

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.

2. Installation Guides for Solvers

For Windows

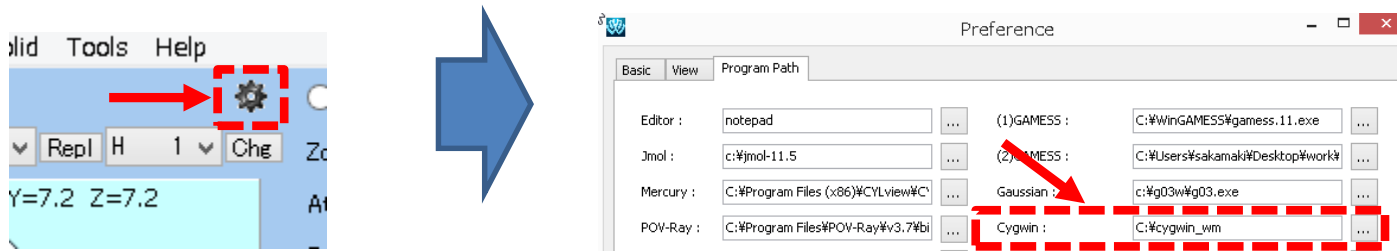
[cygwin_wm_v7_20160926.exe\(413MB\)](#) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(For Experts)[NWChem/Gromacs/Amber Build with Cygwin](#) ※we recomend to use cygwin_wm_v7_20160926.exe

[GAMESS Installation Guide](#)

[LAMMPS Installation Guide](#)

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



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.

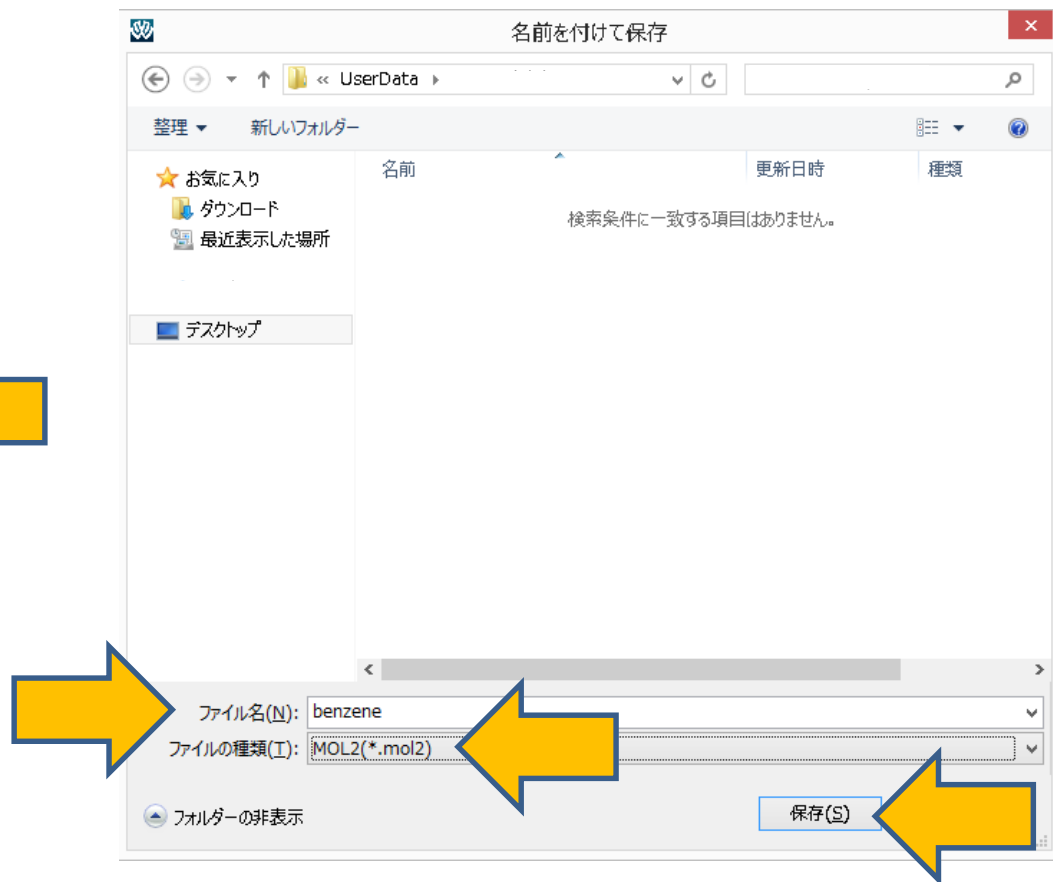
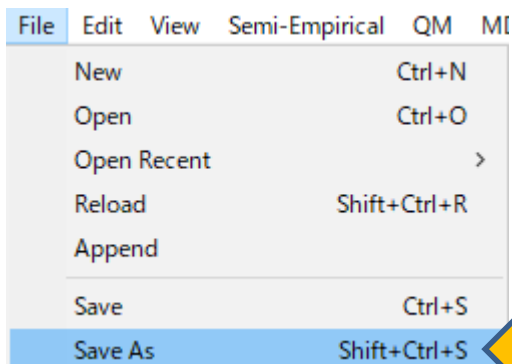
1. Click **-C6H5**.
2. Click **Repl.**

Winmostar 12 C6H5 8.11 1.0997 0 0
2-12-1-2 Leng=4.9804 Ang=0 Dihed=0 Lper=0 H

1	C	0	1	0	1	0	1	0	0	0
2	H	1.099666	1	0	1	0	1	0	0	0
3	C	1.39504	1	120.0019	1	0	1	1	2	0
4	C	1.39504	1	119.9984	1	179.9993	1	1	2	3
5	C	1.39504	1	120.0021	1	0.028	1	4	1	3
6	C	1.39505	1	119.9993	1	0.028	1	3	1	4
7	C	1.39505	1	119.9979	1	-0.0166	1	5	4	1
8	H	1.09967	1	119.998	1	179.972	1	4	1	3
9	H	1.09966	1	120.0066	1	179.9743	1	5	4	1
10	H	1.09966	1	120.0016	1	-0.0044	1	3	1	2
11	H	1.09966	1	120.0033	1	179.9929	1	6	3	1
12	H	1.09966	1	120.0049	1	-179.984	1	7	5	4

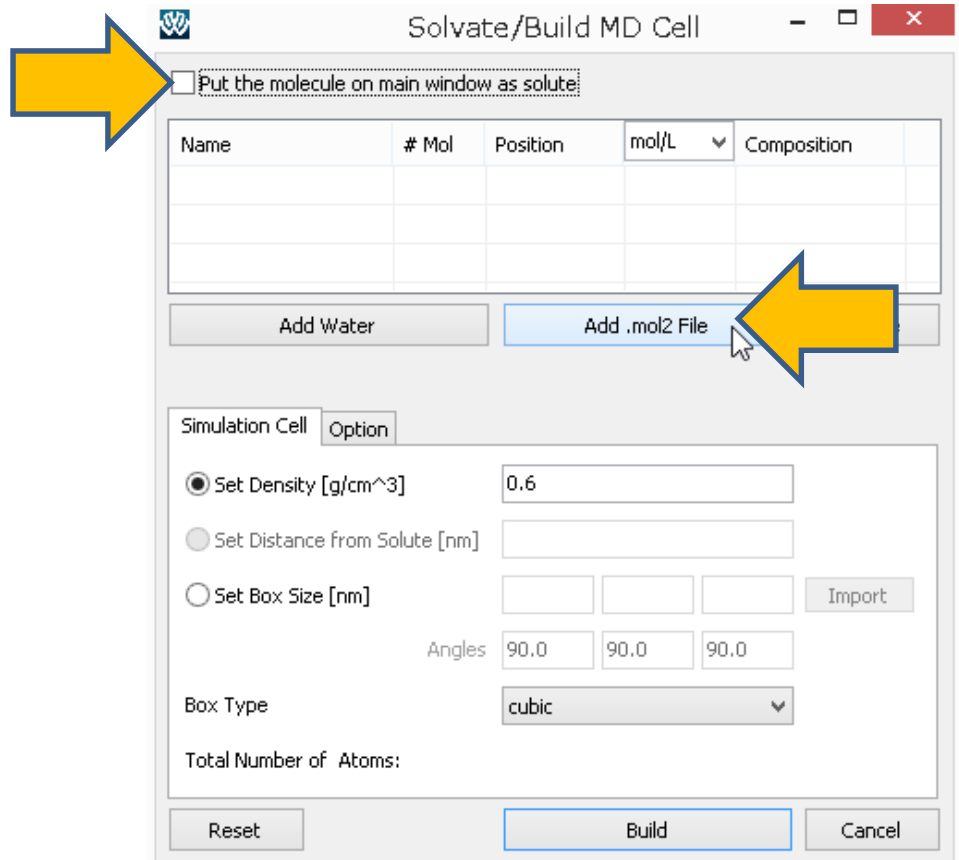
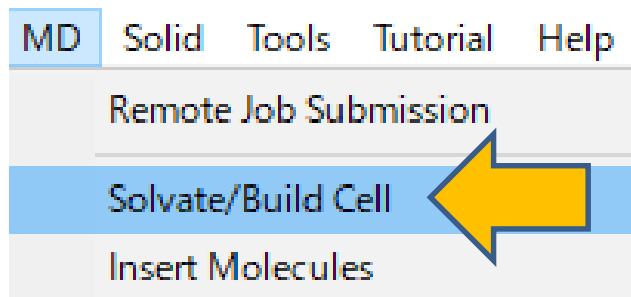
I. MD of component 1 liquid phase (modeling)

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



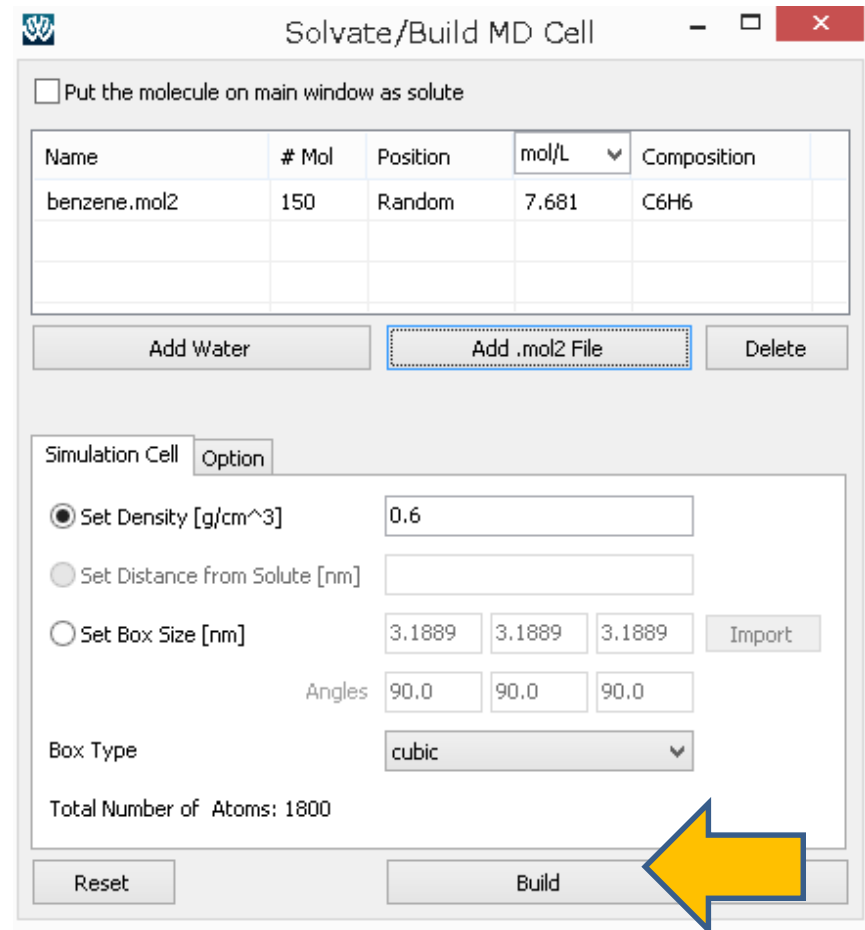
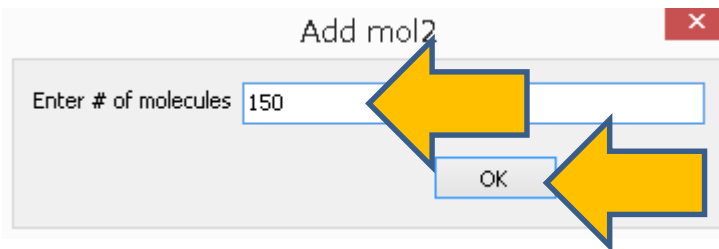
I. MD of component 1 liquid phase (Build Cell)

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**.



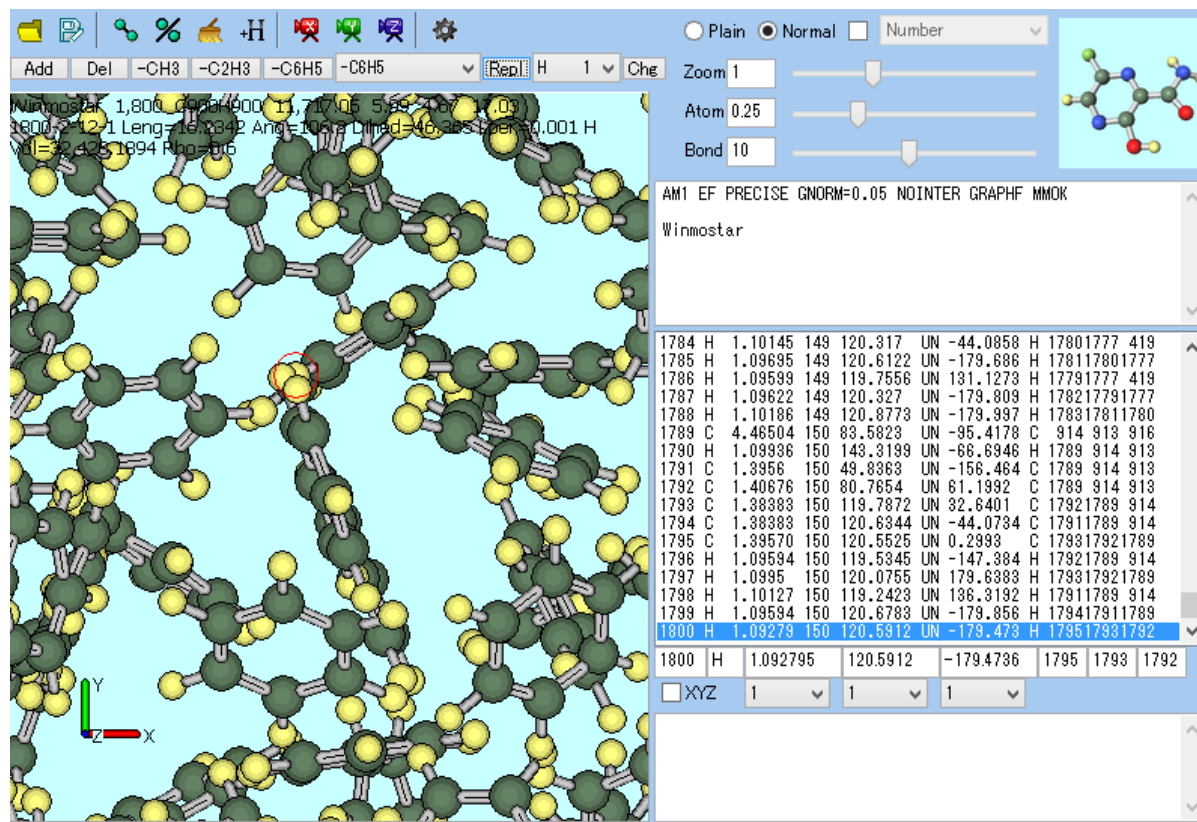
I. MD of component 1 liquid phase (Build Cell)

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



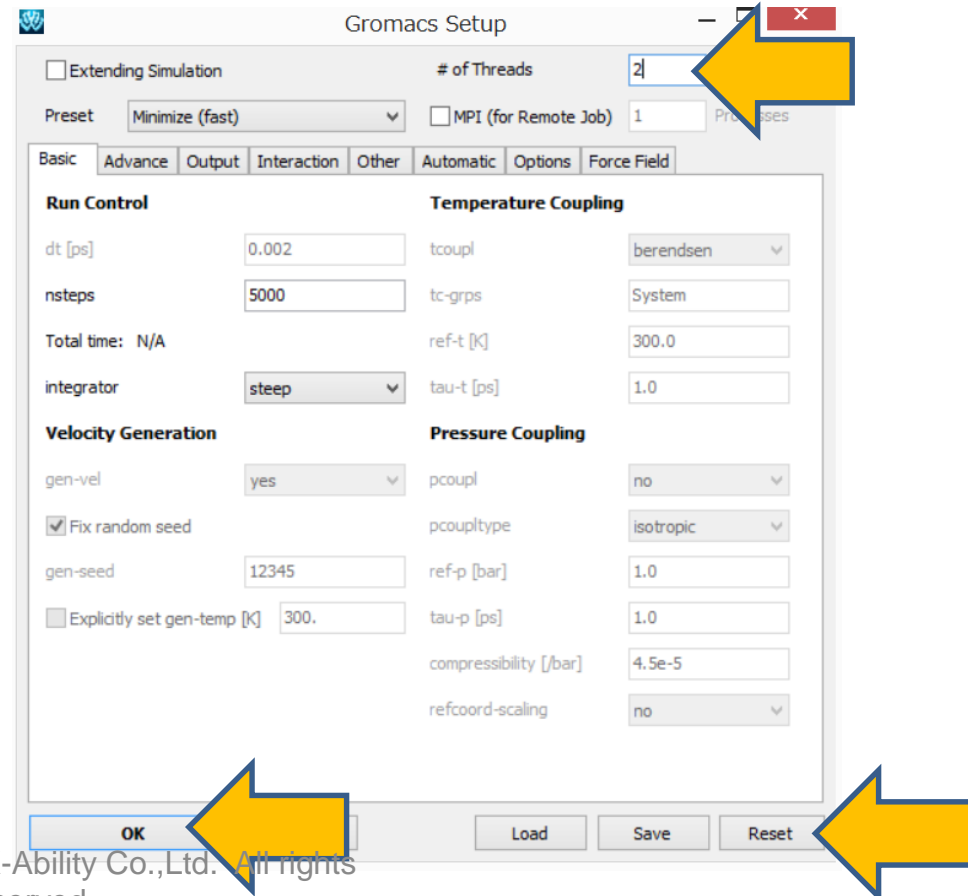
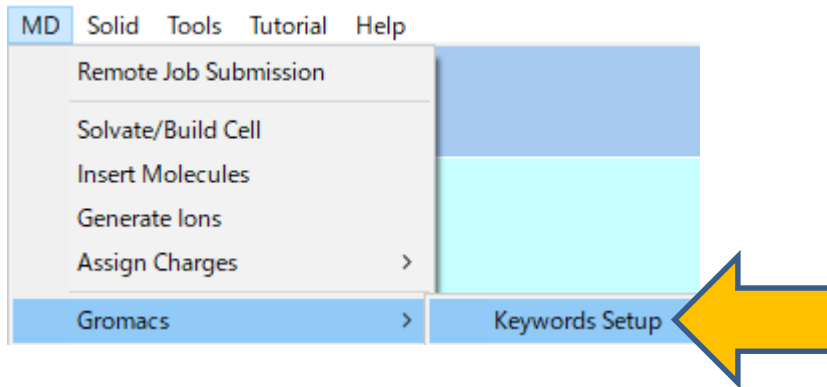
I. MD of component 1 liquid phase (Build Cell)

This will be the simulation cell.



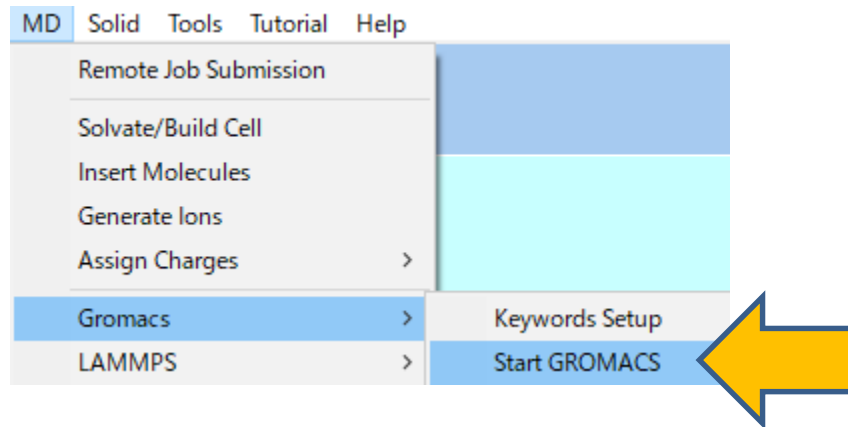
I. MD of component 1 liquid phase (Equilibration 1)

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



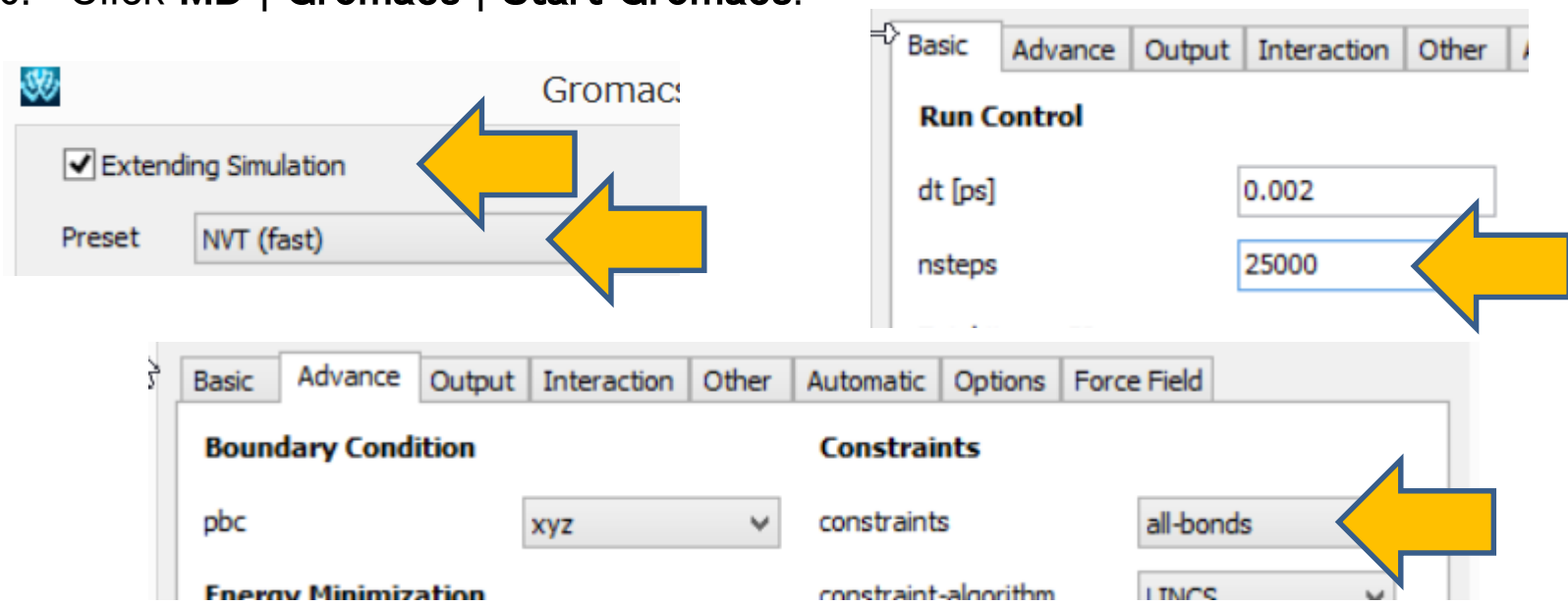
I. MD of component 1 liquid phase (Equilibration 1)

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.



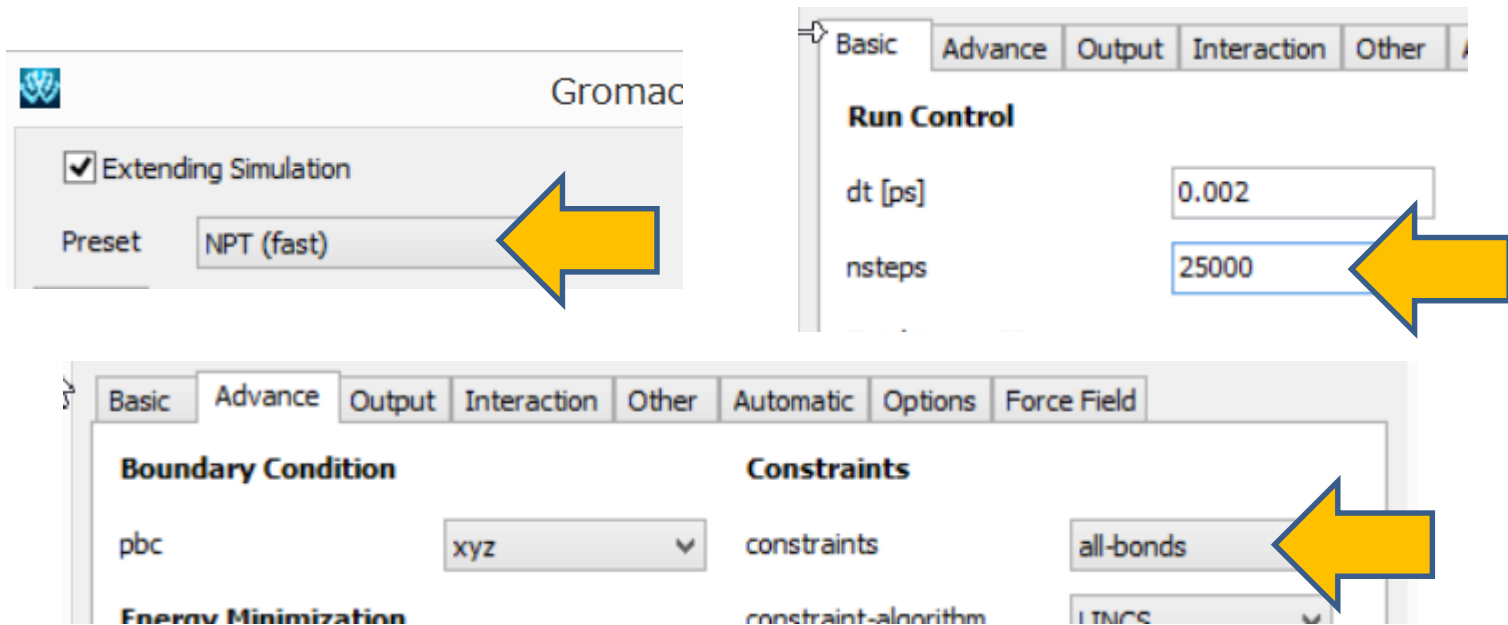
I. MD of component 1 liquid phase (Equilibration 2)

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**.



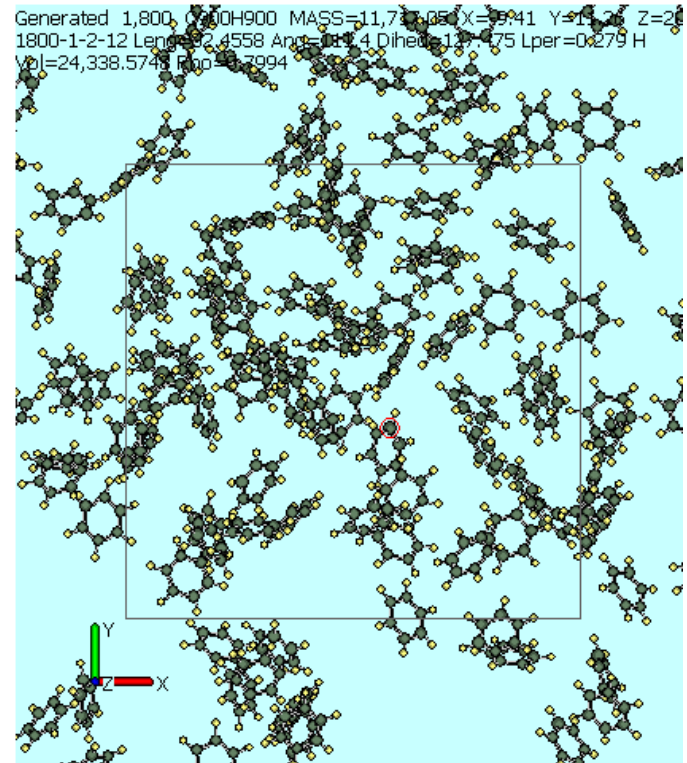
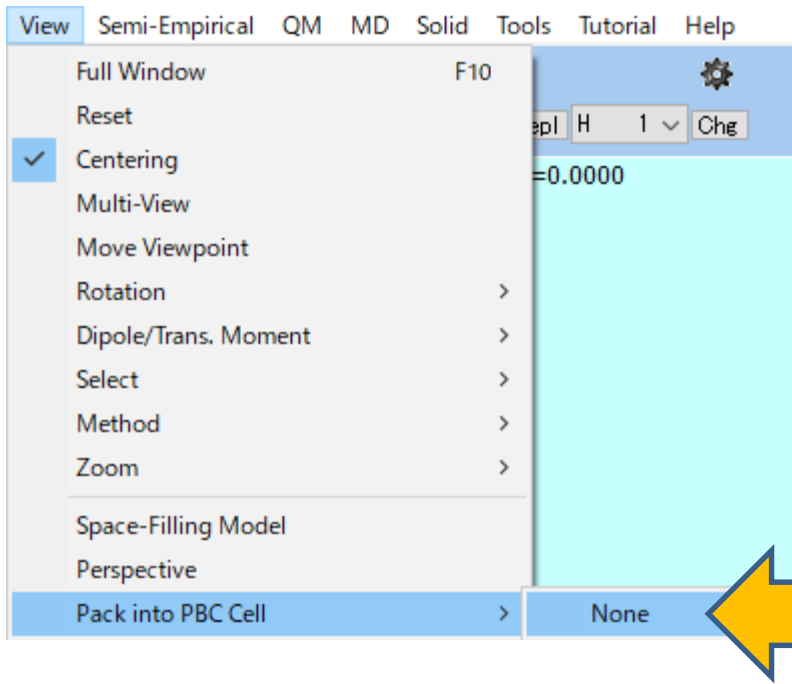
I. MD of component 1 liquid phase (Equilibration 3・Product run)

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**.



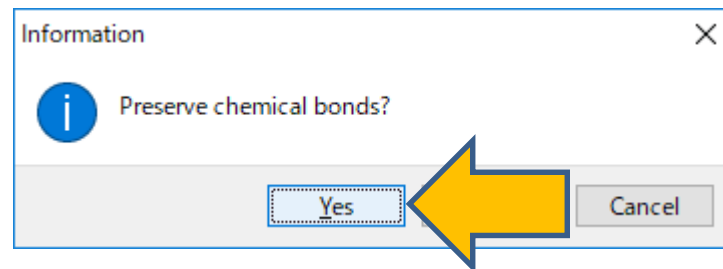
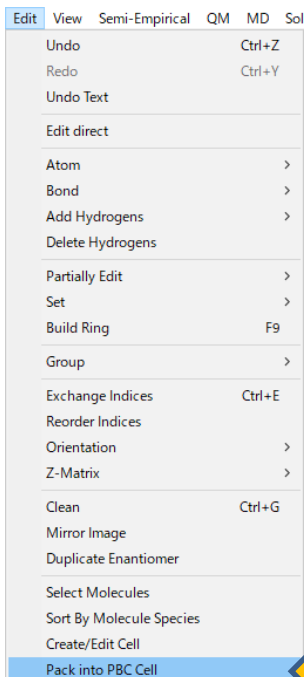
I. MD of component 1 liquid phase (Edit coordinates)

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**.

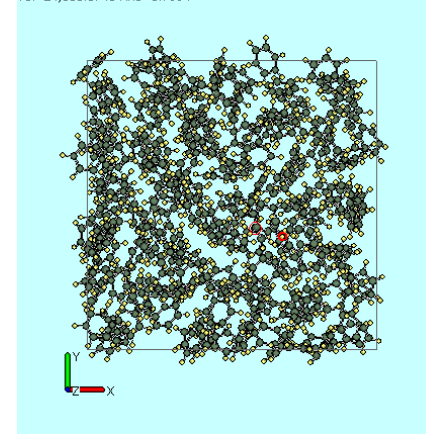


I. MD of component 1 liquid phase (Edit coordinates)

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**.

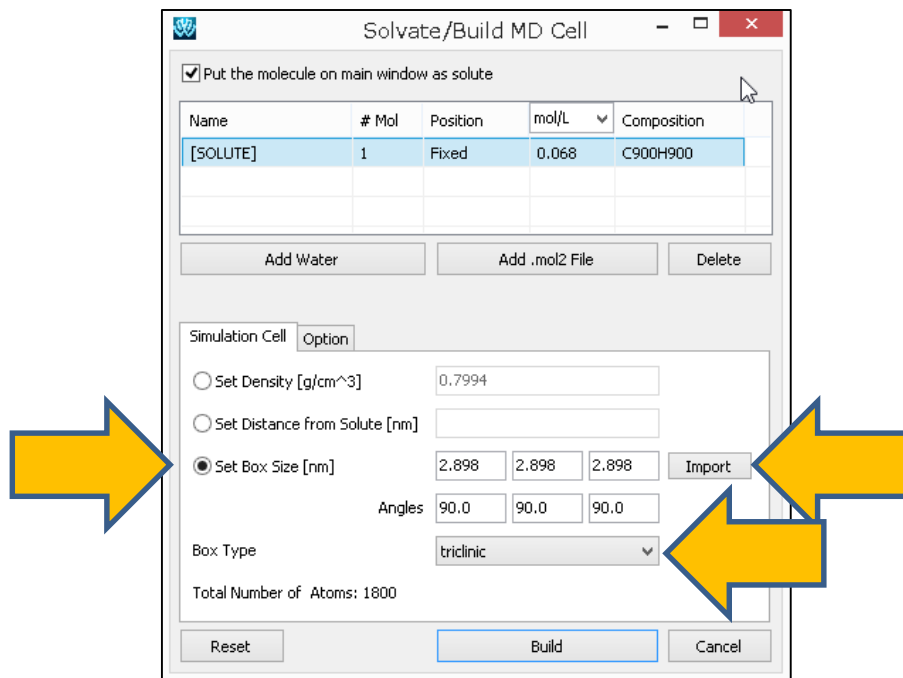


Generated 1,800 C900H900 MASS=11,717.05 X=19.57 Y=11.26 Z=2
1800-1-2-12 Leng=19.206 Ang=99.9 Dihed=63.625 Lper=0.315 H
Vol=24,338.5748 Rho=0.7994



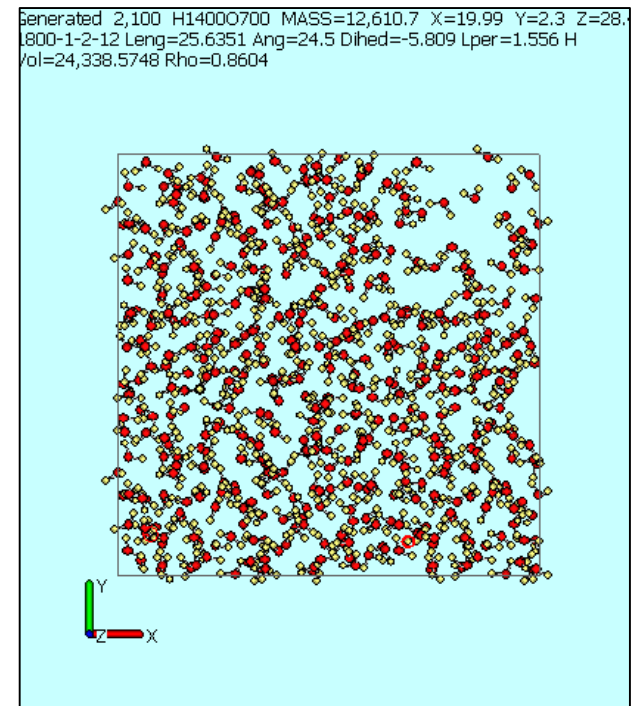
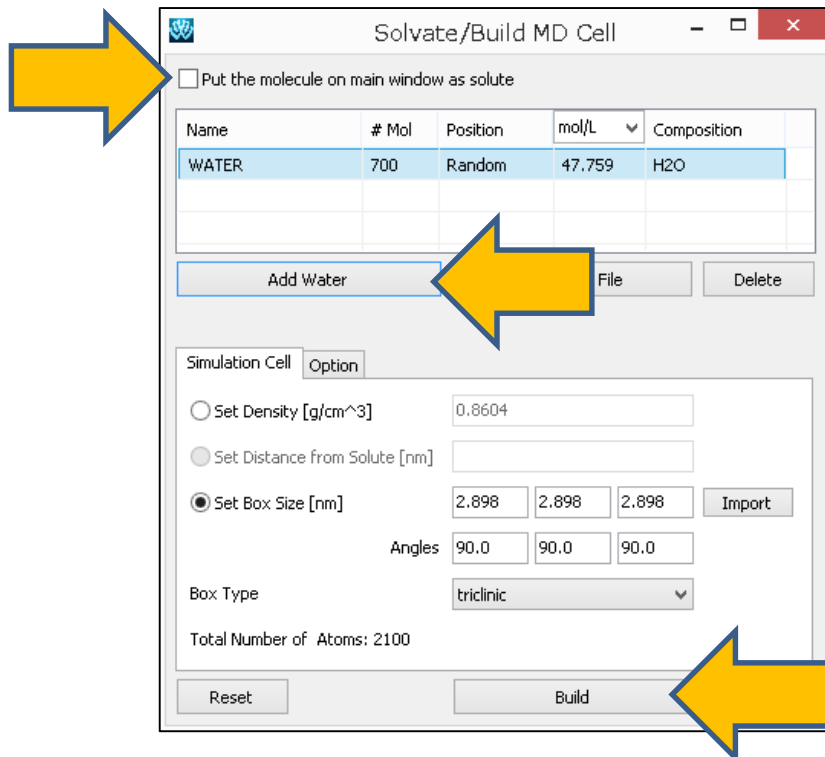
II. MD of component 2 liquid phase (Build cell)

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**.

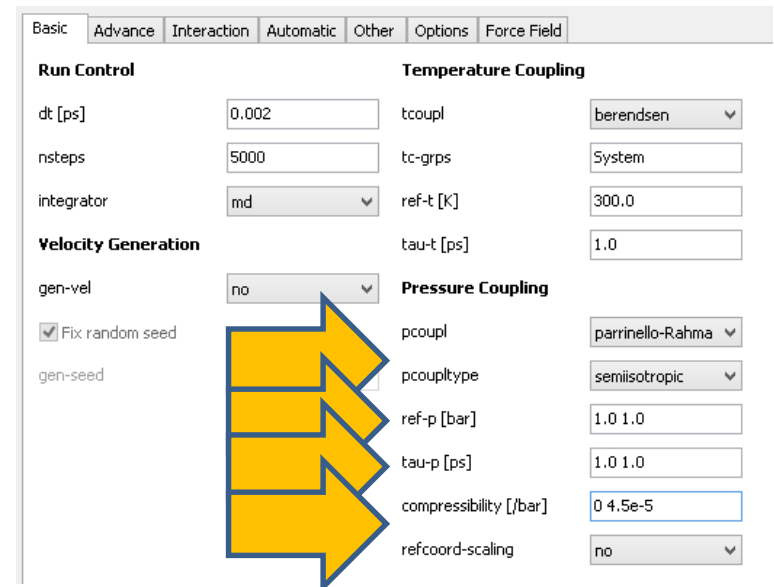
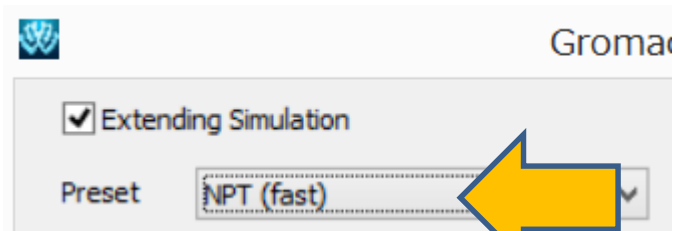


II. MD of component 2 liquid phase (Equilibration 1&2)

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**.

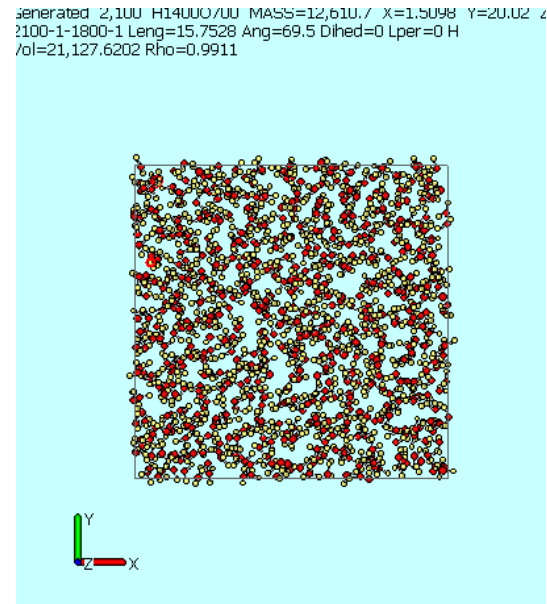
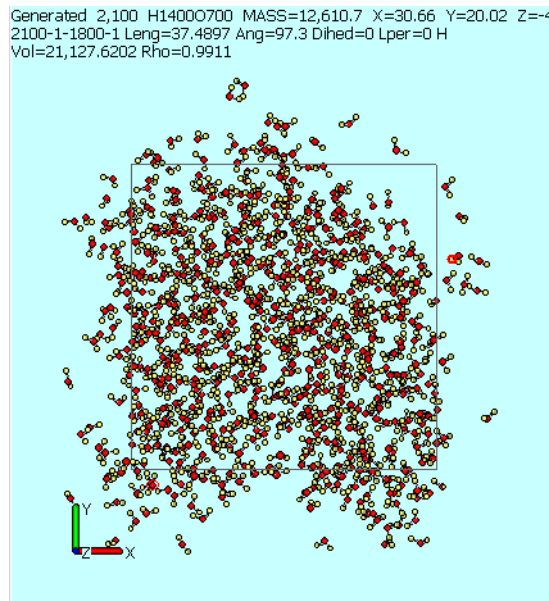
II. MD of component 2 liquid phase (Equilibration 3)

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**.



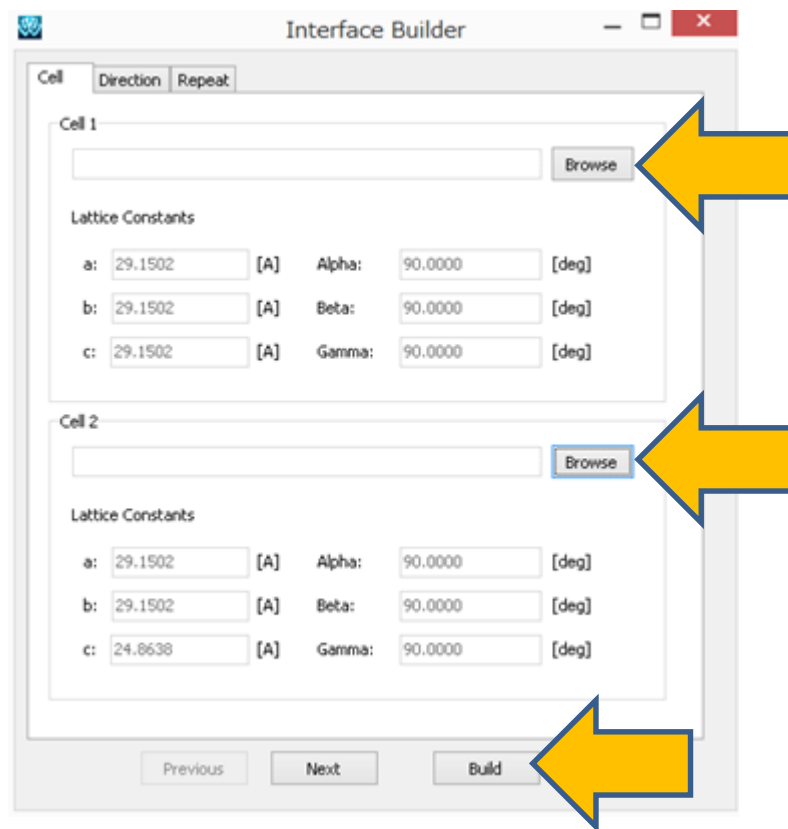
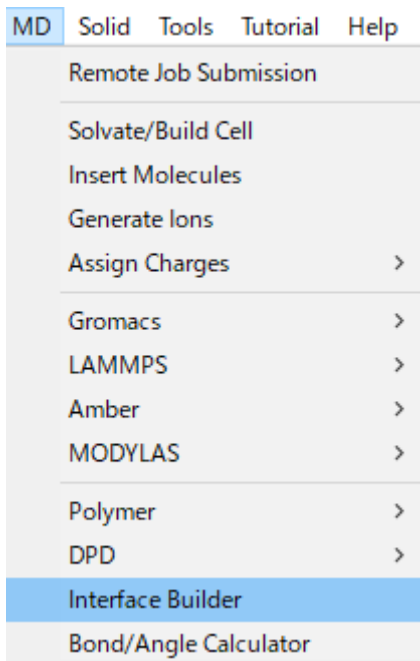
II. MD of component 2 liquid phase (Edit coordinates)

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**.



III. MD of interfacial system (Build cell)

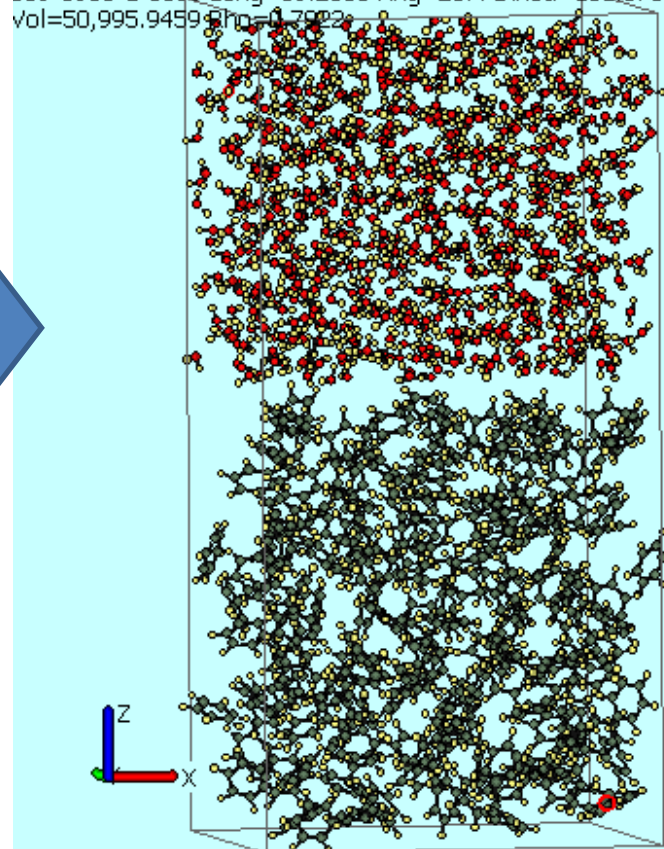
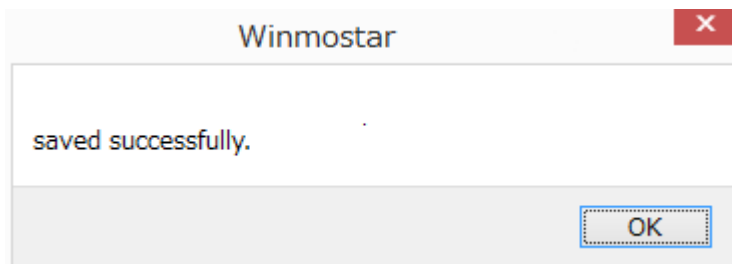
1. Click **MD | Interface Builder**.
2. Click **Browse** of **Cell 1**, then open **benzene_eq.mol2**.
3. Click **Browse** of **Cell 2**, then open **water_eq.mol2**.
4. Click **Build**.



III. MD of interface system (Build cell)

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

Generated 3,900 C900H2300O700 MASS=24,327.74 X=29.5 Y=23.73
589-3900-1-3899 Leng=59.2363 Ang=26.4 Dihed=131.373 Lper=1.144 C
Vol=50,995.9459 Rhc=0.7922

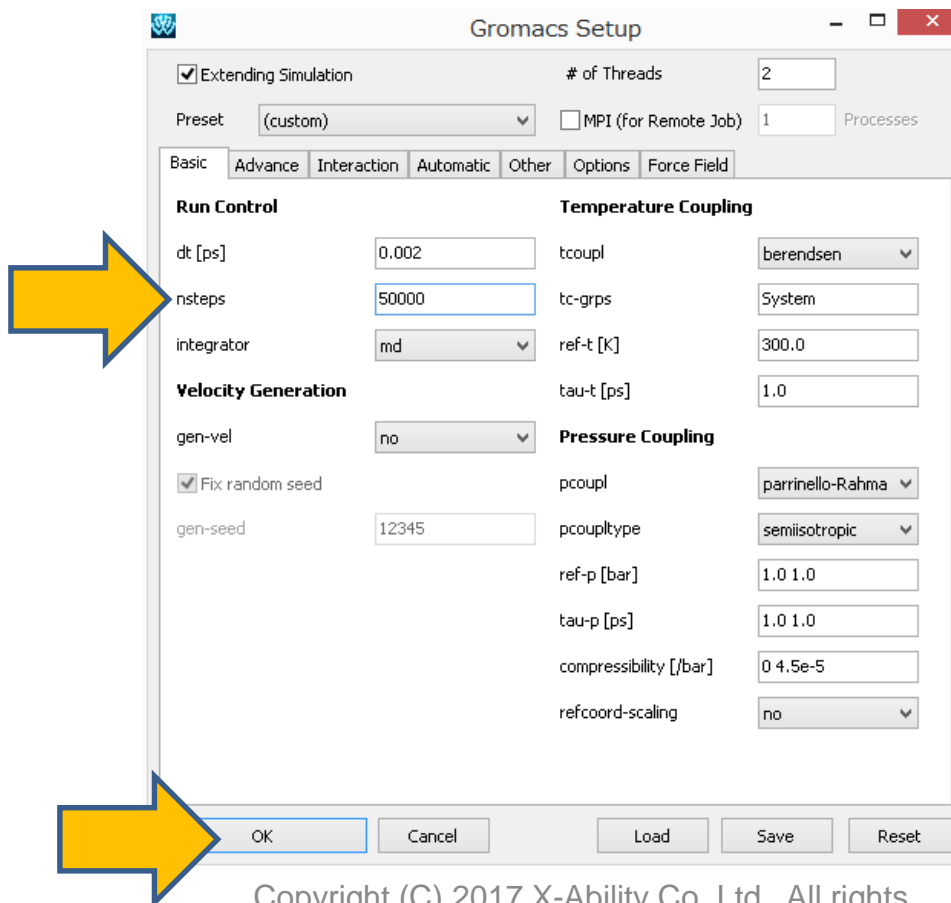


III. MD of interface system (Equilibration 1~3)

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**.

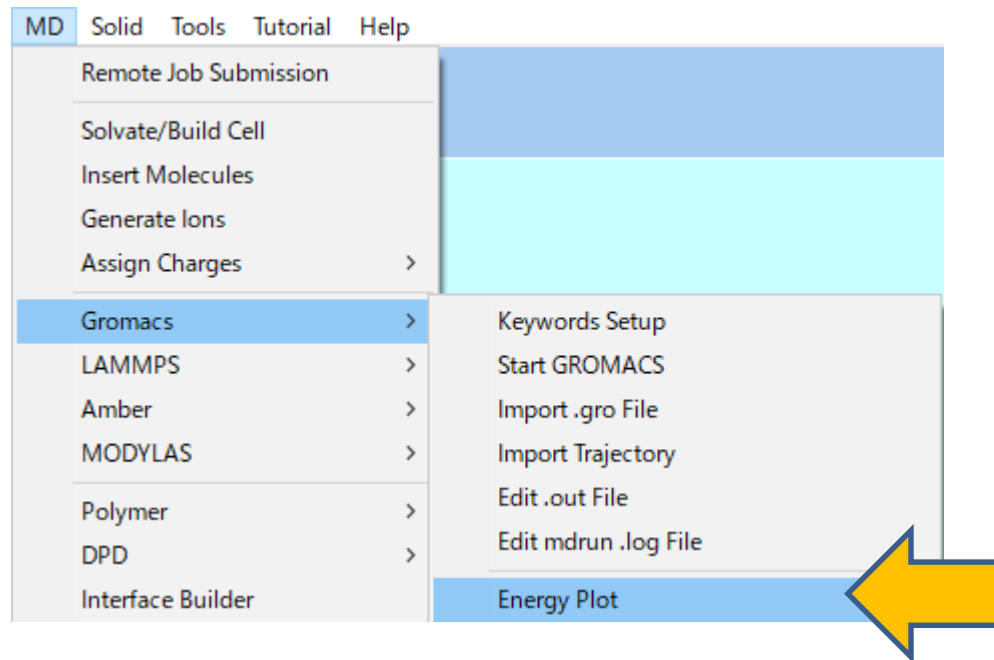
III. MD of interface system (Product run)

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**.



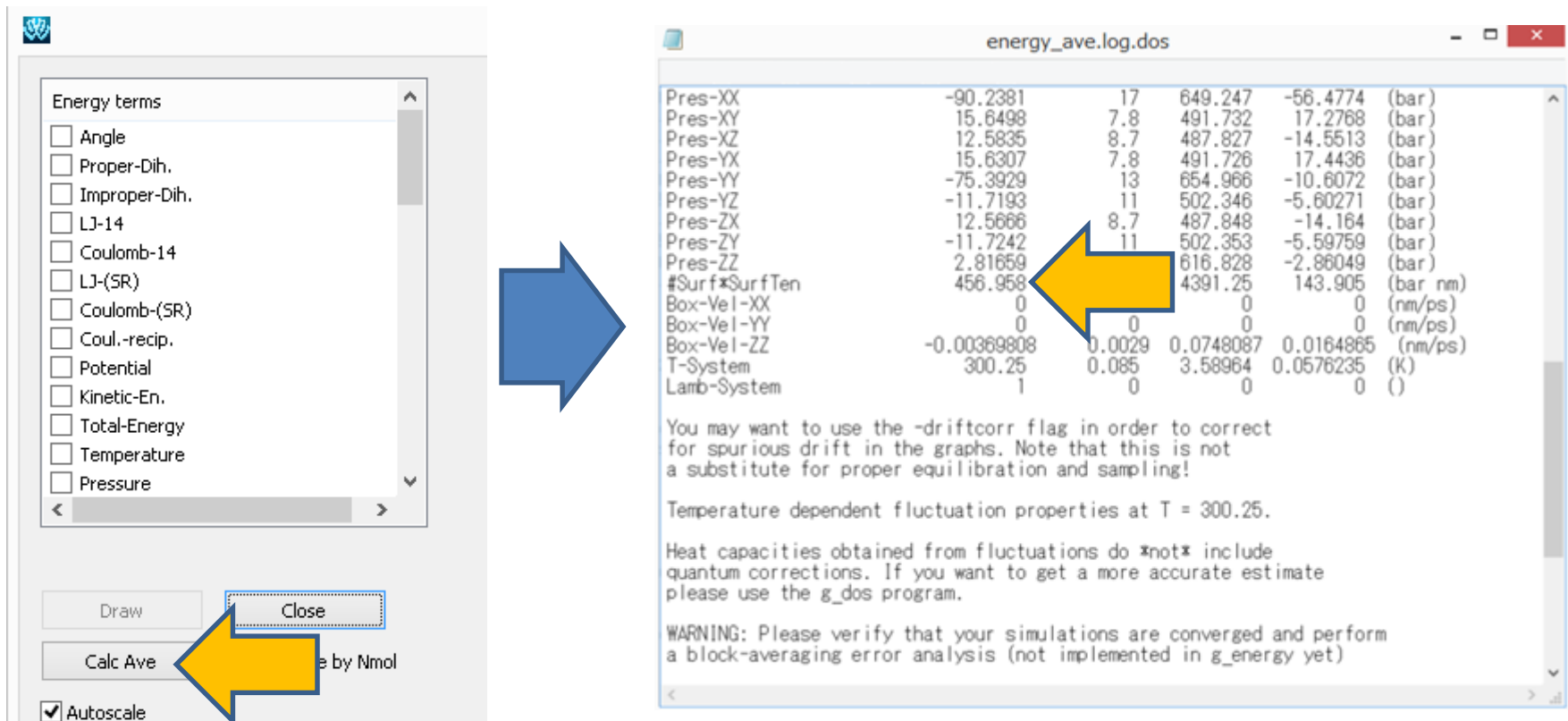
IV. Processing results

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



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 $1 \text{ bar} \cdot \text{nm} = 0.1 \text{ mN/m}$.



The screenshot shows the software interface with the 'Energy terms' dialog box on the left and the 'energy_ave.log.dos' output window on the right. A blue arrow points from the 'Calc Ave' button in the dialog box to the output window. A yellow arrow points to the '#Surf*SurfTen' value in the output window.

Energy terms dialog box:

- Energy terms
- Angle
- Proper-Dih.
- Improper-Dih.
- LJ-14
- Coulomb-14
- LJ-(SR)
- Coulomb-(SR)
- Coul.-recip.
- Potential
- Kinetic-En.
- Total-Energy
- Temperature
- Pressure
- Draw
- Close
- Calc Ave
- Autoscale

energy_ave.log.dos output window:

Pres-XX	-90.2381	17	649.247	-56.4774	(bar)
Pres-XY	15.6498	7.8	491.732	17.2768	(bar)
Pres-XZ	12.5835	8.7	487.827	-14.5513	(bar)
Pres-YX	15.6307	7.8	491.726	17.4436	(bar)
Pres-YY	-75.3929	13	654.966	-10.6072	(bar)
Pres-YZ	-11.7193	11	502.346	-5.60271	(bar)
Pres-ZX	12.5666	8.7	487.848	-14.164	(bar)
Pres-ZY	-11.7242	11	502.353	-5.59759	(bar)
Pres-ZZ	2.81659		616.828	-2.86049	(bar)
#Surf*SurfTen	456.958		4391.25	143.905	(bar nm)
Box-Vel-XX	0	0	0	0	(nm/ps)
Box-Vel-YY	0	0	0	0	(nm/ps)
Box-Vel-ZZ	-0.00369808	0.0029	0.0748087	0.0164865	(nm/ps)
T-System	300.25	0.085	3.58964	0.0576235	(K)
Lamb-System	1	0	0	0	()

You may want to use the -driftcorr flag in order to correct for spurious drift in the graphs. Note that this is not a substitute for proper equilibration and sampling!

Temperature dependent fluctuation properties at T = 300.25.

Heat capacities obtained from fluctuations do *not* include quantum corrections. If you want to get a more accurate estimate please use the g_dos program.

WARNING: Please verify that your simulations are converged and perform a block-averaging error analysis (not implemented in g_energy yet)