winmostar tutorial

Gromacs Basic

V11.5.6

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

About This Document

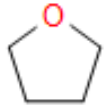
- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- If you are unable to proceed with the operations 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.
-

Overview

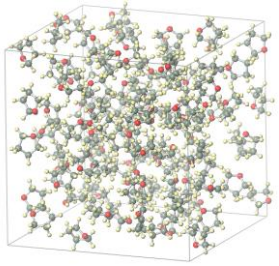
- We will obtain various thermodynamic properties, radial distribution functions, self-diffusion coefficients, specific heats, and compressibility of tetrahydrofuran (THF) liquid under room temperature and atmospheric pressure using molecular dynamics calculations with Gromacs (employing GAFF and AM1-BCC 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:

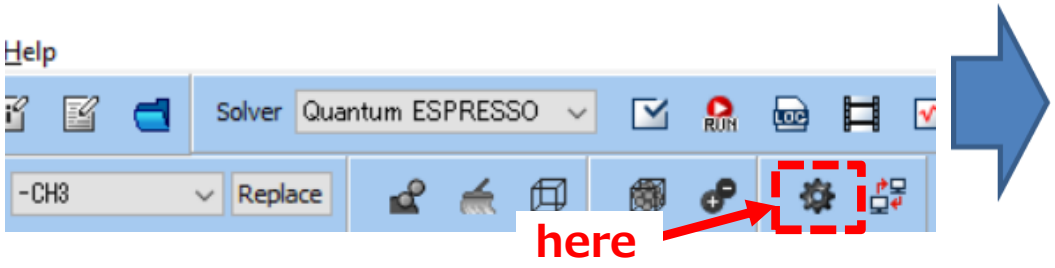
- The number of steps and molecules will vary depending on the type of system, the physical properties you want to calculate, and the desired level of accuracy.
- The choice of force field and type of charges significantly affects the results of the calculations.

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.

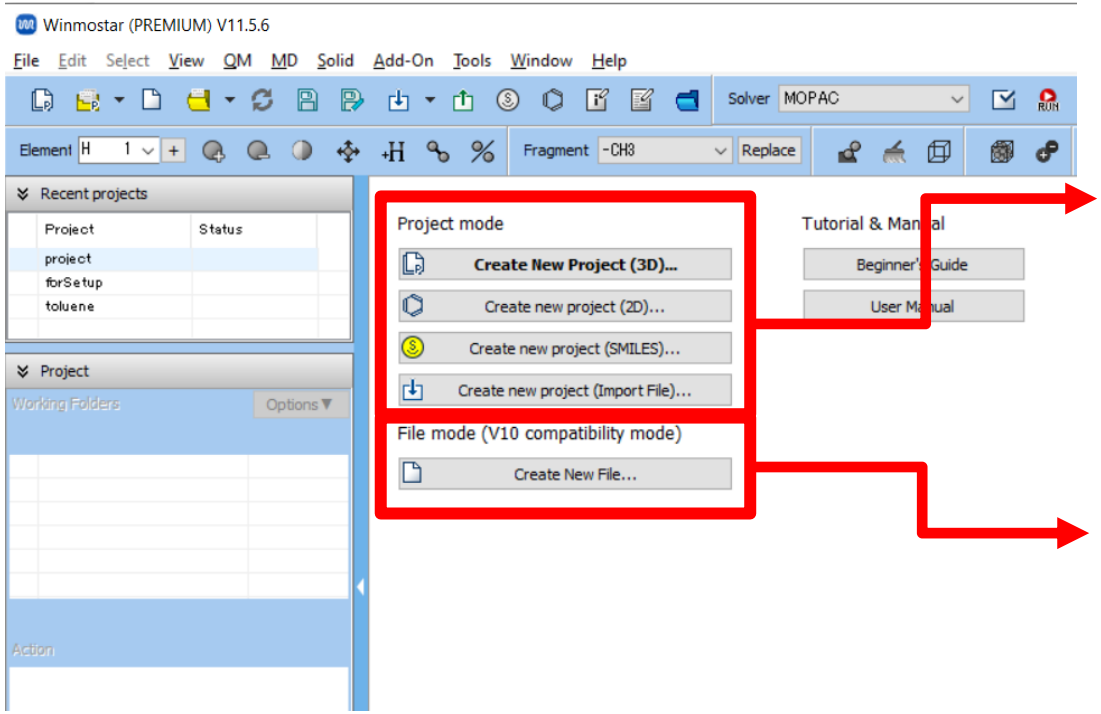
(7) Install Cygwin environment for Winmostar. ← here

- 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

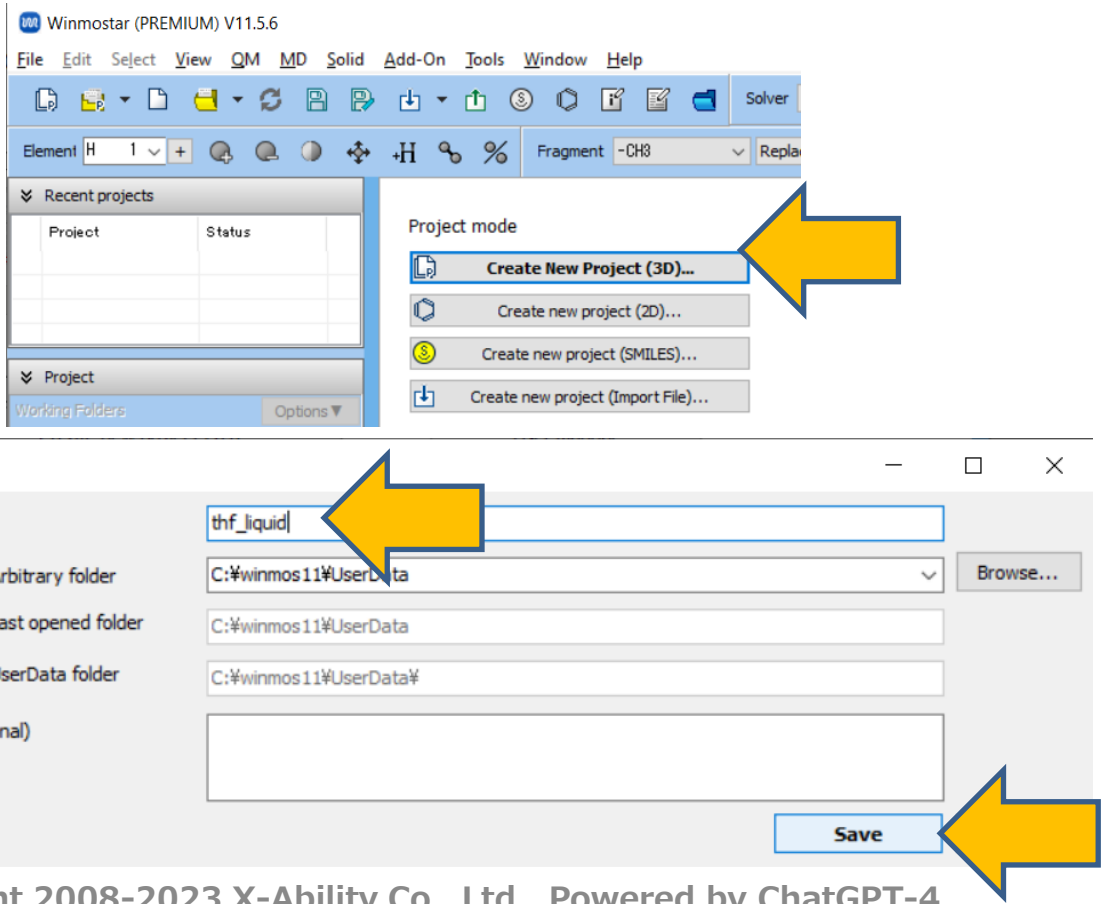
Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

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

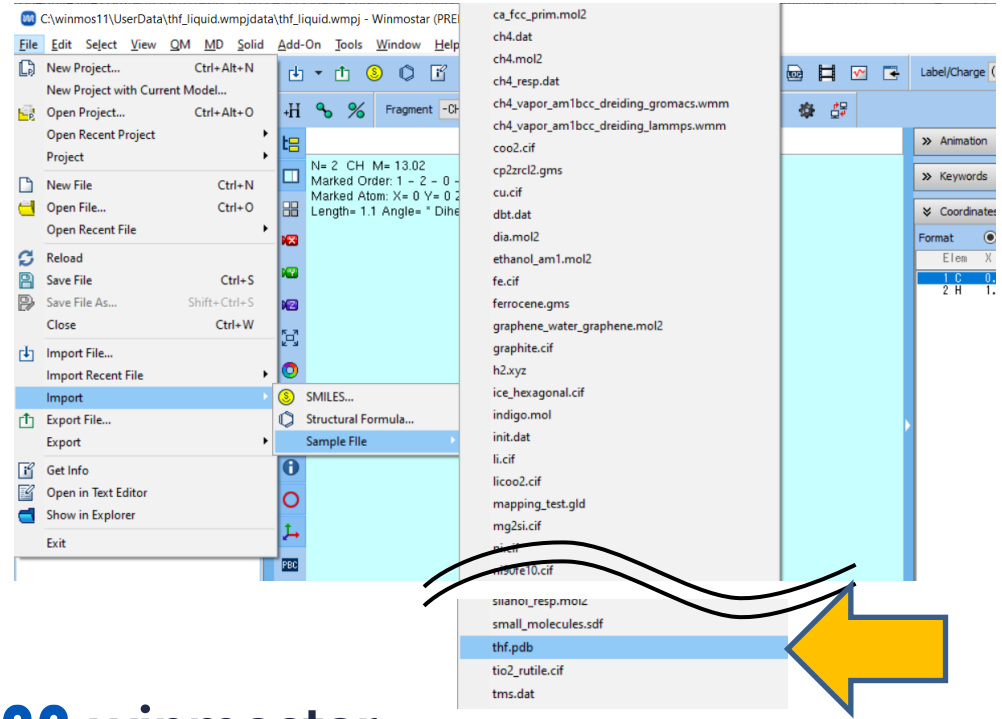
For details on creating an initial structure, please refer to Molecular Modeling Organic Molecules Tutorial.

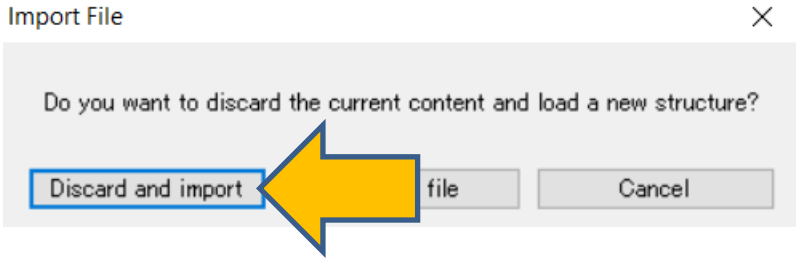
In this section, we will load an existing molecular structure file.

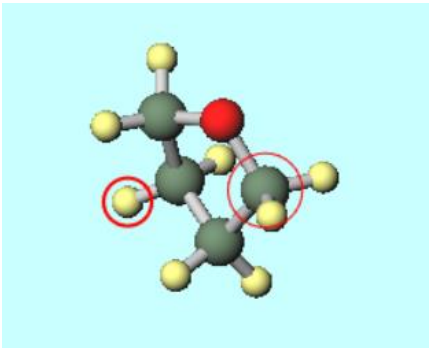
A. Click **File** | **Import** | **Sample File** | **thf.pdb**
   - If you wish to load a different file at this stage, use **File** | **Import File** instead.

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

C. Verify that the desired molecule appears in Viewport.

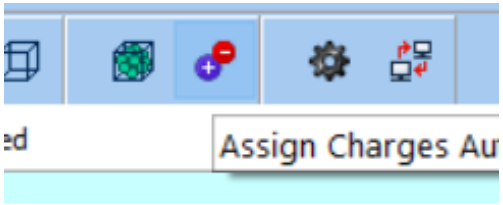


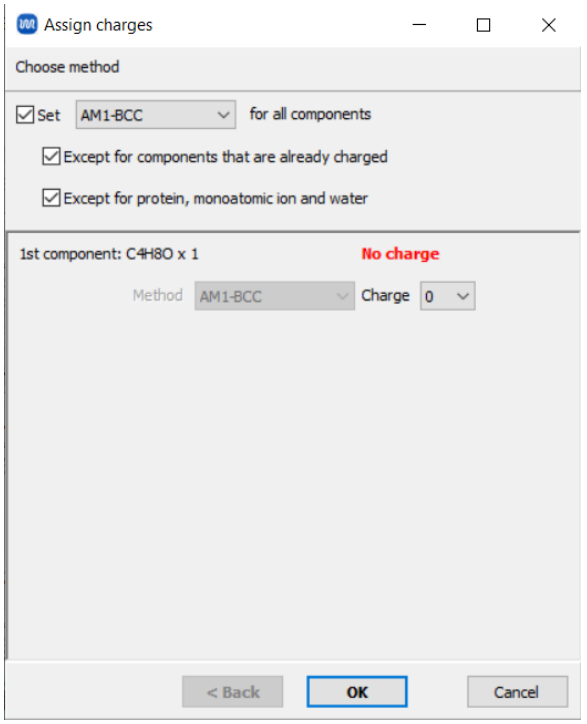


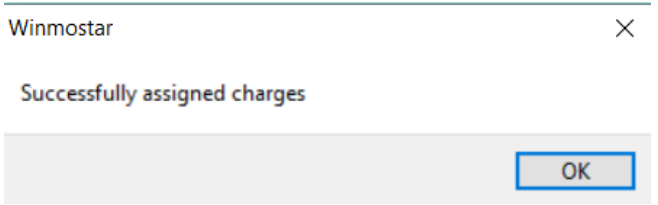


A. System Modeling　(B)Assignment of Charges

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





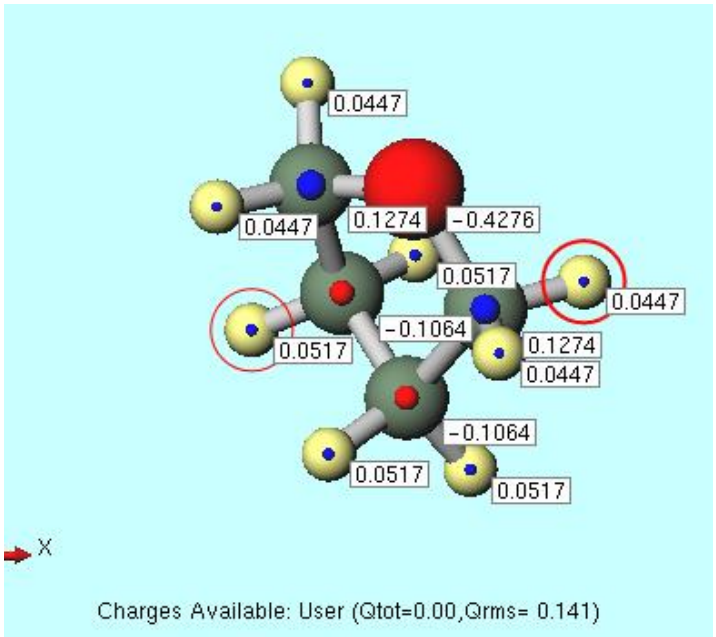


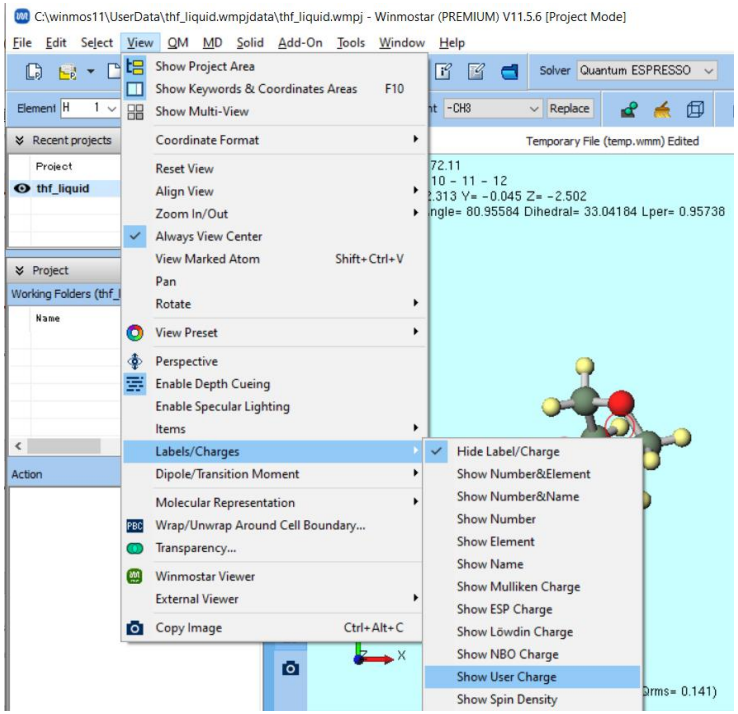
A. System Modeling (B)Assignment of Charges

A. Verify that 'Charges Available: User (Qtot=0.00, Qrms=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**.

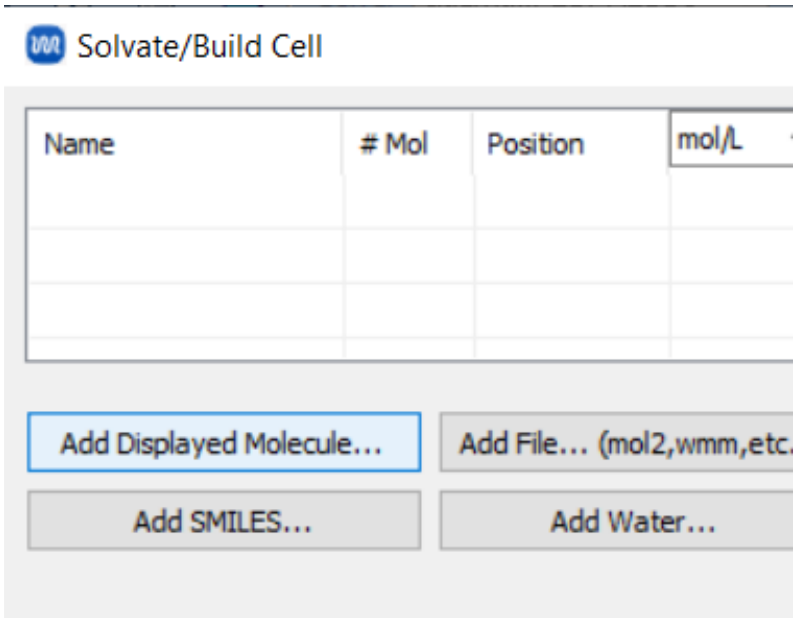
C. To undo step B, click **View** | **Labels/Charges** | **Hide Label/Charge**.

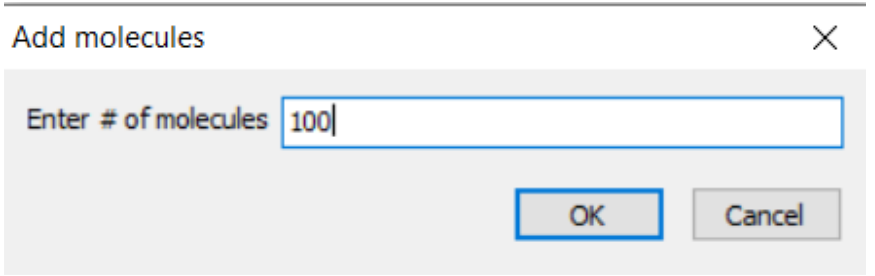




A. System Modeling　(C)Creation of the Liquid Phase

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

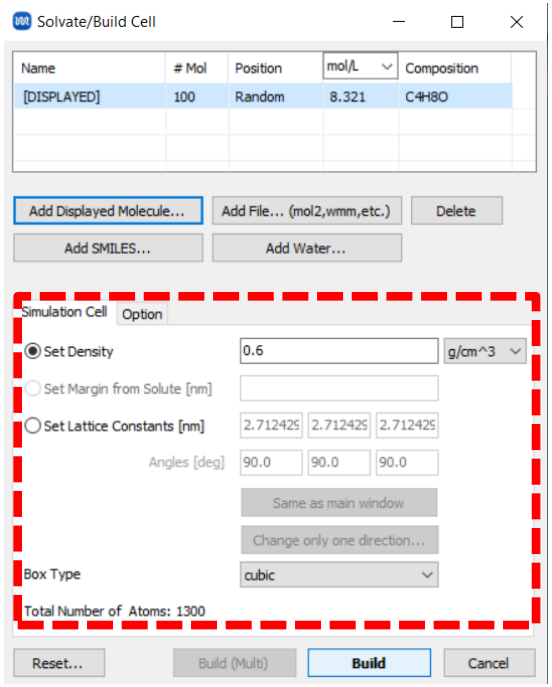


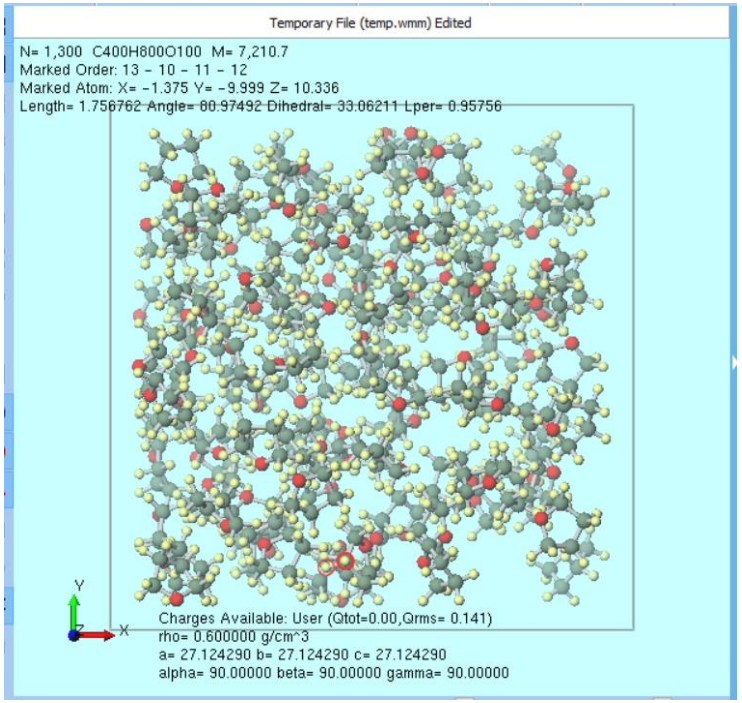


A. System Modeling (C)Creation of the Liquid Phase

A. Verify the settings of **Simulation Cell**. (In this manual, we will proceed without making any specific changes.)

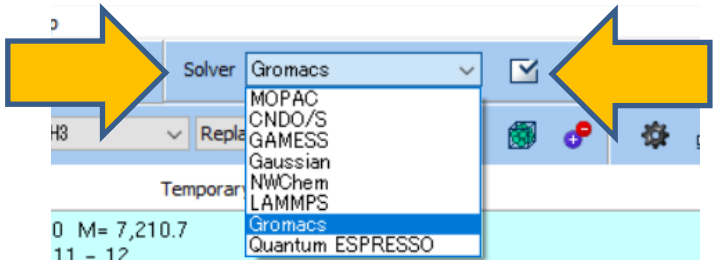
B. When you click **Build**, a black terminal window will appear for a few seconds, and upon successful processing, the message '**The system has been successfully built**' will be displayed. A system with 100 THF molecules aligned at 0.6 g/cm³ will appear. The size and density of the system are displayed at the bottom of Viewport.

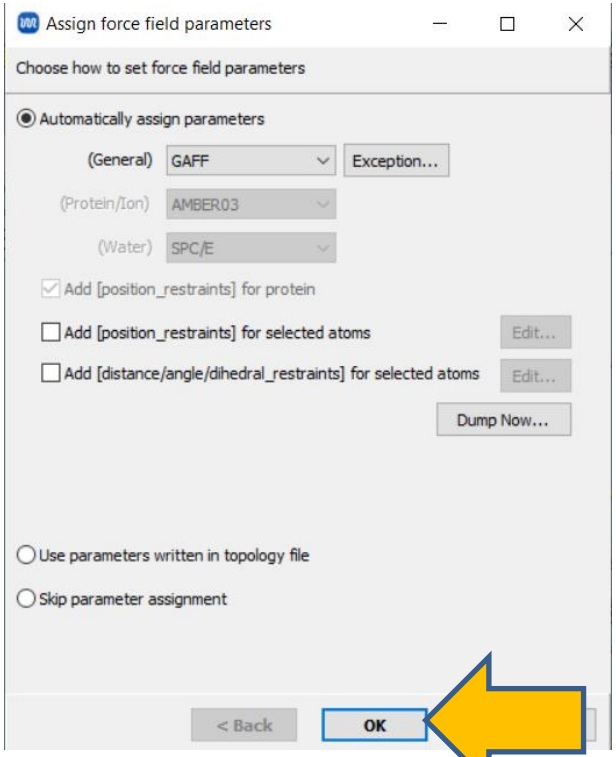


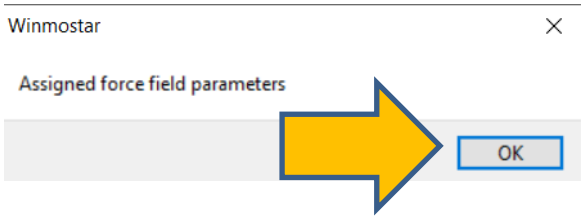


B. Execution of Calculation　(A)Assignment of Force Field

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**.



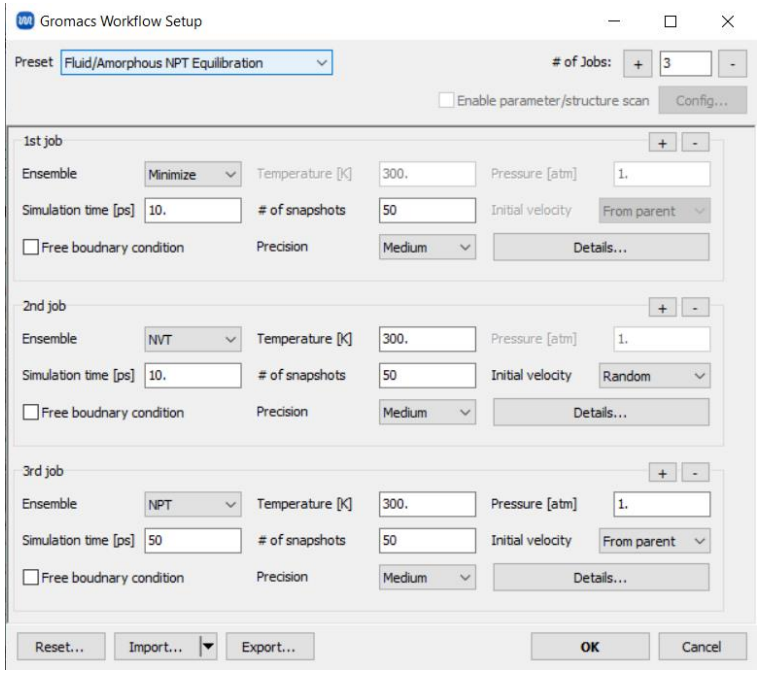




B. Execution of Calculation (B)Equilibration Calculations

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**).

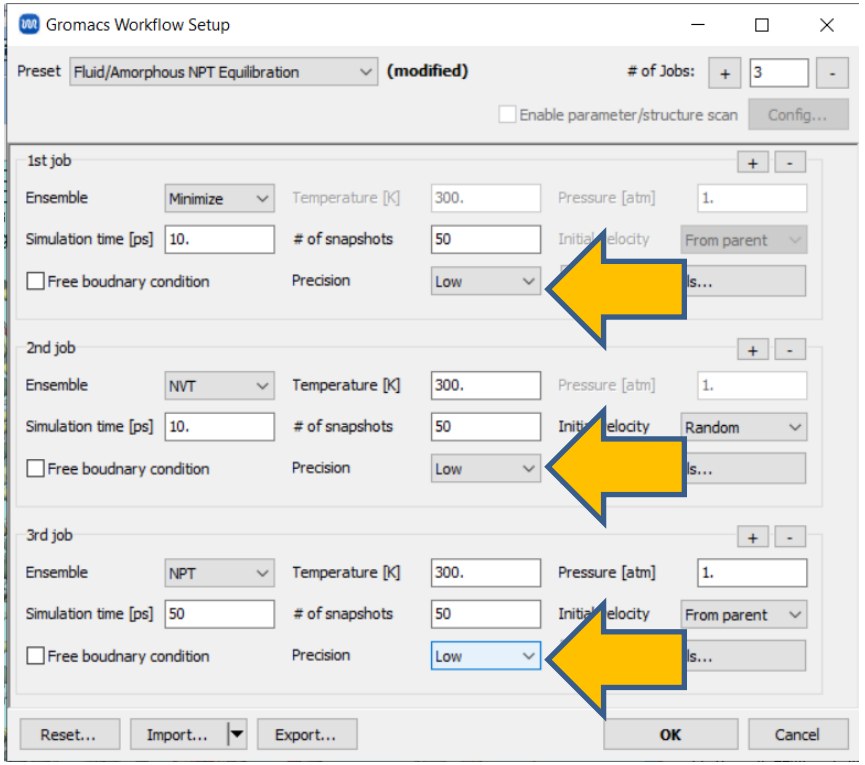
B. If you need to change **Simulation time**, **Temperature**, or **Pressure** for each calculation, modify the relevant sections. (This is not required for the purpose of this manual).



B. Execution of Calculation　(B)Equilibration Calculations

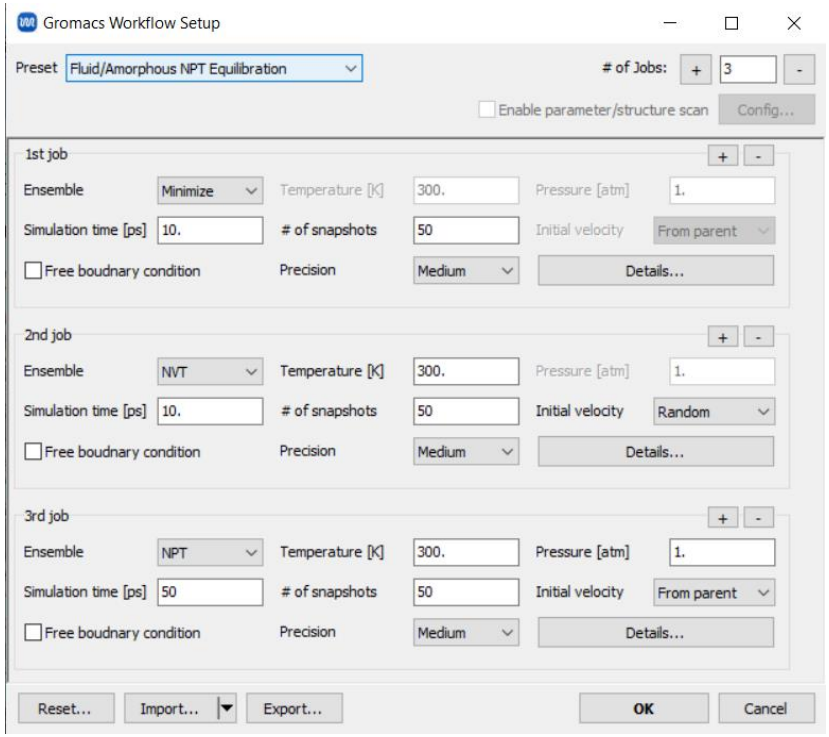
A. If you want to reduce computational accuracy to finish calculations more quickly, change **Precision** setting to '**Low**' for all three jobs: **1st job**, **2nd job**, and **3rd job**. If not, proceed to the next page.

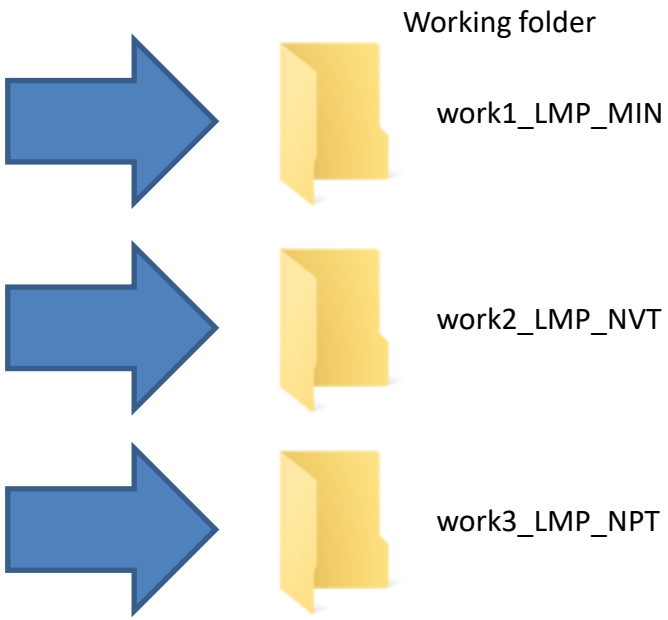
Note: Without reducing computational accuracy, the time taken can range from several hours to half a day depending on machine specifications. However, reducing accuracy can shorten this to just a few minutes. Be aware that reducing accuracy may decrease the stability of the calculations.



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.



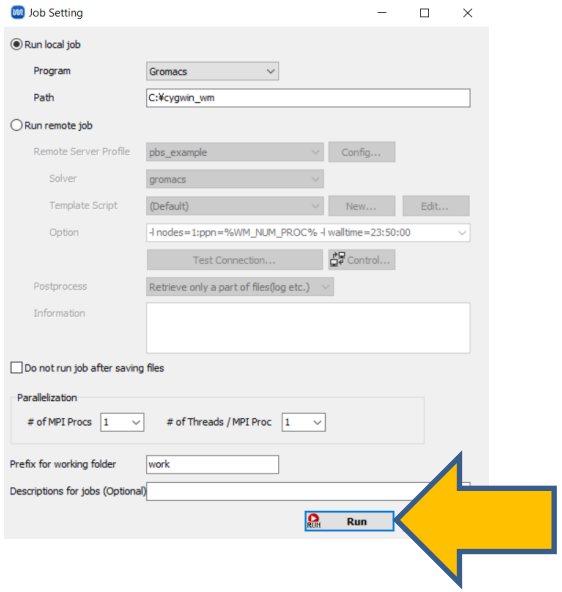


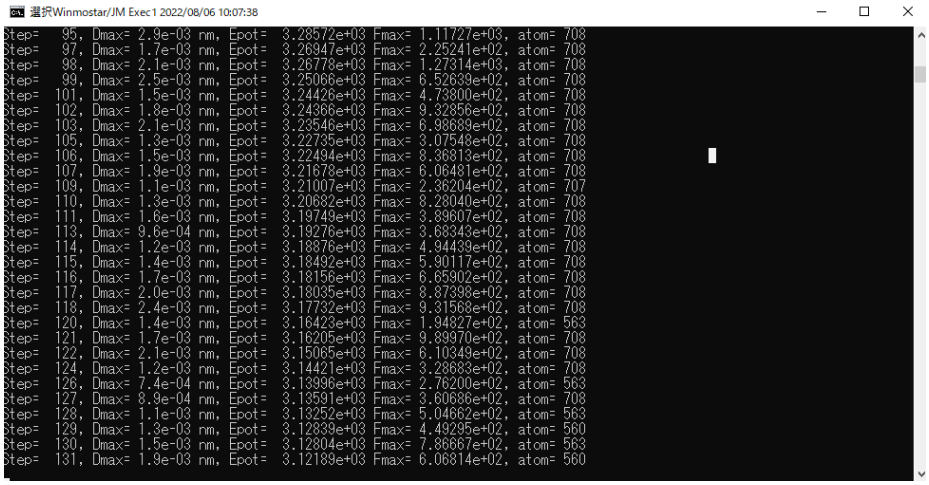
B. Execution of Calculation　(B)Equilibration Calculations

(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.



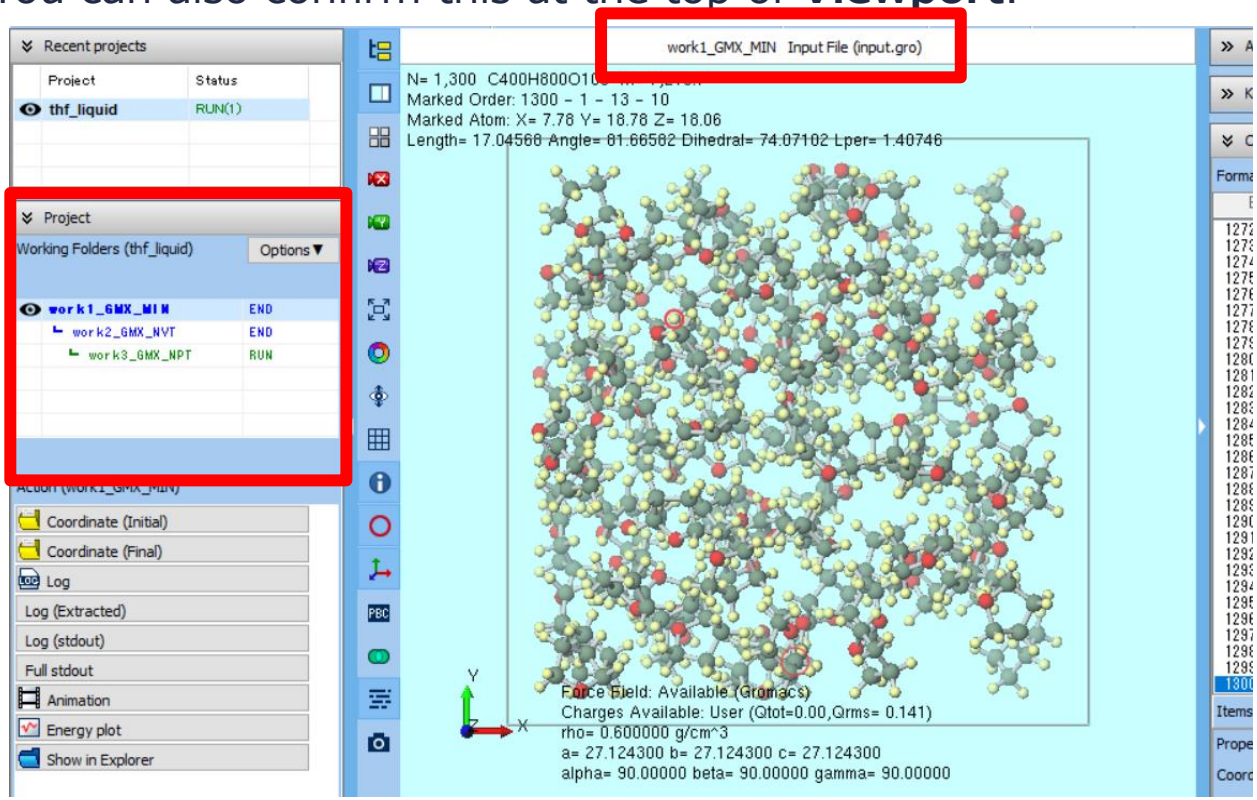


Supplement: If you want to modify the input files yourself or wish to copy them to a remote server for use, check the option '**Do not run job after saving files**' in the job settings window and then click **Run**. To execute the calculations after saving, go to **File** | **Project** | **Selected Woking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

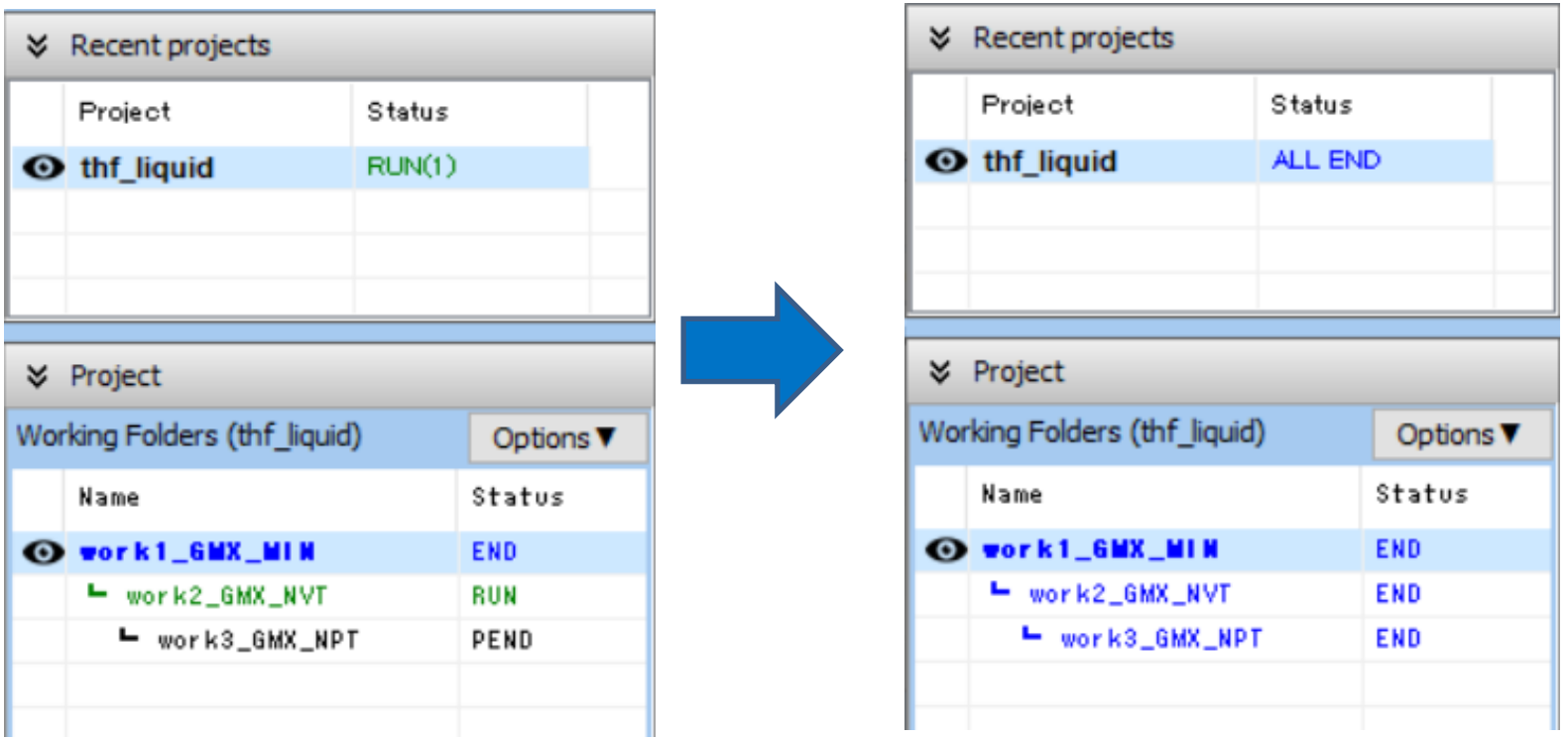
B. In Viewport, the input file of the first work folder (work1_GMX_MIN) will automatically be opened. You can also confirm this at the top of **Viewport**.



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)**.

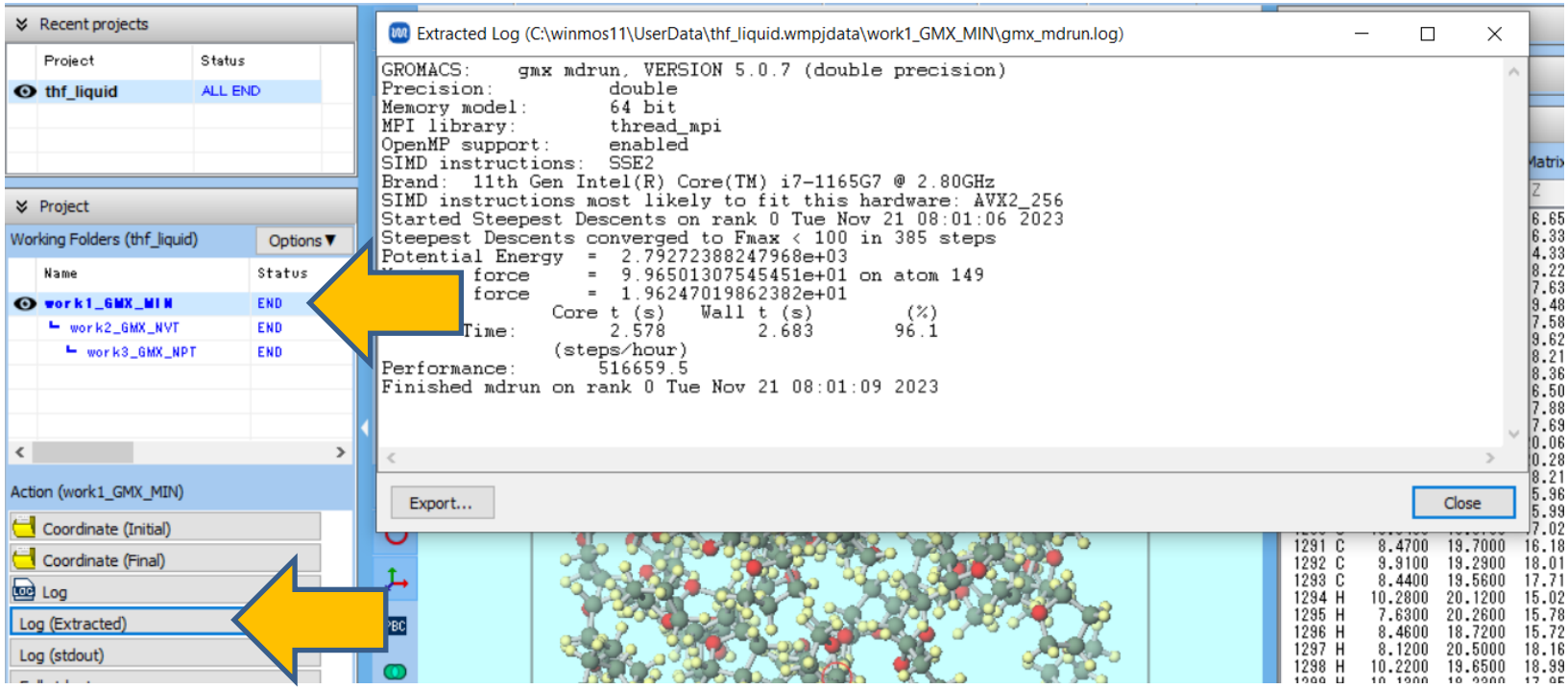
B. Wait until the status of all work folders changes to **END (blue)**. During this time, **the status** of **the recently used project** 'thf_liquid' will also change to ALL **END (blue)**.



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.)

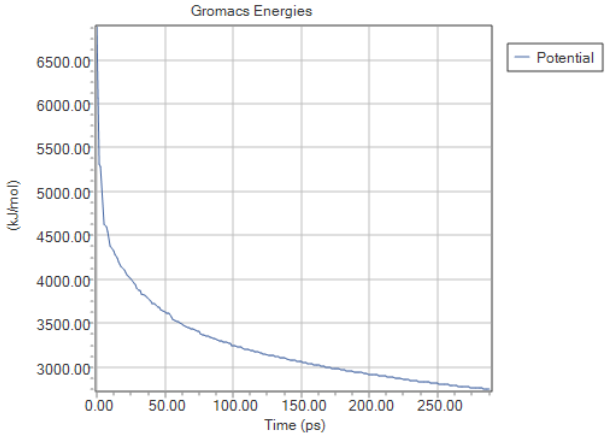
B. If you wish to view the complete log, click **Log**.



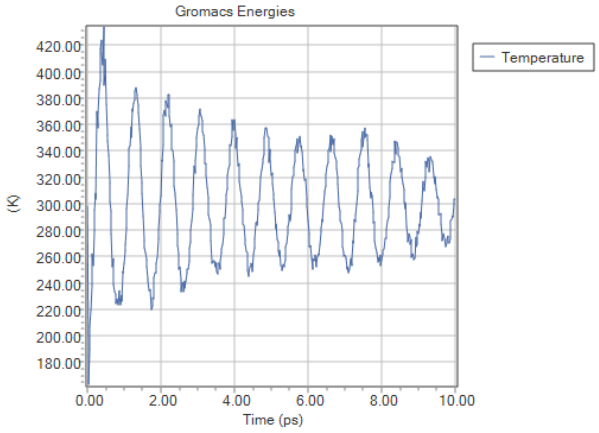
Supplement: Verifying the Convergence of Thermodynamic Quantities in Equilibration Calculations

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.

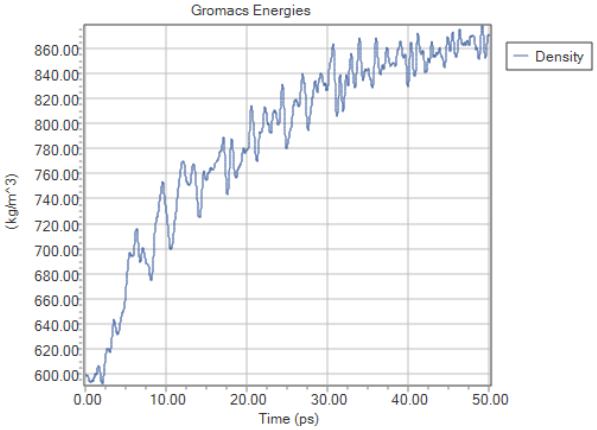
Example:



work1_GMX_MIN (Energy Minimization) for Potential (Potential Energy)



work2_GMX_NVT (Constant Temperature MD) for Temperature (Temperature)

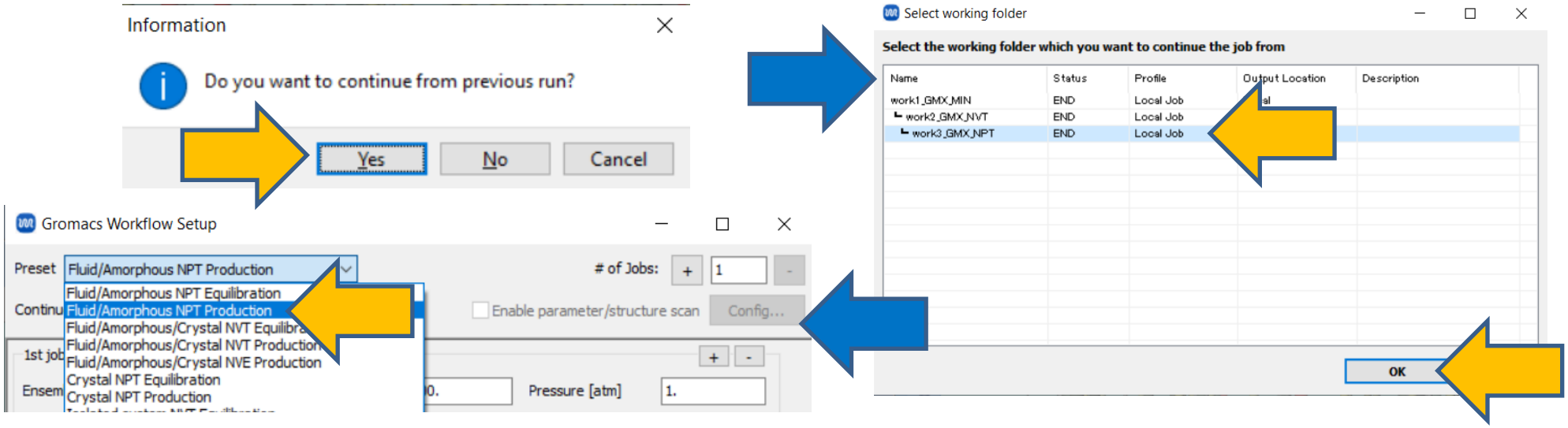


work3_GMX_NPT (Constant Temperature and Pressure MD) for Density (Density)

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.

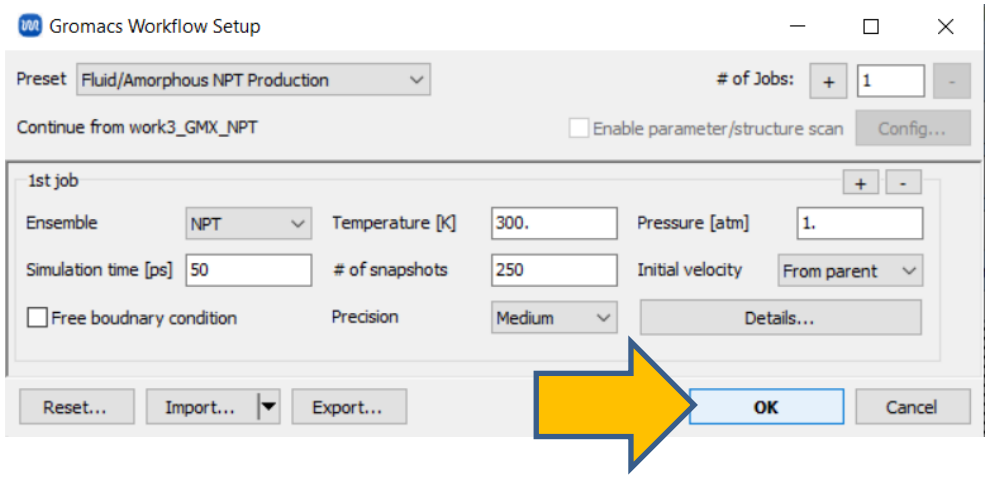
B. Execution of Calculation　(C)The Main Calculation

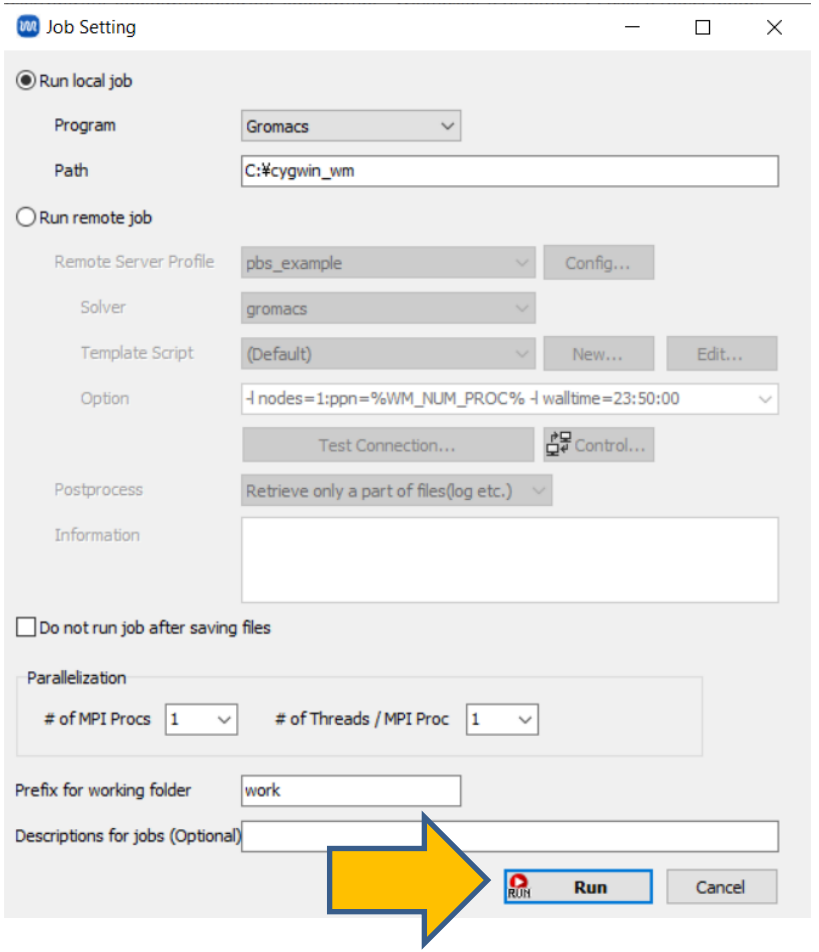
A. After the status of the original work folder (in this case, work3_GMX_NPT) has changed to **END（bulue）** , click (**Workflow Setup**).
B. Click **Yes** in **Information** dialog.
C. Select the original work folder (work3_GMX_NPT) in **Select working folder** and then click **OK**.
D. Select 'Fluid/Amorphous NPT Production' in **Preset**.
E. 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.



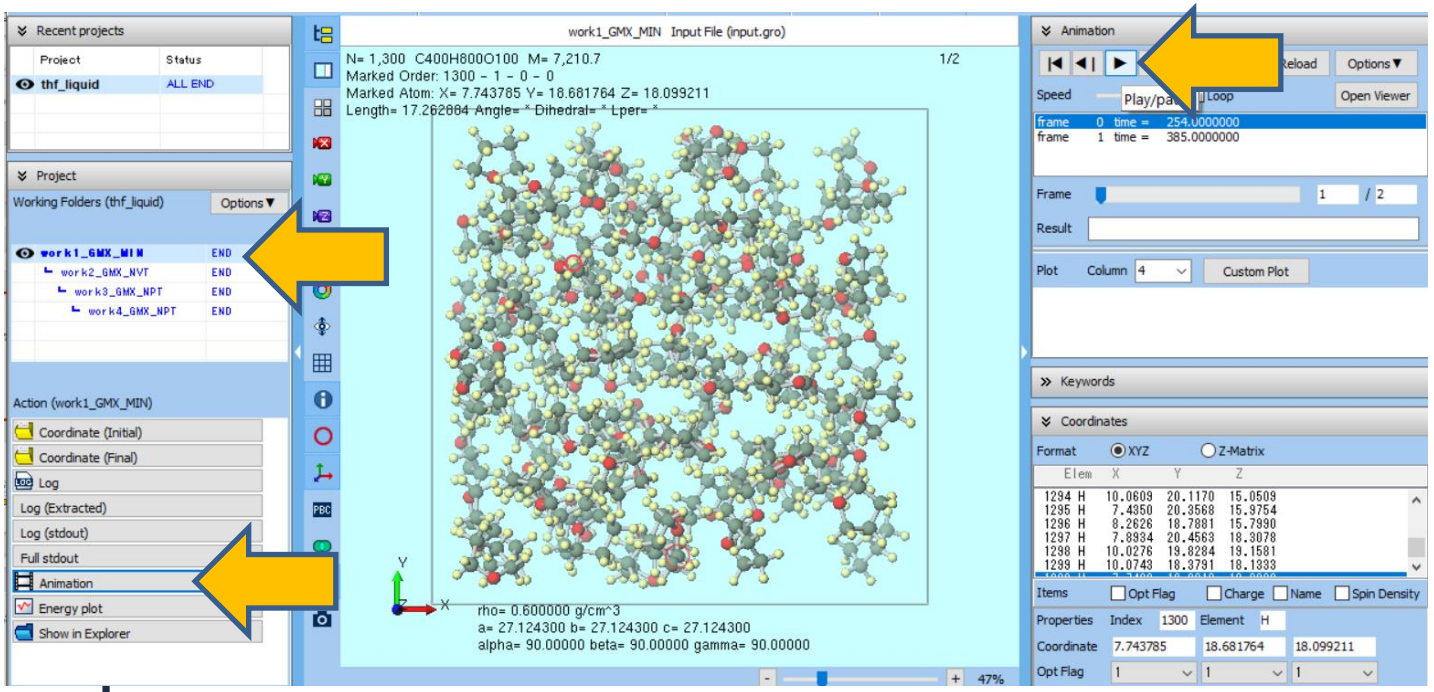


C. Result Analysis Animation

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

A. Click the **relevant work folder** in Project display area (here, we will use 'work1_GMX_MIN').

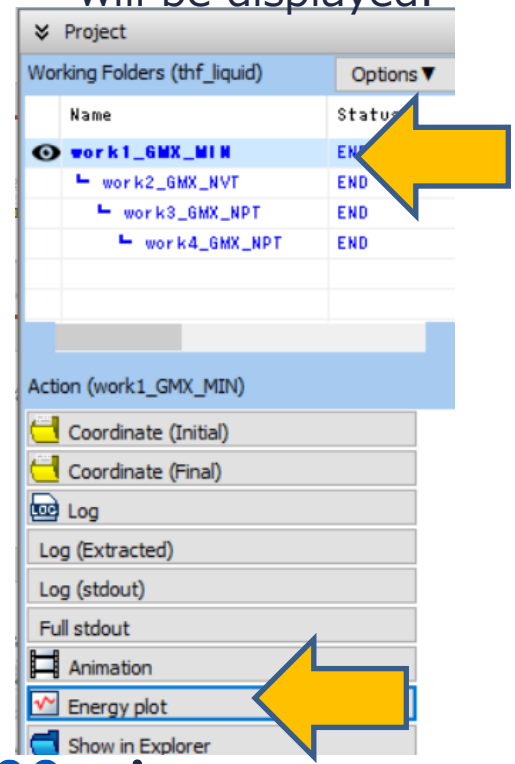
B. When you click **Animation** in **Action**, **Animation display area** will appear on the right side of the main window. Clicking the button  will display the calculation process as an animation.

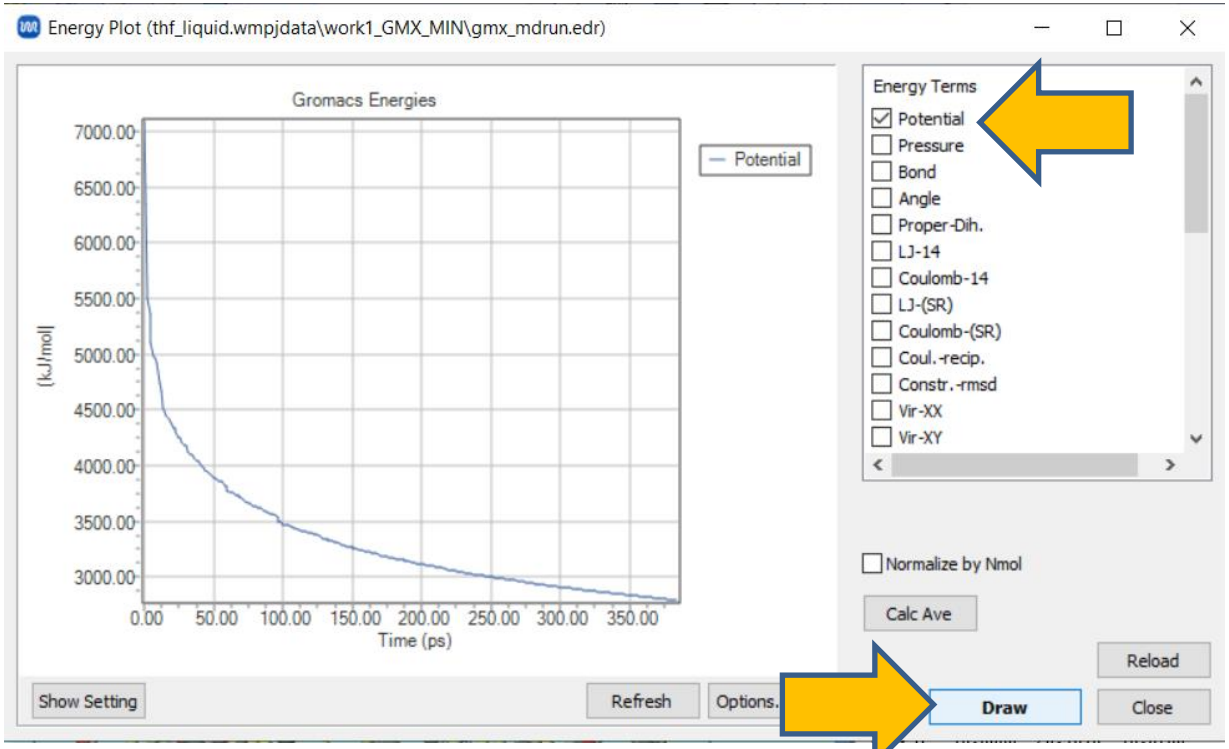


C. Result Analysis Temporal Variation and Averages of Energy and Other Parameters

A. Click **the relevant work folder** in **Project Area** (here we will use 'work1_GMX_MIN').

B. 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.

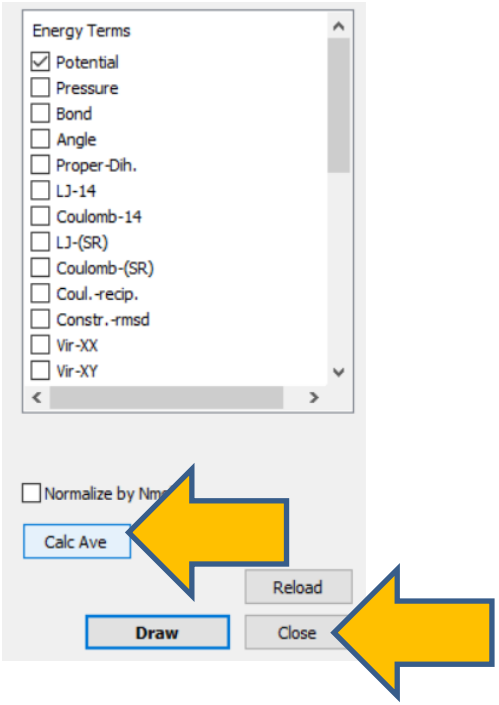


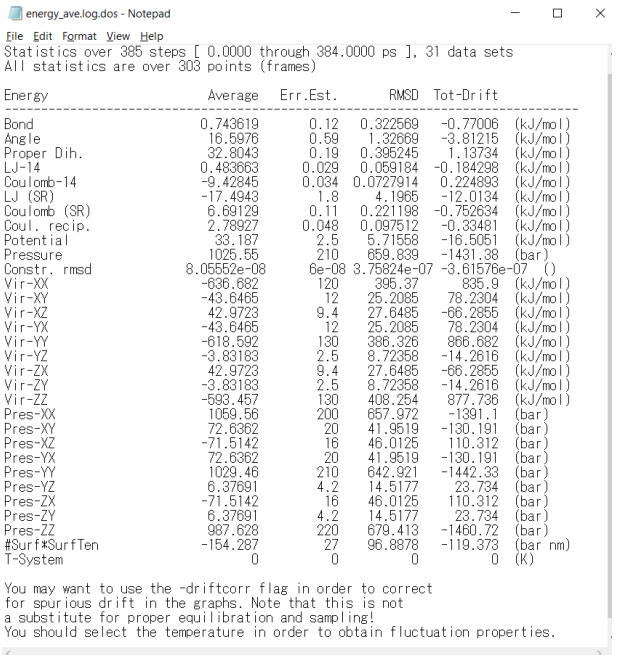


C. Result Analysis Temporal Changes and Averages of Energy and Other Quantities

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.




energy_ave.log.dos - 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)

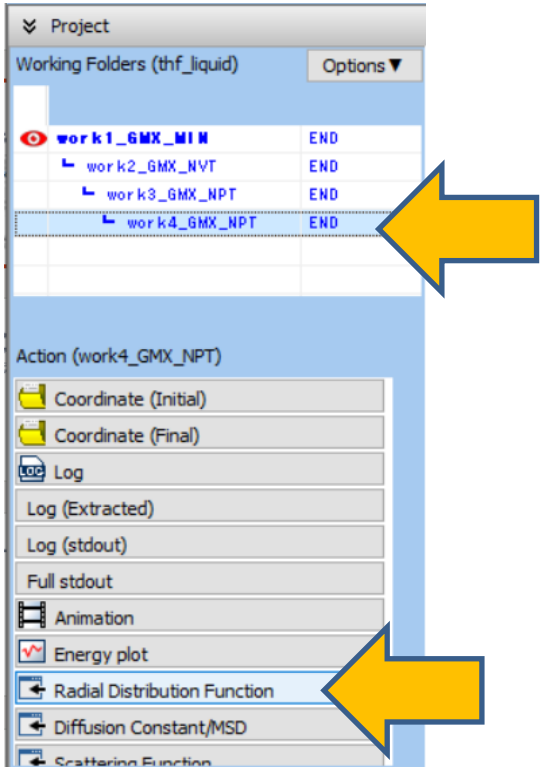
Energy	Average	Err.Est.	RMSD	Tot-Drift	
Bond	0.743619	0.12	0.322569	-0.77006	(kJ/mol)
Angle	16.5976	0.59	1.32669	-3.81215	(kJ/mol)
Proper Dih.	32.8043	0.19	0.395245	1.13734	(kJ/mol)
LJ-14	0.483663	0.029	0.059184	-0.184298	(kJ/mol)
Coulomb-14	-9.42845	0.034	0.0727914	0.224893	(kJ/mol)
LJ (SR)	-17.4943	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	-0.33481	(kJ/mol)
Potential	33.187	2.5	5.71558	-16.5051	(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	386.326	866.682	(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	6.37691	4.2	14.5177	23.734	(bar)
Pres-ZX	-71.5142	16	46.0125	110.312	(bar)
Pres-ZY	6.37691	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)

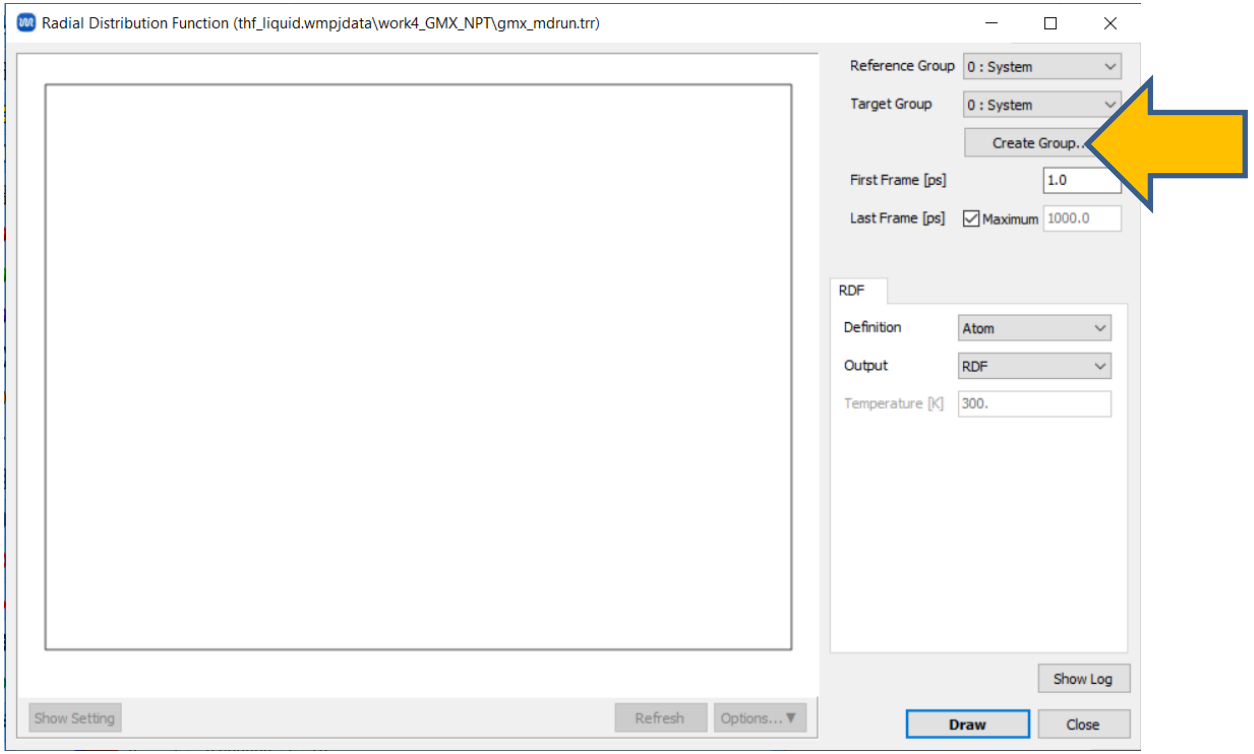
You may want to use the -driftcorr flag in order to correct
for spurious drift in the graphs. Note that this is not
a substitute for proper equilibration and sampling!
You should select the temperature in order to obtain fluctuation properties.

C. Result Analysis Radial Distribution Function

A. Click **the relevant work folder** in **Project Area** (here, we will use 'work4_GMX_NPT').

B. 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**.



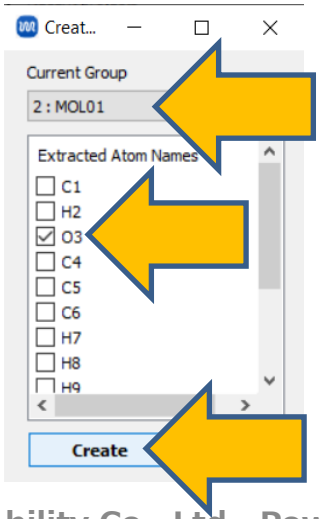


C. Result Analysis Radial Distribution Function

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**.

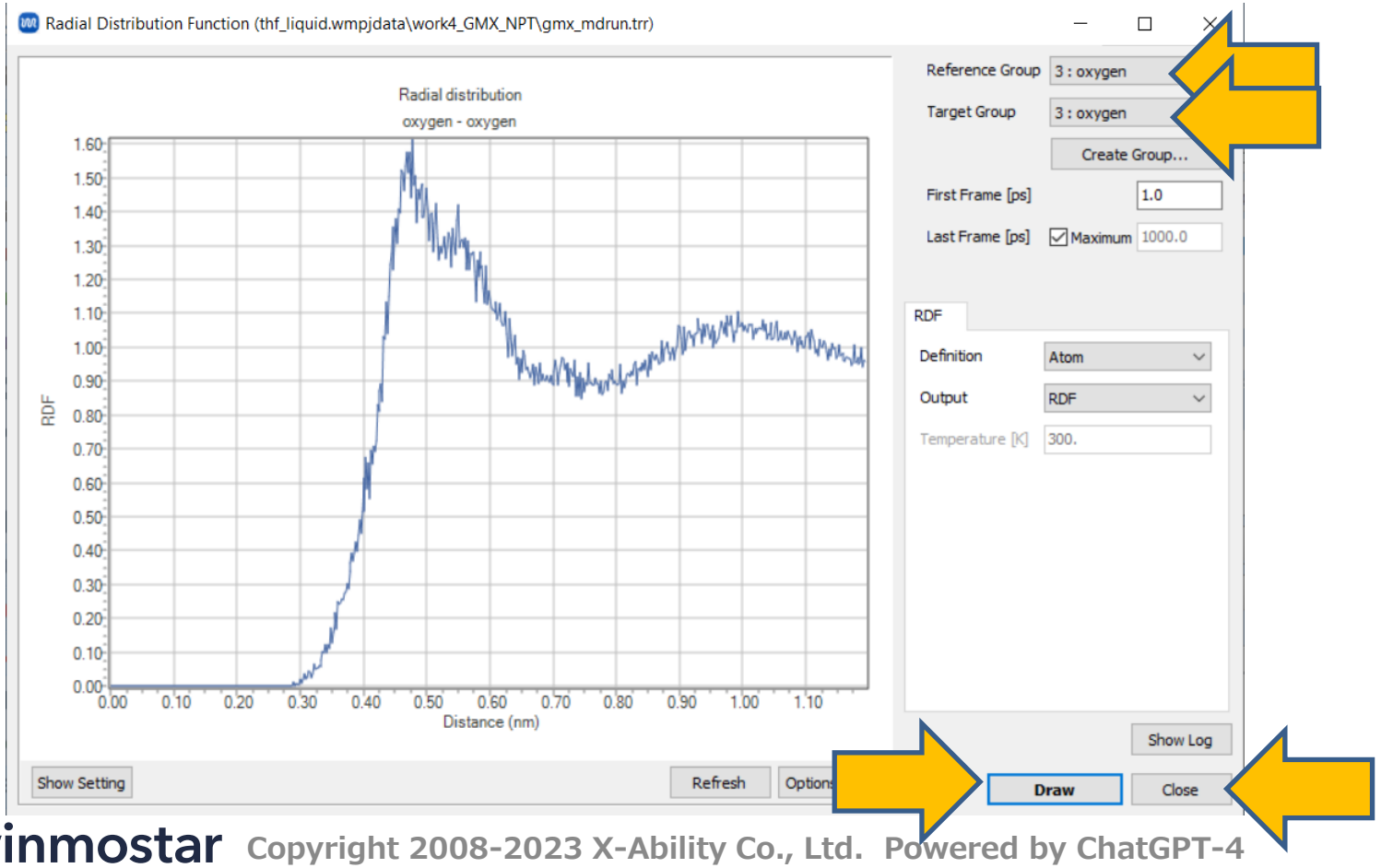
C. Once the terminal window appears and the process is complete, click **Close**.



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**.

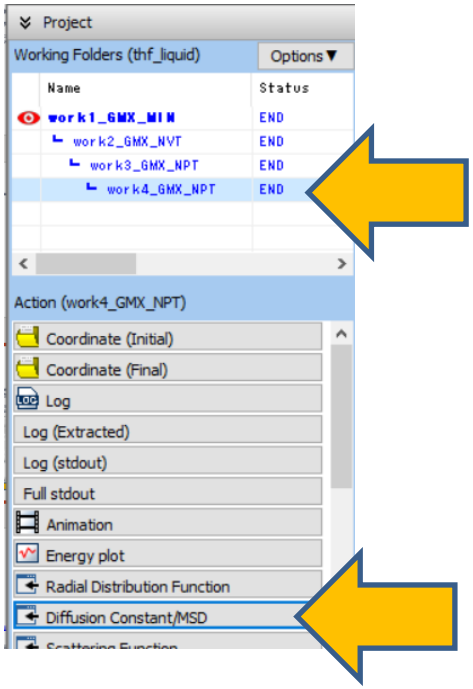


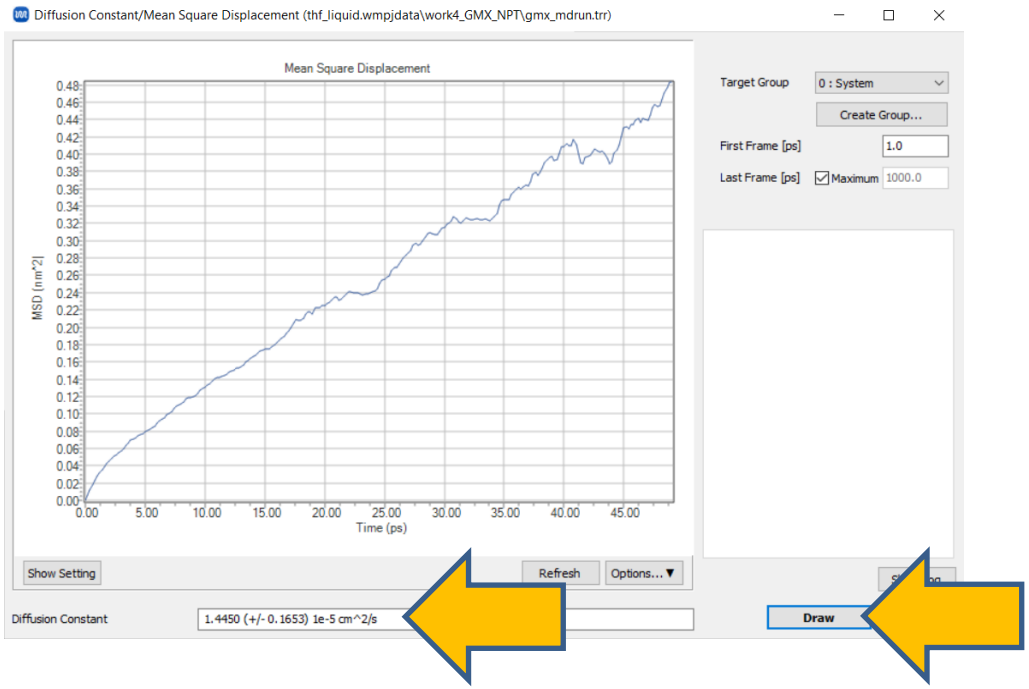
C. Result Analysis Self-Diffusion Coefficient

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**).

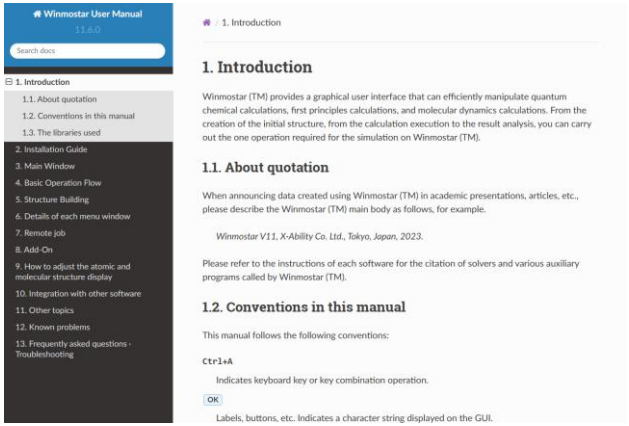
Supplement: Ideally, the self-diffusion coefficient should be determined from NVT calculations, but in this manual, it is simplistically derived from NPT calculations (refer to J. Chem. Phys. 153, 021101 (2020) and similar sources).





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.