winmostar tutorial

Gromacs Viscosity and Dielectric Constant

V11.6.5

31 March 2024 X-Ability Co., Ltd.

About This Manual

- 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.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- 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 using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
-

Overview・Note

- In this tutorial, we introduce a method to calculate the dielectric constant and viscosity of water at ambient temperature and pressure using Gromacs modules. Here, we apply an equilibration procedure (below) to perform NVE (constant number of particles, volume, and energy) calculations at the target temperature and pressure. (It is not always necessary to calculate under NVE conditions; it is also possible to validate the results and calculate under NPT (constant number of particles, pressure, and temperature) or NVT (constant number of particles, volume, and temperature) conditions.)

  A. Energy Minimization: Removal of coordinate overlaps

  B. NVT Constant: Equilibration of particle velocities

  C. NPT Constant: Density equilibration

  D. NPT Constant: Calculation of average density → Scaling the system to the average density

  E. Energy Minimization: Removal of coordinate overlaps

  F. NVT Constant: Equilibration of particle velocities

  G. NVE Constant: Calculation of average temperature → Scaling the system to the average temperature

  H. NVE Constant: Main calculation

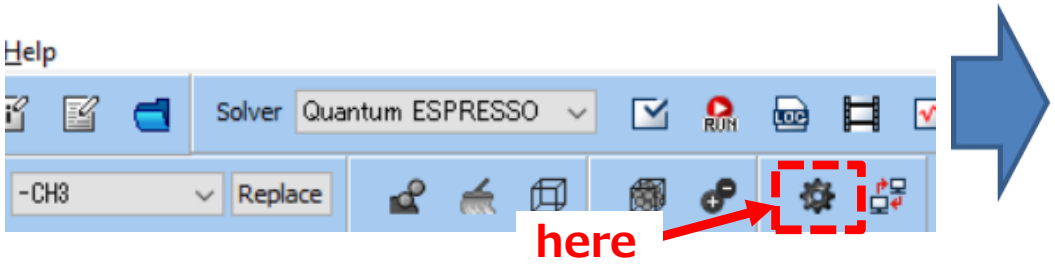
- The number of steps required for equilibration depends on the type of substance and its initial density. Particularly, slow-relaxing substances (such as high-viscosity materials) may not yield valid values with this method.
- The calculation method of interactions, the force field, and the method of calculating charges also affect the results.
- Due to the tutorial nature, we do not perform calculations with a sufficient number of steps to ensure convergence of physical quantities.

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.

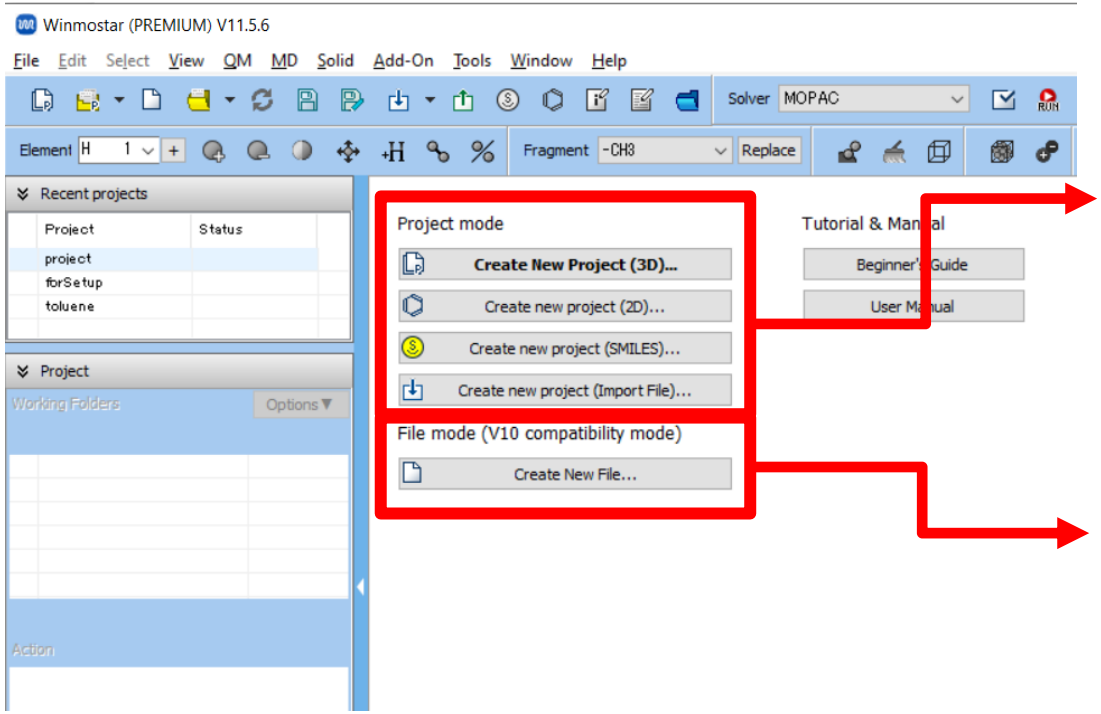
(7) Install Cygwin environment for Winmostar. ← here

- 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.
For operations in File Mode, please refer to LAMMPS Tutorial for V10.



Project Mode New Features in V11

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

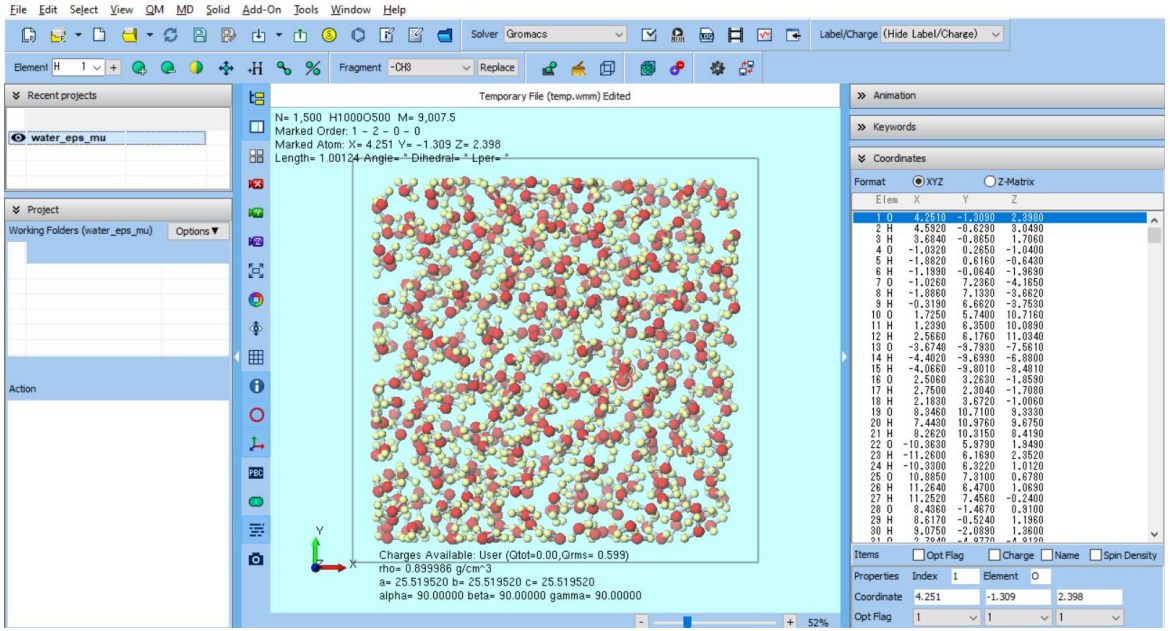
File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

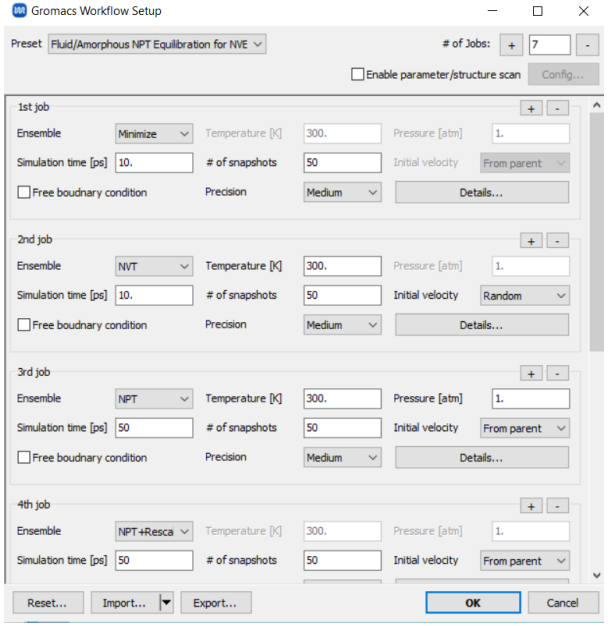
For basic operations, please refer to Gromacs Basics tutorial.

A. Click **File | New Project**, enter '`water_eps_mu`' in **Project name**, and click **Save**.
B. Click  **Solvate/Build Cell**.
C. Click **Add Water**, enter '500', and click **OK**.
D. Enter '0.9' in **Set Density** to the right of **Simulation Cell** and click **Build**.
E. Click **OK** when 'The system has been successfully built.' is displayed.



B. Execution of Calculations (Equilibration)

A. Select **Gromacs** from **Solver**, and open **(Workflow Setup)**.
B. Click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.
C. Change **Preset** to 'Fluid/Amorphous NPT Equilibration for NVE.'
D. Adjust **Simulation time**, **Temperature**, **Pressure** as needed (no changes needed for this tutorial).
E. If you want to finish the calculation quickly by reducing computational accuracy, change **Precision** of **all jobs** from **1st** to **7th** to 'Low'.
F. Click **OK**, adjust settings in **Job Setting** window as needed, and then click **Run**.

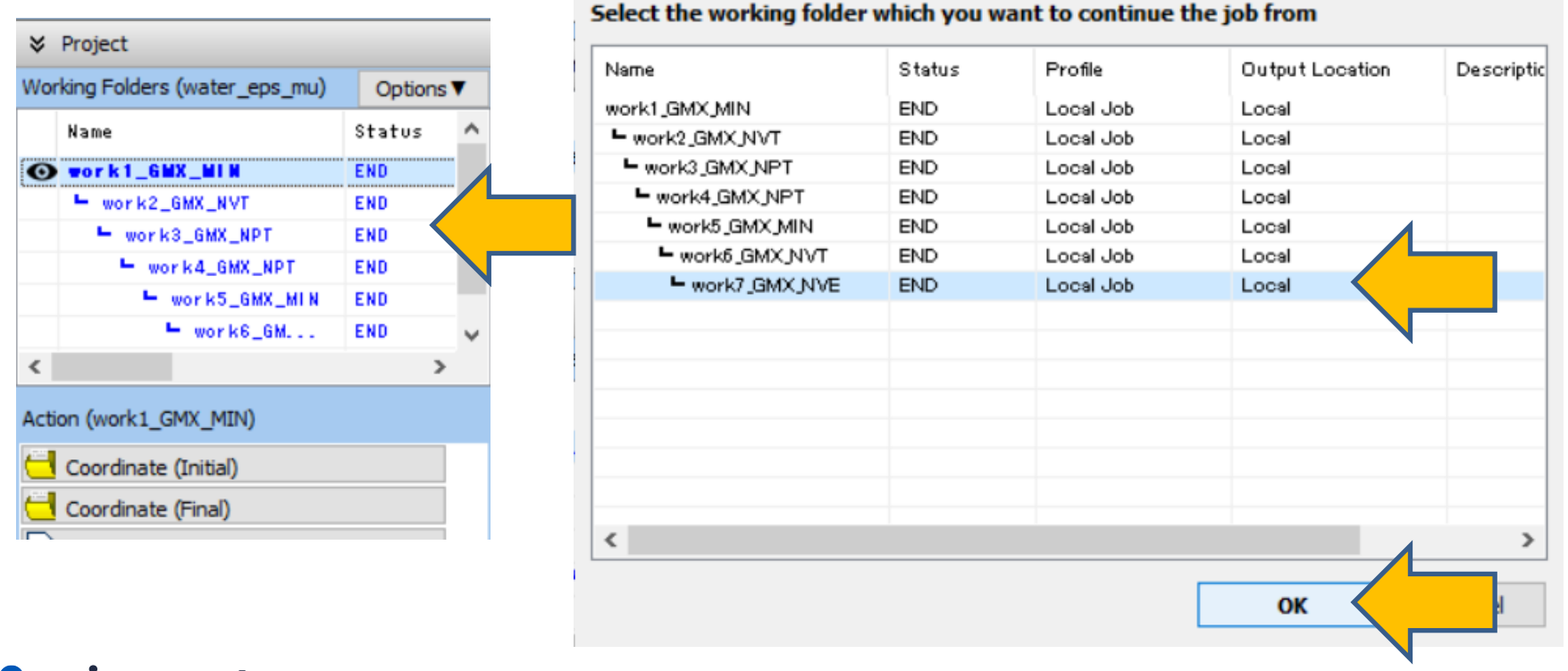


B. Execution of Calculations (Main Calculation)

A. Once **the status** of the work folders from work1_GMX_MIN to work7_GMX_NVE changes to **END** or **END(-)**, click **(Workflow Setup)** again.

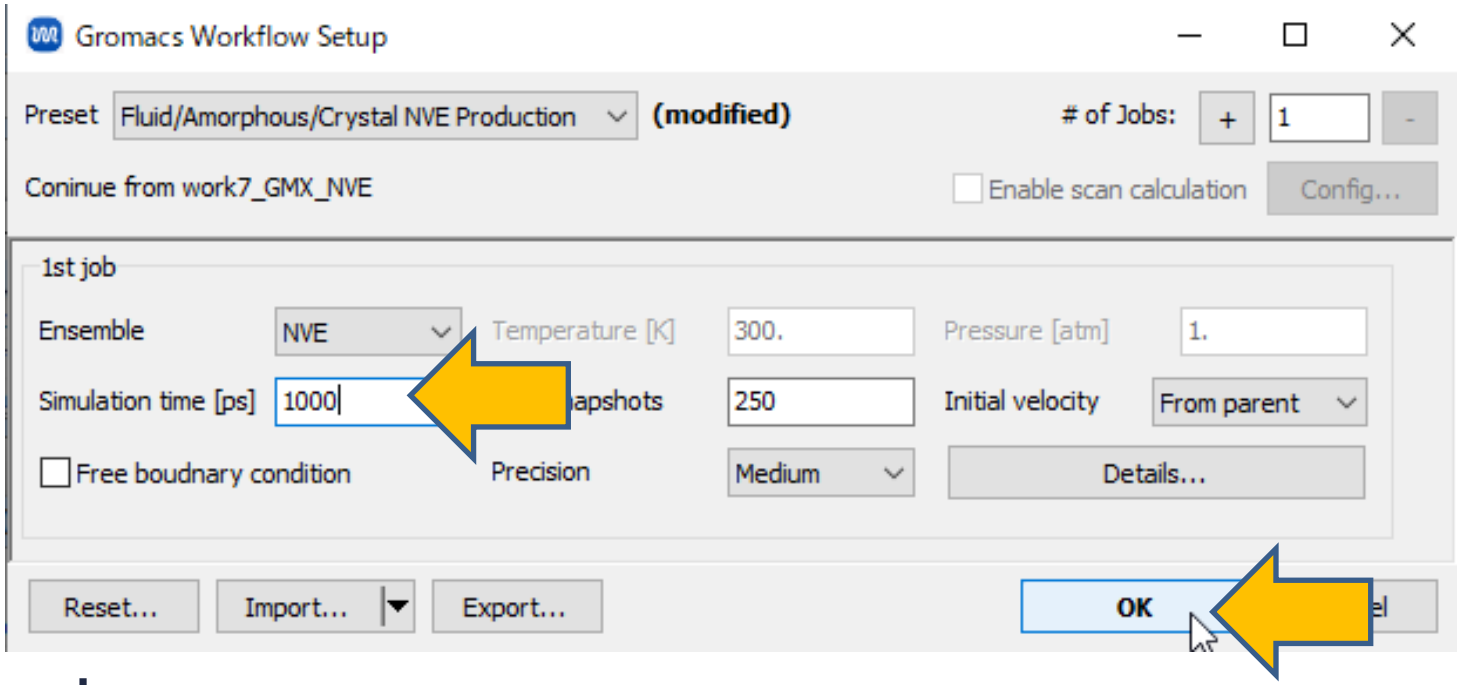
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.

C. Select work7_GMX_NVE and click **OK**.



B. Execution of Calculations (Main Calculation)

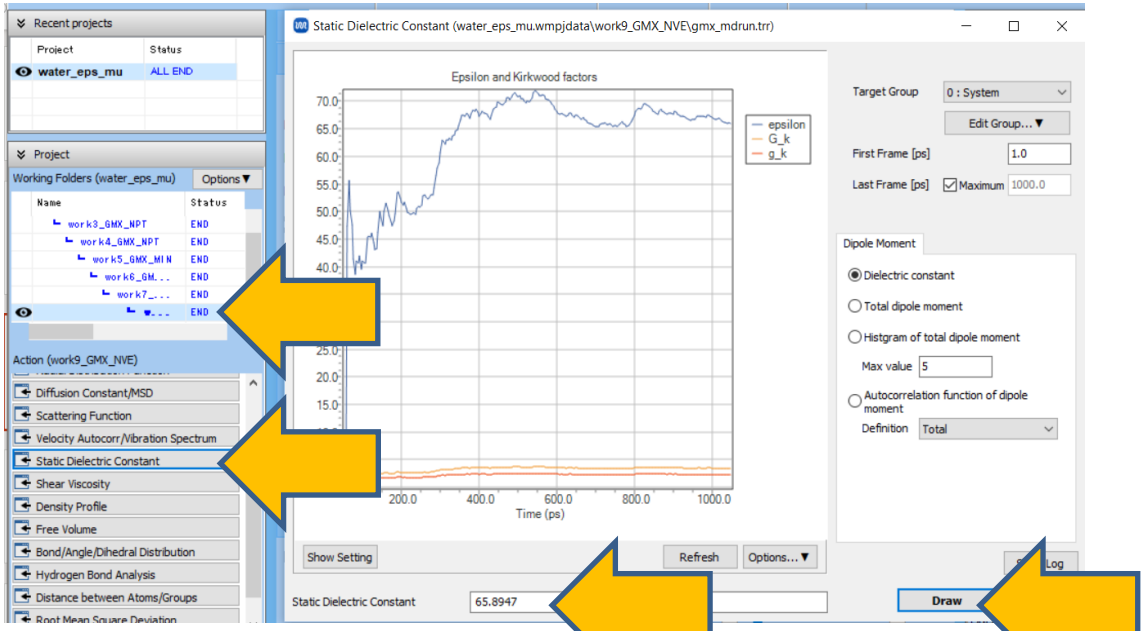
A. Change **Preset** to 'Fluid/Amorphous/Crystal NVE Production.'
B. Adjust **Simulation time** to '1000' (or a larger value if possible).
C. If you wish to shorten the calculation time by reducing accuracy, change **Precision** to 'Low' and **Simulation time** to '50.'
D. Click **OK**.
E. In **Job Setting** window, adjust the settings as necessary and then click **Run**.



C. Result Analysis Dielectric Constant

A. Once **the status** of the work folder 'work8_GMX_NVE' changes to **END**, click on 'work8_GMX_NVE' within **Working Folders**, then click **Static Dielectric Constant** under **Action**.

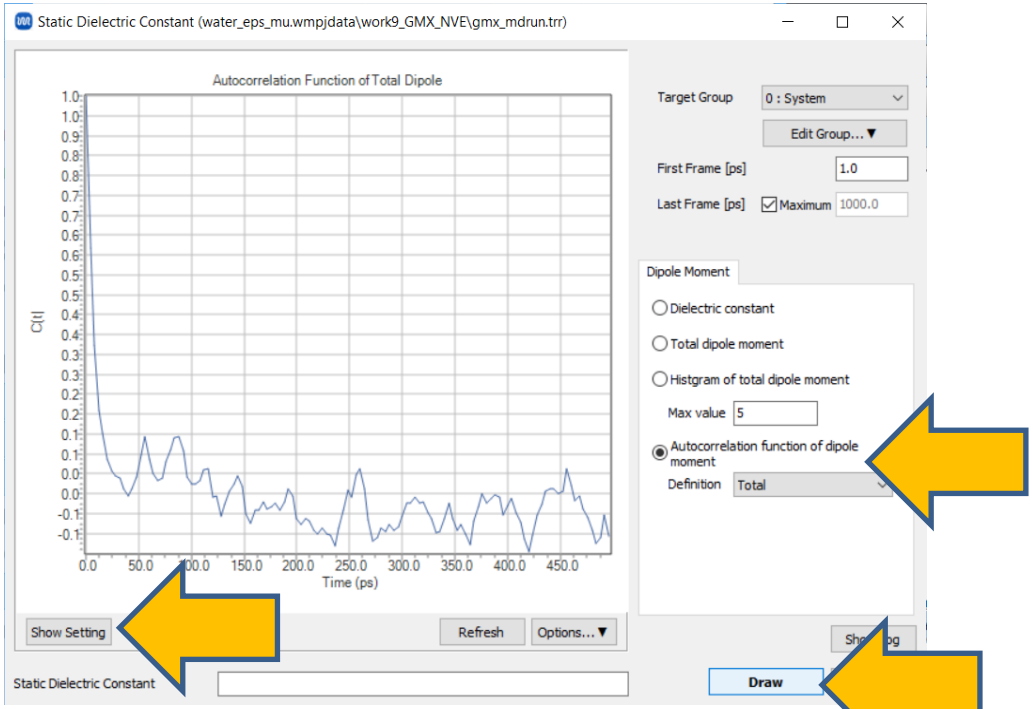
B. Click **Draw**, and when prompted to 'Enter Temperature,' type '300' (the target temperature for this instance) and click **OK**. The final value of **epsilon** in the graph and the number below the graph represent the relative dielectric constant. (Note that in this calculation, the results have not fully converged, and a longer calculation time is required for convergence.)



C. Result Analysis Autocorrelation Function (Related to Dielectric Constant)

A. Check **Autocorrelation function of dipole moment** and click **Draw**.

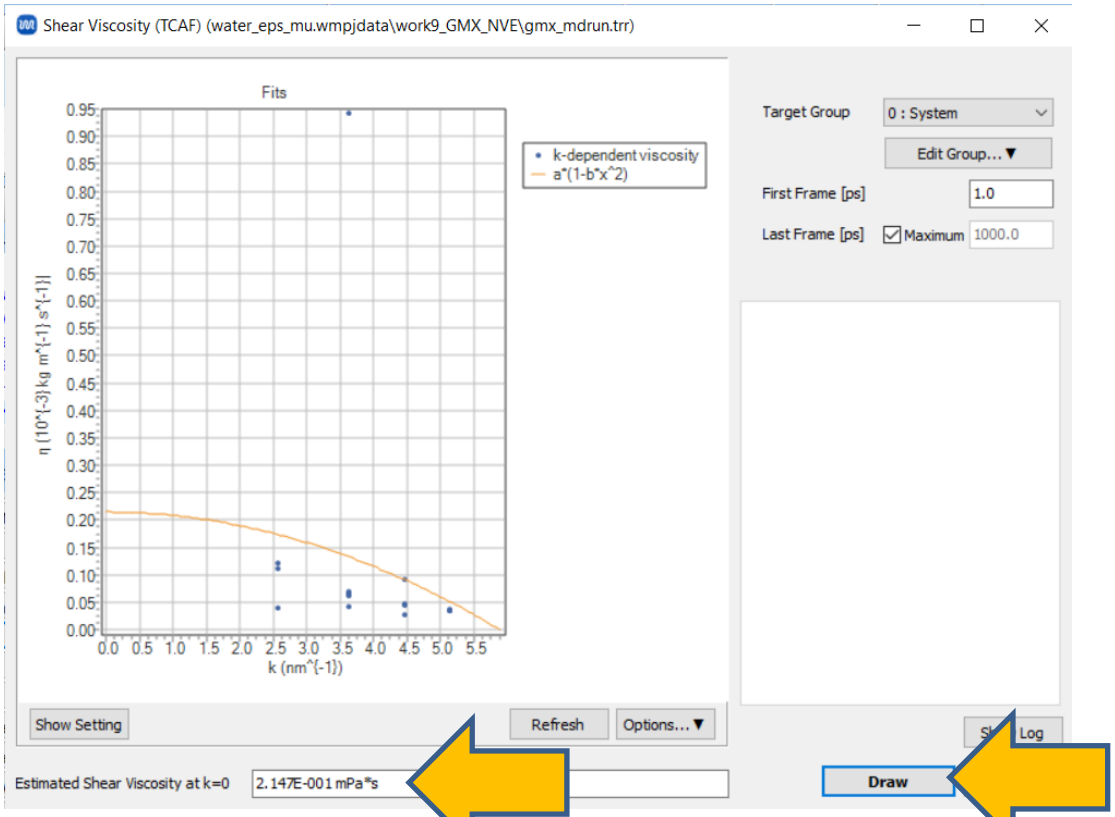
B. The autocorrelation function of the dipole moment will be displayed. This serves as one criterion for determining the convergence of the dielectric constant calculation. If necessary, click **Show Setting** and check **Logarithm** to view the shape in a logarithmic plot. (Note that in this calculation, the results have not sufficiently converged, and a longer calculation time is required for convergence.)



C. Result Analysis Viscosity

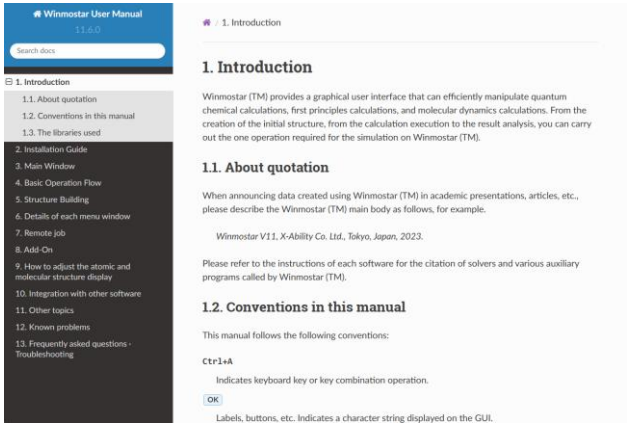
A. In **Working Folders**, click work8_GMX_NVE and then click **Shear Viscosity** under **Action**.

B. Click **Draw** to display the estimated value of the viscosity below. (In this case, due to insufficient calculation time, the accuracy of the calculated viscosity is not high.)



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.