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Winmostar tutorial

Gromacs

Viscosity・Dielectric constant

V8.007

X-Ability Co., Ltd.

question@winmostar.com

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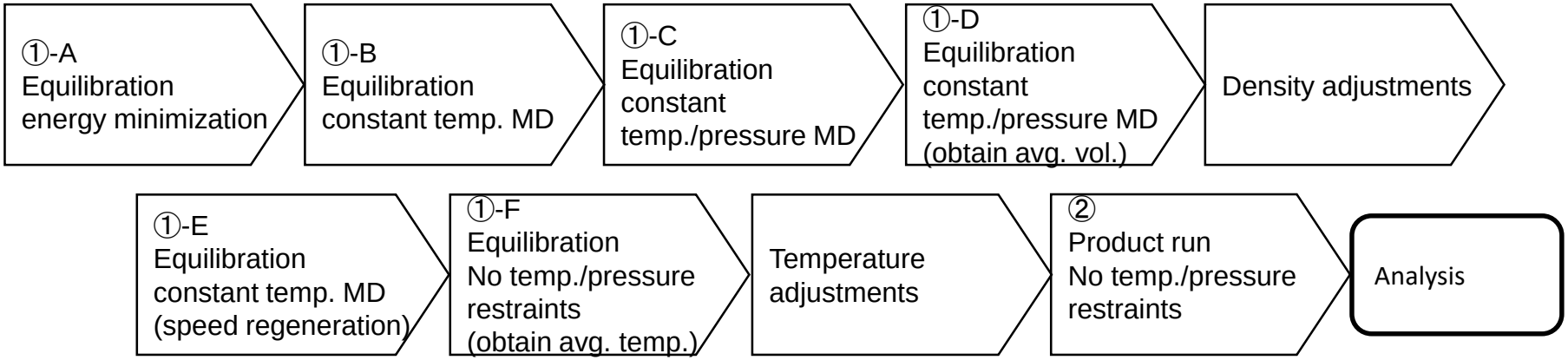
Summary

In this tutorial, we will calculate viscosity and dielectric constant of liquid of water. Product run will be executed on a NVE ensemble (no restraints on temperature/pressure) to calculate physical properties sensitive to delicate movements of molecules. We will also show equilibration procedure for calculating NVE ensemble under target temperature/pressure.



Notes:

- The number of steps required for equilibration depends on the type of molecule and initial density varies and may be different from this example.
- To obtain accurate and reproducible results, the calculation requires long simulation times.
- The method for interaction calculations and/or the force field also affect the simulation results.

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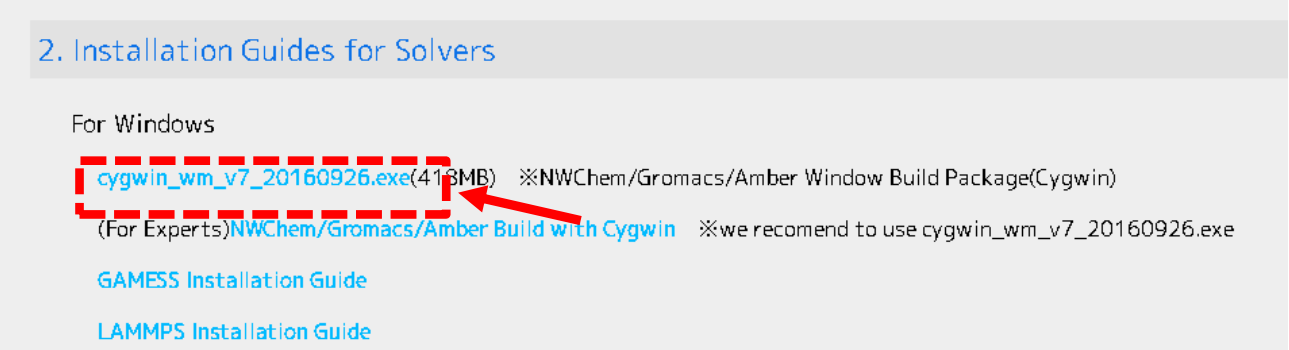
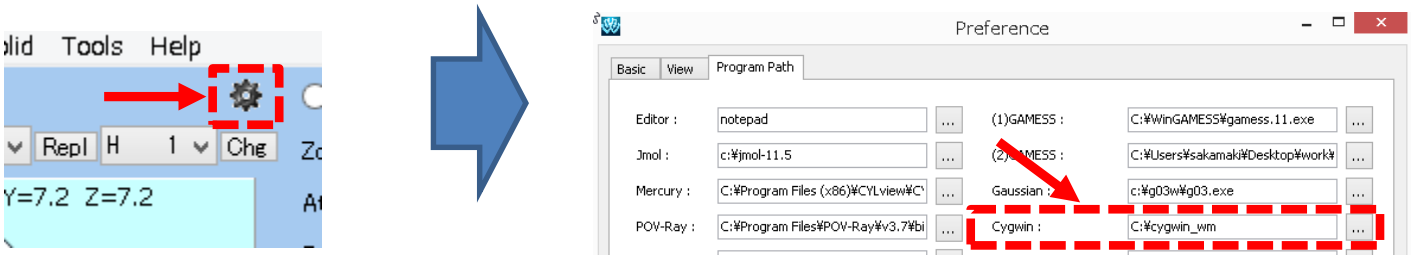
Configuration

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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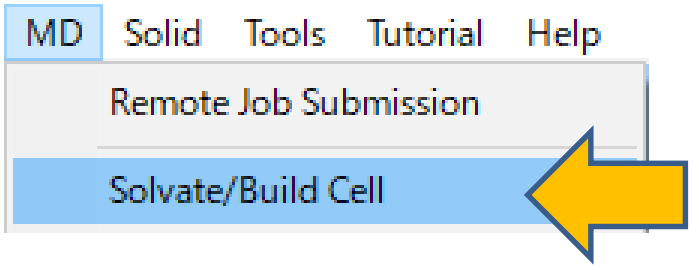
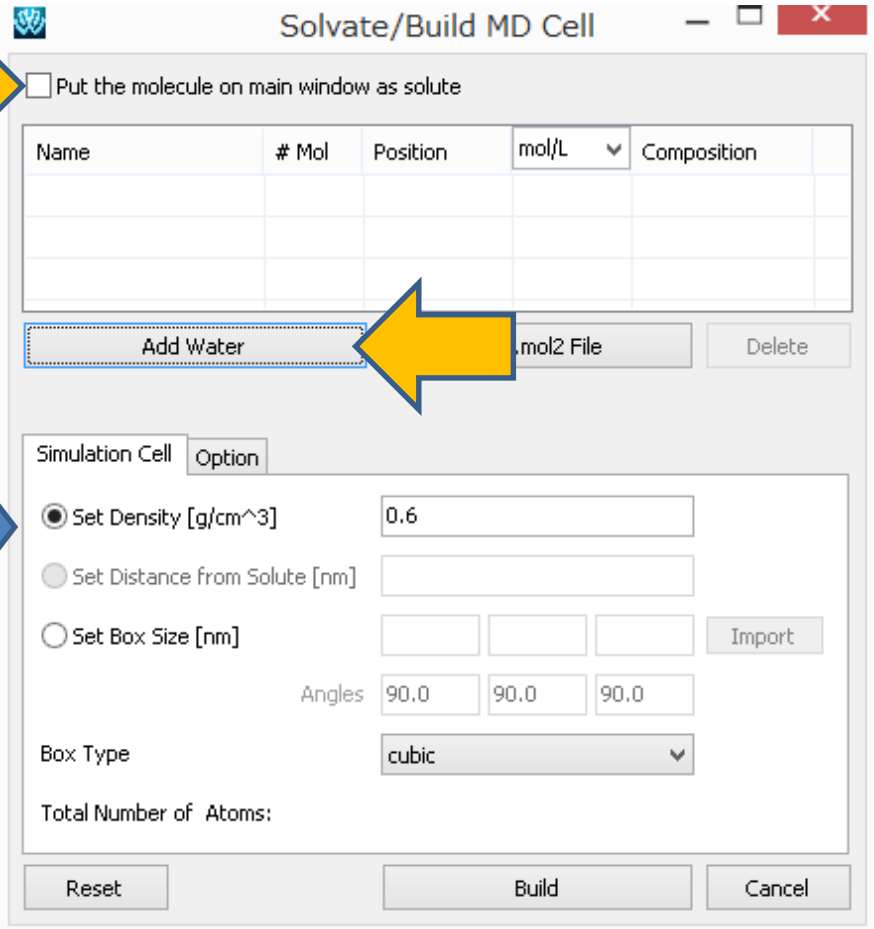
I. Build a simulation cell

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





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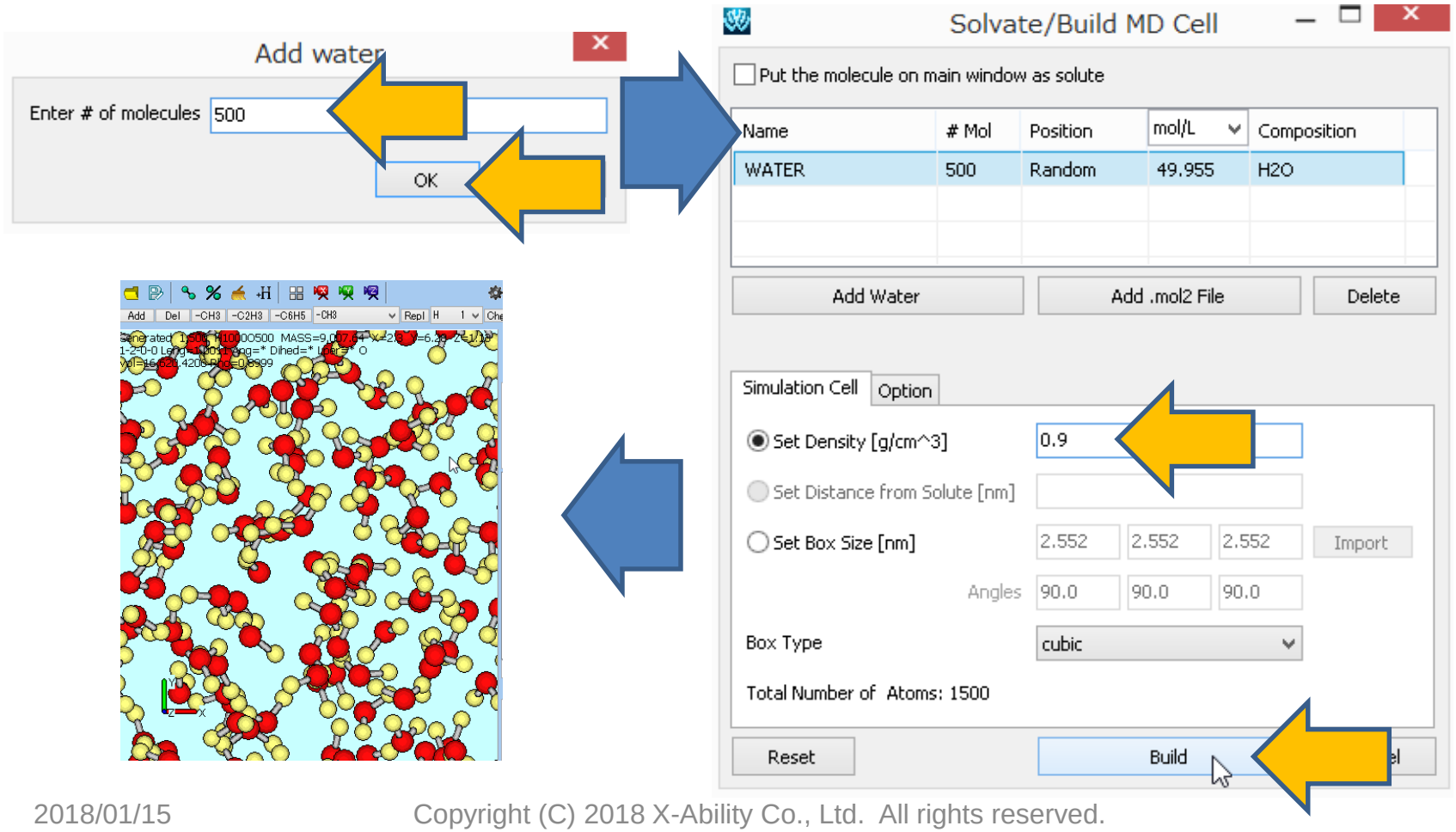
I. Build a simulation cell

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



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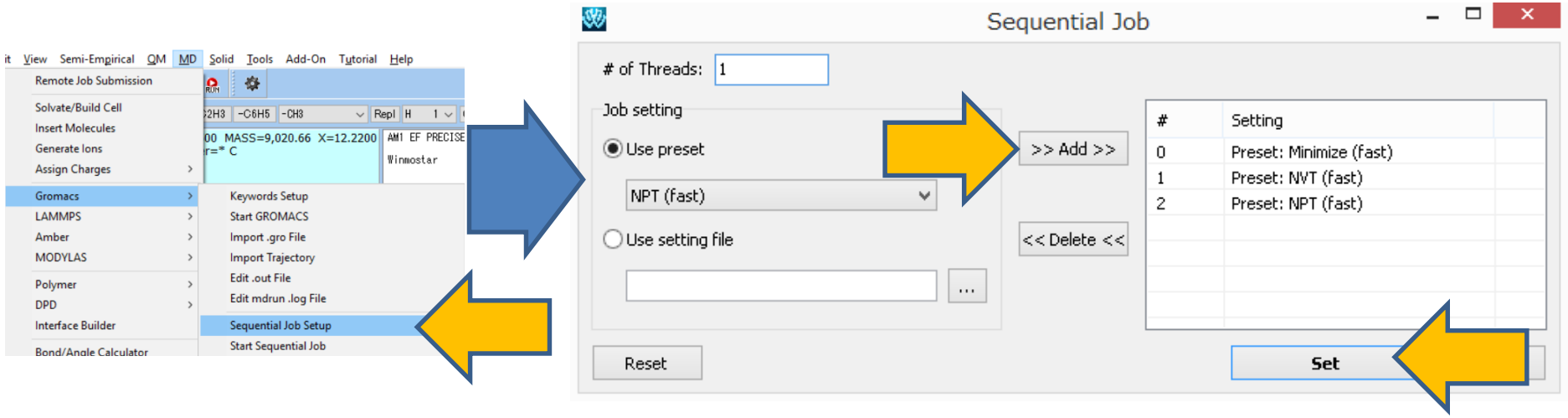
II. Equilibration (A - C)

1. Select **MD** | **Gromacs** | **Sequential Job Setup**.
2. Set Use **preset** to **Minimize (fast)** and click **>>> Add >>>**
3. Set Use **preset** to **NVT (fast)** and click **>>> Add >>>**
4. Set Use **preset** to **NPT (fast)** and click **>>> Add >>>**
5. After sequentially setting **Use presets**, click **Set**.
6. Next, select **MD** | **Gromacs** | **Start Sequential Job** and save files to begin job.



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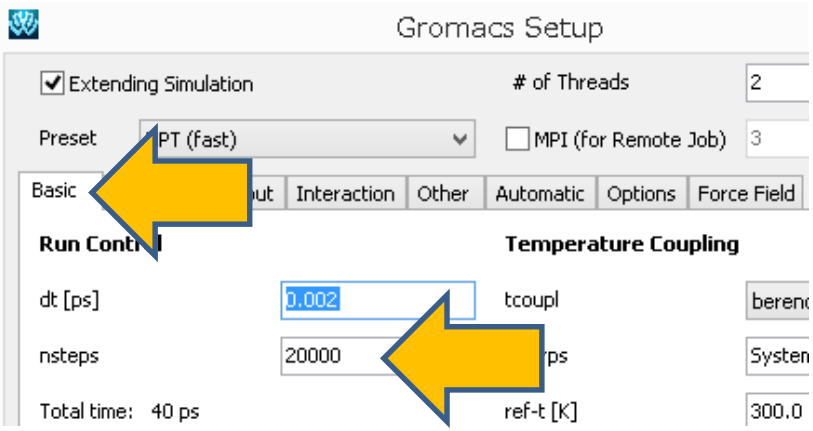
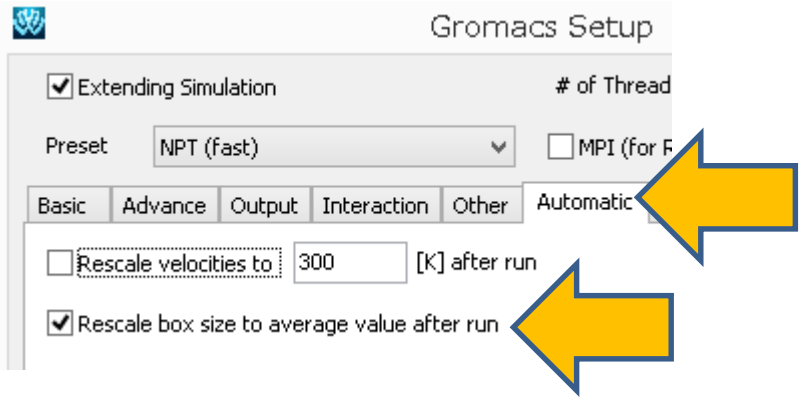
II. Equilibration (D) + Density Adjustment

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. In the **Basic** tab, set **nsteps** to **25000**.
3. In the **Automatic** tab, check box for **Rescale box size…**
3. Click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.





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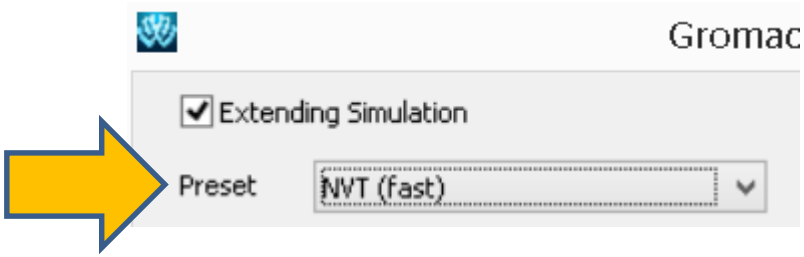
II. Equilibration (E)

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



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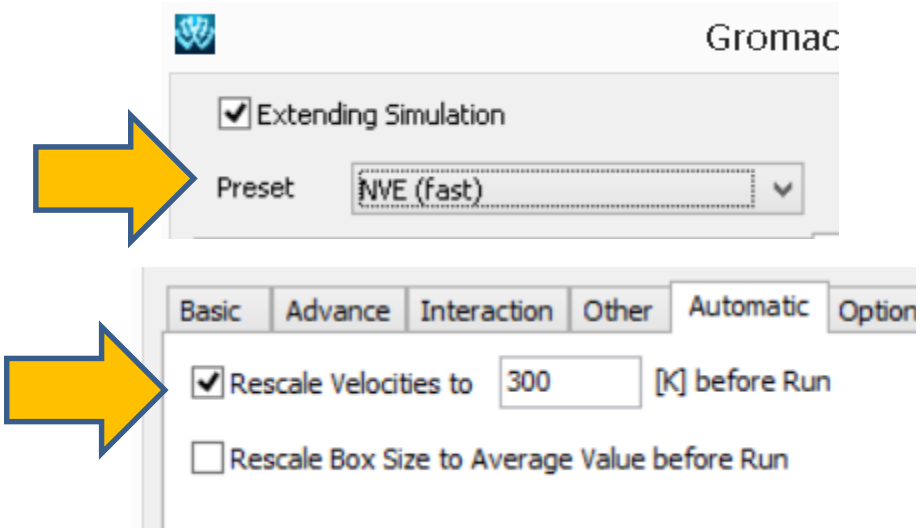
II. Equilibration (F)

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



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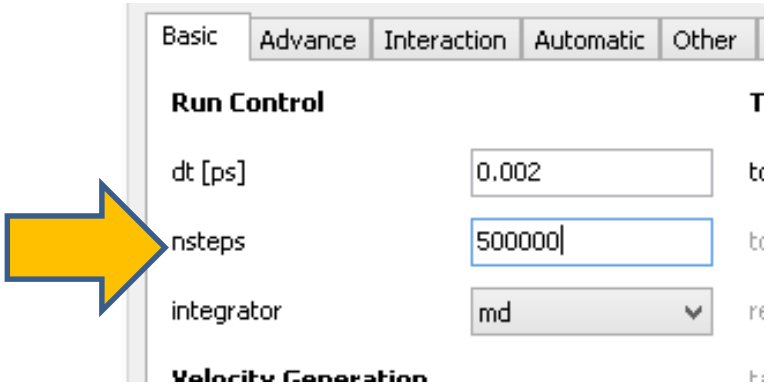
III. Product Run

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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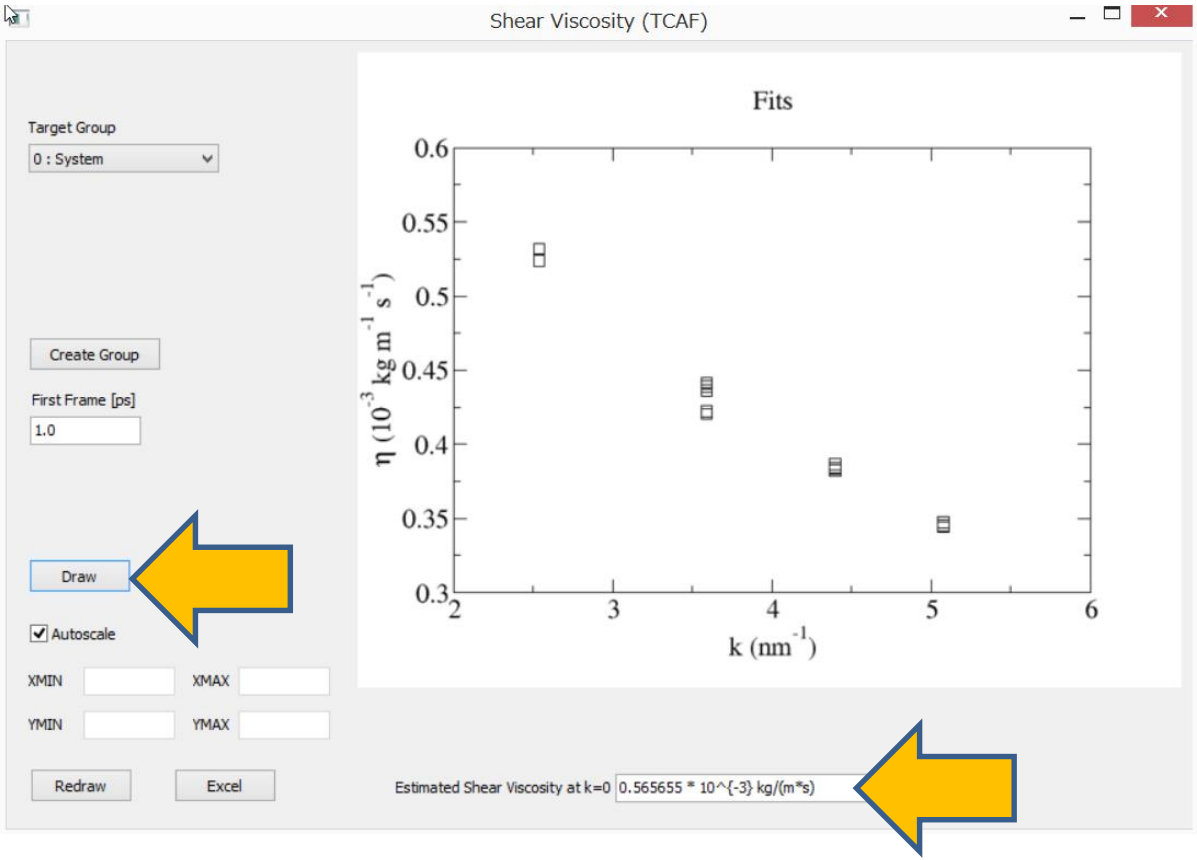
IV. Prediction of Viscosity

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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V. 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.