

Winmostar tutorial

Gromacs

Protein

V7.025

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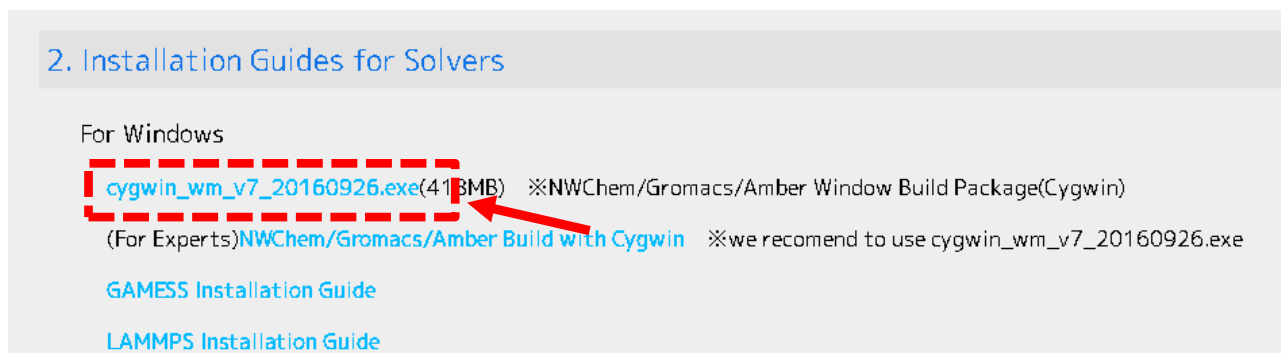
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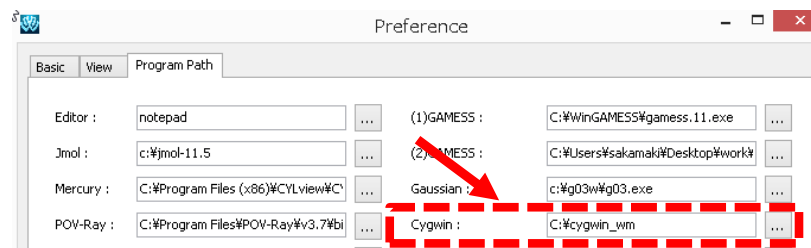
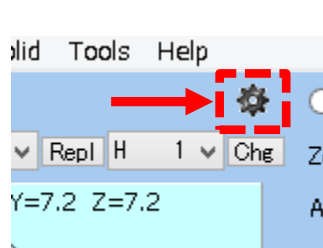
Configure

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.

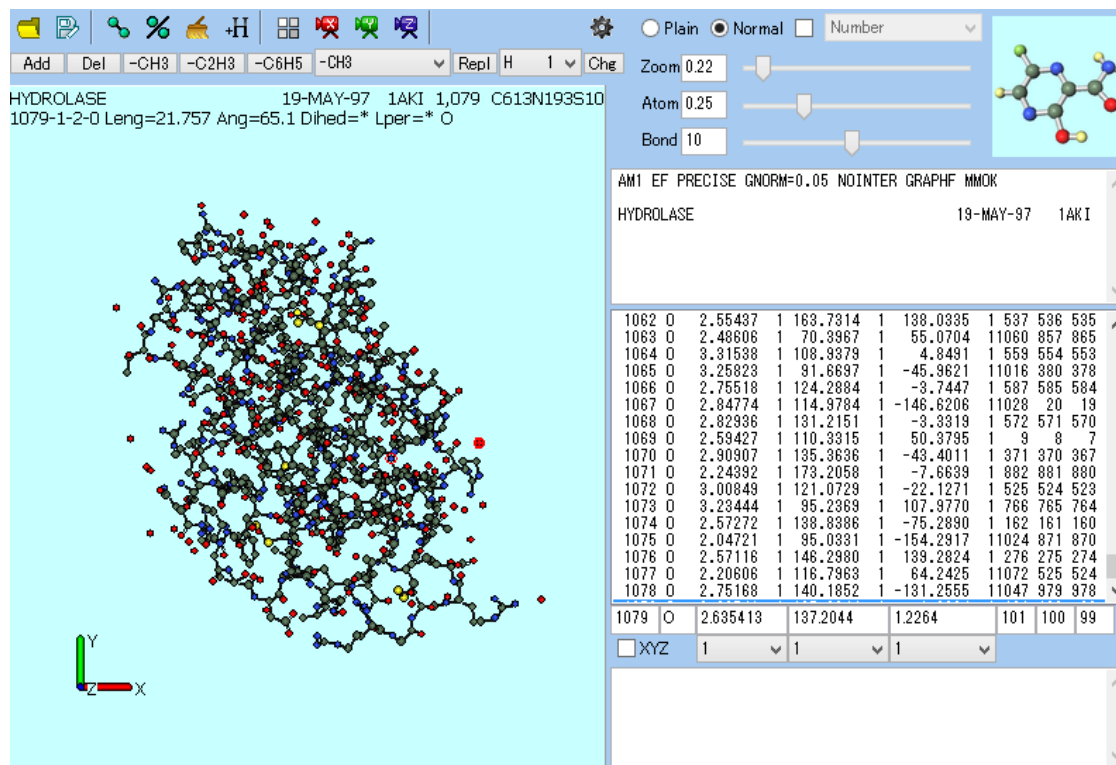


Note

- 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.

I. Build a simulation cell

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



I. Build a simulation cell

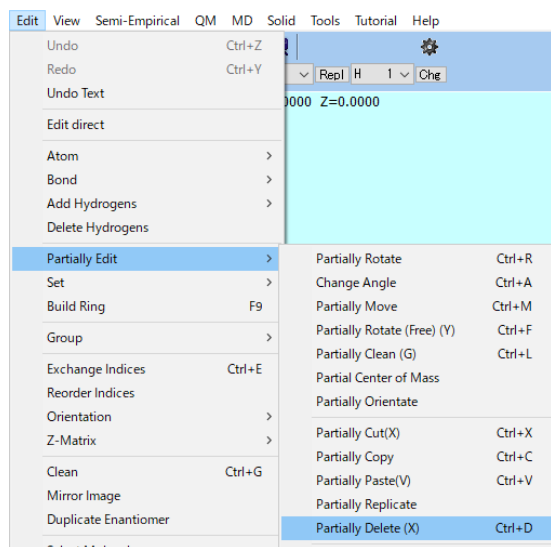
1. Click **Edit | Select Molecules**.
2. On **Select Molecules** window, check "**O 78.**" This will add blue circles around oxygen atoms of crystallization water as shown below (i.e. partial selection).

The screenshot displays the X-Ability software interface. On the left, the 'Edit' menu is open, with 'Select Molecules' highlighted. A yellow arrow points from this menu item to the 'Select Molecules' window on the right. The 'Select Molecules' window shows a table with columns 'Composition' and '# Mol'. The entry 'O 78.' is selected, indicated by a yellow arrow. The main window shows a 3D molecular model of a protein-ligand complex. A blue arrow points from the 'Edit' menu to the 3D model. The bottom right of the interface shows a table of coordinates and other data.

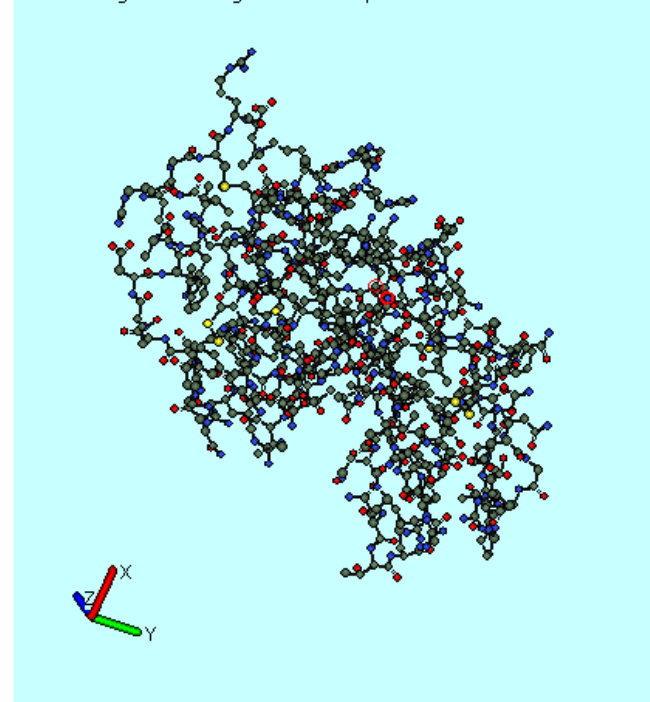
Atom	X	Y	Z	Occupancy	B-factor
1079 O	2.685413	137.2044	1.2264	101	100
1080 O	2.685413	137.2044	1.2264	101	100
1081 O	2.685413	137.2044	1.2264	101	100

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.

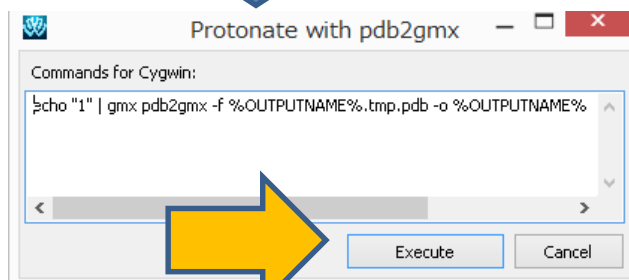
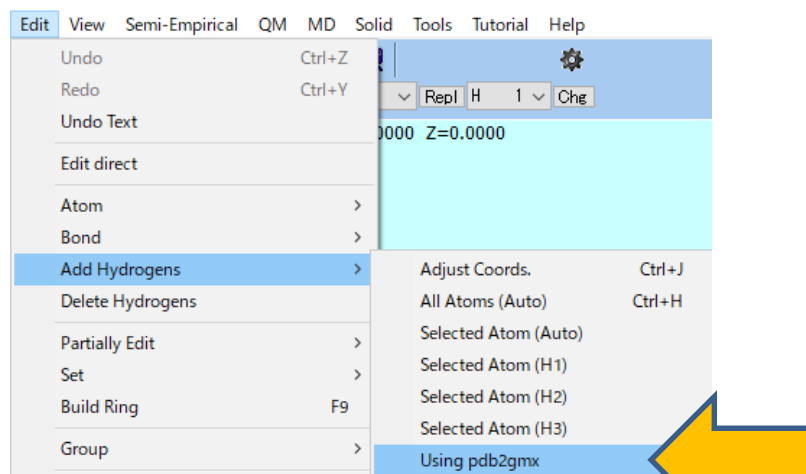


HYDROLASE 19-MAY-97 1AKI 1,001 C613N193S1C
1-2-0-0 Leng=1.4812 Ang=* Dihed=* Lper=* N

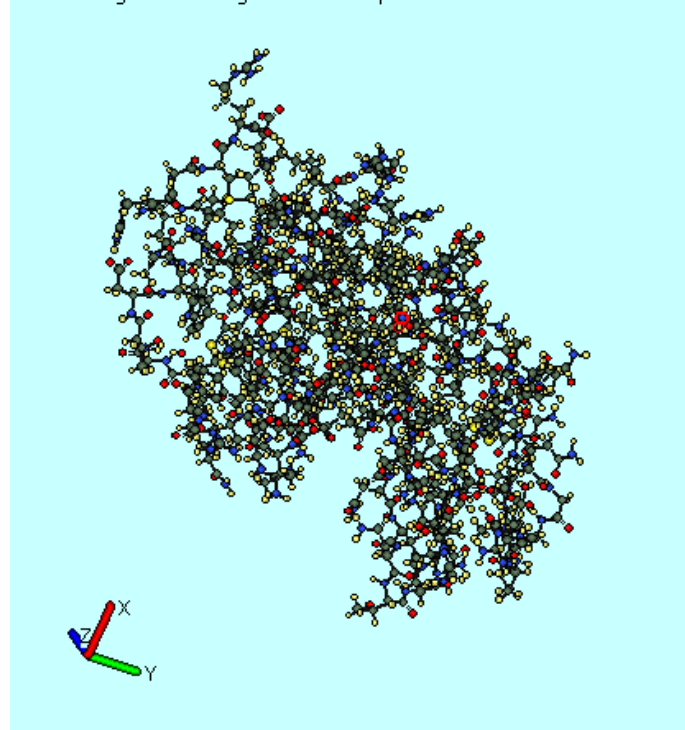


I. Build a simulation cell

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.

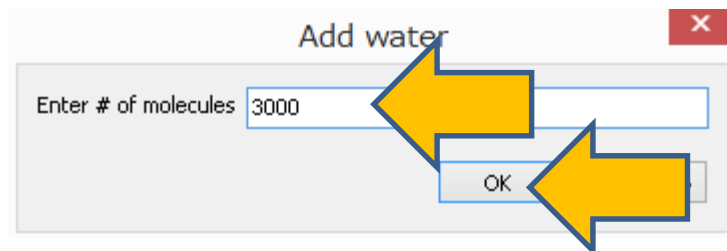
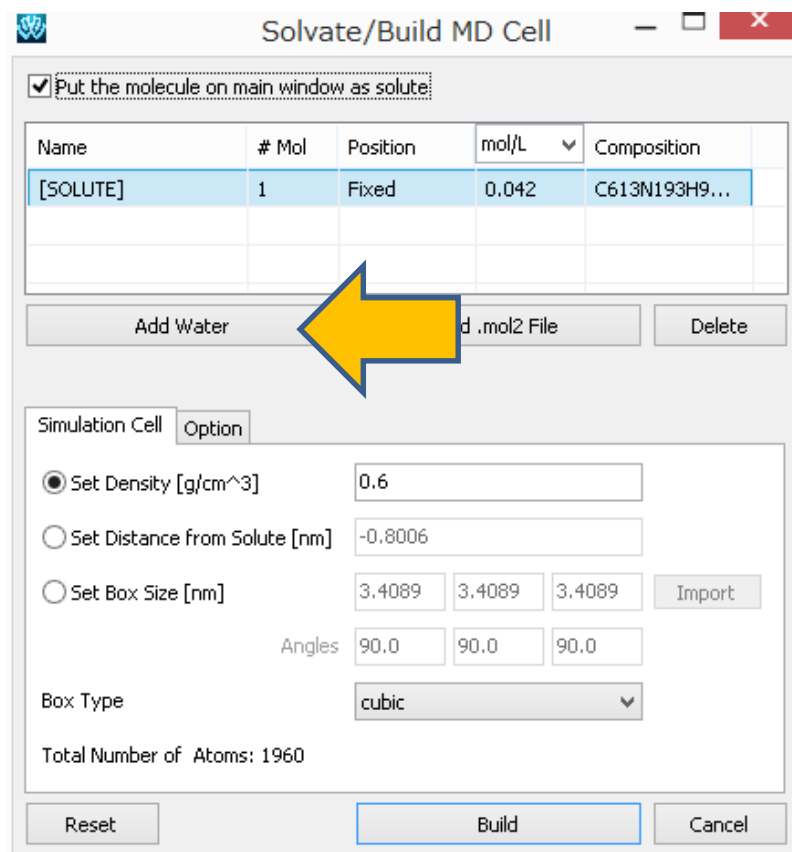
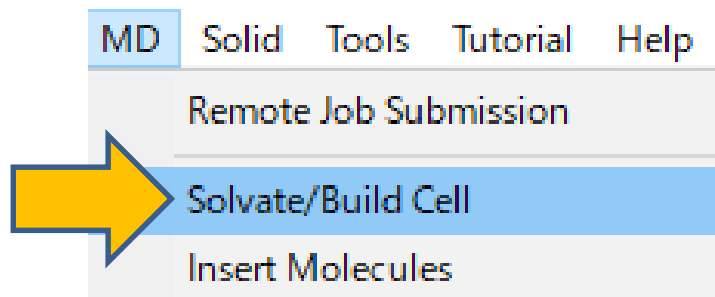


HYDROLASE 1,960 C613N193H959S100185 MASS=14,313.21 X=35.36
L-2-O-0 Leng=0.9986 Ang=* Dihed=* Lper=* N



I. Build a simulation cell

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



I. Build a simulation cell

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

Solvate/Build MD Cell

☒ Put the molecule on main window as solute

Name	# Mol	Position	mol/L	Composition
[SOLUTE]	1	Fixed	0.013	C613N193H9...
WATER	3000	Random	39.496	H2O

Add Water Add .mol2 File Delete

Simulation Cell Option

☒ Set Density [g/cm³] 0.9

☐ Set Distance from Solute [nm] 0.0025

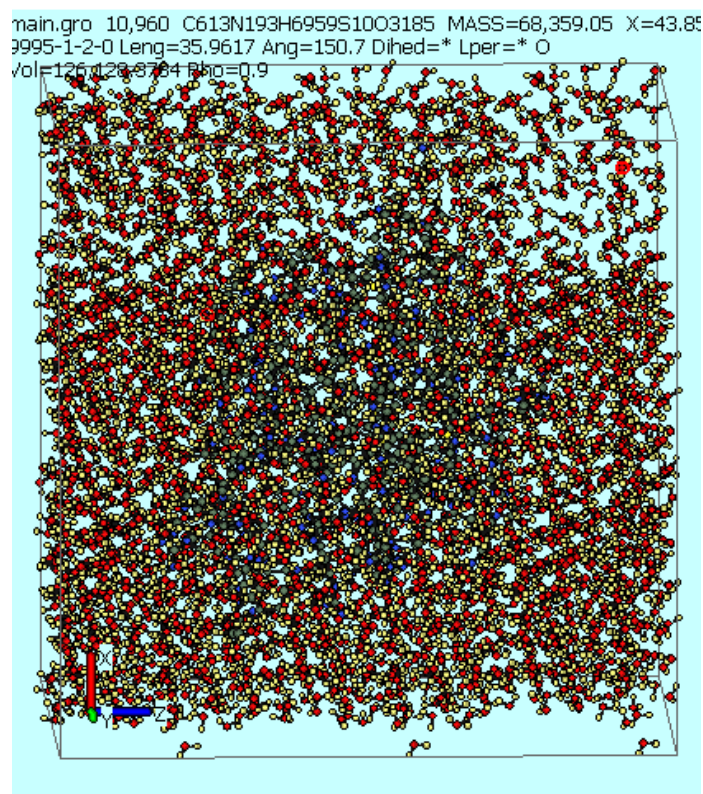
☐ Set Box Size [nm] 5.015 5.015 5.015 Import

Angles 90.0 90.0 90.0

Box Type cubic

Total Number of Atoms: 10960

Reset Build



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.

The screenshot illustrates the process of building a simulation cell. On the left, the 'MD' menu is open, and 'Generate Ions' is highlighted. A yellow arrow points to this option. Below it, the 'Generate Ions' window is shown. A yellow arrow points to the 'Execute' button in this window. A large blue arrow points from the 'Execute' button to the right, where a 3D visualization of the simulation cell is displayed. The cell is a rectangular box filled with a dense arrangement of atoms, represented by small spheres of various colors (red, white, grey, blue, green). Above the 3D visualization, the following text is displayed:

```
generated 10,900 Na11C613N193H6899S1003155Cl19 MASS=68,745.0
9995-1-2-0 Leng=10.6997 Ang=105.6 Dihed=* Lper=* O
Vol=126,128.3784 Rho=0.9051
```

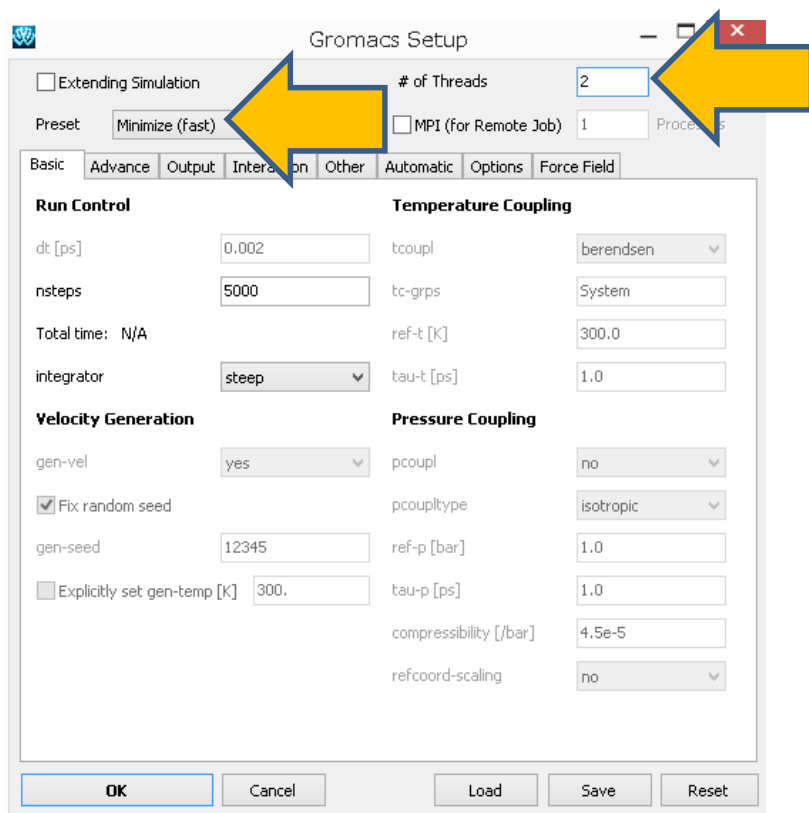
Below the 'Execute' button, a table shows the parameters for the generated system:

Item	Value
Neutral	True
Concentration [mol/L]	0.15
Cations	NA
Number of Cations	0
Anions	CL
Number of Anions	0

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**.



Gromacs Setup

☐ Extending Simulation

Preset: **Minimize (fast)**

of Threads: **2**

☐ MPI (for Remote Job) 1

Basic | **Advance** | Output | Interaction | Other | Automatic | Options | Force Field

Run Control

dt [ps]: 0.002

nsteps: 5000

Total time: N/A

integrator: steep

Velocity Generation

gen-vel: yes

☒ Fix random seed

gen-seed: 12345

☐ Explicitly set gen-temp [K]: 300.

Temperature Coupling

tcoupl: berendsen

tc-grps: System

ref-t [K]: 300.0

tau-t [ps]: 1.0

Pressure Coupling

pcoupl: no

pcoupltype: isotropic

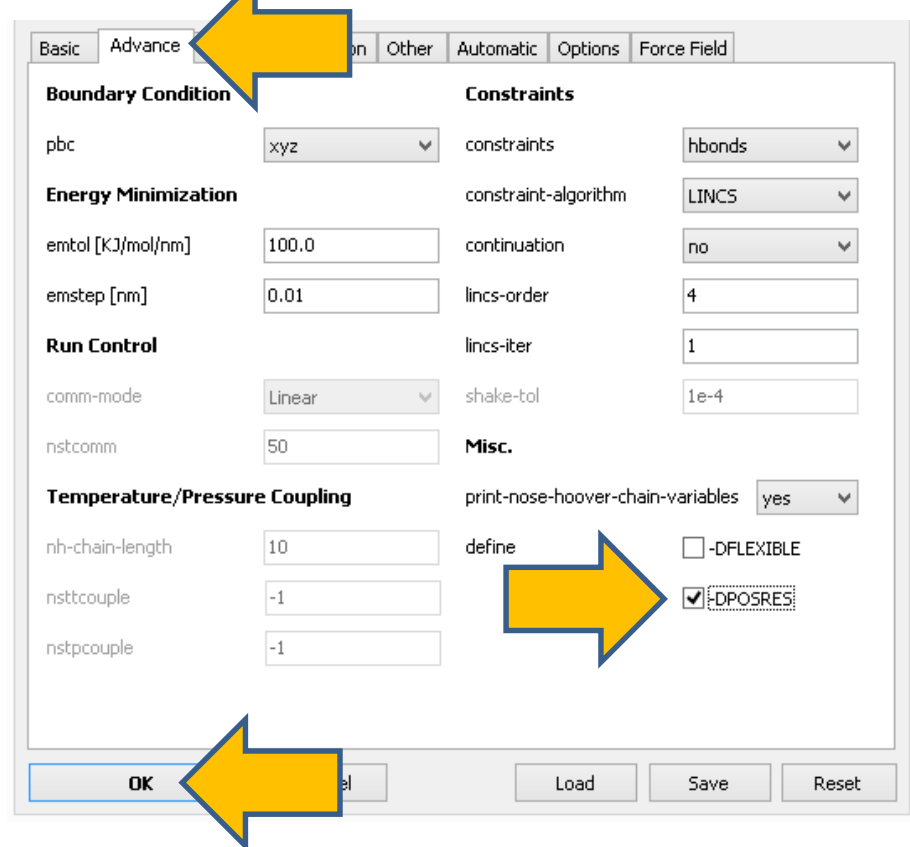
ref-p [bar]: 1.0

tau-p [ps]: 1.0

compressibility [/bar]: 4.5e-5

refcoord-scaling: no

OK Cancel Load Save Reset



Basic | **Advance** | Output | Interaction | Other | Automatic | Options | Force Field

Boundary Condition

abc: xyz

Energy Minimization

emtol [KJ/mol/nm]: 100.0

emstep [nm]: 0.01

Run Control

comm-mode: Linear

nstcomm: 50

Temperature/Pressure Coupling

nh-chain-length: 10

nsttcouple: -1

nstpcouple: -1

Constraints

constraints: hbonds

constraint-algorithm: LINCS

continuation: no

lincs-order: 4

lincs-iter: 1

shake-tol: 1e-4

Misc.

print-nose-hoover-chain-variables: yes

define: ☐ -DFLEXIBLE ☒ **-DPOSRES**

OK Cancel Load Save Reset

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.

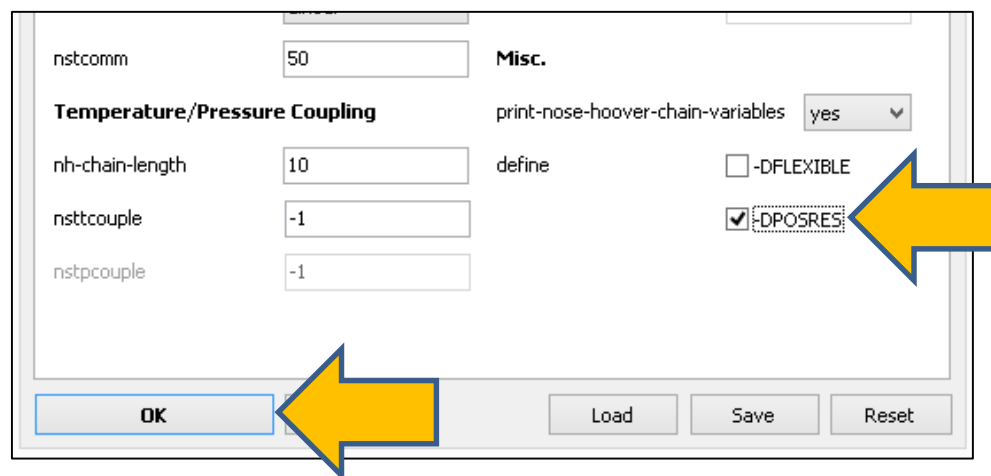
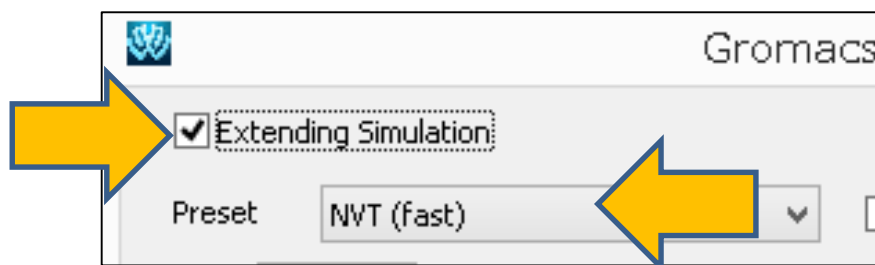
The image shows the Winmostar JM software interface. On the left, the 'MD' menu is open, displaying options: Remote Job Submission, Solvate/Build Cell, Insert Molecules, Generate Ions, Assign Charges, Gromacs, and LAMMPS. The 'Gromacs' option is highlighted in blue, and a yellow arrow points to the 'Start GROMACS' sub-option. A blue arrow points from the 'Start GROMACS' option to a terminal window on the right. The terminal window displays simulation progress data for steps 2333 through 2358, including Dmax, Epot, and Fmax values.

Step	Dmax	Epot	Fmax
2333	3.1e-03 nm	-1.81631e+05	1.34236e+
2335	1.8e-03 nm	-1.81633e+05	1.47046e+
2336	2.2e-03 nm	-1.81635e+05	1.91499e+
2337	2.7e-03 nm	-1.81637e+05	2.13751e+
2338	3.2e-03 nm	-1.81638e+05	2.73518e+
2339	3.8e-03 nm	-1.81639e+05	3.10191e+
2341	2.3e-03 nm	-1.81645e+05	4.05734e+
2342	2.8e-03 nm	-1.81649e+05	3.77722e+
2343	3.3e-03 nm	-1.81657e+05	1.27366e+
2345	2.0e-03 nm	-1.81659e+05	1.74990e+
2346	2.4e-03 nm	-1.81661e+05	1.88865e+
2347	2.9e-03 nm	-1.81662e+05	2.46743e+
2348	3.4e-03 nm	-1.81663e+05	2.76982e+
2349	4.1e-03 nm	-1.81663e+05	3.50483e+
2350	4.9e-03 nm	-1.81664e+05	4.03403e+
2352	3.0e-03 nm	-1.81673e+05	4.84224e+
2354	1.8e-03 nm	-1.81676e+05	2.23965e+
2355	2.1e-03 nm	-1.81680e+05	1.01263e+
2356	2.6e-03 nm	-1.81680e+05	2.90177e+
2357	3.1e-03 nm	-1.81685e+05	1.78256e+
2358	3.7e-03 nm	-1.81682e+05	3.84875e+

II. Execute simulations

1. Equilibration (*NVT* with restraint)

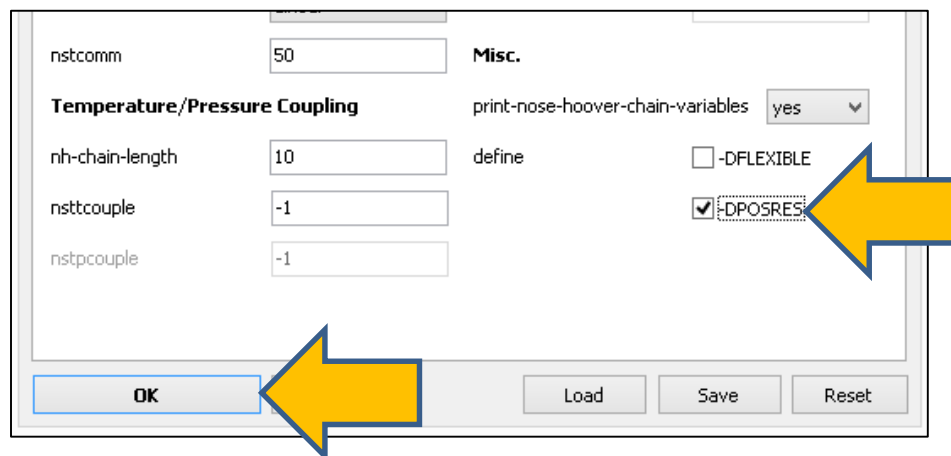
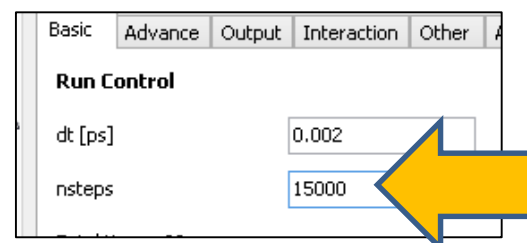
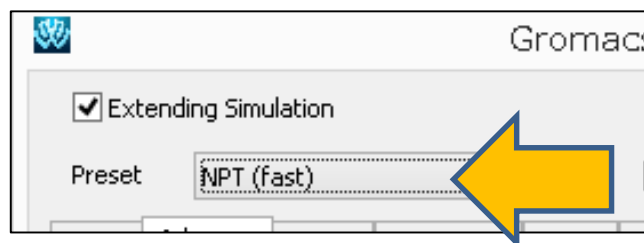
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVT (fast)**, check **Extending Simulation**.
3. On **Advance** tab, check **-DPOSRES**, then click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



II. Execute simulations

1. Equilibration (*NPT* with restraint)

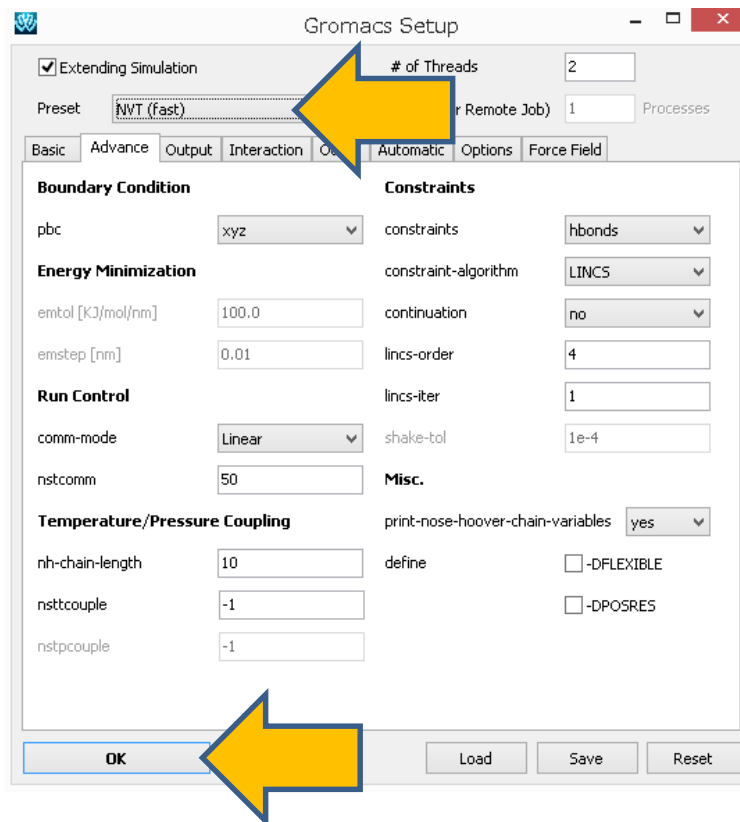
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NPT (fast)**.
3. On **Basic** tab, set **nsteps** to **15000**.
4. On **Advance** tab, check **-DPOSRES**, then click **OK**.
5. Click **MD | Gromacs | Start Gromacs**.



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.



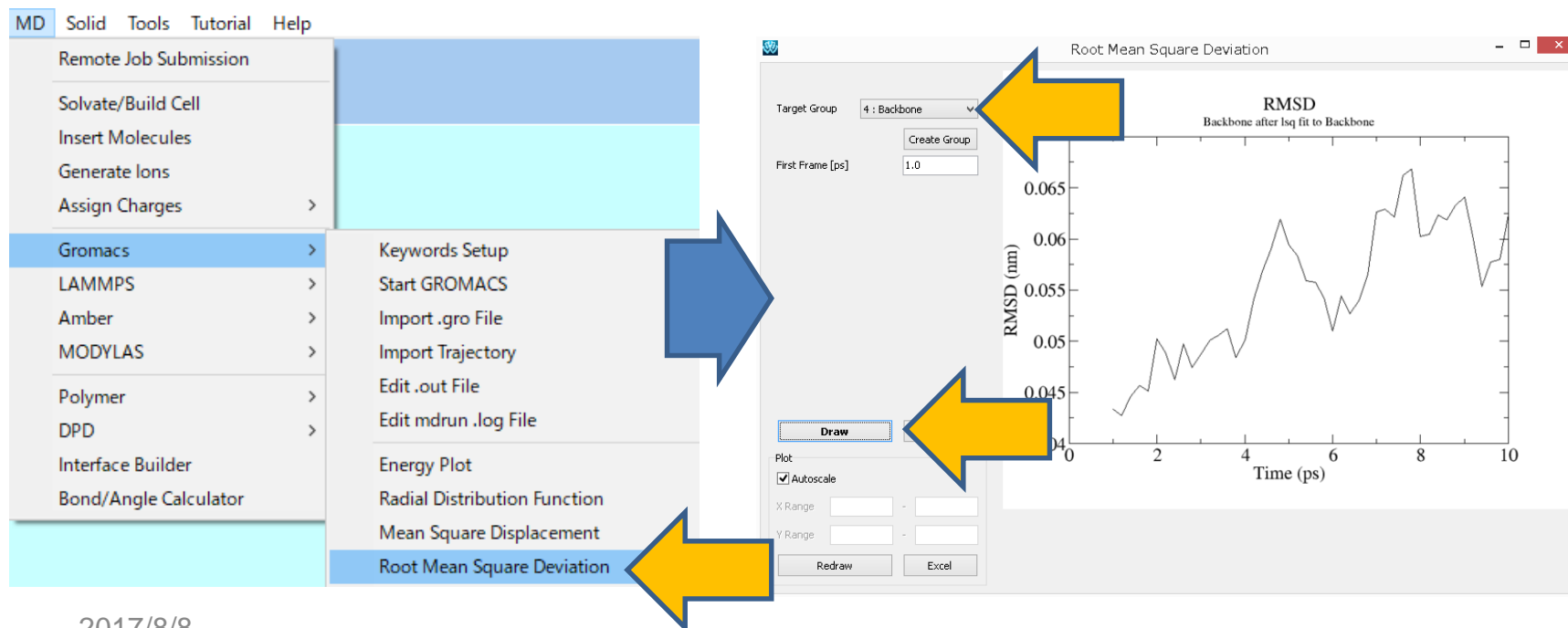
II. Execute simulations

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.

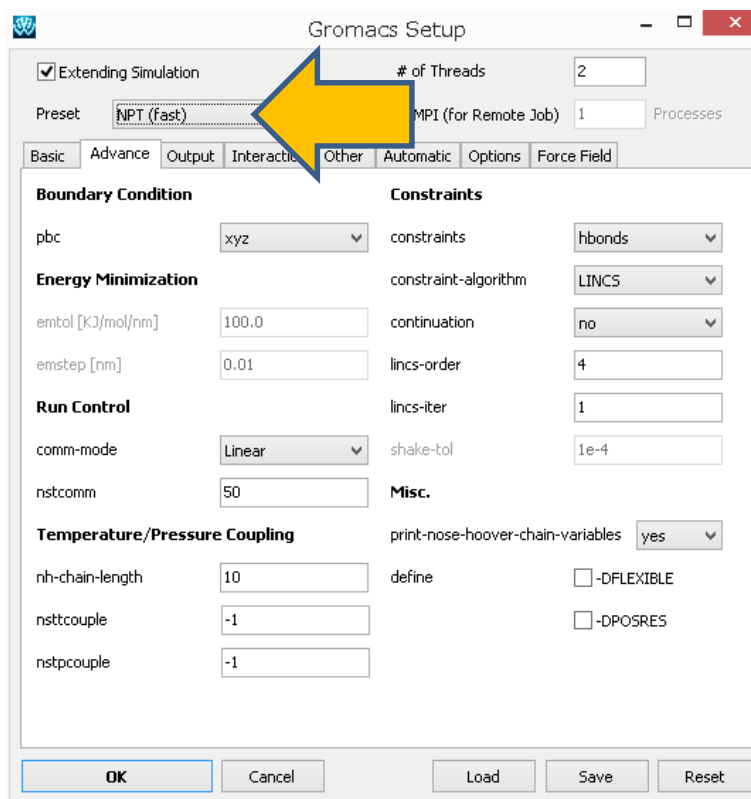
The radius of gyration can be obtained in the same way.



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**.



Gromacs Setup

☒ Extending Simulation

Preset: **NPT (fast)** # of Threads: 2 MPI (for Remote Job): 1 Processes

Basic Advance Output Interactive **Other** Automatic Options Force Field

Boundary Condition

pbx xyz

Energy Minimization

emtol [KJ/mol/nm] 100.0

emstep [nm] 0.01

Run Control

comm-mode Linear

nstcomm 50

Temperature/Pressure Coupling

nh-chain-length 10

nsttcouple -1

nstpcouple -1

Constraints

constraints hbonds

constraint-algorithm Lincs

continuation no

lincs-order 4

lincs-iter 1

shake-tol 1e-4

Misc.

print-nose-hoover-chain-variables yes

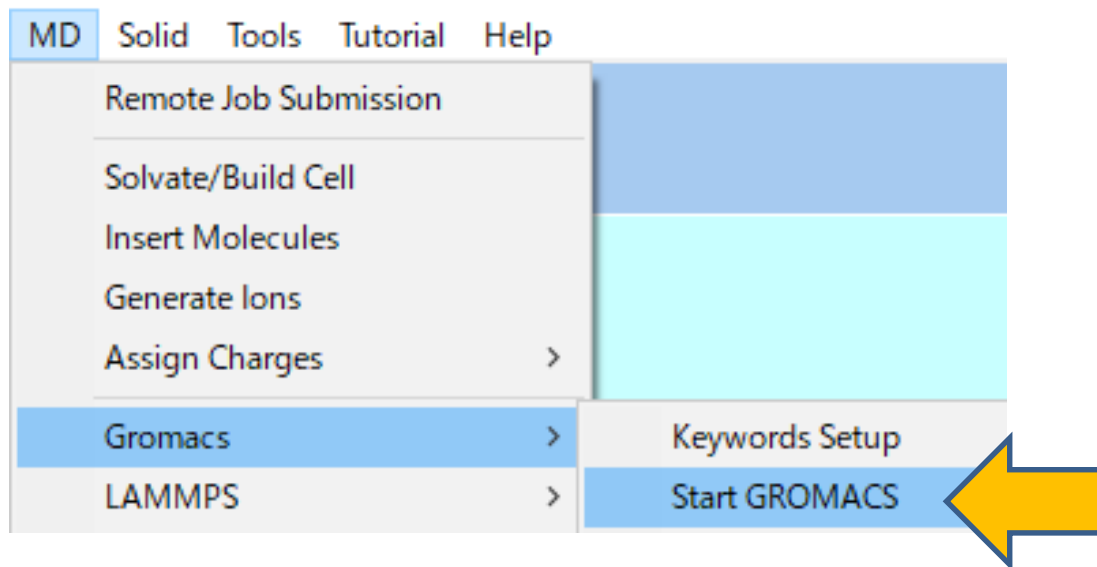
define ☐ -DFLEXIBLE ☐ -DPOSRES

OK Cancel Load Save Reset

II. Execute simulations

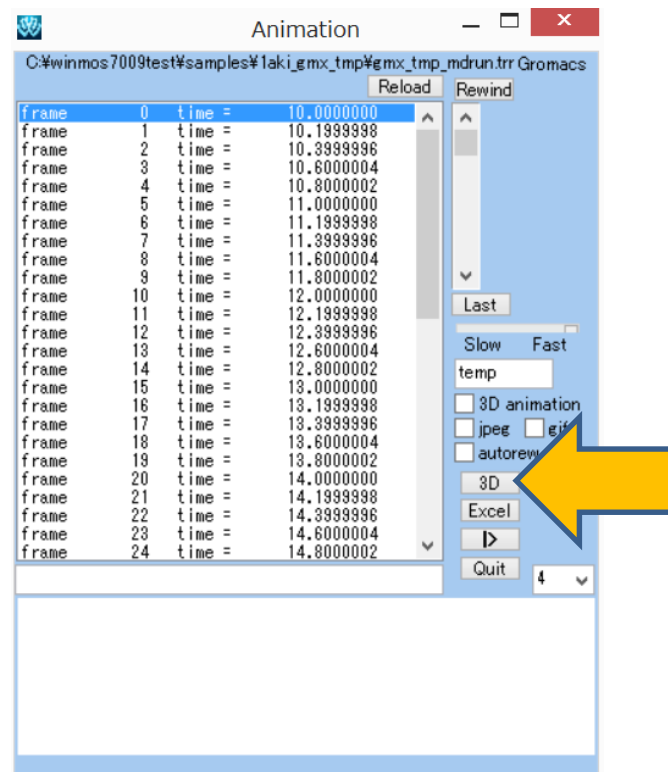
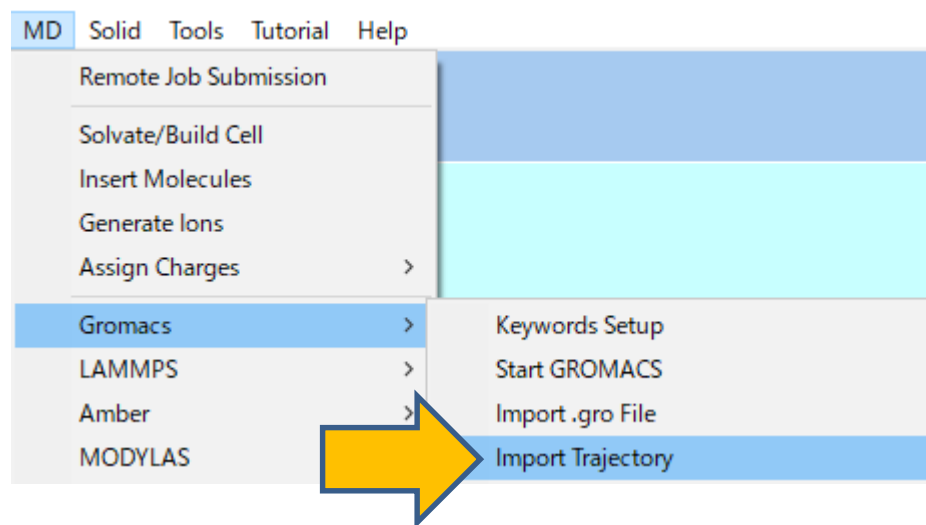
1. Product run

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



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**.



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.

The screenshot shows the Winmostar 3D interface. The 'View' menu is open, showing options like Model, Background, Preferences, Perspective, Debug, and Animation. A yellow arrow points to the 'View' menu. The 'Preferences' dialog box is open, showing various settings. A yellow arrow points to the 'Preferences' dialog. A red dashed box highlights the 'Mol. Weight' option in the 'Boundary Condition' section of the Preferences dialog.

Preferences

Rotation
☒ Free ☐ X ☐ Y ☐ Z

Boundary Condition
☐ None ☐ Atom ☒ Mol.

☐ Rainbow ☐ Gold

☐ By turn ☒ Mol. Weight

1 ☒ BS Blue
 2 ☐ Red
 3 ☒ Magenta
 4 ☒ Lime
 5 ☒ Cyan
 6 ☒ Yellow
 7 ☒ White
 8 ☒ Brown
 9 ☒ Gray

☐ Stereo ☐ Enantiomer
☒ Para ☐ Cross ☐ Anag

Shift < > 1.0
 Rot < > 1.0

☒ H ☒ Dum. ☐ Backbone

Atom < > 1.00
 Bond < > 1.00
 Zclip < > 1.00

MO Format Solid

color (+) < >

Trans < > 0.00

☐ X < > 1
☐ Y < > 1
☐ Z < > 1