

 winmostar tutorial

Gromacs Basic

V11.5.6

29 November, 2023 X-Ability Co., Ltd.

About This Document

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult [Beginner's Guide](#).
- For those who wish to explore the details of each feature, please refer to [Winmostar User Manual](#).
- If you are unable to proceed with the operations as outlined in this manual, please first consult [Frequently asked questions](#).
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us from [Contact](#). Attach files generated at the time of the issue and provide steps to reproduce the problem.
- The copyright for this document is held by X-Ability Co., Ltd. Any copying or duplication of the content in any form without the express permission of X-Ability Co., Ltd. is strictly prohibited.

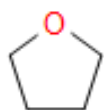
Overview

- We will obtain various thermodynamic properties, radial distribution functions, self-diffusion coefficients, specific heats, and compressibility of tetrahydrofuran (THF) liquid under room temperature and atmospheric pressure using molecular dynamics calculations with Gromacs (employing GAFF and AM1-BCC charges). For equilibration, we will perform energy minimization, constant temperature MD, and constant temperature-pressure MD. Following this, the main calculation will again be executed under constant temperature and pressure conditions using MD.

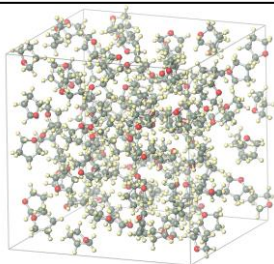
Procedure Overview:

A. System Modeling

- (A) Creation of a single molecule.
- (B) Assignment of charges.
- (C) Creation of the liquid phase.



THE Molecule



B. Execution of Calculations

- (A) Assignment of the force field.
- (B) Equilibration calculations.
(Energy minimization →
Constant temperature MD →
Constant temperature and pressure MD)
- (C) Main calculation.
(constant temperature and pressure MD)

C. Result Analysis

Various thermodynamic properties.
Radial distribution functions.
Self-diffusion coefficients.
Specific heat and compressibility.

Note:

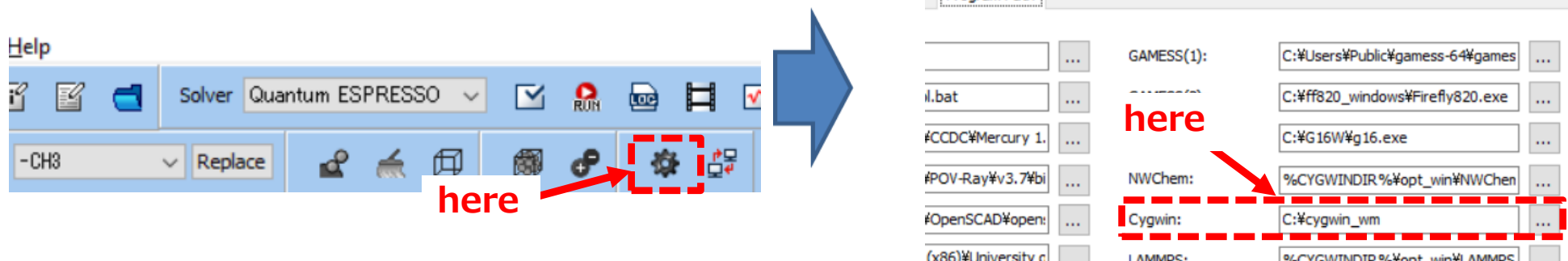
- The number of steps and molecules will vary depending on the type of system, the physical properties you want to calculate, and the desired level of accuracy.
- The choice of force field and type of charges significantly affects the results of the calculations.

Operating Environment Settings

- To use this feature, it is necessary to set up Cygwin.
- <https://winmostar.com/en/installation/> Set up Cygwin by following the configuration steps outlined in the installation instructions.

(7) Install **Cygwin environment for Winmostar.** ← **here**

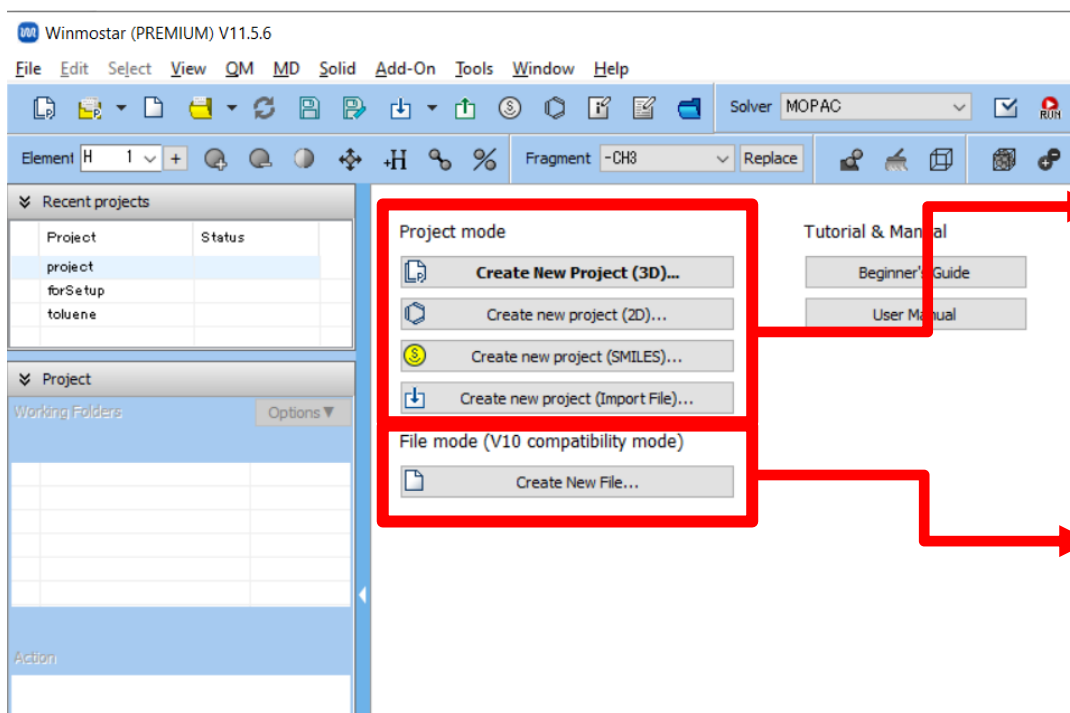
- By default, it is installed directly under C:, but you can install it in a location of your choice by changing the 'Program Path' > 'Cygwin' in Winmostar Preference.



Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.

This manual focuses on operations in Project Mode.



Project Mode **New Features in V11**

Users can manage jobs without having to manage individual files.

We generally recommend using this mode.

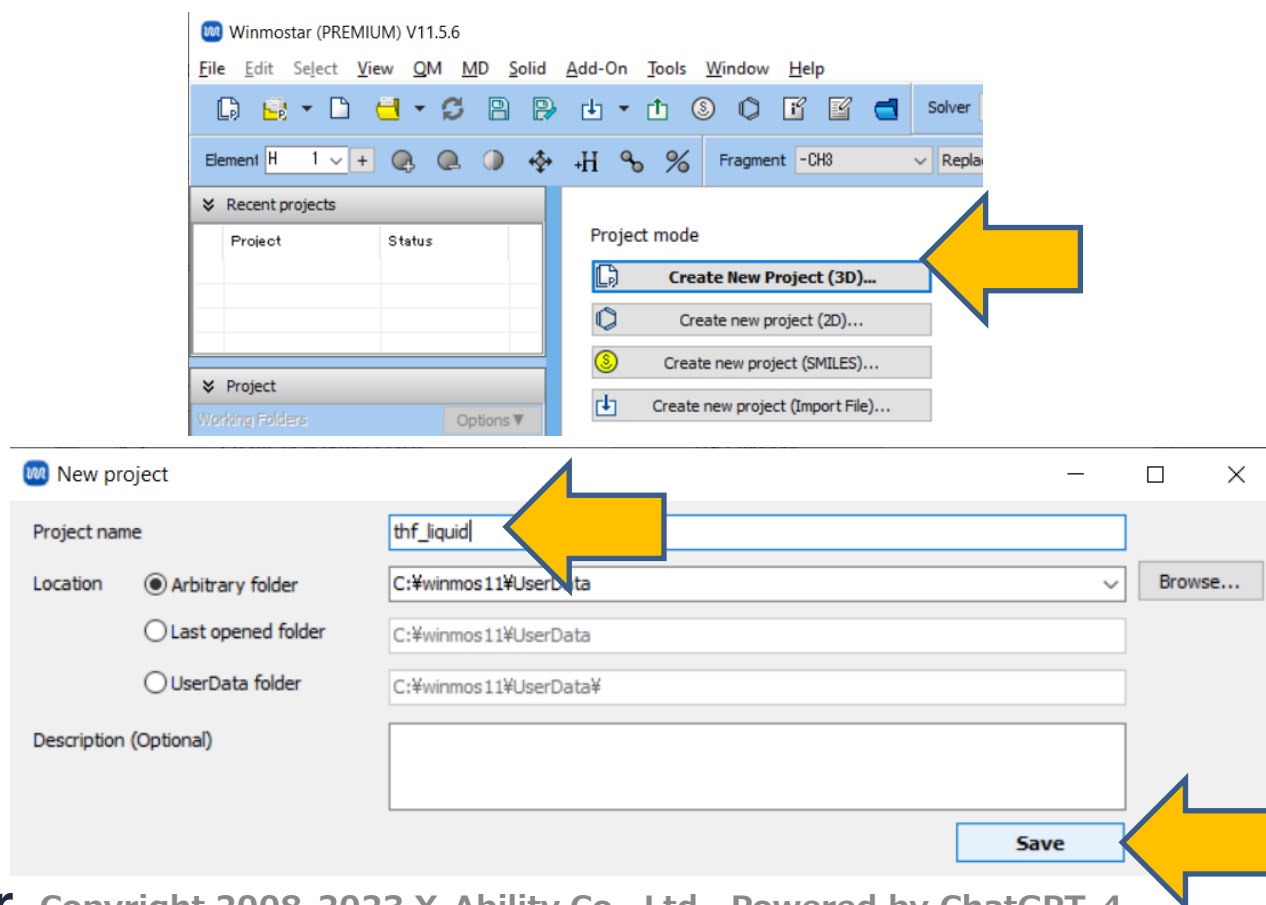
File Mode

Users explicitly create and manage individual files.

The operational procedure is the same as from V10 and earlier versions.

A. System Modeling (A)Creation of a Single Molecule

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.
- B. Enter 'thf_liquid' for **Project name** and click **Save**.



A. System Modeling (A)Creation of a Single Molecule

For details on creating an initial structure, please refer to [Molecular Modeling Organic Molecules Tutorial](#).

In this section, we will load an existing molecular structure file.

A. Click **File | Import | Sample File | thf.pdb**

- If you wish to load a different file at this stage, use **File | Import File** instead.

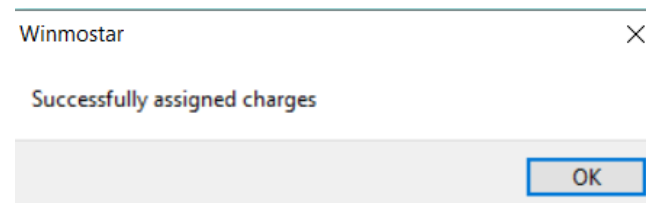
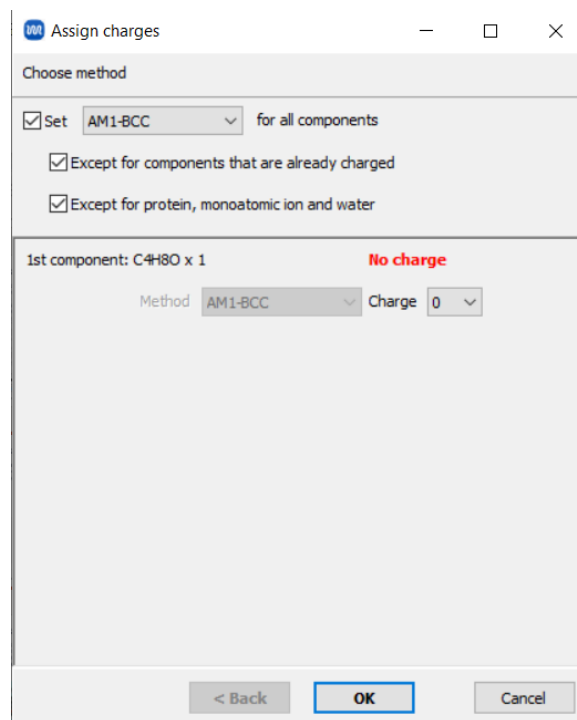
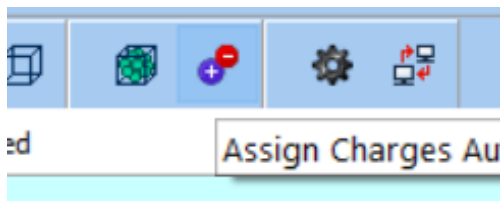
B. In **Import File** dialog, click **Discard and import**.

C. Verify that the desired molecule appears in Viewport.

The screenshot displays the Winmostar software interface. The 'File' menu is open, showing the path 'File > Import > Sample File > thf.pdb'. A yellow arrow points to 'thf.pdb' in the file list. Another yellow arrow points to the 'Discard and import' button in the 'Import File' dialog box, which asks 'Do you want to discard the current content and load a new structure?'. Below the dialog box, a 3D ball-and-stick model of a molecule is shown in the viewport.

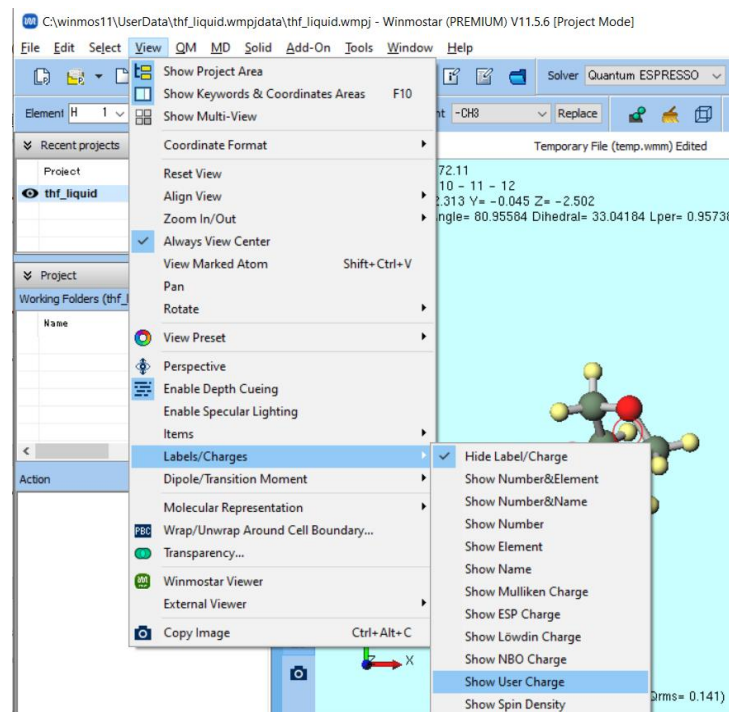
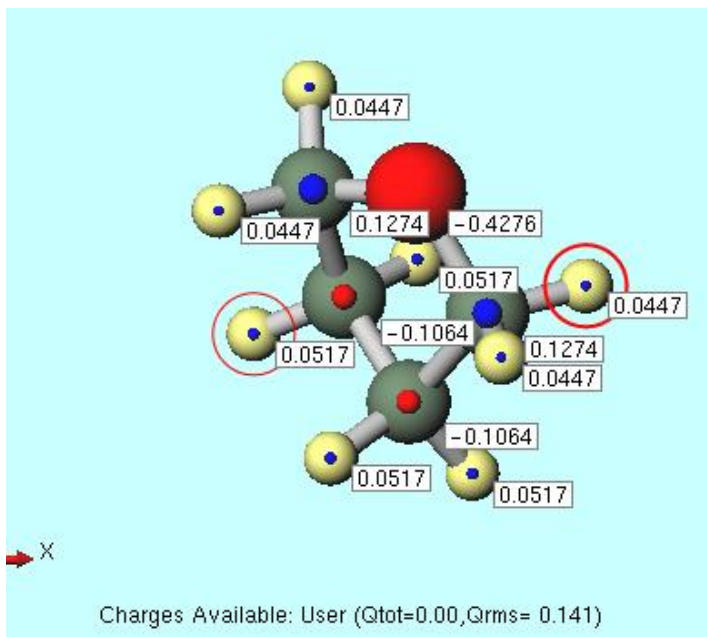
A. System Modeling (B)Assignment of Charges

- Click **Assign Charges Automatically**.
- Click OK in **Assign charges** window.
- After a black window appears several times, click **OK** when the message 'Successfully assigned charges' is displayed.



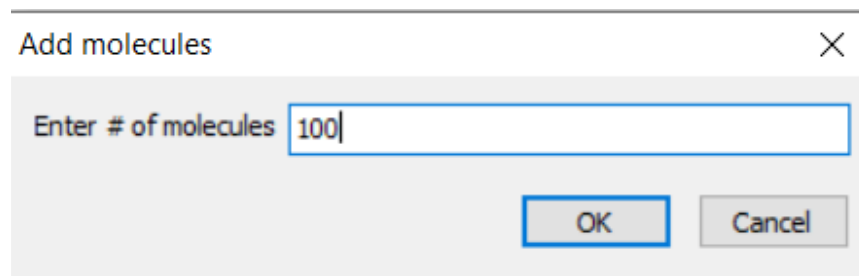
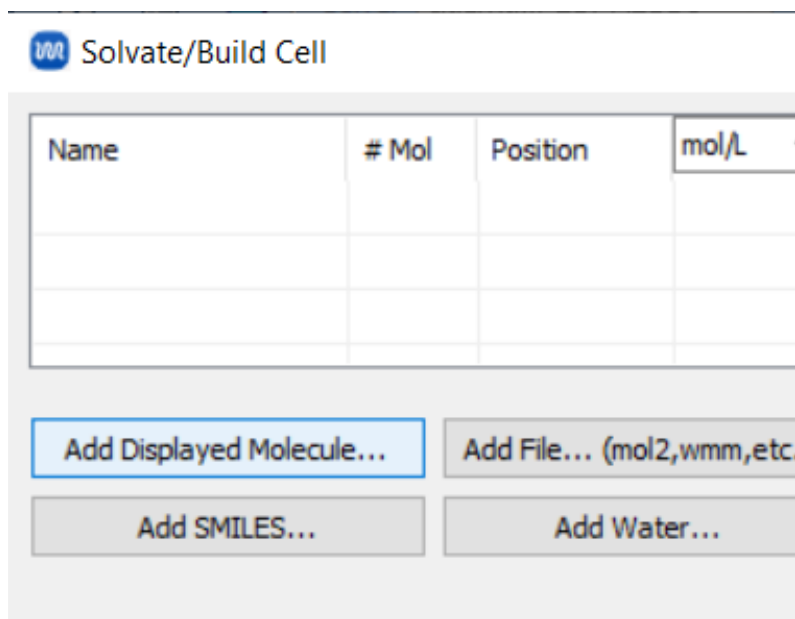
A. System Modeling (B) Assignment of Charges

- A. Verify that 'Charges Available: User ($Q_{\text{tot}}=0.00$, $Q_{\text{rms}}=0.141$)' is displayed at the bottom of Viewport, ensuring that the total value is 0 and each atom has been assigned a non-zero User charge.
- B. To graphically display the charges, click **View | Labels/Charges | Show User Charge**.
- C. To undo step B, click **View | Labels/Charges | Hide Label/Charge**.



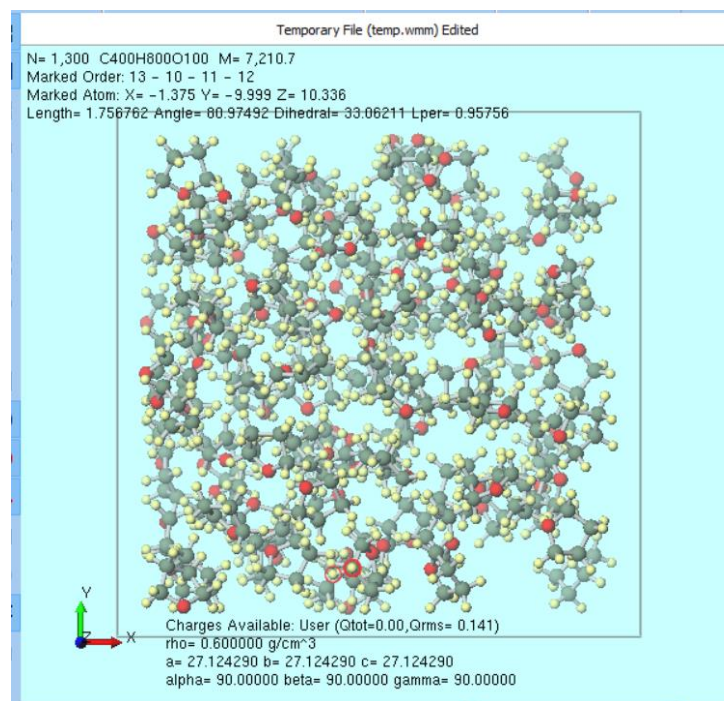
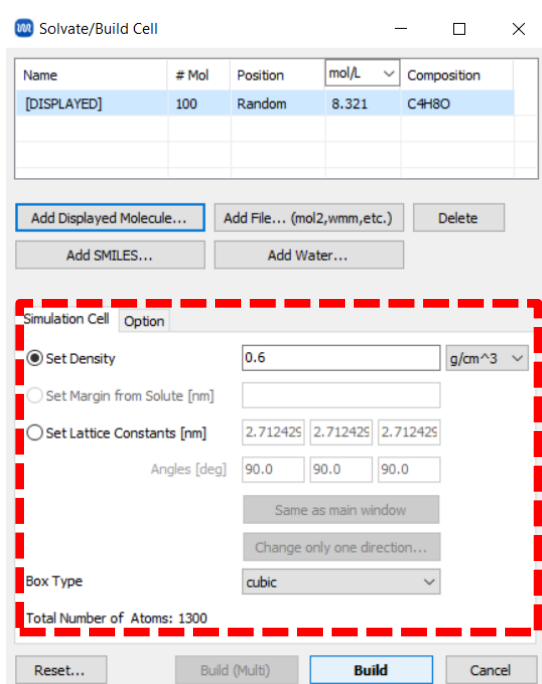
A. System Modeling (C)Creation of the Liquid Phase

- A. Click  **Solvate/Build cell**.
- B. Click **Add Displayed Molecule**, enter '100' in the dialog that appears, and then click **OK**.



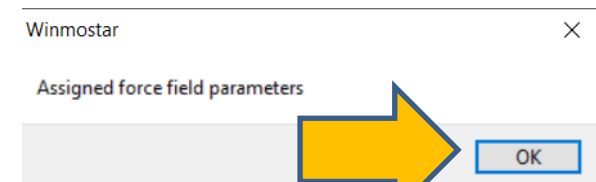
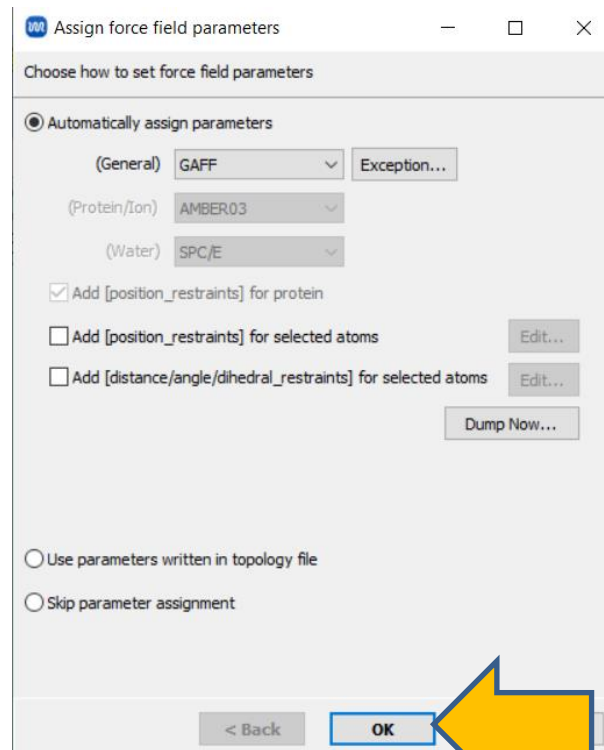
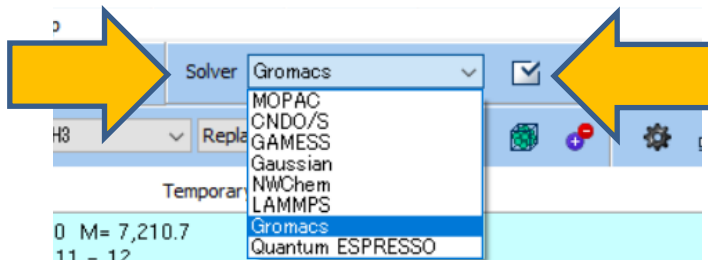
A. System Modeling (C)Creation of the Liquid Phase

- A. Verify the settings of **Simulation Cell**. (In this manual, we will proceed without making any specific changes.)
- B. When you click **Build**, a black terminal window will appear for a few seconds, and upon successful processing, the message '**The system has been successfully built**' will be displayed. A system with 100 THF molecules aligned at 0.6 g/cm³ will appear. The size and density of the system are displayed at the bottom of Viewport.



B. Execution of Calculation (A) Assignment of Force Field

- A. Select **Gromacs** from Toolbar's **Solver**.
- B. ☒ Click **Workflow Setup**.
- C. When **Assign force field parameters** window opens, click **OK** at the bottom right. A black terminal window will appear for a few seconds. Once the processing is successful and the message '**Assigned force field parameters**' is displayed, click **OK**.



B. Execution of Calculation (B)Equilibration Calculations

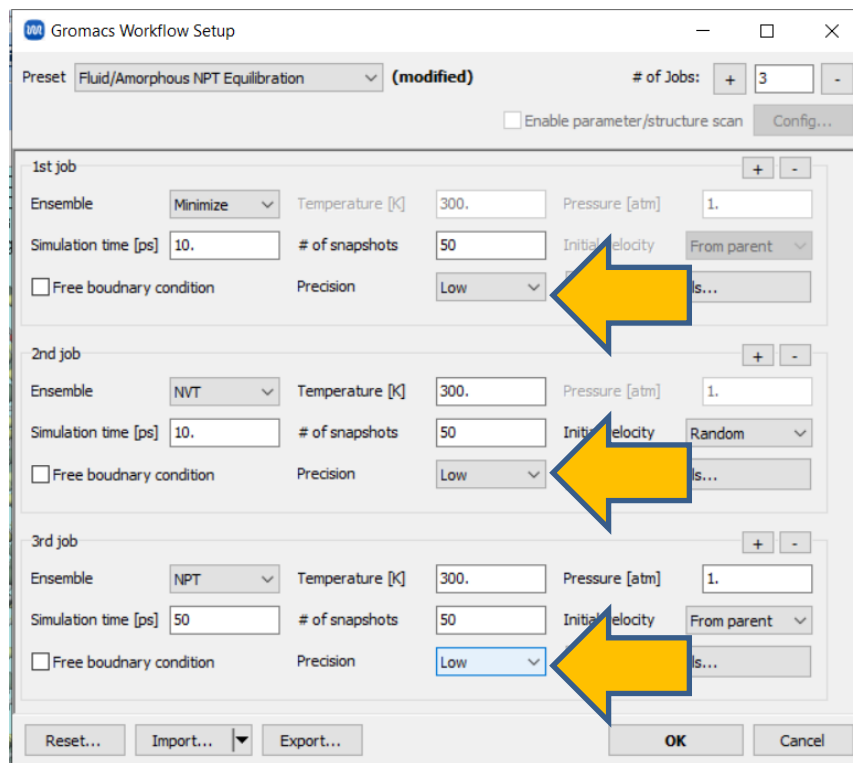
- A. In **Gromacs Workflow Setup** window, verify the computation flow. No specific settings are changed here. With this setup, a total of three jobs are executed consecutively: Energy Minimization (**Minimize**), Constant Temperature MD (**NVT**), and Constant Temperature and Pressure MD (**NPT**).
- B. If you need to change **Simulation time**, **Temperature**, or **Pressure** for each calculation, modify the relevant sections. (This is not required for the purpose of this manual).

The screenshot shows the 'Gromacs Workflow Setup' window. At the top, the 'Preset' is set to 'Fluid/Amorphous NPT Equilibration' and the '# of Jobs' is 3. Below this, there are three job configuration sections. Each section has a '+' and '-' button to the right. The first job is '1st job' with 'Ensemble' set to 'Minimize', 'Temperature [K]' at 300, 'Pressure [atm]' at 1, 'Simulation time [ps]' at 10, '# of snapshots' at 50, 'Initial velocity' set to 'From parent', and 'Precision' set to 'Medium'. The second job is '2nd job' with 'Ensemble' set to 'NVT', 'Temperature [K]' at 300, 'Pressure [atm]' at 1, 'Simulation time [ps]' at 10, '# of snapshots' at 50, 'Initial velocity' set to 'Random', and 'Precision' set to 'Medium'. The third job is '3rd job' with 'Ensemble' set to 'NPT', 'Temperature [K]' at 300, 'Pressure [atm]' at 1, 'Simulation time [ps]' at 50, '# of snapshots' at 50, 'Initial velocity' set to 'From parent', and 'Precision' set to 'Medium'. At the bottom, there are buttons for 'Reset...', 'Import...', 'Export...', 'OK', and 'Cancel'.

B. Execution of Calculation (B)Equilibration Calculations

- A. If you want to reduce computational accuracy to finish calculations more quickly, change **Precision** setting to '**Low**' for all three jobs: **1st job**, **2nd job**, and **3rd job**. If not, proceed to the next page.

Note: Without reducing computational accuracy, the time taken can range from several hours to half a day depending on machine specifications. However, reducing accuracy can shorten this to just a few minutes. Be aware that reducing accuracy may decrease the stability of the calculations.



The screenshot shows the 'Gromacs Workflow Setup' window. At the top, the 'Preset' is 'Fluid/Amorphous NPT Equilibration' (modified) and the '# of Jobs' is 3. Below this, there are three sections for '1st job', '2nd job', and '3rd job'. Each section has a 'Precision' dropdown menu. In all three sections, the 'Precision' is set to 'Low'. Three large yellow arrows point to these 'Low' settings. Other settings visible include 'Ensemble' (Minimize for 1st job, NVT for 2nd and 3rd), 'Temperature [K]' (300), 'Pressure [atm]' (1), 'Simulation time [ps]' (10 for 1st and 2nd, 50 for 3rd), and '# of snapshots' (50). The 'Initial velocity' is set to 'From parent' for the 1st and 3rd jobs, and 'Random' for the 2nd job. The 'Free boundary condition' checkbox is unchecked for all jobs. At the bottom, there are buttons for 'Reset...', 'Import...', 'Export...', 'OK', and 'Cancel'.

Supplement: Flow of Executing Calculations

In this case, after the calculation for (A) Minimize is executed, the calculation for (B) NVT will be performed. The information on atomic coordinates and velocities is automatically transferred between the consecutively executed calculations, ensuring that the final structure of (A) matches the initial structure of (B). Similarly, following the (B) NVT calculation, the (C) NPT calculation is executed. Each calculation is performed within its respective work folder.

Gromacs Workflow Setup

Preset: Fluid/Amorphous NPT Equilibration

of Jobs: 3

Enable parameter/structure scan

1st job

Ensemble: Minimize

Temperature [K]: 300.

Pressure [atm]: 1.

Simulation time [ps]: 10.

of snapshots: 50

Initial velocity: From parent

Free boundary condition: ☐

Precision: Medium

Details...

2nd job

Ensemble: NVT

Temperature [K]: 300.

Pressure [atm]: 1.

Simulation time [ps]: 10.

of snapshots: 50

Initial velocity: Random

Free boundary condition: ☐

Precision: Medium

Details...

3rd job

Ensemble: NPT

Temperature [K]: 300.

Pressure [atm]: 1.

Simulation time [ps]: 50

of snapshots: 50

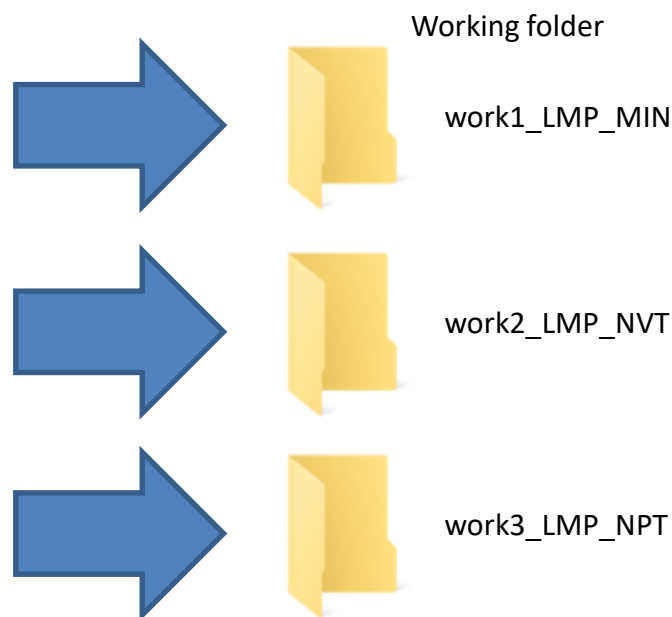
Initial velocity: From parent

Free boundary condition: ☐

Precision: Medium

Details...

Reset... Import... Export... OK Cancel

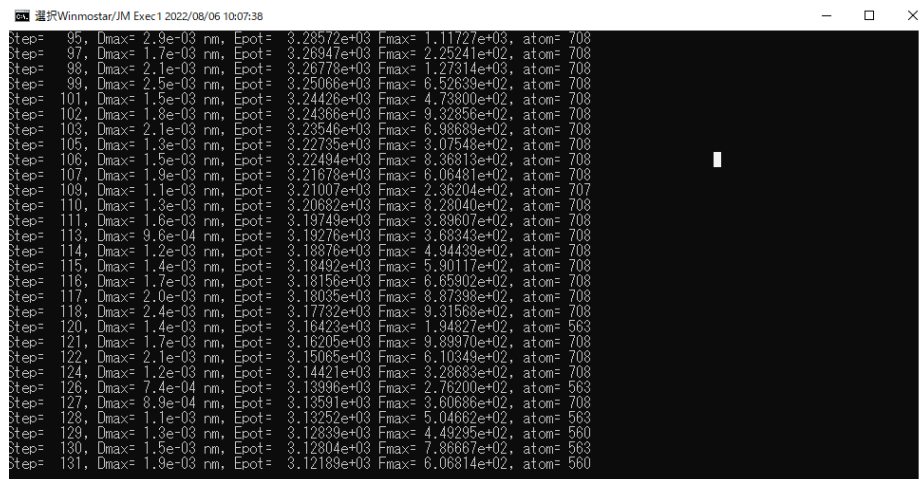
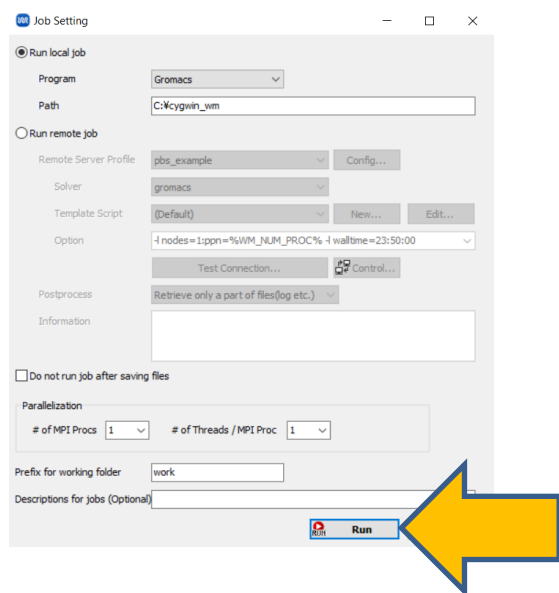


B. Execution of Calculation (B)Equilibration Calculations

(If working with remote jobs, please proceed [here](#) first.)

A. Click **OK** at the bottom right of **Gromacs Workflow Setup** window.

B. Click **Run** in **Job Setting** window. **Winmostar Job Manager** will start in the background, and a black console window, as shown in the right figure, will appear, indicating the start of the calculation.



Supplement: If you want to modify the input files yourself or wish to copy them to a remote server for use, check the option '**Do not run job after saving files**' in the job settings window and then click **Run**. To execute the calculations after saving, go to **File | Project | Selected Working Folder | Run**.

B. Execution of Calculation (B)Equilibration Calculations

- A. Upon returning to the main window (it's fine even if the calculations are still running), the parent-child relationship of the three work folders corresponding to each job in the **Gromacs Workflow Setup** window will be displayed in a tree structure in **Project Area**.
- B. In Viewport, the input file of the first work folder (work1_GMX_MIN) will automatically be opened. You can also confirm this at the top of **Viewport**.

The screenshot displays the Gromacs Workflow Setup interface. On the left, the 'Project Area' shows a tree structure of working folders for the project 'thf_liquid'. The 'work1_GMX_MIN' folder is selected and highlighted with a red box. Below it, the 'work2_GMX_NVT' and 'work3_GMX_NPT' folders are listed. The 'work1_GMX_MIN' folder is marked as 'END', 'work2_GMX_NVT' as 'END', and 'work3_GMX_NPT' as 'RUN'. The 'Recent projects' list at the top left shows 'thf_liquid' with status 'RUN(1)'. The 'Action (work1_GMX_MIN)' list on the bottom left includes 'Coordinate (Initial)', 'Coordinate (Final)', 'Log', 'Log (Extracted)', 'Log (stdout)', 'Full stdout', 'Animation', 'Energy plot', and 'Show in Explorer'. The 'Viewport' on the right shows a 3D molecular model of a liquid system. Above the model, the text 'work1_GMX_MIN Input File (input.gro)' is highlighted with a red box. Below the model, the text 'Force field: Available (Gromacs)' is visible. The 'Viewport' also displays various simulation parameters and coordinates.

Recent projects

Project	Status
thf_liquid	RUN(1)

Project

Working Folders (thf_liquid)

Folder	Status
work1_GMX_MIN	END
work2_GMX_NVT	END
work3_GMX_NPT	RUN

Action (work1_GMX_MIN)

- Coordinate (Initial)
- Coordinate (Final)
- Log
- Log (Extracted)
- Log (stdout)
- Full stdout
- Animation
- Energy plot
- Show in Explorer

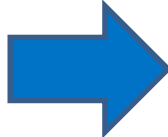
work1_GMX_MIN Input File (input.gro)

N= 1,300 C400H800O10
Marked Order: 1300 - 1 - 13 - 10
Marked Atom: X= 7.78 Y= 18.78 Z= 18.06
Length= 17.04566 Angle= 81.66582 Dihedral= 74.07102 Lper= 1.40746

Force field: Available (Gromacs)
Charges Available: User (Qtot=0.00,Qrms= 0.141)
rho= 0.600000 g/cm³
a= 27.124300 b= 27.124300 c= 27.124300
alpha= 90.00000 beta= 90.00000 gamma= 90.00000

B. Execution of Calculation (B)Equilibration Calculations

- A. Based on the progress of the calculation, **the status** of each working folder in **Project Area** changes from **PEND (black)** → **RUN (green)** → **END (blue)**.
- B. Wait until the status of all work folders changes to **END (blue)**. During this time, **the status of the recently used project 'thf_liquid'** will also change to ALL **END (blue)**.



Recent projects	
Project	Status
thf_liquid	RUN(1)

Project	
Working Folders (thf_liquid) Options ▼	
Name	Status
work1_GMX_MIN	END
work2_GMX_NVT	RUN
work3_GMX_NPT	PEND

Recent projects	
Project	Status
thf_liquid	ALL END

Project	
Working Folders (thf_liquid) Options ▼	
Name	Status
work1_GMX_MIN	END
work2_GMX_NVT	END
work3_GMX_NPT	END

B. Execution of Calculation (B)Equilibration Calculations

- A. If you want to view the main contents of each calculation's log, select the relevant calculation's working folder in **Working Folders section of Project Area**, then click **Log(Extracted)** under **Action**. (This feature is exclusive to the Professional Premium Edition.)
- B. If you wish to view the complete log, click **Log**.

Recent projects

Project	Status
thf_liquid	ALL END

Project

Working Folders (thf_liquid)

Name	Status
work1_GMX_MIN	END
work2_GMX_NVT	END
work3_GMX_NPT	END

Action (work1_GMX_MIN)

- Coordinate (Initial)
- Coordinate (Final)
- Log
- Log (Extracted)**
- Log (stdout)

Extracted Log (C:\winmos11\UserData\thf_liquid.wmpjdata\work1_GMX_MIN\gmxdmrun.log)

```
GROMACS: gmxdmrun, VERSION 5.0.7 (double precision)
Precision: double
Memory model: 64 bit
MPI library: thread_mpi
OpenMP support: enabled
SIMD instructions: SSE2
Brand: 11th Gen Intel(R) Core(TM) i7-1165G7 @ 2.80GHz
SIMD instructions most likely to fit this hardware: AVX2_256
Started Steepest Descents on rank 0 Tue Nov 21 08:01:06 2023
Steepest Descents converged to Fmax < 100 in 385 steps
Potential Energy = 2.79272388247968e+03
Force = 9.96501307545451e+01 on atom 149
Force = 1.96247019862382e+01
Time: Core t (s) Wall t (s) (%)
(steps/hour)
Performance: 516659.5
Finished mdrun on rank 0 Tue Nov 21 08:01:09 2023
```

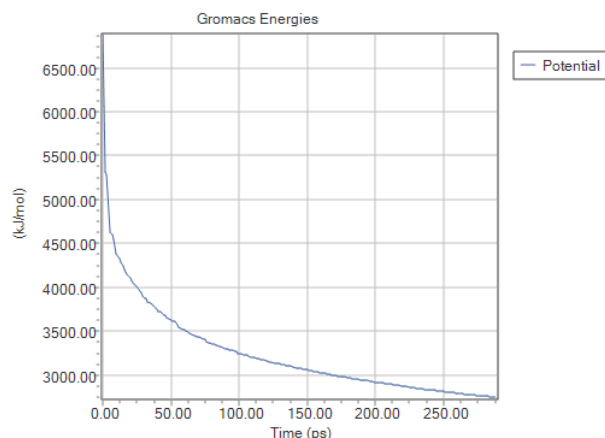
Export... Close

1291 C 8.4700 19.7000 16.18
1292 C 9.9100 19.2900 18.01
1293 C 8.4400 19.5600 17.71
1294 H 10.2800 20.1200 15.02
1295 H 7.6300 20.2600 15.78
1296 H 8.4600 18.7200 15.72
1297 H 8.1200 20.5000 18.16
1298 H 10.2200 19.6500 18.99

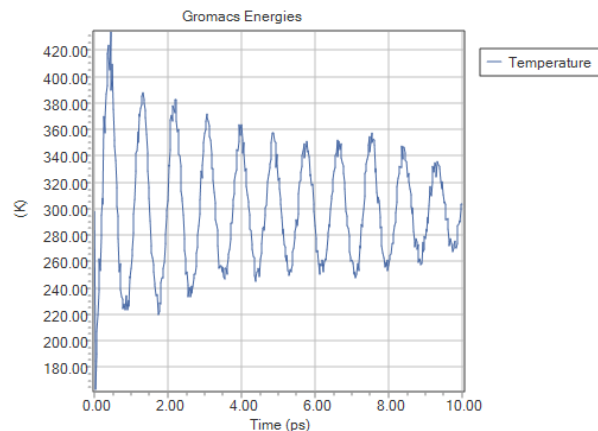
Supplement: Verifying the Convergence of Thermodynamic Quantities in Equilibration Calculations

According to the procedure on page 24, it is necessary to confirm that temperature, potential energy, pressure, and density have converged in the equilibration calculations. If they have not converged, continue to execute additional calculations while appropriately adjusting the conditions as per the procedure on pages 21-22 until convergence is achieved.

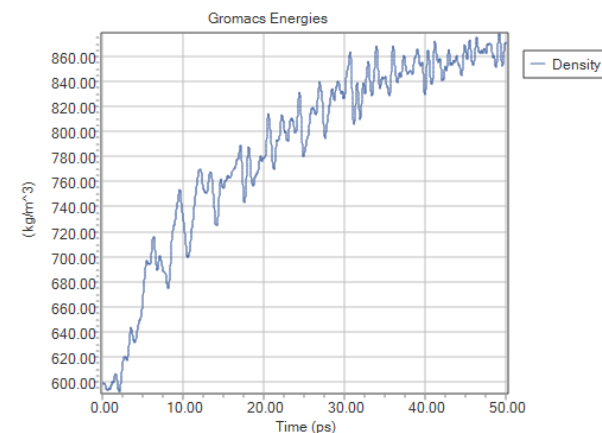
Example:



work1_GMX_MIN (Energy Minimization)
for Potential (Potential Energy)



work2_GMX_NVT (Constant
Temperature MD) for
Temperature (Temperature)



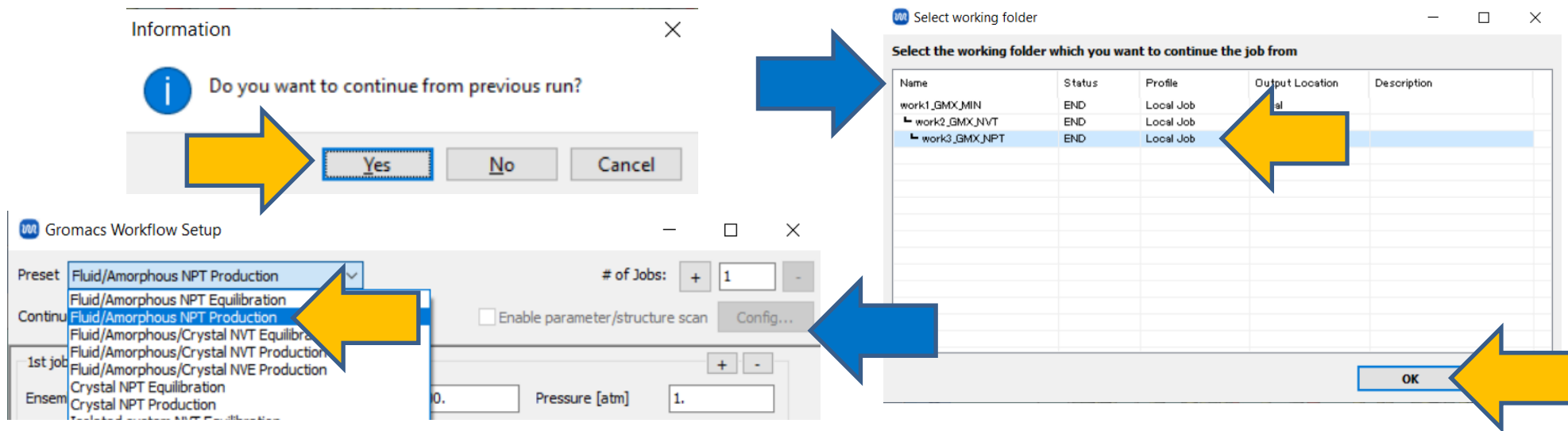
work3_GMX_NPT (Constant
Temperature and Pressure MD) for
Density (Density)

Note: Be aware that the convergence of density can be particularly slow.

Also note that in the examples given in this manual, the determination of convergence may be insufficient, thus longer duration calculations are preferable.

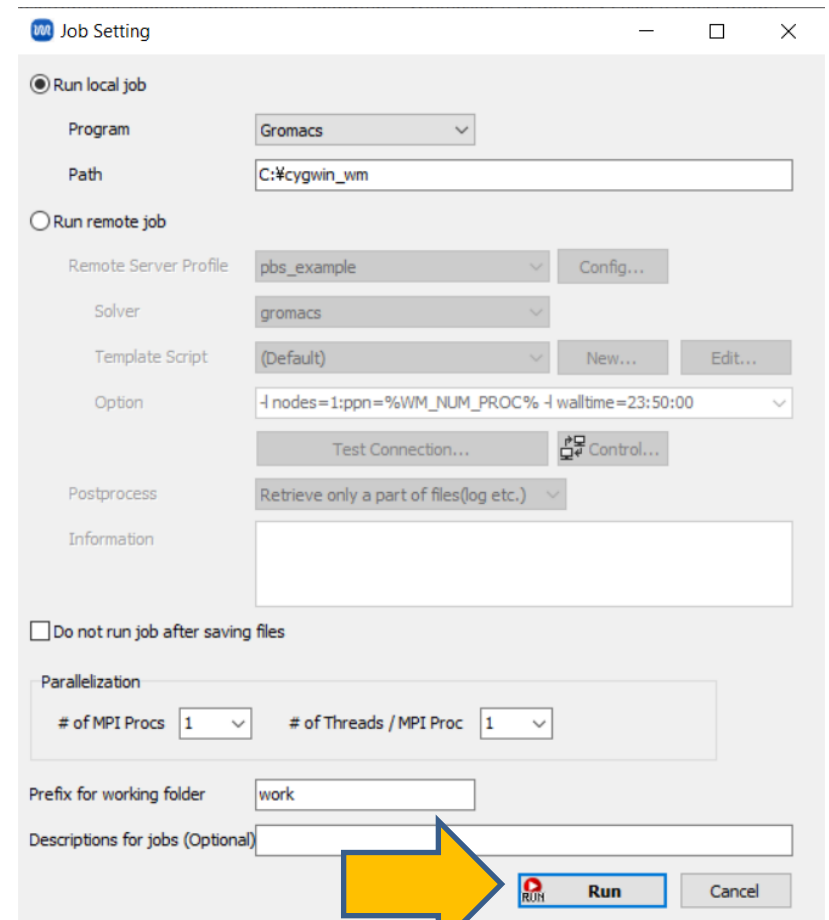
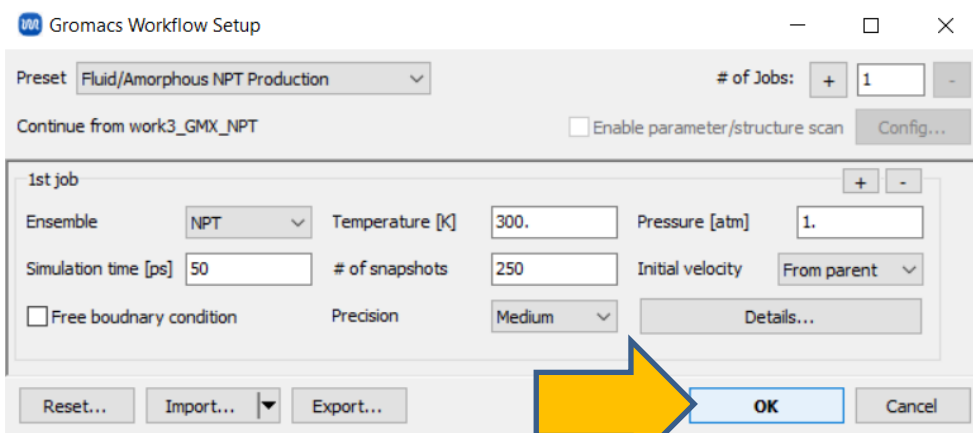
B. Execution of Calculation (C)The Main Calculation

- After the status of the original work folder (in this case, work3_GMX_NPT) has changed to **END (blue)**, click ☒ (**Workflow Setup**).
- Click **Yes** in **Information** dialog.
- Select the original work folder (work3_GMX_NPT) in **Select working folder** and then click **OK**.
- Select 'Fluid/Amorphous NPT Production' in **Preset**.
- If you want to decrease the computational accuracy to speed up the calculation, change **Precision** to 'Low'.




B. Execution of Calculation (C)The Main Calculation

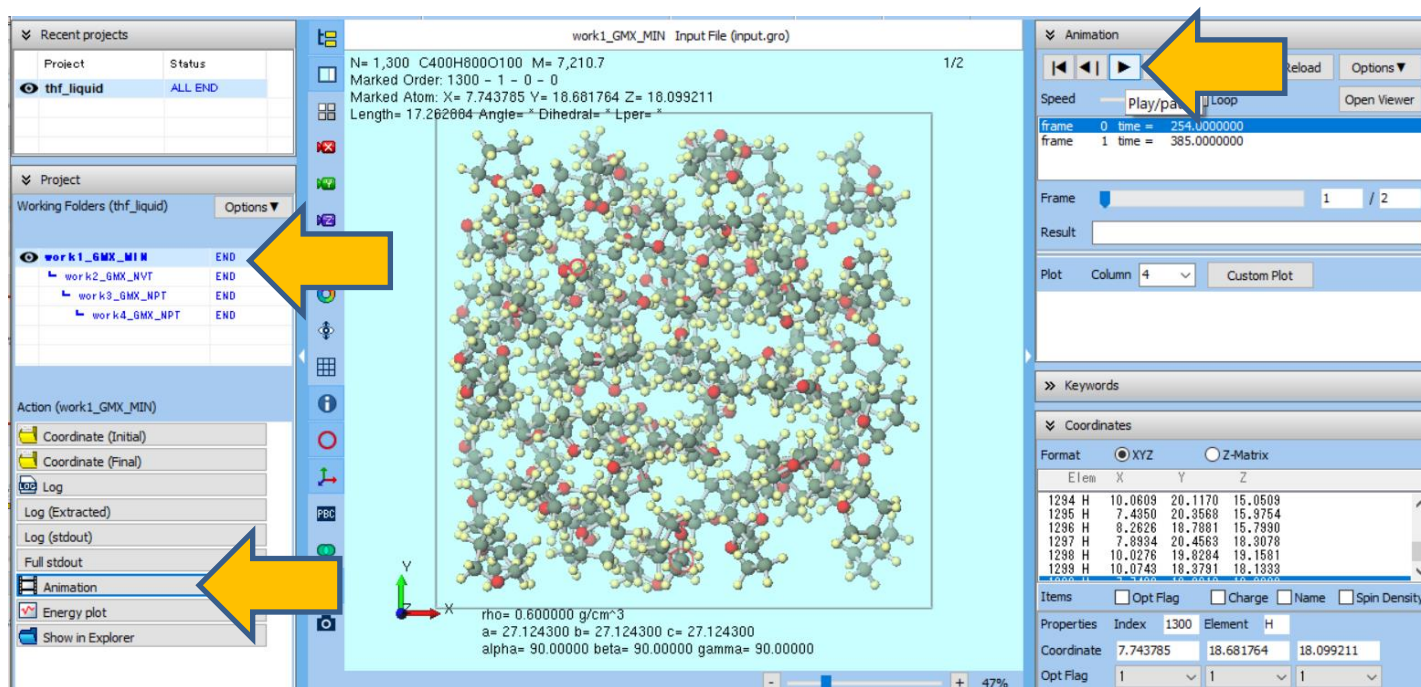
A. Click **OK** and then click **Run** in **Job Setting** window.



C. Result Analysis Animation

From this point onward, it is possible to skip steps that do not pertain to the analysis items you wish to check.

- Click the **relevant work folder** in Project display area (here, we will use 'work1_GMX_MIN').
- When you click **Animation** in **Action**, **Animation display area** will appear on the right side of the main window. Clicking the button  will display the calculation process as an animation.

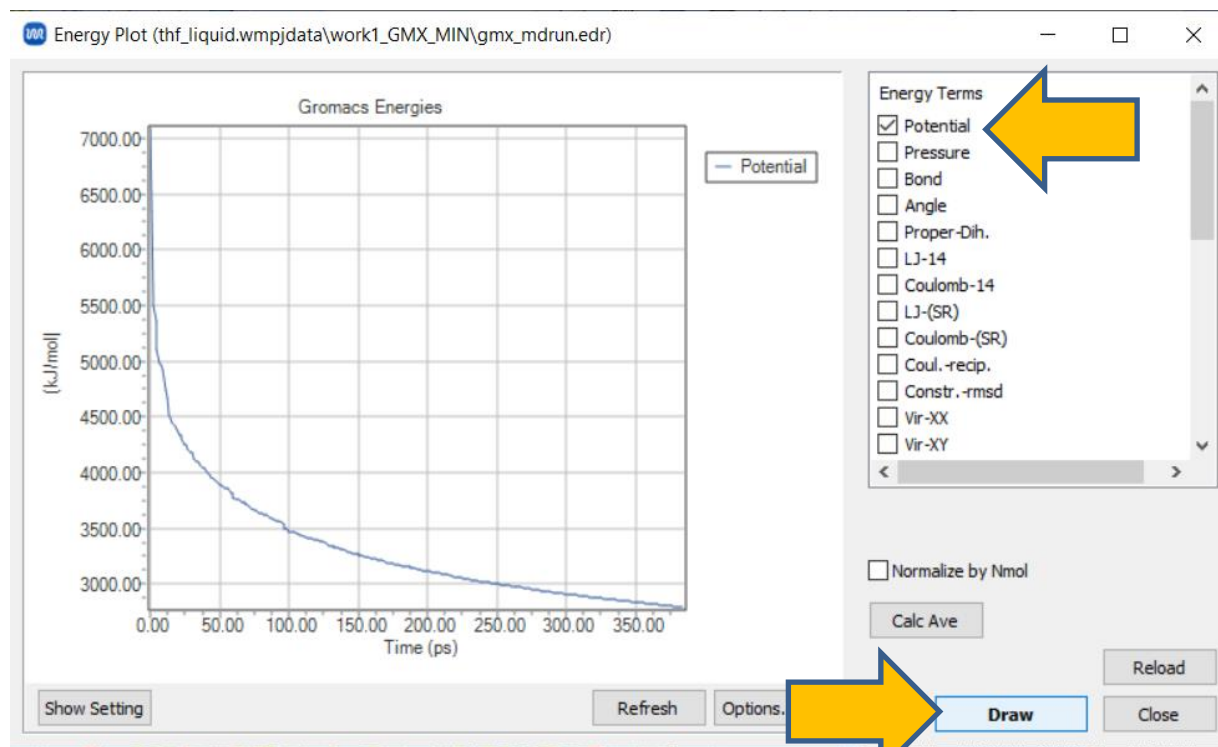
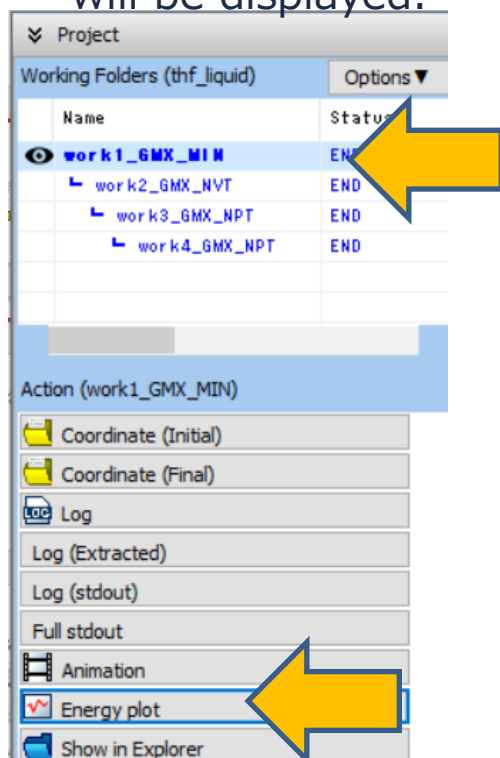


The screenshot displays the winmostar software interface. The central window shows a 3D molecular model of a protein-ligand complex. The left sidebar contains the 'Project' panel with a list of working folders, including 'work1_GMX_MIN', 'work2_GMX_MVT', 'work3_GMX_NPT', and 'work4_GMX_NPT'. Below this is the 'Action' panel for 'work1_GMX_MIN', which includes options like 'Coordinate (Initial)', 'Coordinate (Final)', 'Log', 'Log (Extracted)', 'Log (stdout)', 'Full stdout', 'Animation', 'Energy plot', and 'Show in Explorer'. The 'Animation' option is highlighted with a yellow arrow. The right sidebar features the 'Animation' panel, which includes playback controls (play, stop, previous, next, reload, options), a speed slider, a frame range selector (frame 0 to 1), a result field, and a plot column selector. Below this is the 'Coordinates' panel, which displays a table of atom coordinates in XYZ format. The table has columns for Element, X, Y, and Z. The data rows show coordinates for atoms 1294 through 1299. The 'Items' section below the table includes checkboxes for Opt Flag, Charge, Name, and Spin Density. The 'Properties' section at the bottom shows the Index (1300), Element (H), and Coordinate (7.743785, 18.681764, 18.099211). The 'Opt Flag' section shows values for 1, 1, and 1. A yellow arrow points to the 'Animation' button in the top right corner of the main window.

Element	X	Y	Z
1294 H	10.0609	20.1170	15.0509
1295 H	7.4350	20.3568	15.9754
1296 H	8.2626	18.7881	15.7990
1297 H	7.8994	20.4563	18.3078
1298 H	10.0276	19.8284	18.1581
1299 H	10.0743	18.3791	18.1333

C. Result Analysis Temporal Variation and Averages of Energy and Other Parameters

- Click the **relevant work folder** in **Project Area** (here we will use 'work1_GMX_MIN').
- When you click **Energy plot** in **Action**, **Energy Plot** window will appear. Check the physical quantity you want to visualize in **Energy Terms** (here we choose 'Potential' for potential energy), and when you click **Draw**, a graph showing the time variation will be displayed.



C. Result Analysis Temporal Changes and Averages of Energy and Other Quantities

- A. When you want to check the average values, click **Calc Ave**. Click **OK** when prompted with 'Enter first frame to read'. A text file will open, displaying the average values and standard errors of various physical quantities. Please note that average values, except for calculations that have reached a certain degree of equilibration (in this manual, corresponding to 'work4_GMX_NPT'), may not have physical significance.
- B. After confirming, click **Close** to close **Energy Plot** window.

The image shows two windows. On the left is the 'Energy Terms' dialog box with a list of energy components and buttons at the bottom. On the right is a Notepad window showing the contents of 'energy_ave.log'.

Energy Terms Dialog Box:

- ☒ Potential
- ☐ Pressure
- ☐ Bond
- ☐ Angle
- ☐ Proper-Dih.
- ☐ LJ-14
- ☐ Coulomb-14
- ☐ LJ-(SR)
- ☐ Coulomb-(SR)
- ☐ Coul.-recip.
- ☐ Constr.-rmsd
- ☐ Vir-XX
- ☐ Vir-XY
- ☐ Vir-YZ
- ☐ Vir-ZX
- ☐ Vir-ZY
- ☐ Vir-ZZ
- ☐ Pres-XX
- ☐ Pres-XY
- ☐ Pres-XZ
- ☐ Pres-YX
- ☐ Pres-YY
- ☐ Pres-YZ
- ☐ Pres-ZX
- ☐ Pres-ZY
- ☐ Pres-ZZ
- ☐ Surf*SurfTen
- ☐ T-System

Buttons: **Calc Ave**, **Reload**, **Draw**, **Close**

energy_ave.log - Notepad:

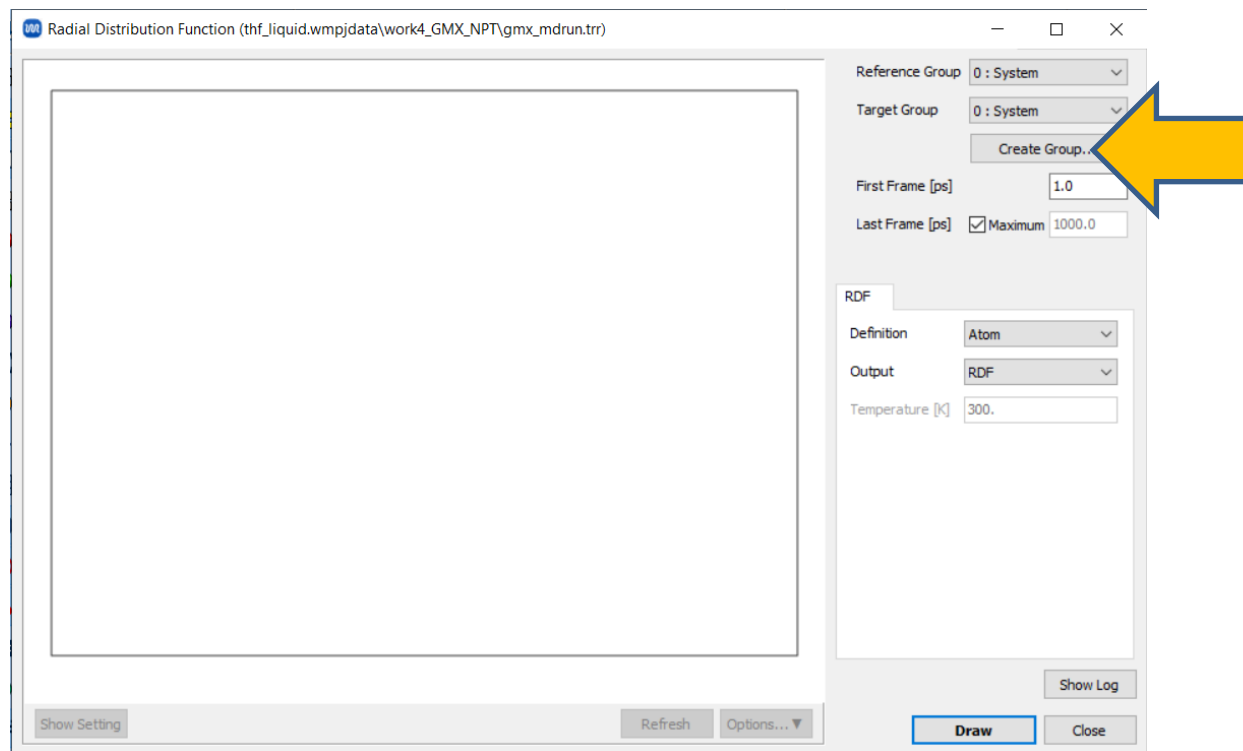
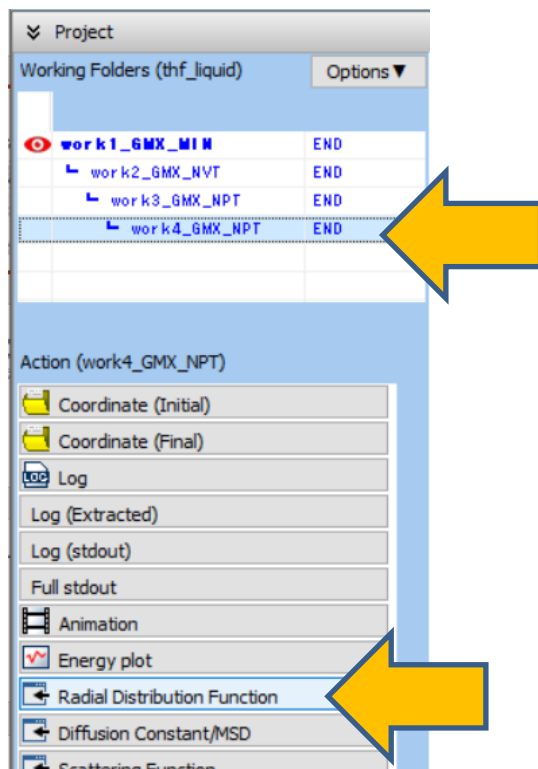
File Edit Format View Help
Statistics over 385 steps [0.0000 through 384.0000 ps], 31 data sets
All statistics are over 303 points (frames)

Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	0.743619	0.12	0.322569	-0.77006	(kJ/mol)
Angle	16.5976	0.59	1.32669	-3.81215	(kJ/mol)
Proper Dih.	32.8043	0.19	0.395245	1.13734	(kJ/mol)
LJ-14	0.483663	0.029	0.059184	-0.184298	(kJ/mol)
Coulomb-14	-9.42845	0.034	0.0727914	0.224893	(kJ/mol)
LJ (SR)	-17.4943	1.8	4.1965	-12.0134	(kJ/mol)
Coulomb (SR)	6.69129	0.11	0.221198	-0.752634	(kJ/mol)
Coul. recip.	2.78927	0.048	0.097512	-0.53481	(kJ/mol)
Potential	33.187	2.5	5.71558	-18.5061	(kJ/mol)
Pressure	1025.55	210	659.839	-1431.38	(bar)
Constr. rmsd	8.05552e-08	6e-08	3.75824e-07	-3.61576e-07	()
Vir-XX	-636.682	120	395.37	835.9	(kJ/mol)
Vir-XY	-43.6465	12	25.2085	78.2304	(kJ/mol)
Vir-XZ	42.9723	9.4	27.6485	-66.2855	(kJ/mol)
Vir-YX	-43.6465	12	25.2085	78.2304	(kJ/mol)
Vir-YY	-618.592	130	396.326	866.882	(kJ/mol)
Vir-YZ	-3.83183	2.5	8.72358	-14.2616	(kJ/mol)
Vir-ZX	42.9723	9.4	27.6485	-66.2855	(kJ/mol)
Vir-ZY	-3.83183	2.5	8.72358	-14.2616	(kJ/mol)
Vir-ZZ	-593.457	130	408.254	877.736	(kJ/mol)
Pres-XX	1059.56	200	657.972	-1391.1	(bar)
Pres-XY	72.6362	20	41.9519	-130.191	(bar)
Pres-XZ	-71.5142	16	46.0125	110.312	(bar)
Pres-YX	72.6362	20	41.9519	-130.191	(bar)
Pres-YY	1029.46	210	642.921	-1442.33	(bar)
Pres-YZ	6.37891	4.2	14.5177	23.734	(bar)
Pres-ZX	-71.5142	16	46.0125	110.312	(bar)
Pres-ZY	6.37891	4.2	14.5177	23.734	(bar)
Pres-ZZ	987.628	220	679.413	-1460.72	(bar)
#Surf*SurfTen	-154.287	27	96.8878	-119.373	(bar nm)
T-System	0	0	0	0	(K)

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!
You should select the temperature in order to obtain fluctuation properties.

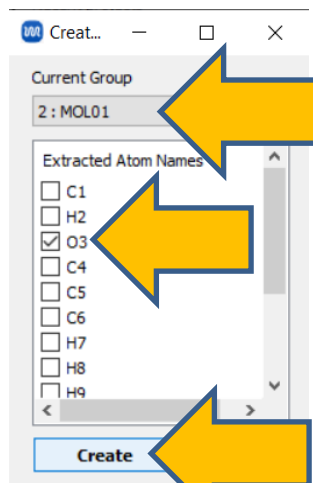
C. Result Analysis Radial Distribution Function

- Click **the relevant work folder** in **Project Area** (here, we will use 'work4_GMX_NPT').
- When you click **Radial Distribution Function** in **Action**, **Radial Distribution Function** window will appear. To obtain the radial distribution function not for all atoms but specifically between certain atoms, click **Create Group**.



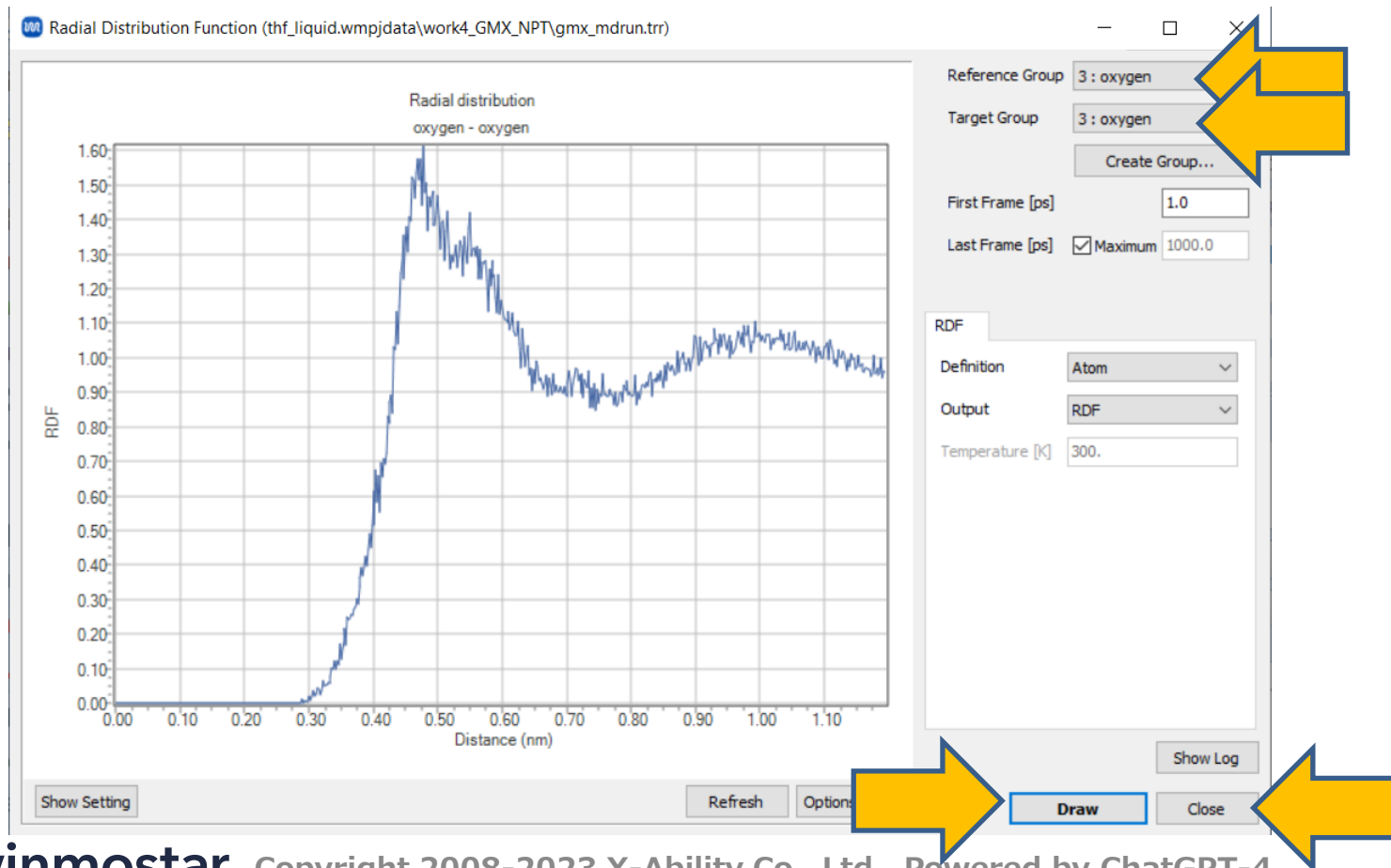
C. Result Analysis Radial Distribution Function

- A. In **Create Group** window, select '**2: MOL01**' (which refers to THF in this case) in **Current Group**, choose '**O3**' in Extracted Atom Names, and click **Create**.
- Beforehand, by checking **View | Labels/Charges | Show Name** in the main window, you can verify the Atom Names of each atom in Viewport.
 - Also, by clicking **MD | Gromacs | Analysis | Radial Distribution Function** and selecting a pre-created .ndx file, you can further fine-tune the analysis target groups. .ndx files can be created from **Select menu** in the main window. (Refer to the user manual for details)
- B. When prompted with 'New Group Name', enter 'oxygen' and click **OK**.
- C. Once the terminal window appears and the process is complete, click **Close**.



C. Result Analysis Radial Distribution Function

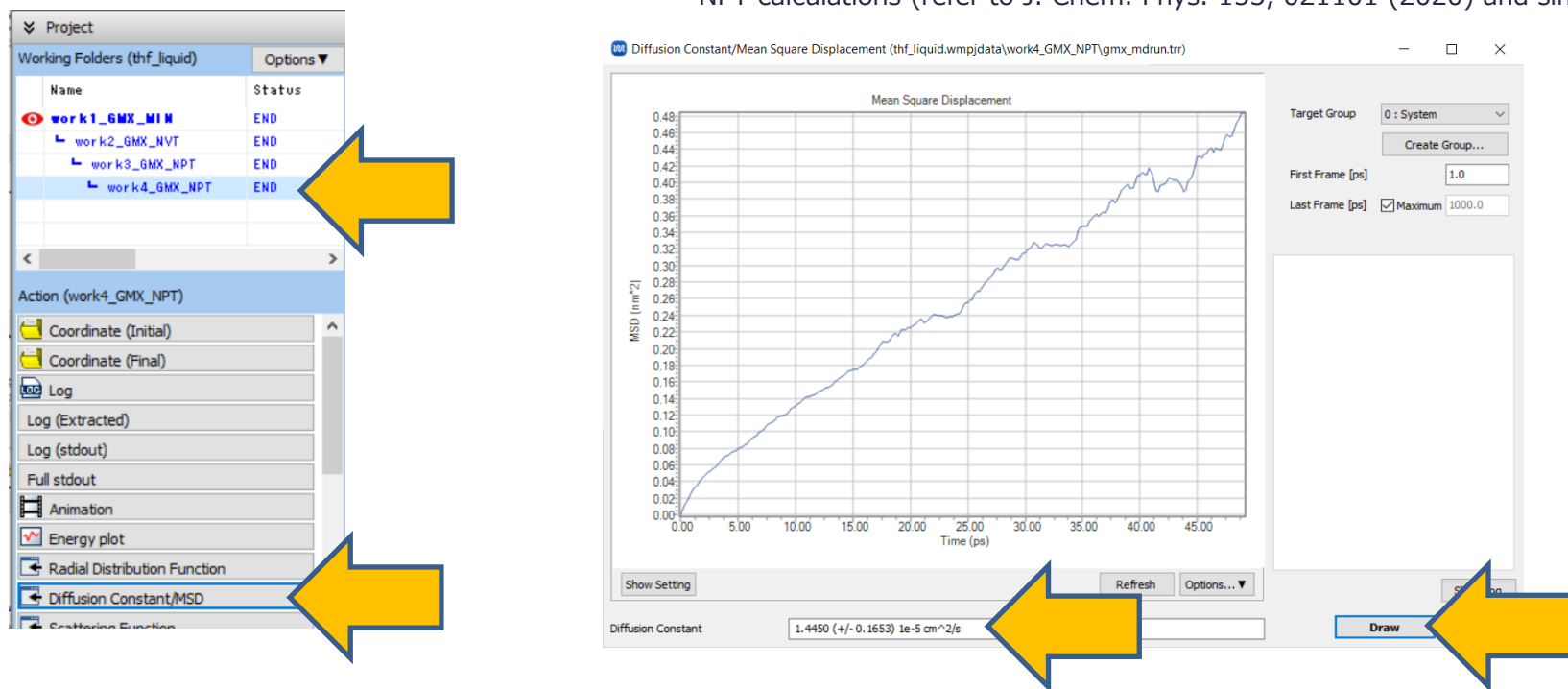
- A. Select the recently created '**oxygen**' for both **Reference Group** and **Target Group**, and click **Draw** to output the radial distribution function between oxygen atoms.
- B. After reviewing the graph, click **Close**.



C. Result Analysis Self-Diffusion Coefficient

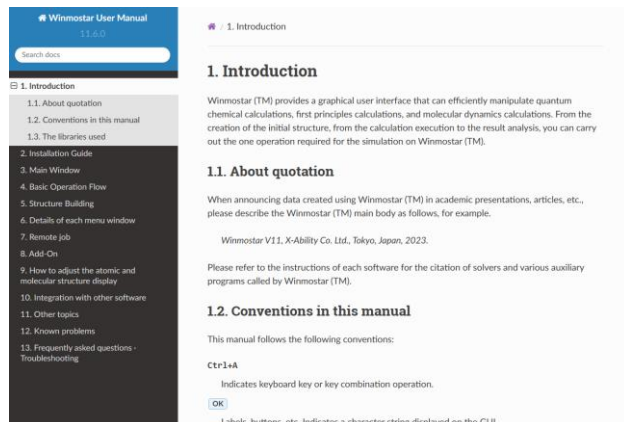
- A. Click the relevant work folder in **Project Area** (here we will use 'work4_GMX_MIN').
- B. When you click **Diffusion Constant/MSD** in **Action, Diffusion Constant/Mean Square Displacement** window will appear. Clicking **Draw** will display the graph of the mean square displacement and the self-diffusion coefficient (**Diffusion Constant**).

Supplement: Ideally, the self-diffusion coefficient should be determined from NVT calculations, but in this manual, it is simplistically derived from NPT calculations (refer to J. Chem. Phys. 153, 021101 (2020) and similar sources).



Troubleshooting and Additional Resources

- For detailed information on each feature, please refer to [Winmostar User Manual](#).



[Winmostar User Manual](#)

- If you are unable to proceed as instructed in this guide, please first refer [Frequently asked questions](#).
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through [Contact](#), detailing the steps to reproduce the issue and attaching any generated files at that time.