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Winmostar tutorial

Gromacs

Viscosity・Dielectric constant

V7.025

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Contents

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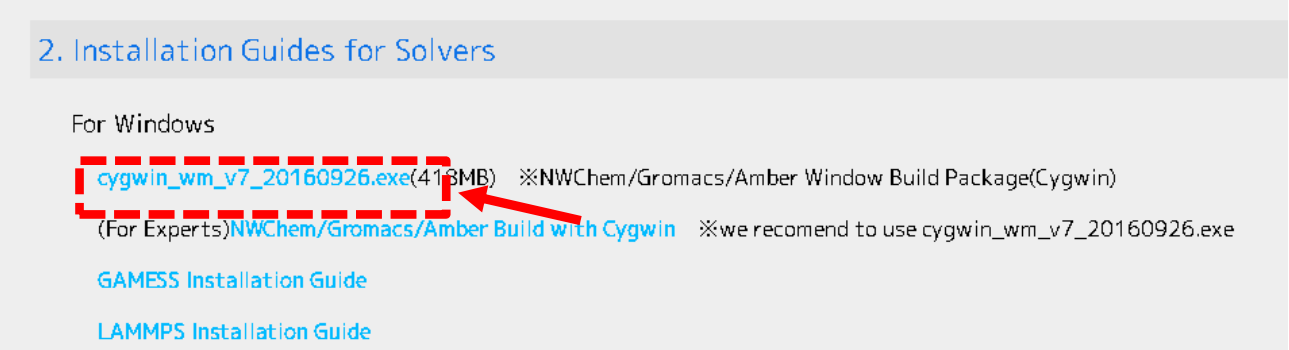
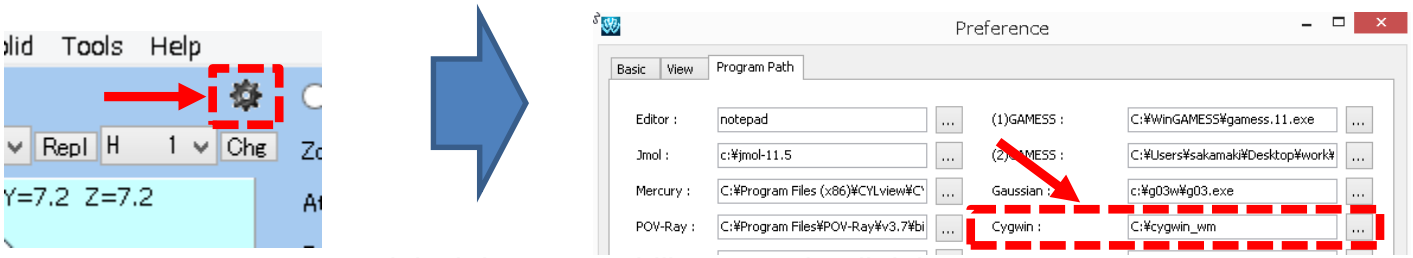
Configure

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.



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Note

- The simulation steps required are dependent on molecular species and initial density.
- To obtain accurate and reproducible results, you have to set long simulation time.
- The method for interaction calculations and/or the force field also affect the simulation results.

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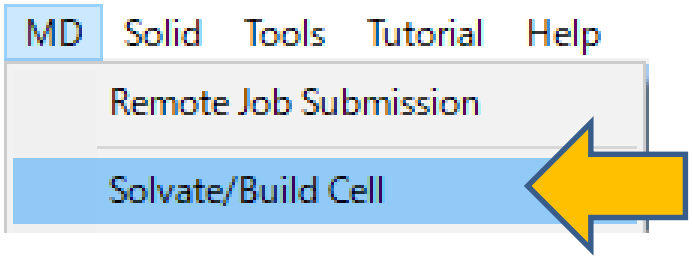
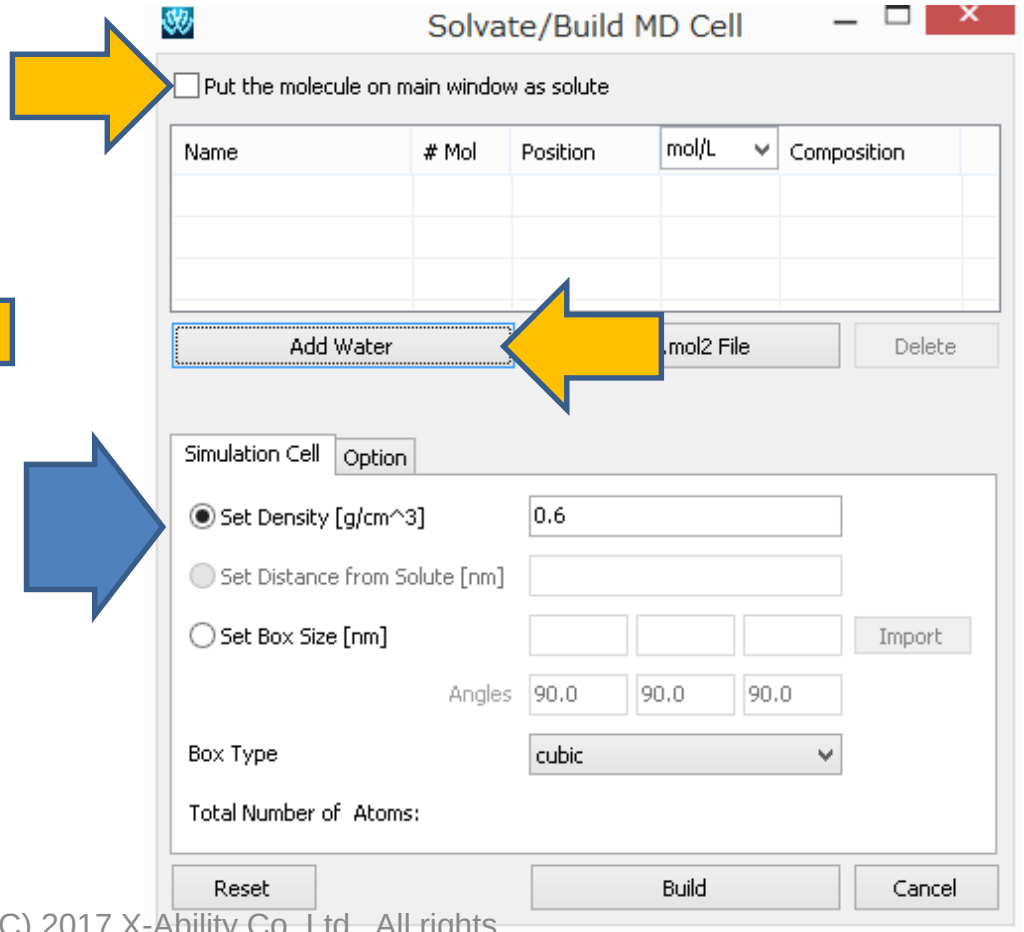
I. Build a simulation cell

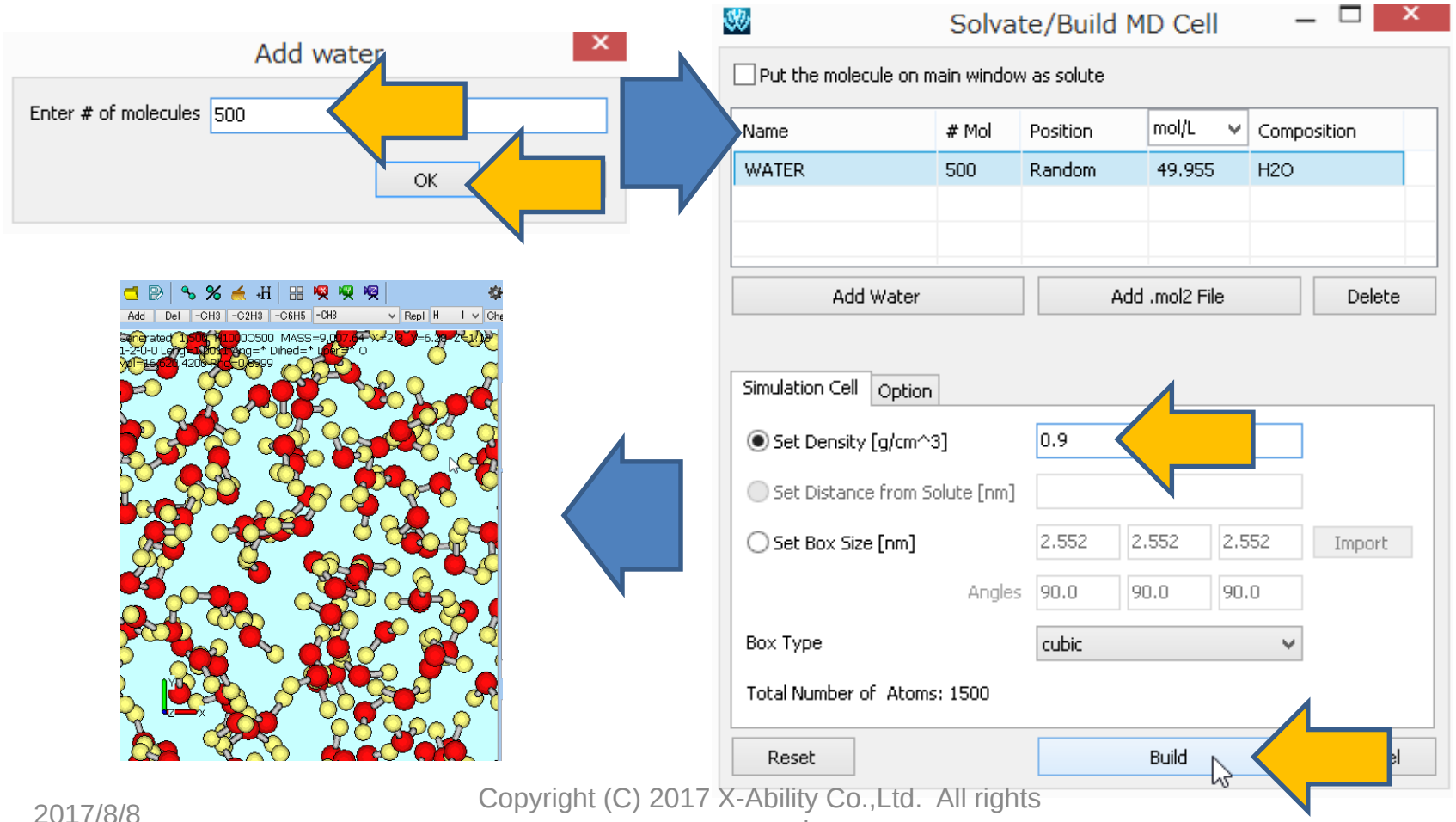
1. Click **MD | Solvate/Build Cell**.
2. Uncheck **Put the molecule on main window as solute**.
3. Click **Add Water**.





I. Build a simulation cell

1. Set **Enter # of molecules** to **500**, then click **OK**.
2. Set **Set Density** to **0.9**, then click **Build**.



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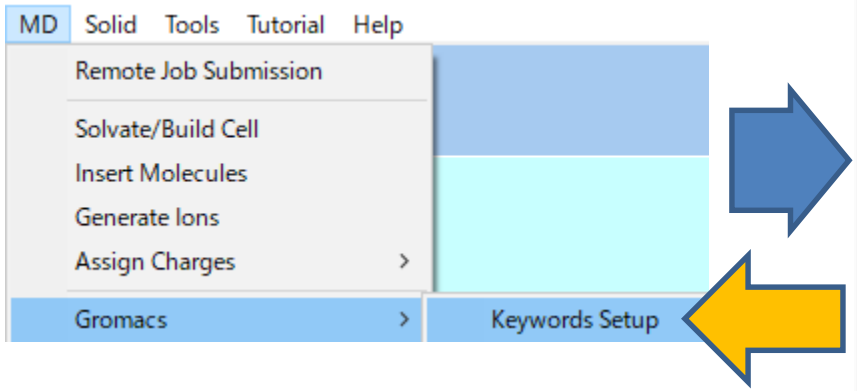
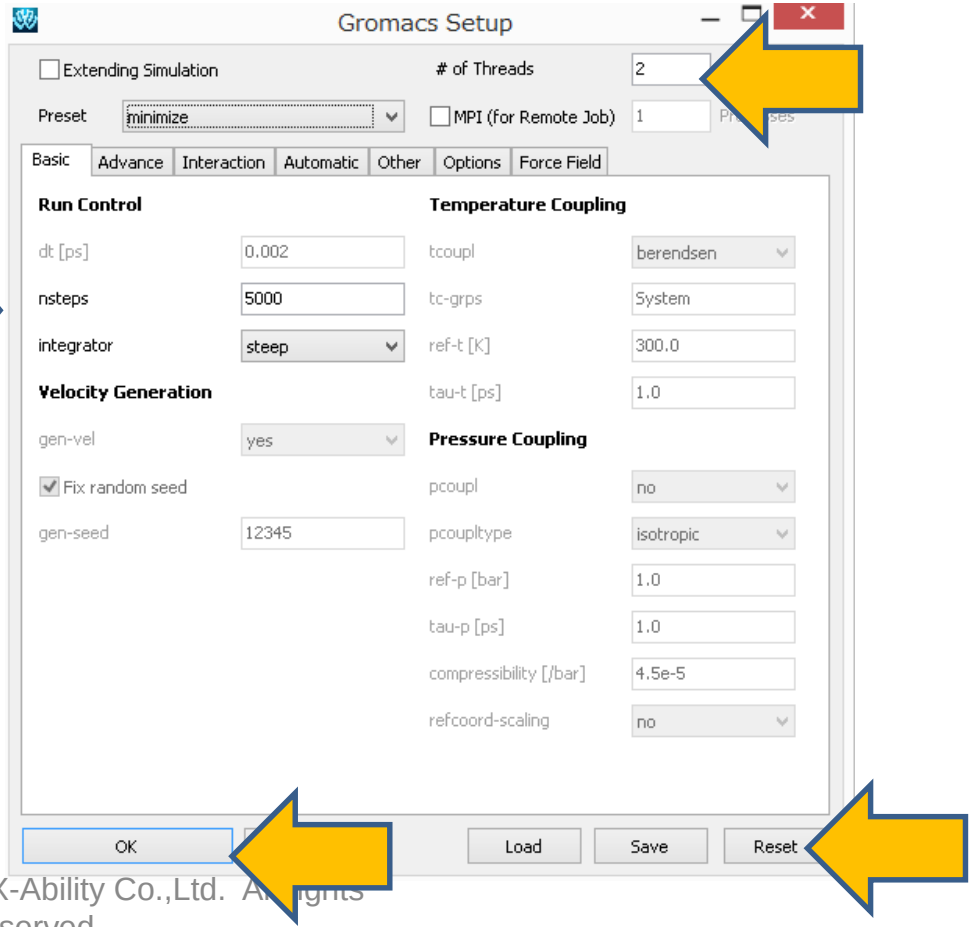
II. Execute simulations

1. Equilibration（Energy minimization）

1. Click **MD | Gromacs | Keywords Setup**.
2. Click **Reset**.
3. Set **# of Threads** to a parallel number, then click **OK**.





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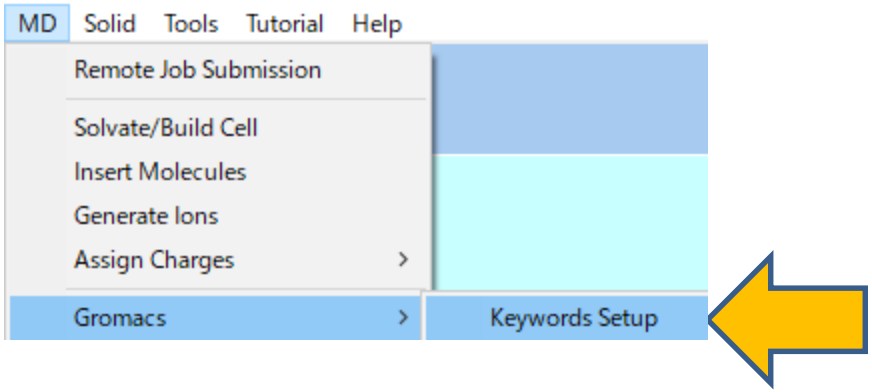
II. Execute simulations
1. Equilibration（Energy minimization）

1. Click **MD | Gromacs | Start Gromacs**.
2. Save the coordination file as **water.gro**, topology file as **water.top**. Then Cygwin will be launched and Gromacs process will begin.



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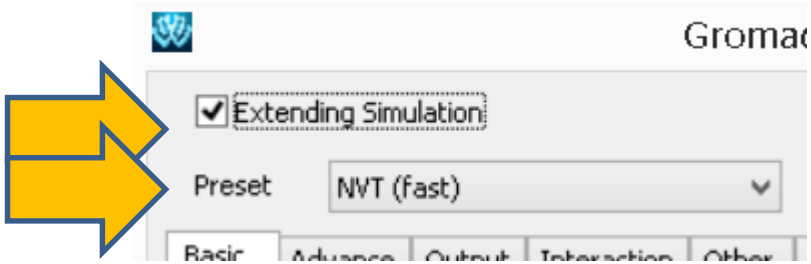
II. Execute simulations
1. Equilibration（*NVT*）

1. After the calculation, Click **MD** | **Gromacs** | **Keywords Setup**.
2. Check **Extending Simulation**, set **Preset** to **NVT （fast)**.
3. Click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.



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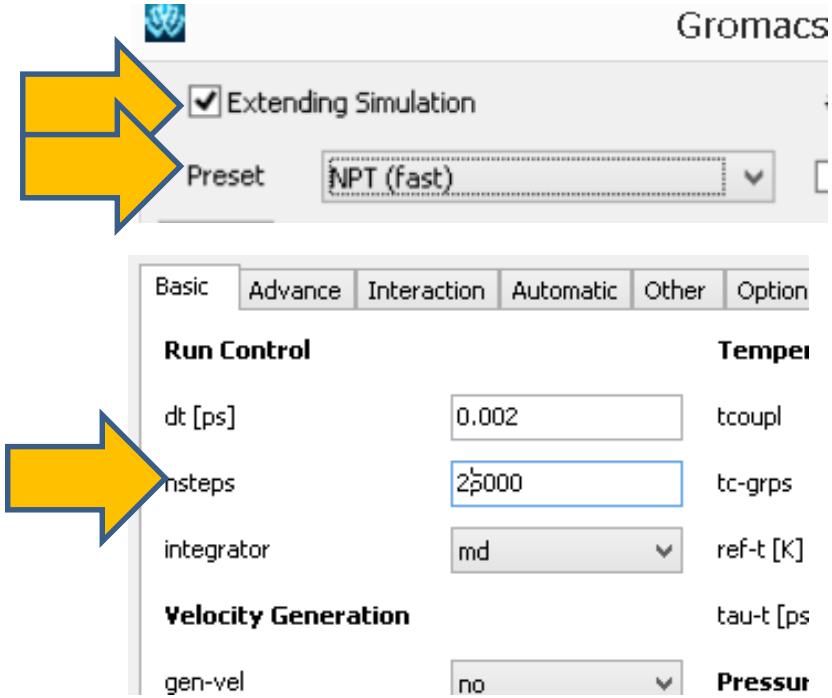
II. Execute simulations
1. Equilibration (*NPT*)

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NPT (fast)**, **nsteps** to **25000**.

(when **nsteps** is modified, **Preset** will be automatically set to **(custom)**.)

3. Click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.



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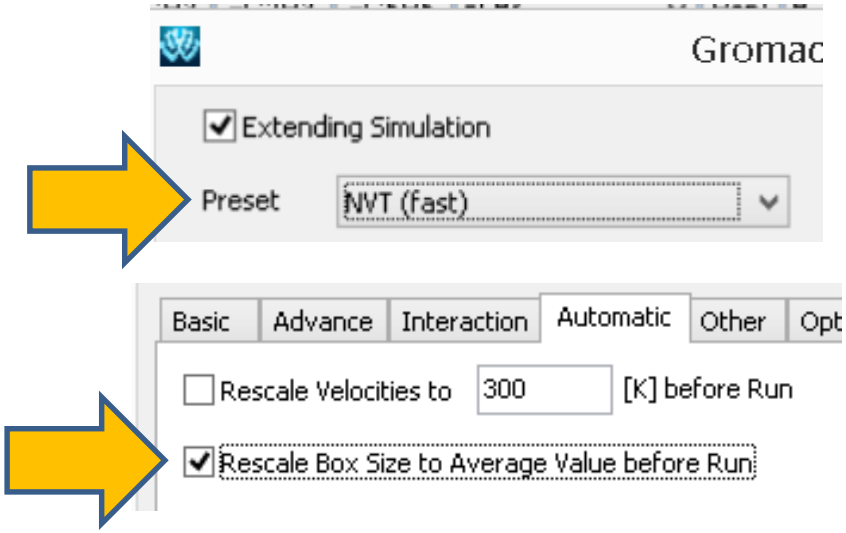
II. Execute simulations
1. Equilibration（*NVT* 2）

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NVT (fast)**.
3. On **Automatic** tab, check **Rescale Box Size to Average Value before Run**.
4. Click OK.
5. Click **MD** | **Gromacs** | **Start Gromacs**.



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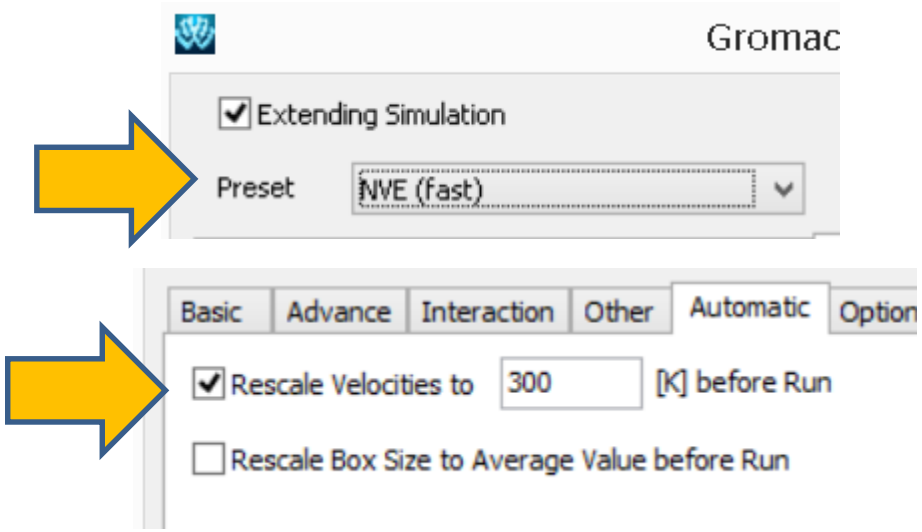
II. Execute simulations

1. Equilibration（No Temperature and Pressure control）

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVE (fast)**.
3. On **Automatic** tab, check **Rescale Velocities to ...** .
4. Click **OK**.
5. Click **MD | Gromacs | Start Gromacs**.



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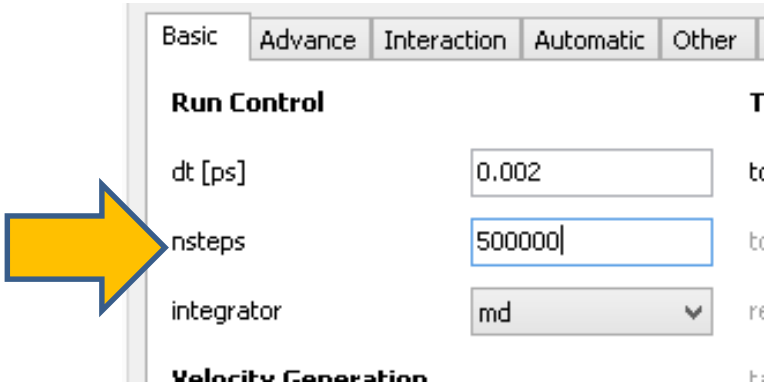
II. Execute simulations
2. Product run

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. On **Basic** tab, set **nsteps** to **500000**.
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



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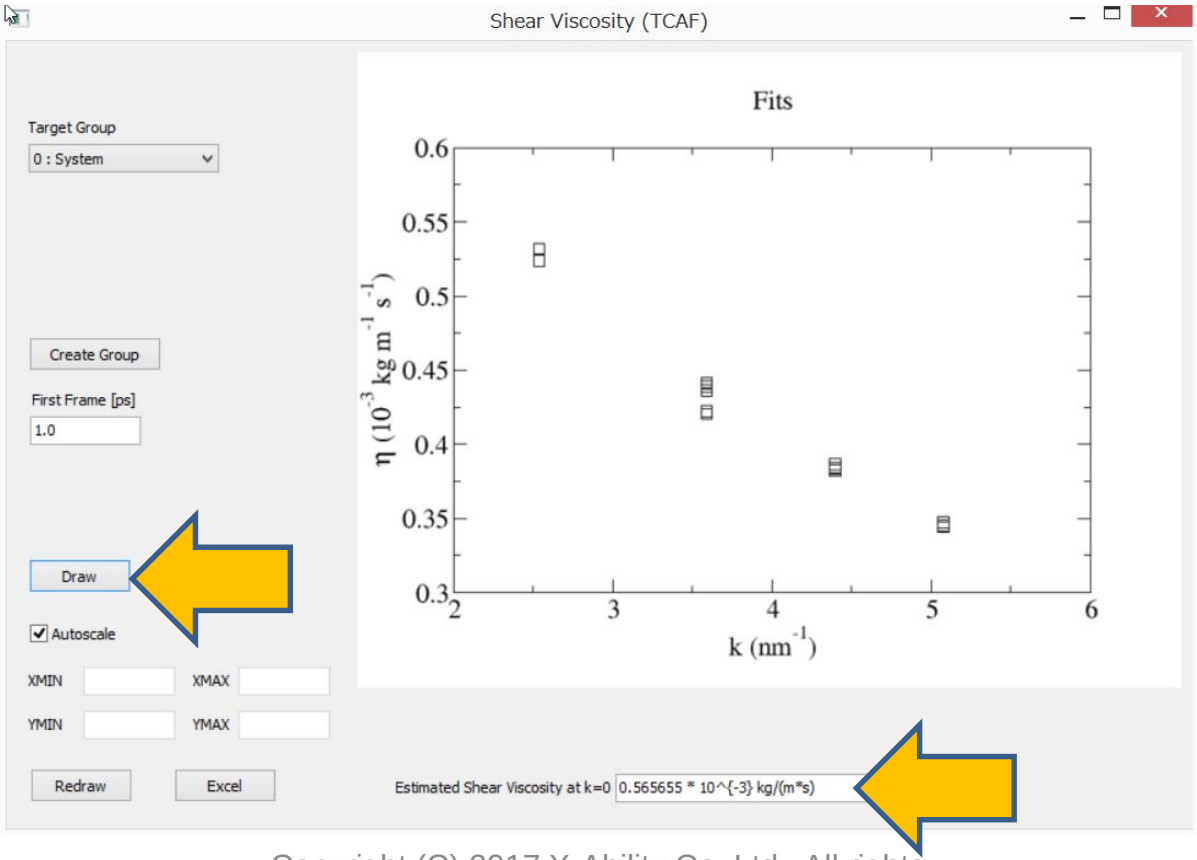
III. Analyze
1. Prediction of Viscosity

1. After the calculation, click **MD | Gromacs | Shear Viscosity**.
2. Open the default files; repeat 3 times.
3. Click **Draw** to draw the predicted value of Viscosity.



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III. Analyze
2. Prediction of dielectric constant

1. After the calculation, click **MD | Gromacs | Static Dielectric Constant**.
2. Open the default files; repeat 3 times.
3. Click **Draw** and set **Tempareture [K]** to **300**, then click **OK**.
   The predicted value of dielectric constant will be displayed.