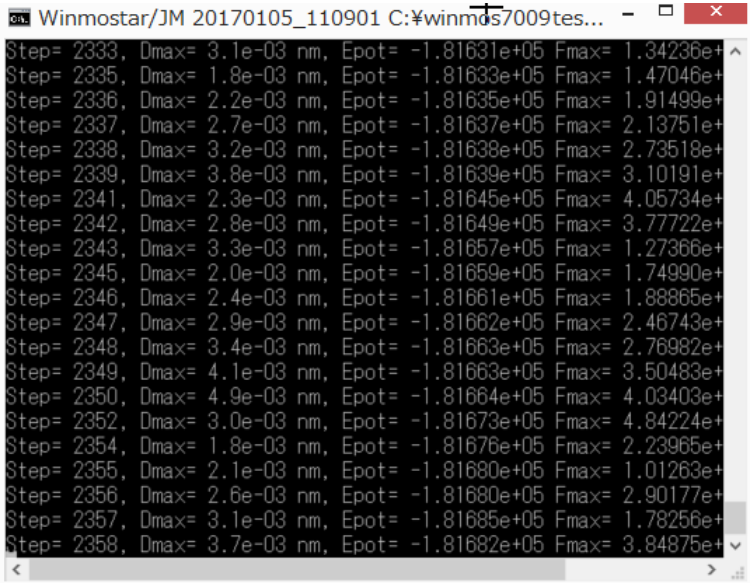
X-Ability
クロスアビリティ

# II. Execute simulations

## 1. Equilibration (Energy minimization with restraint)

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



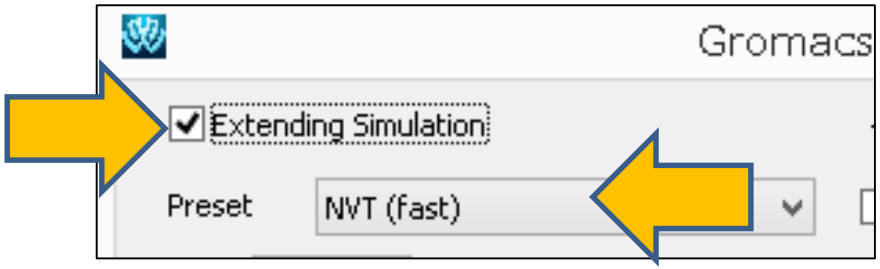



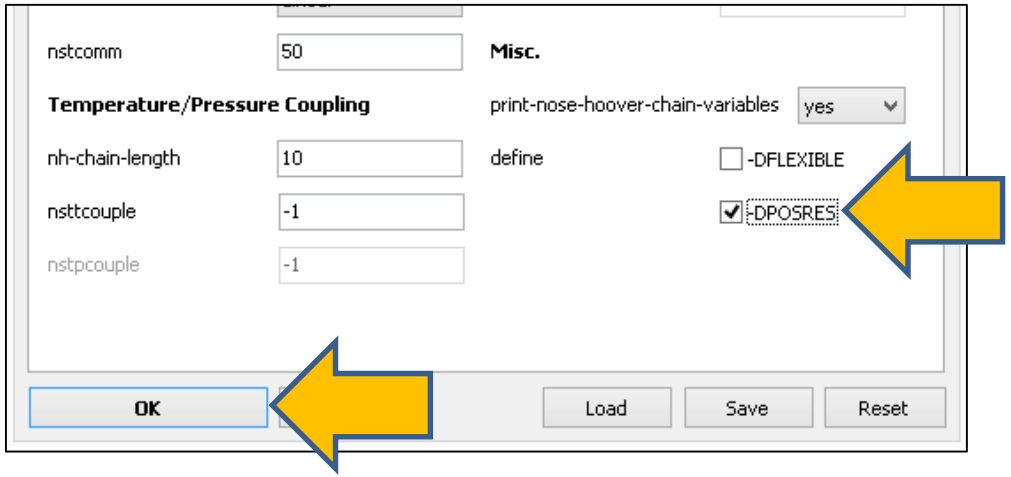
X-Ability
クロスアビリティ

# 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**.



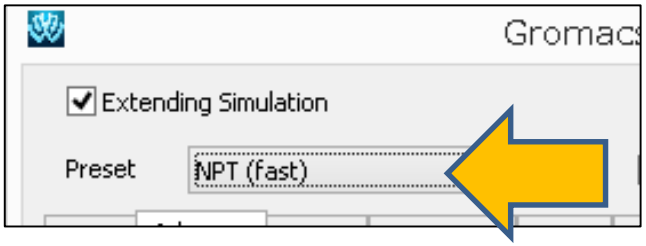



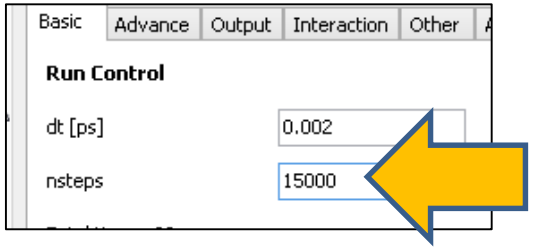
X-Ability
クロスアビリティ

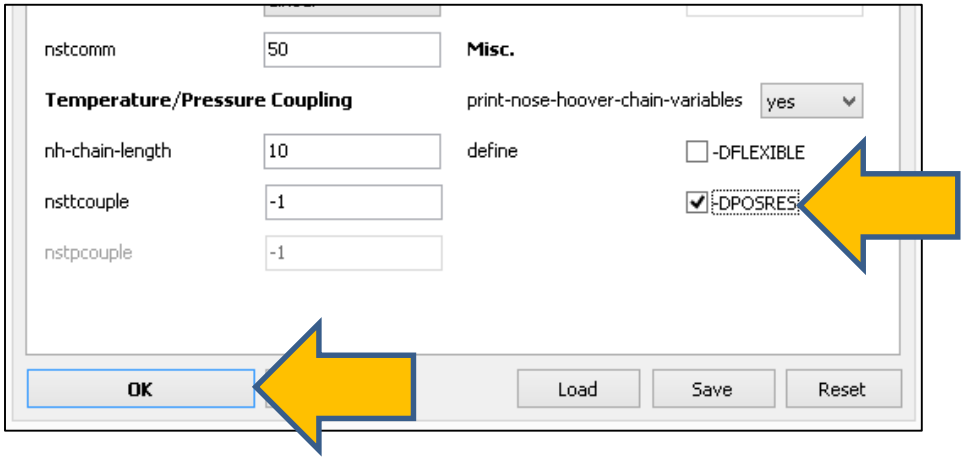
# II. Execute simulations

## 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**.



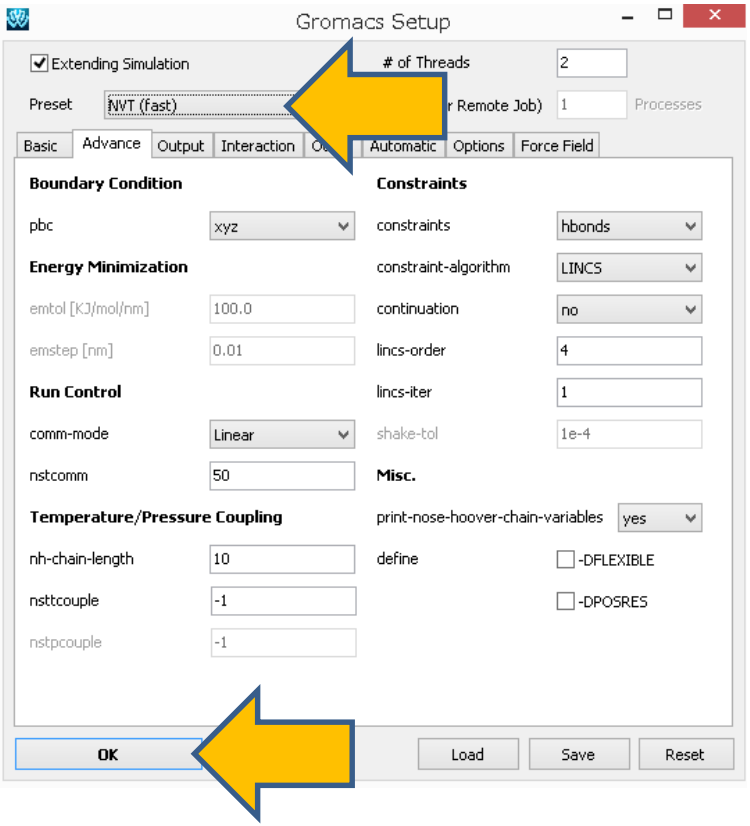



X-Ability
クロスアビリティ

# II. Execute simulations

## 1. Equilibration (*NVT*)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NVT (fast)**, then click **OK**.
3. Click **MD** | **Gromacs** | **Start Gromacs**. Calculation will start without any restraints.



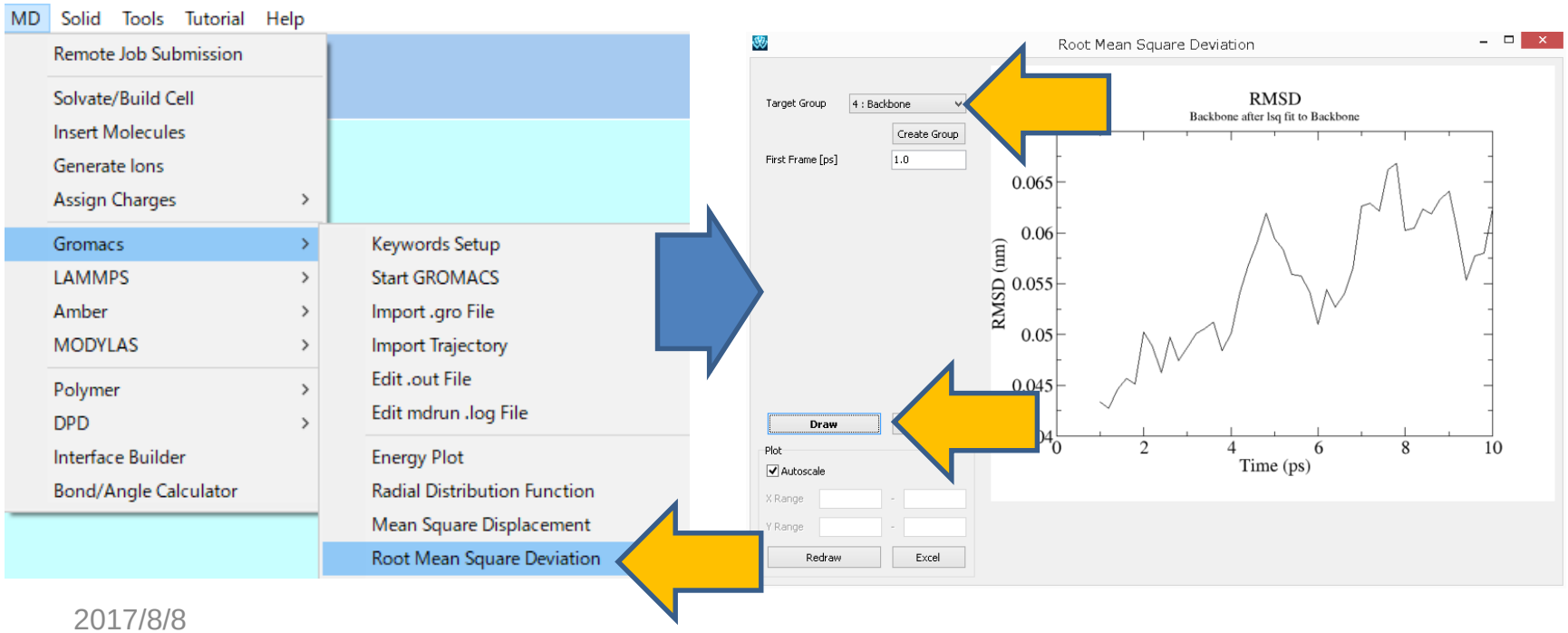
X-Ability
クロスアビリティ

# 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.

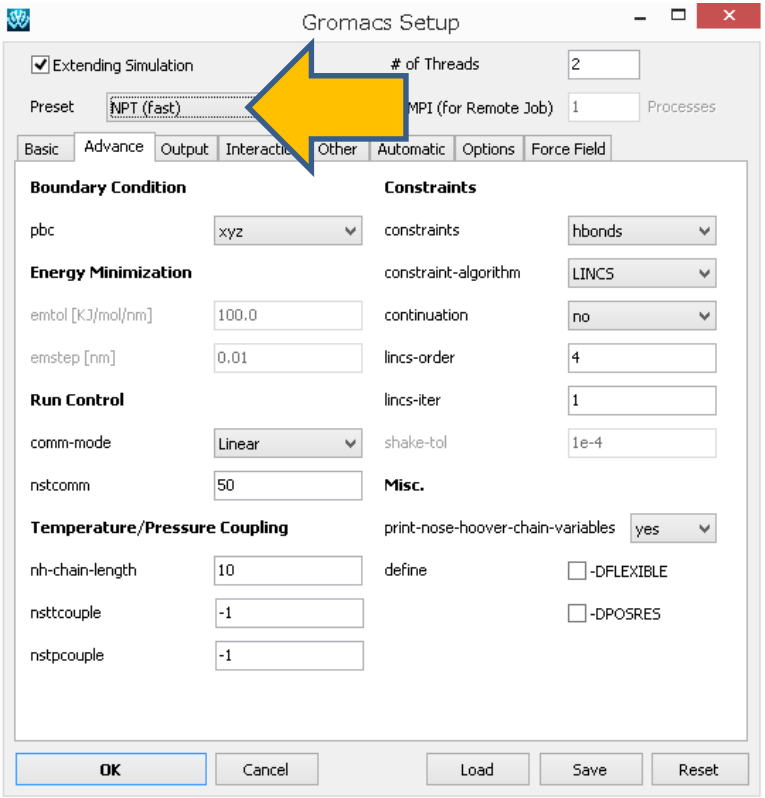


X-Ability
クロスアビリティ

# 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**.

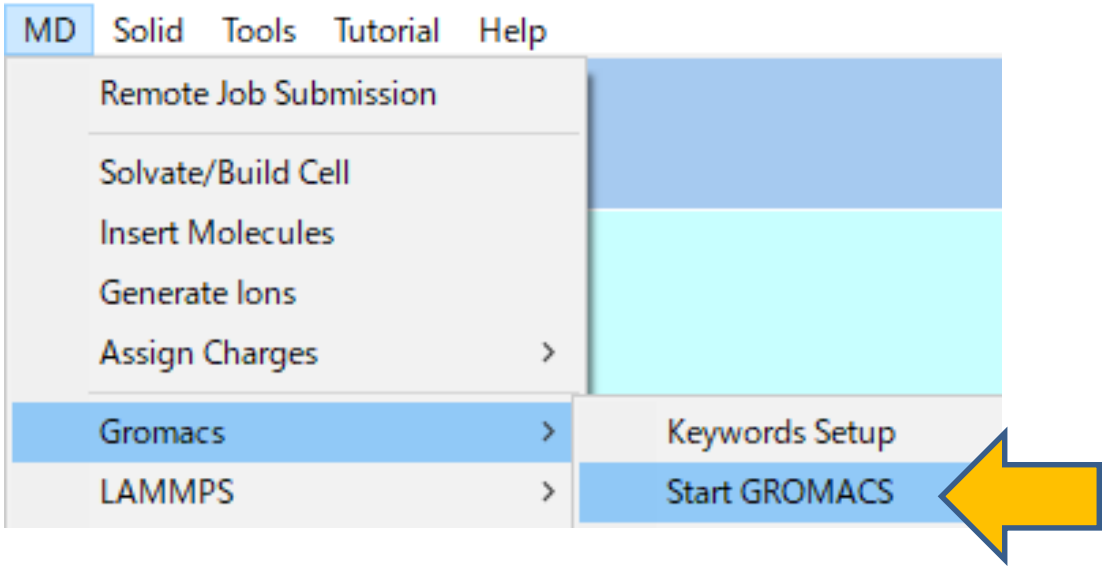


X-Ability
クロスアビリティ

# II. Execute simulations

## 1. Product run

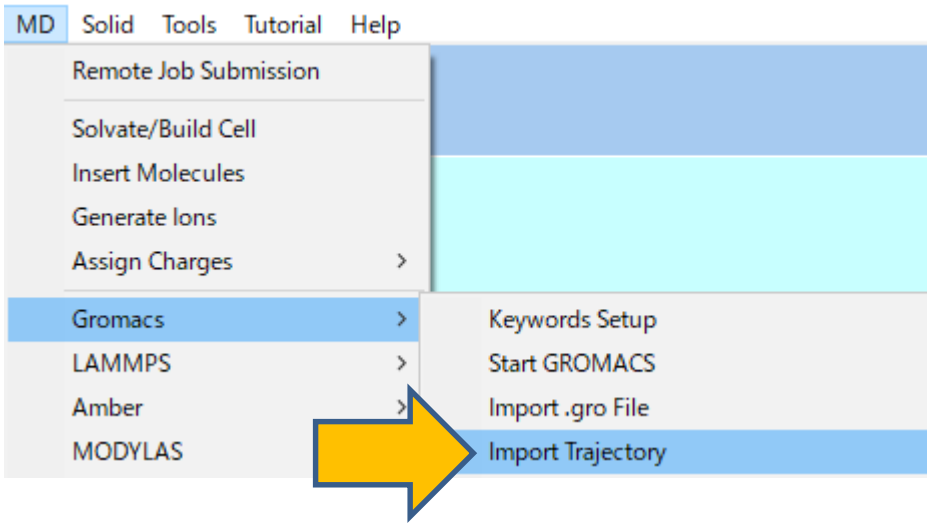
1. After the calculation, click **MD** | **Gromacs** | **Start Gromacs**.
   (The same condition as the last calculation for equilibration.)

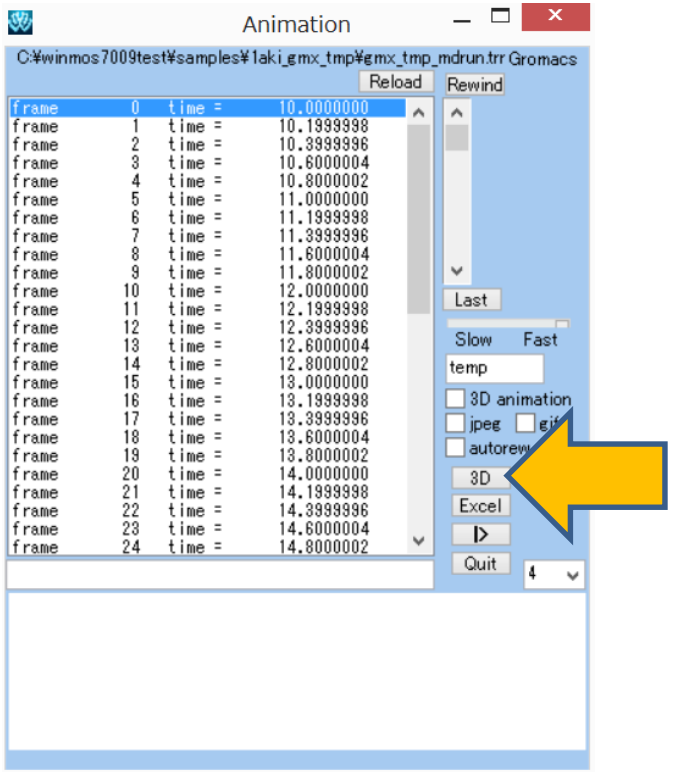


X-Ability
クロスアビリティ

# III. 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**.



X-Ability
クロスアビリティ

# III. 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.