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Winmostar tutorial

Gromacs

Interfacial Tension

V7.025

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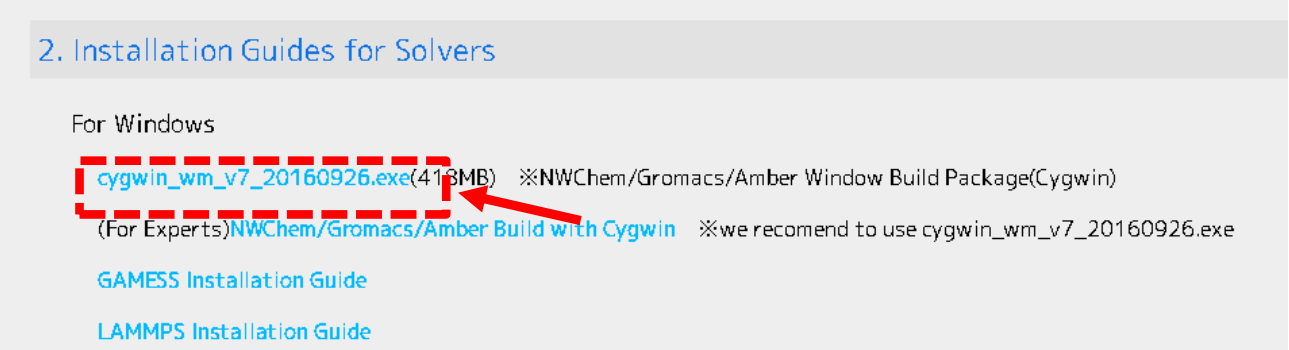
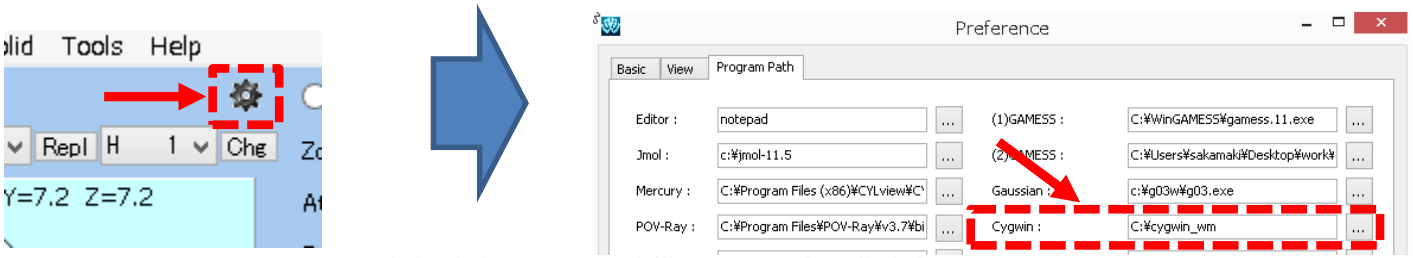
Configure

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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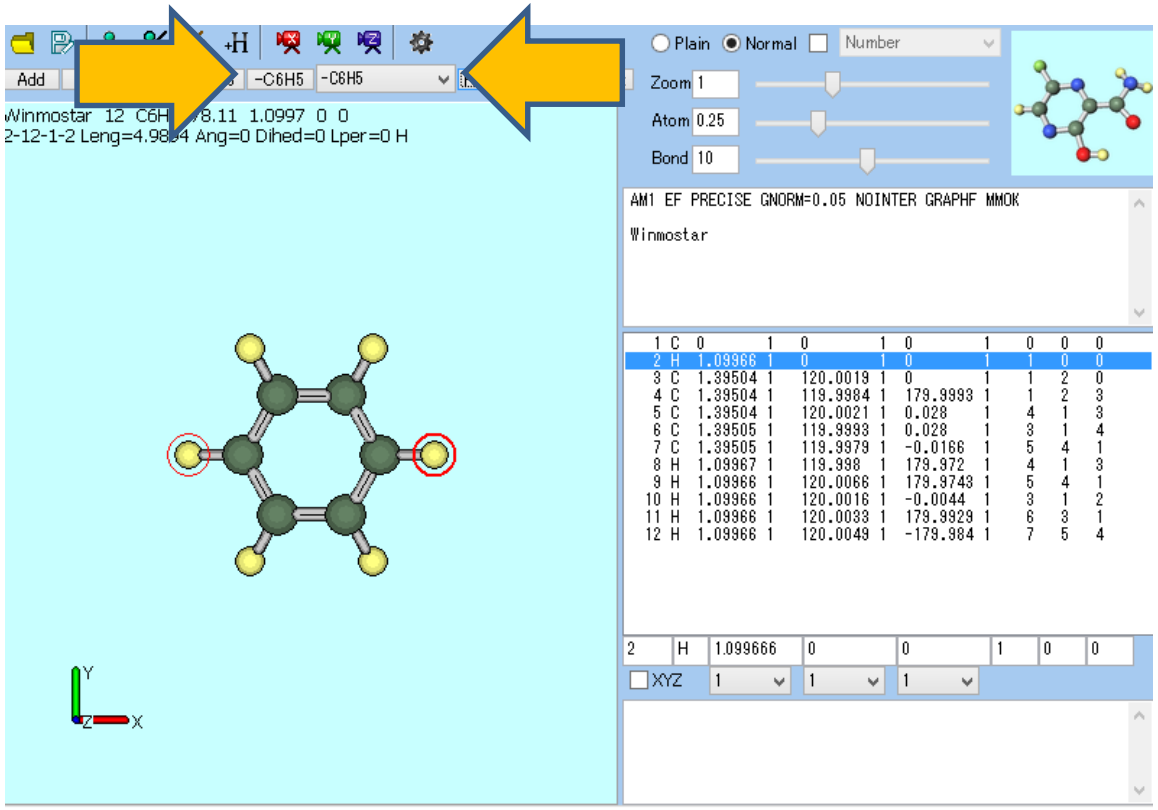
Note

- The simulation steps required are depend on the 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.

I. MD of component 1 liquid phase (modeling)

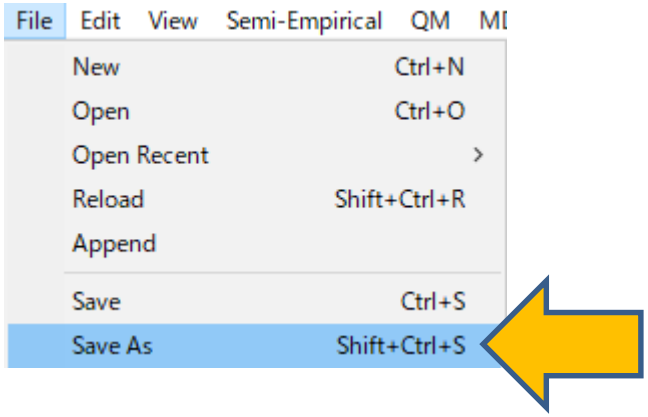
In this tutorial, the component 1 is benzene.

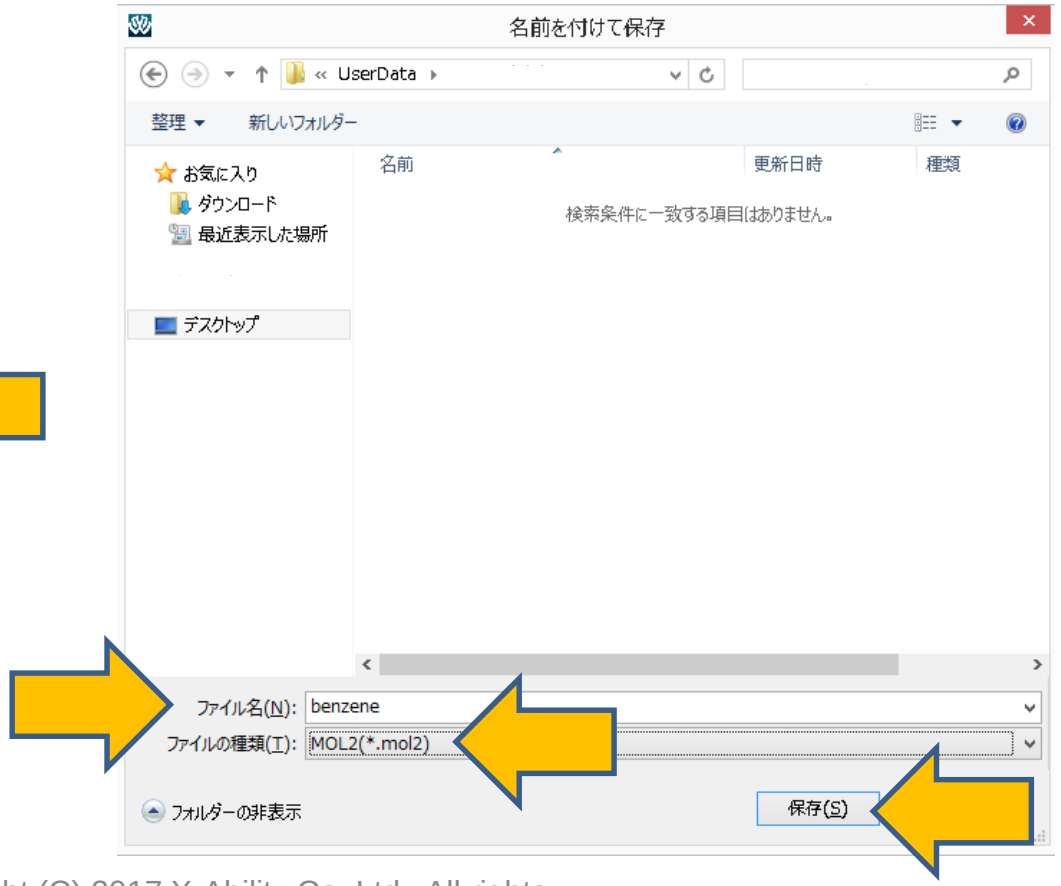
1. Click **−C6H5**.
2. Click **Repl**.



I. MD of component 1 liquid phase (modeling)

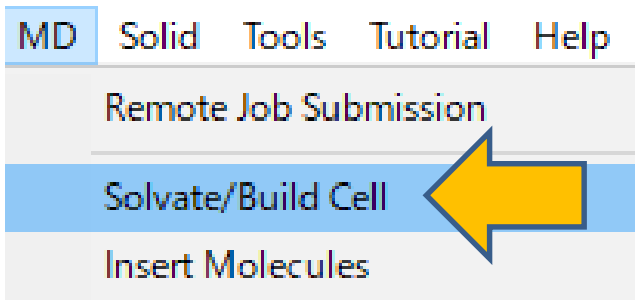
1. Click **File | Save as**.
2. Save as **benzene**. The file extension should be **MOL2**.

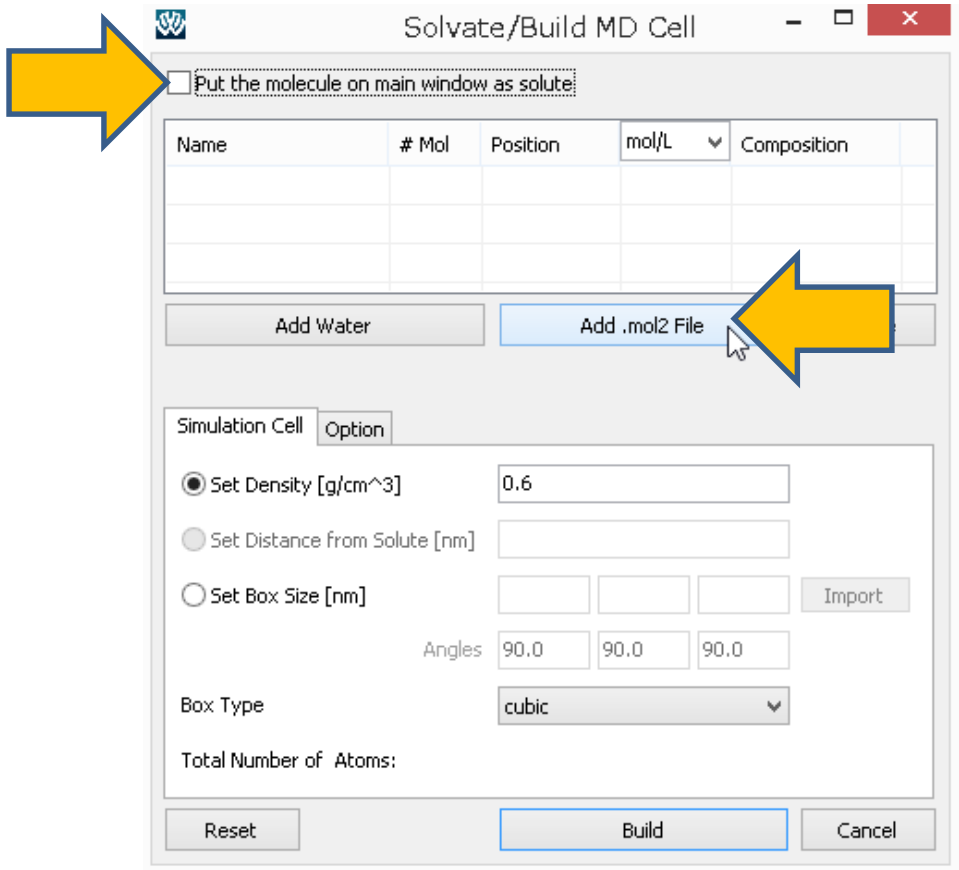




I. MD of component 1 liquid phase (Build Cell)

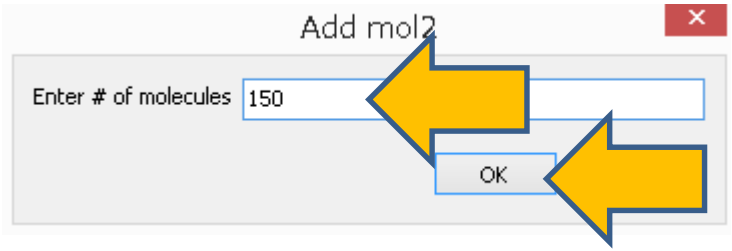
1. Click **MD | Solvate/Build Cell**.
2. Uncheck **Put the molecule on main window as solute**.
3. Click **Add mol2 File**, then select **benzene.mol2**.

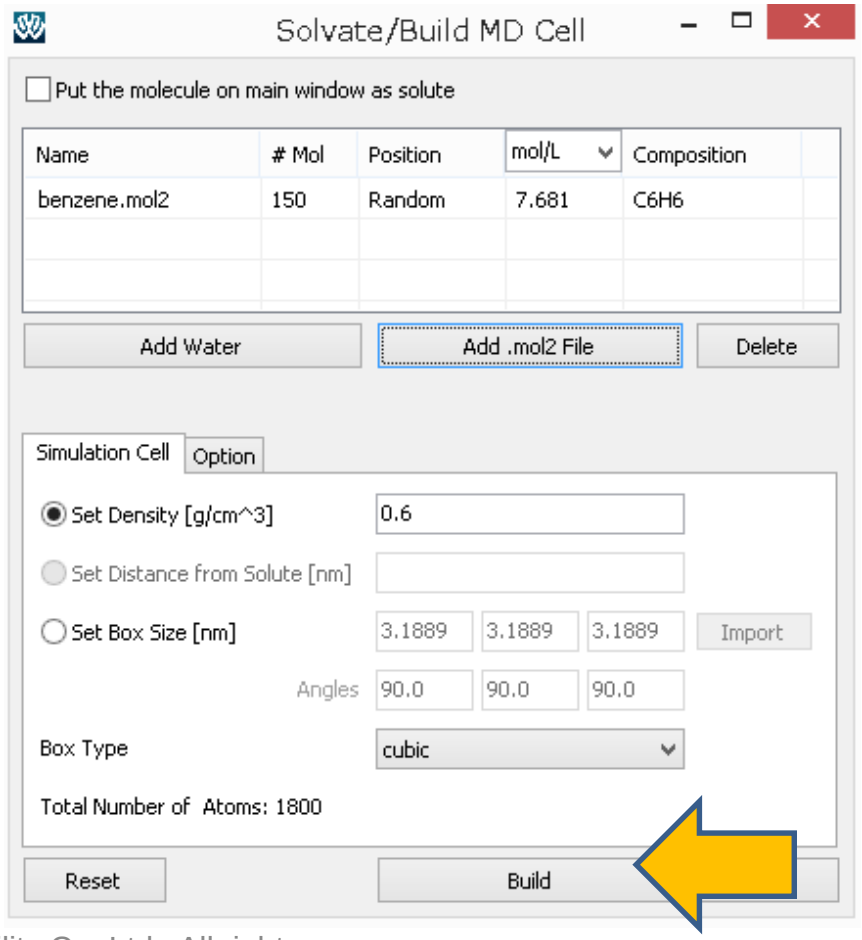




I. MD of component 1 liquid phase (Build Cell)

1. Set **Enter # of molecules** to **150**, then click **OK**.
2. Click **Build**.





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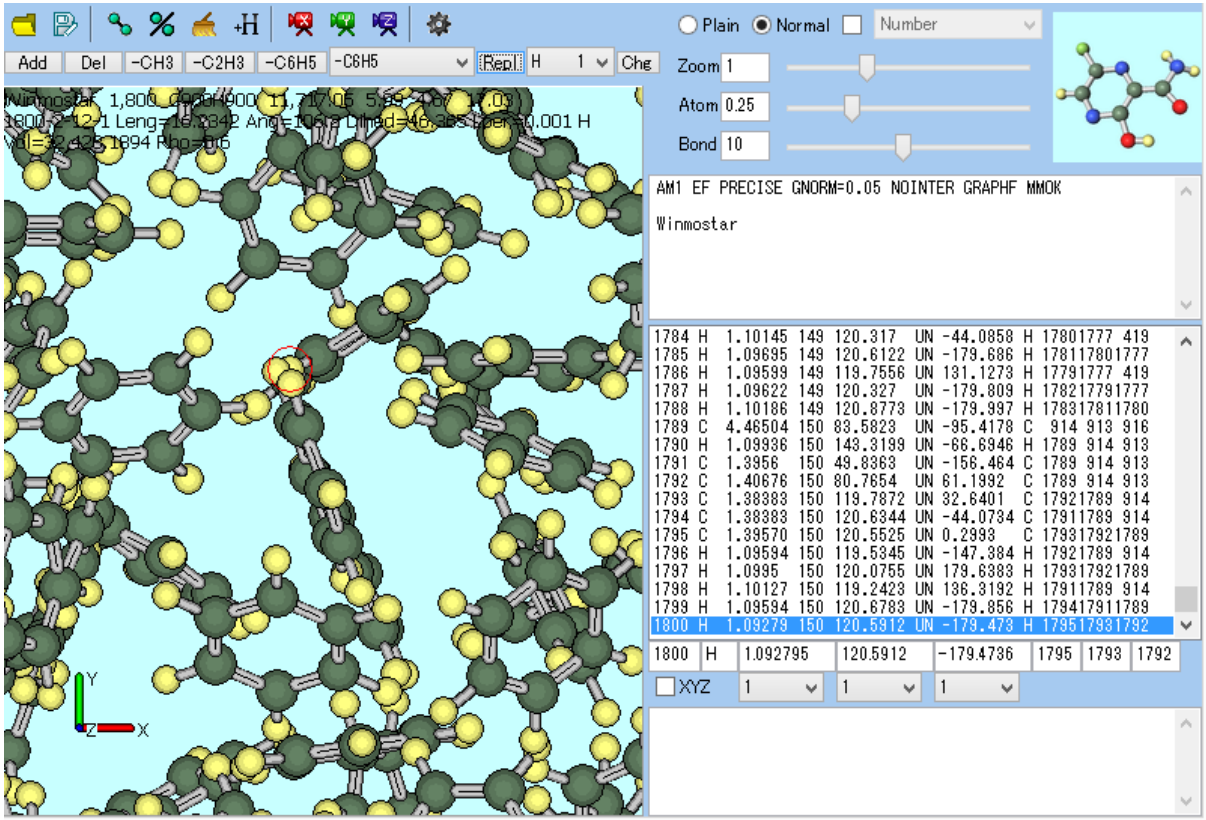
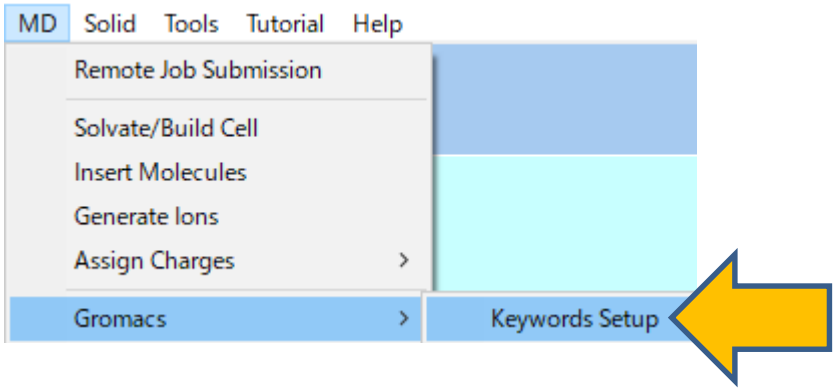
I. MD of component 1 liquid phase （Build Cell）

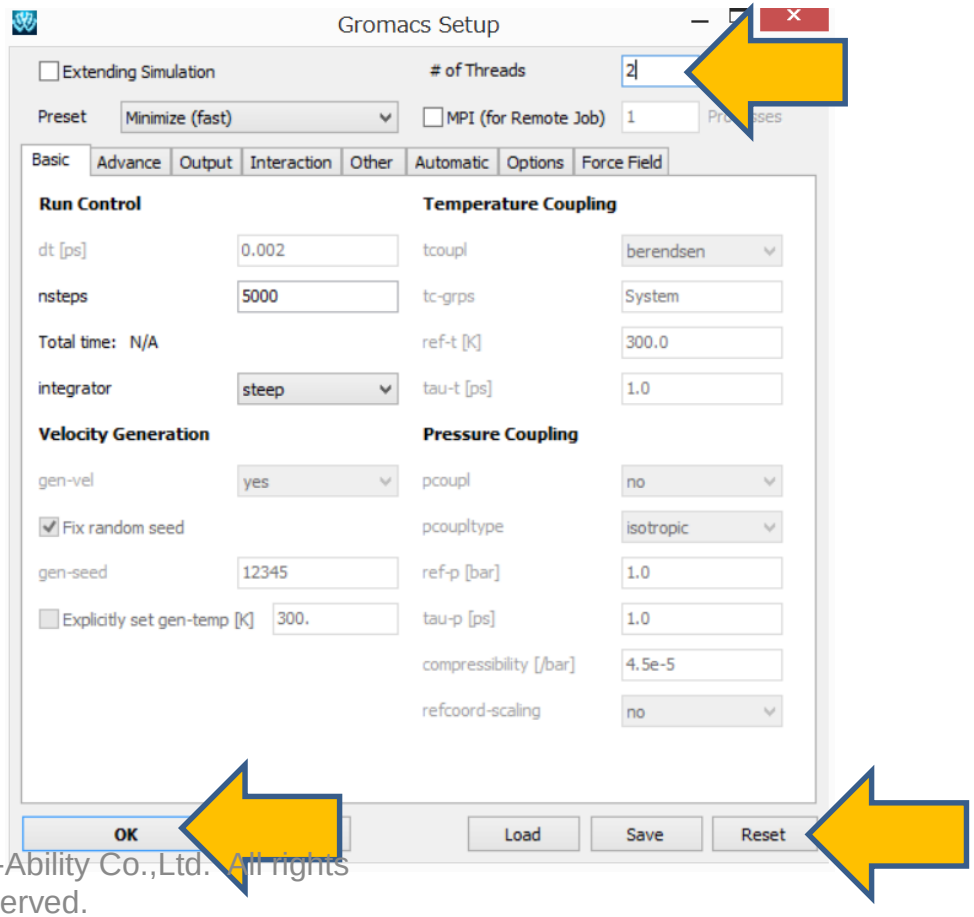
This will be the simulation cell.



I. MD of component 1 liquid phase (Equilibration 1)

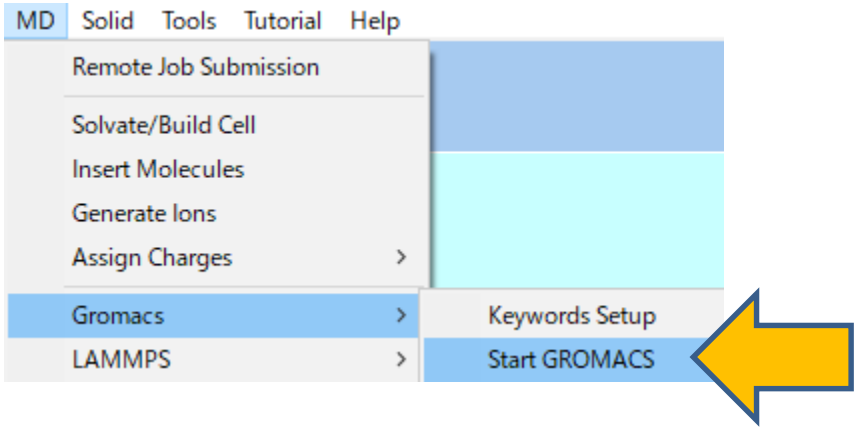
1. Click **MD | Gromacs | Keywords Setup**.
2. Click **Reset**.
3. Set **Preset** to **Minimize (fast)**, **# of Threads** to **parallel number**.
4. Click **OK**.





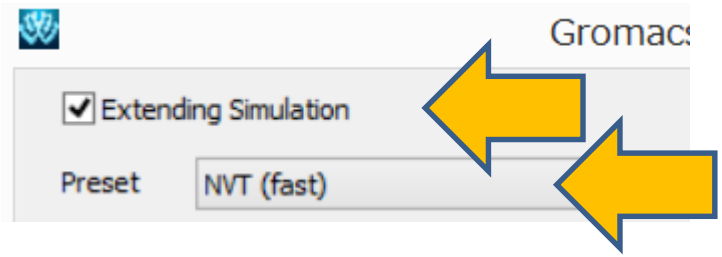
I. MD of component 1 liquid phase （Equilibration 1）

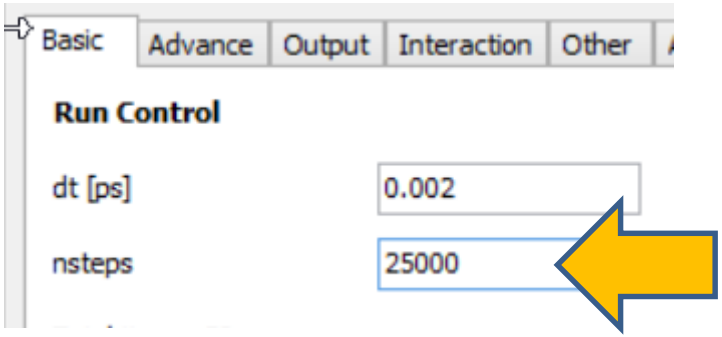
1. Click **MD** | **Gromacs** | **Start Gromacs**.
2. Open the coordinate file **benzene.gro**, and topology file **benzene.top**. Cygwin will launch and Gromacs process will begin.



I. MD of component 1 liquid phase (Equilibration 2)

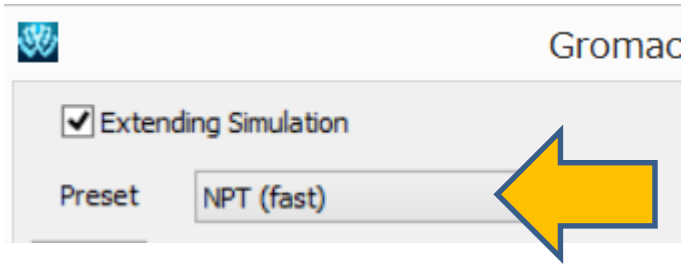
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Check **Extending Simulation**.
3. Set **Preset** to **NVT (fast)**.
4. On **Basic** tab, set **nsteps** to **25000**.
5. On **Advance** tab, set **constraints** to **all-bonds**, then click **OK**.
6. Click **MD | Gromacs | Start Gromacs**.

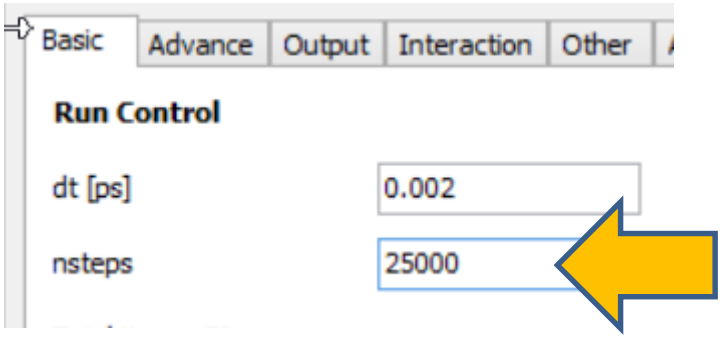




I. MD of component 1 liquid phase (Equilibration 3・Product run)

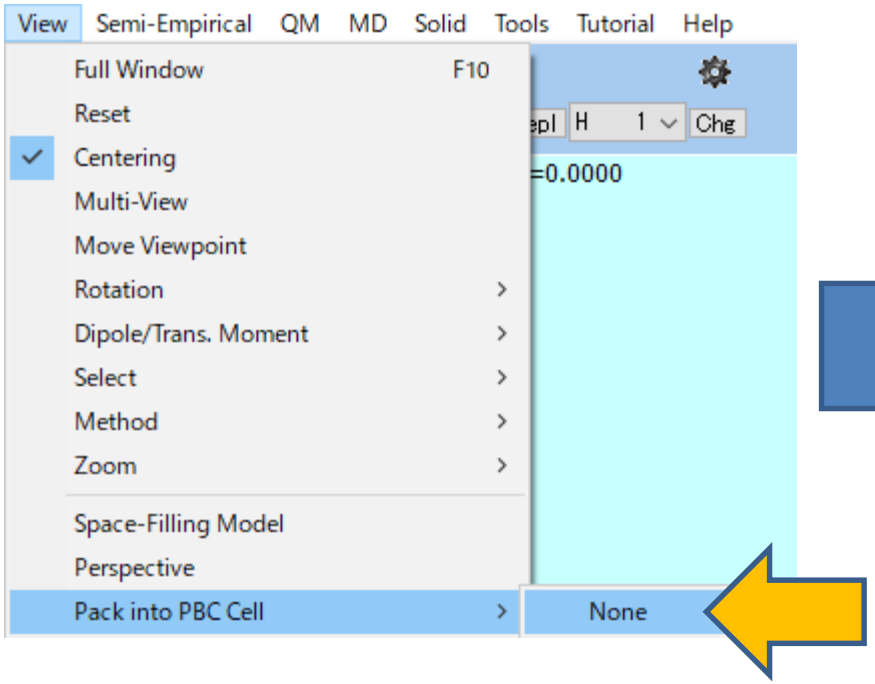
1. Click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NPT (fast)**.
3. On **Basic** tab, set **nsteps** to **25000**.
4. On **Advance** tab, **constraints** to **all-bonds**, then click **OK**.
5. Click **MD** | **Gromacs** | **Start Gromacs**.

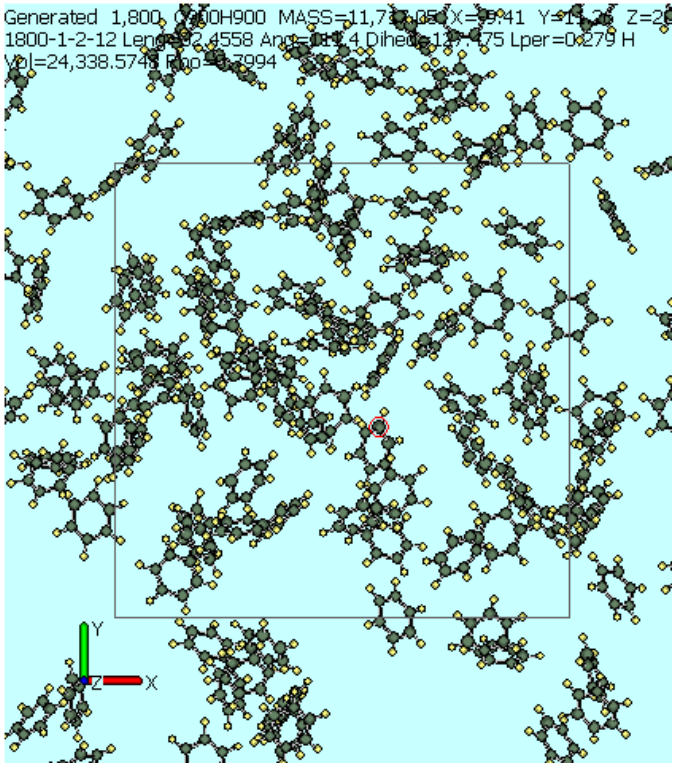




I. MD of component 1 liquid phase (Edit coordinates)

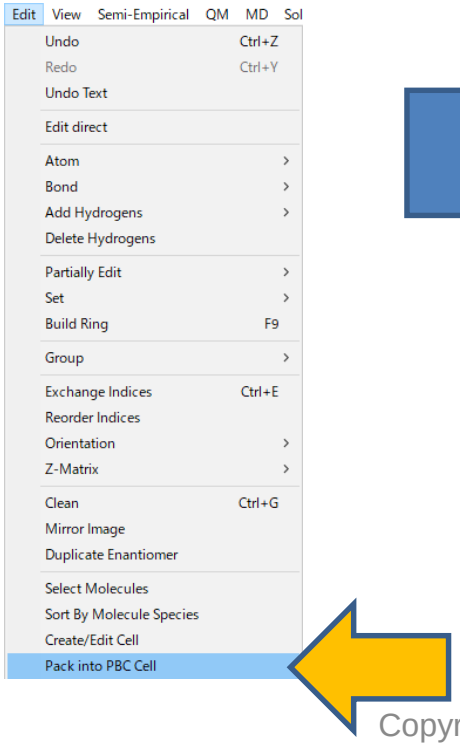
1. Click **MD** | **Gromacs** | **Import .gro File**.
2. Open the file selected by default.
3. Display the final step coordinates.
4. Click **View** | **Pack into PBC Cell** | **None**.

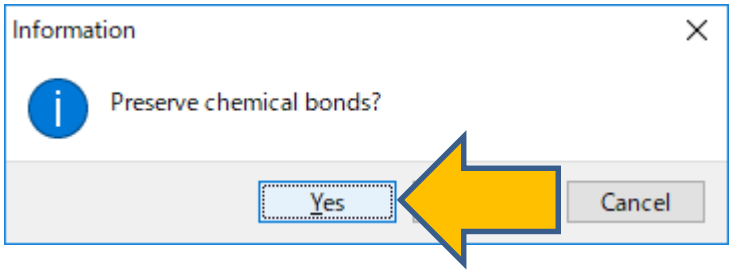


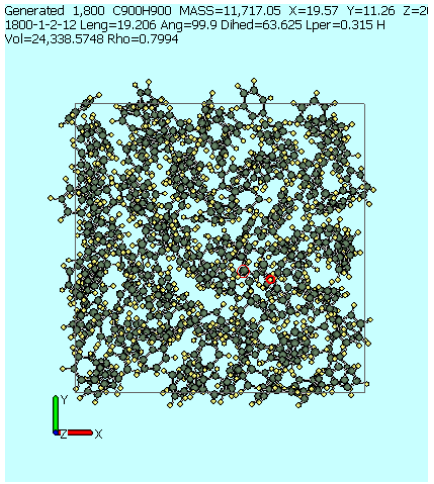


I. MD of component 1 liquid phase (Edit coordinates)

1. Click **Edit | Pack into PBC Cell**.
2. Click **Yes** on the dialog, **“Preserve chemical bonds?”**.
   Confirm that all molecules were packed into the cell.
3. Click **File | Save as**.
4. Save as **benzene_eq.mol2**.

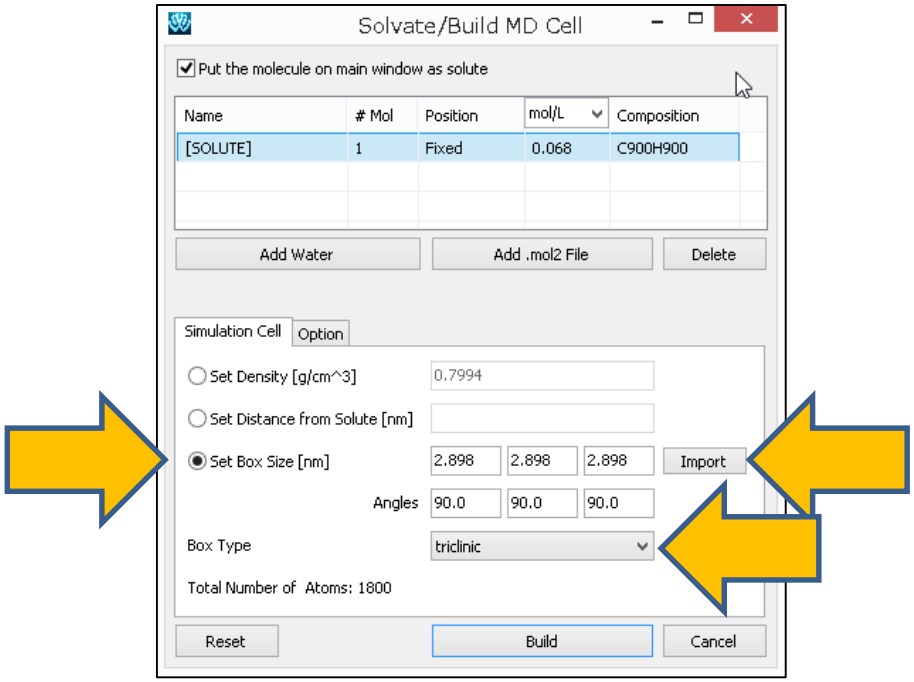






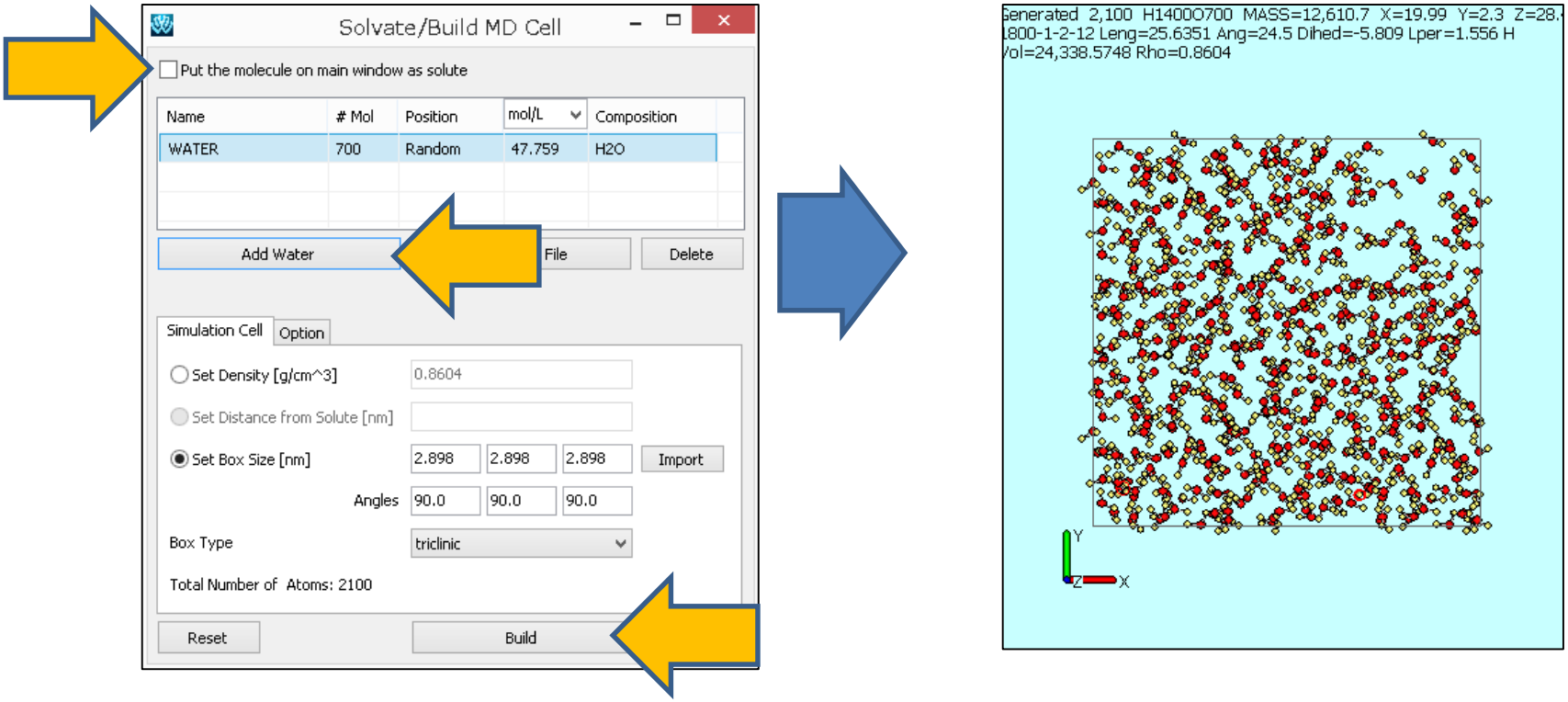
II. MD of component 2 liquid phase (Build cell)

1. Click **MD | Solvate/Build Cell**.
2. Click **Set Box Size**.
3. Click Import.
4. Set **Box Type** to **Triclinic**.



II. MD of component 2 liquid phase (Build cell)

1. Uncheck **Put the molecule on main window as solute**.
2. Click **Add Water**.
3. Set **Enter # of molecules** to **700**, then click **OK**.
4. Click **Build**.



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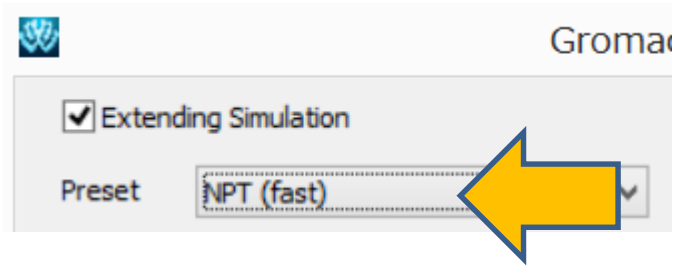
II. MD of component 2 liquid phase （Equilibration 1&2）

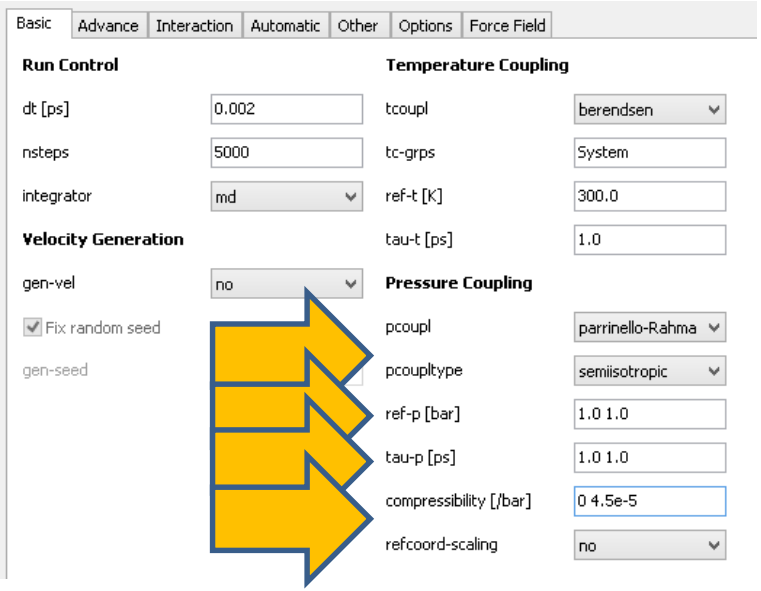
1. Click **MD | Gromacs | Keywords Setup**.
2. Uncheck **Extending Simulation**.
3. Set **Preset** to **Minimize (fast)**.
4. Click **OK**.
5. Click **MD | Gromacs | Start Gromacs**.
6. Save as **water.gro**, and **water.top**.

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

II. MD of component 2 liquid phase (Equilibration 3)

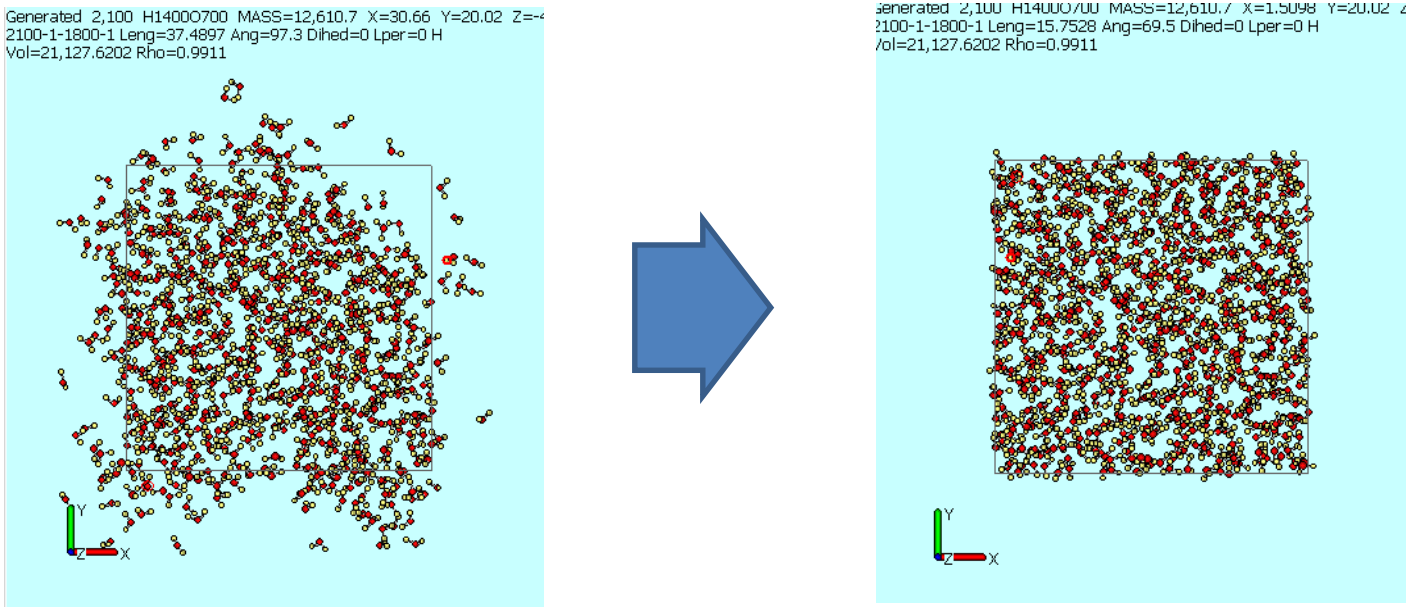
1. Click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NPT (fast)**.
   - Set **pcoupltype** to **semiisotropic**.
   - Set **ref-p** to **1.0 1.0**.
   - Set **tau-p** to **1.0 1.0**.
   - Set **compressibility** to **0 4.5e-5**.
3. Click **MD | Gromacs | Start Gromacs**.





II. MD of component 2 liquid phase (Edit coordinates)

1. Click **MD | Gromacs | Import .gro File**.
2. Open the file selected by default.
3. Display the final step coordinates.
4. Click **Edit | Pack into PBC Cell**.
5. Click **Yes** on the dialog, "**Preserve chemical bonds?**"
6. Click **File | Save as**.
7. Save as **water_eq.mol2**.



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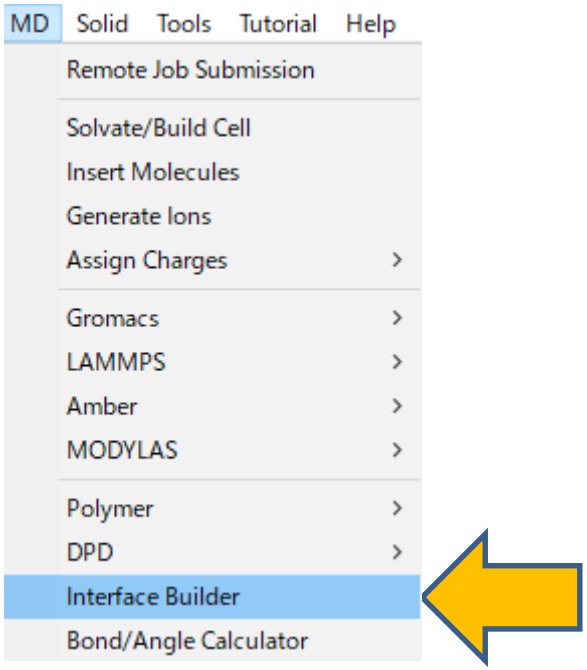
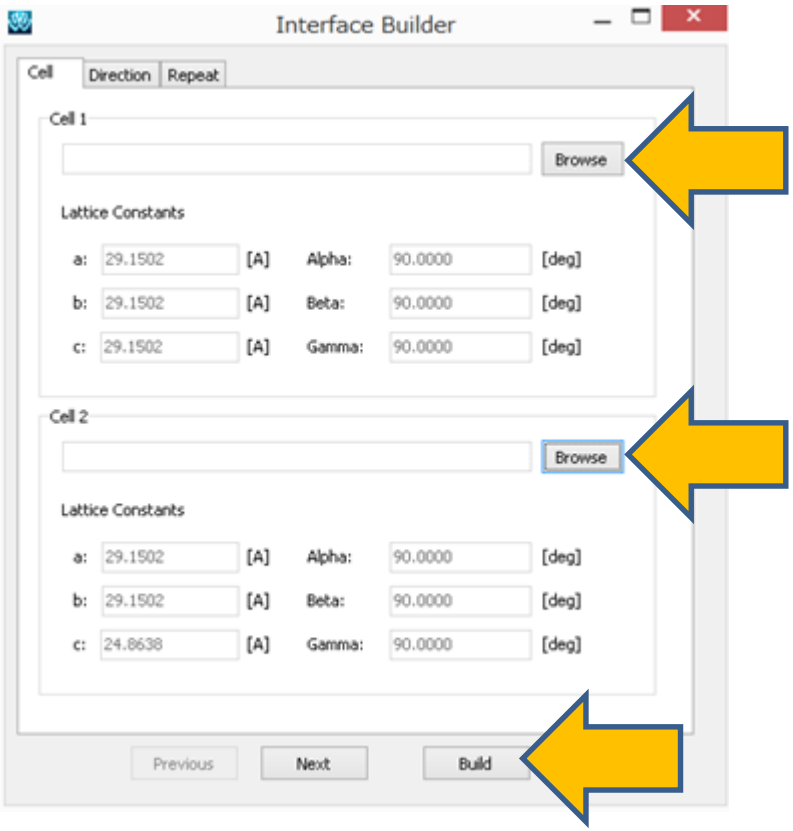
III. MD of interfacial system (Build cell)

1. Click **MD | Interface Builder**.
2. Click **Browse** of **Cell 1**, then open **benzene_eq.mol2**.
3. Click **Browse** of **Cell 2**, then open **water_eq.mol2**.
4. Click **Build**.





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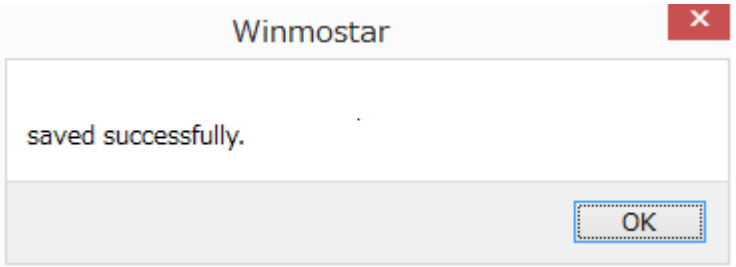
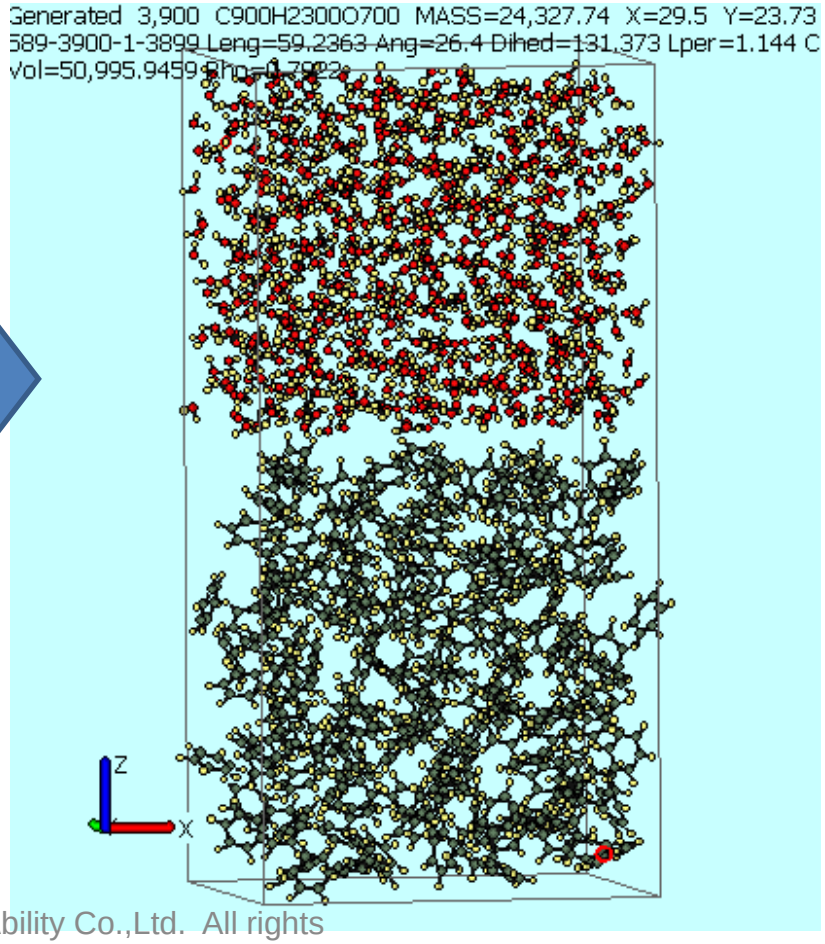
III. MD of interface system (Build cell)

1. Save as **interface.mol2**.
2. After the dialog “saved successfully,”
   Click **Close** of **Interface Builder**.





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III. MD of interface system (Equilibration 1~3)

1. Click **MD** | **Gromacs** | **Keywords Setup**.
2. Uncheck **Extending Simulation**.
3. Set **Preset** to **Minimize (fast)**, then click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.
5. Save as **interface.gro** and **interface.top**.

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Check **Extending Simulation**.
3. Set **Preset** to **NVT (fast)**.
4. On **Advance** tab, set **constraints** to **all-bonds**, then click **OK**.
5. Click **MD** | **Gromacs** | **Start Gromacs**.

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **Preset** to **NPT**.
3. On **Basic** tab, set **pcoupltype** to **semiisotropic**,
   ref-p to **1.0 1.0**, **tau-p** to **1.0 1.0**., **compressibility** to **0 4.5e-5**.
4. On **Advance** tab, set **constraints** to **all-bonds**, then click **OK**.
5. Click **MD** | **Gromacs** | **Start Gromacs**.

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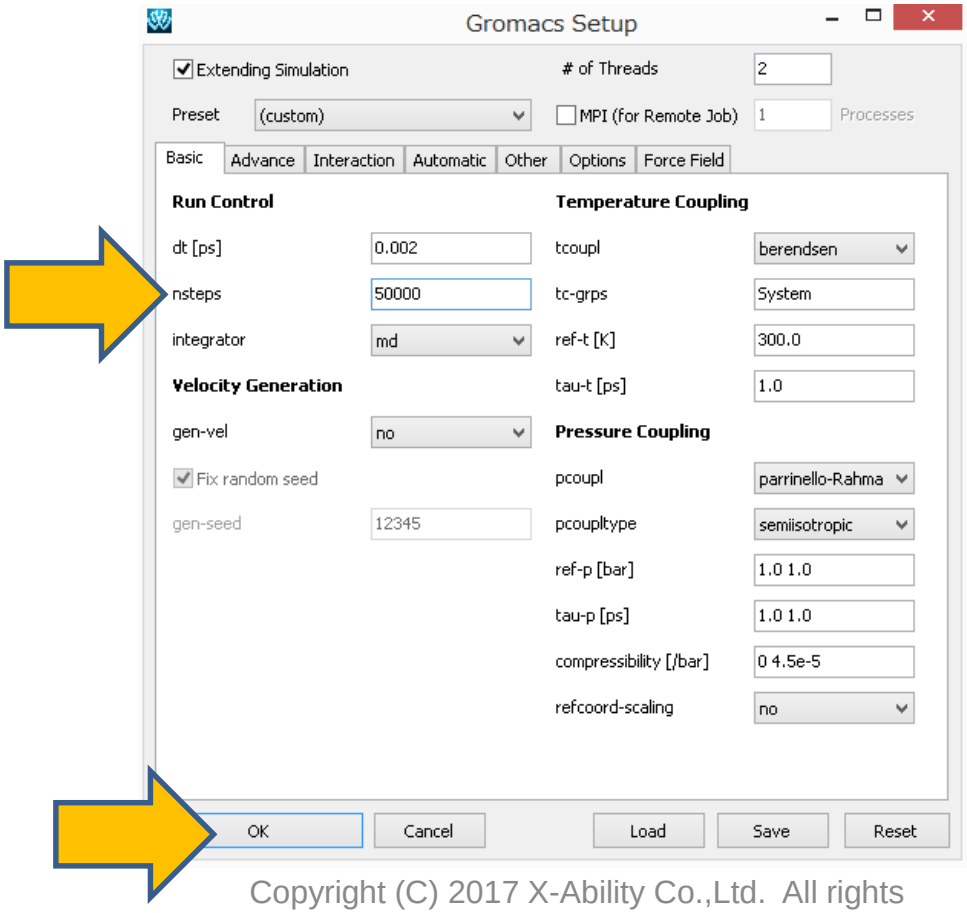
III. MD of interface system （Product run）

1. After the calculation, Click **MD | Gromacs | Keywords Setup**.
2. On **Basic** tab, set **nsteps** to **50000**, then click **OK**.
3. Click **MD | Gromacs | Start Gromacs**.



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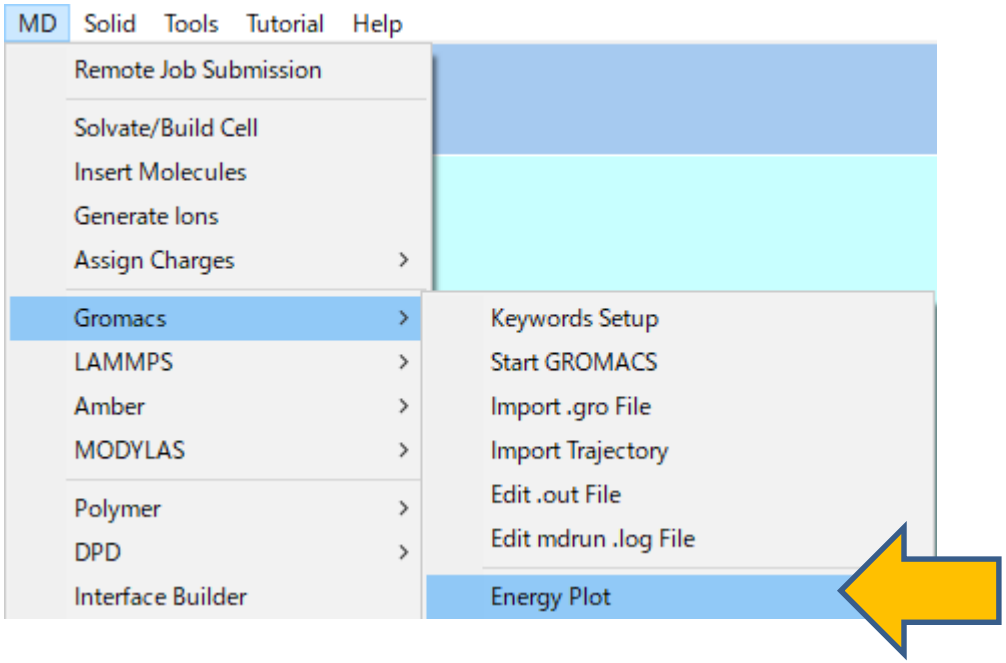
IV. Processing results

1. Click **MD** | **Gromacs** | **Energy Plot**.
2. Open the file selected by default.



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IV. Processing results

1. Click Calc Ave.
2. Open the file selected by default.
3. The value at "#Surf*SurfTen" shows the product of interfacial tension and number of interfaces within a system in the unit of 1 bar*nm = 0.1 mN/m.