winmostar tutorial

Gromacs
Solvation Free Energy
(Energy Representation Method)

V11.6.5

17 April 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.
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Overview

- We will calculate the solvation free energy of ethanol in water using the Energy Representation (ER) method. After conducting MD calculations for the solute + solvent, solvent only, and solute only, we will calculate the energy distribution functions and free energy.
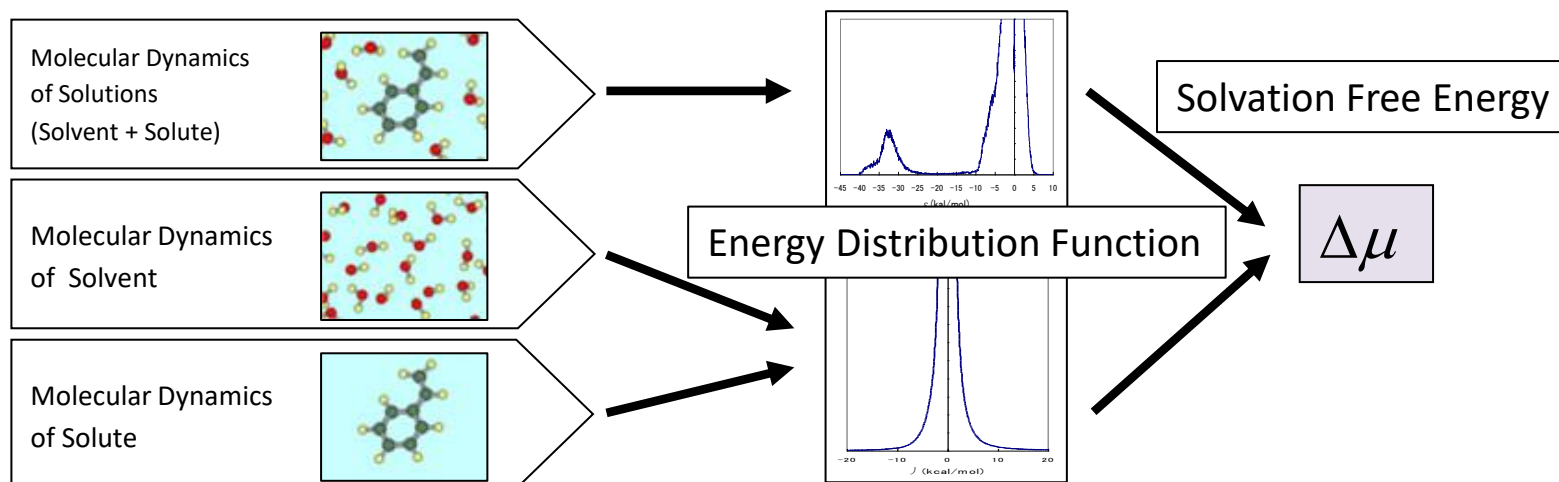

Note:

- The number of steps required for equilibration varies depending on the type of molecules and initial density.

- The larger the number of steps for this calculation, the better the reproducibility and the more reliable the results obtained. The frequency and number of coordinate outputs also affect the results.

- The type of force field, interaction calculation conditions, and the size of the system significantly impact the results.

- ER method calculations use pseudorandom numbers, which can cause results to vary each time.

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.
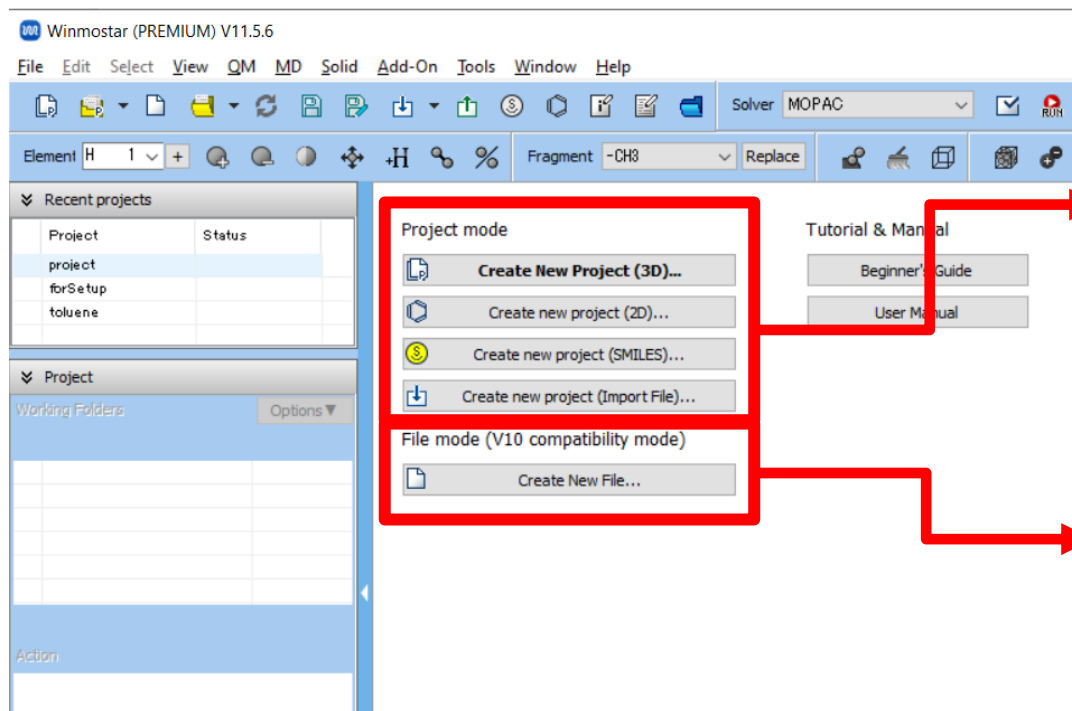

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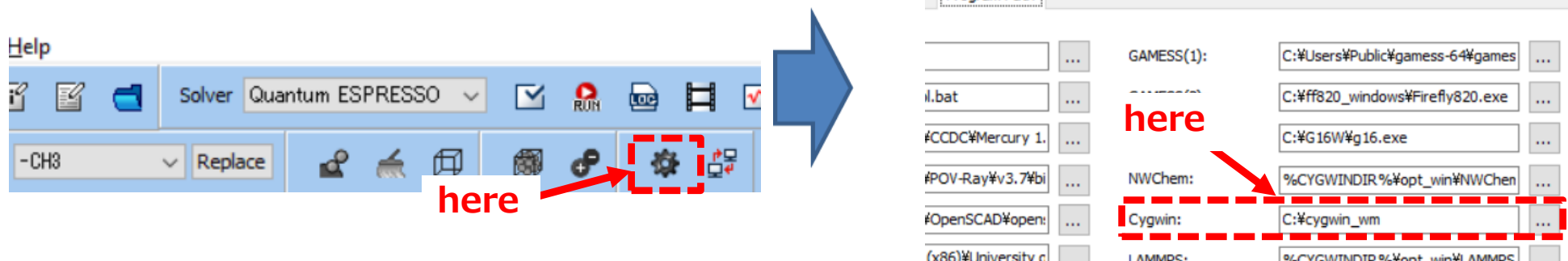
Operating Modes of Winmostar V11

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 [tutorial for version 10.](#)

Project Mode **New Features in V11**
Users can manage jobs without having to manage individual files.
<u>We generally recommend using this mode.</u>

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 (Solution System)

Please refer to [Gromacs Basics Tutorial](#) for basic operational methods.

A. Click **File | New Project**, enter `'etohaq_er'` in **Project name** , and click **Save**.
B. Select '-CH3' **Fragment** and click **Replace** twice to create ethane.
C. Select '-OH' **Fragment** and click **Replace** once to create ethanol.
D. Click **Assign Charges Automatically** and then click **OK**.
E. Click **Export File** and save as `'etoh_am1bcc.mol2'`.
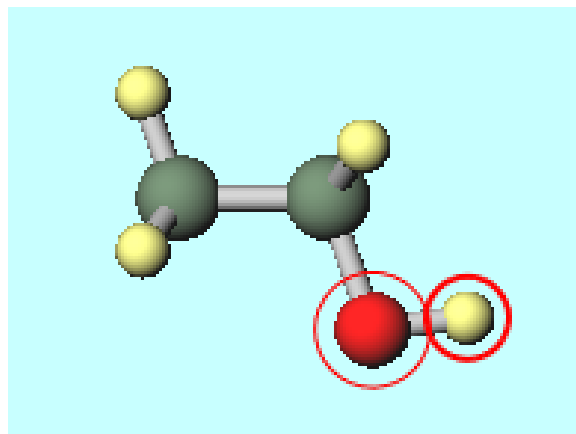
A. Modeling of the System (Solution System)

A. Click 🔲 **Solvate/Build Cell**.
B. Click **Add Displayed Molecule**, enter '**1**', and click **OK**.
C. Click **Add Water**, enter '500', and click **OK**.
D. Enter '0.9' in **Set Density** and click **Build**.

B. Execution of Calculate (Solution System)

A. Select **Gromacs** from **Solver**, and open 　☑ **(Workflow Setup)**.

B. Click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.

C. Click **+** once under **# of jobs**.

D. Change **Simulation time** for **4th job** to '100'.

E. Adjust **Simulation time**, **Temperature**, and **Pressure** as needed (no changes required for this tutorial).

F. If you want to finish the calculation faster by reducing the accuracy, change all Precision settings from **1st job** to **3rd job** to 'Low'.

G. Click **Details** for **4th job**, make the following changes, then click **OK**:

  – In **Output** tab, change **nstxout-compressed** to '10'.

H. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

C. Modeling of the System (Solvent System)

A. Click [icon] **Solvate/Build Cell**.

B. Click **Add Water**, enter '500', and click **OK**.
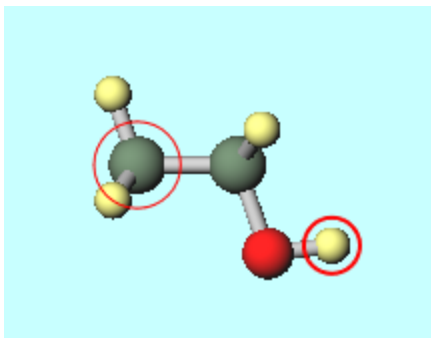
C. Enter '0.9' in **Set Density** and click **Build**.
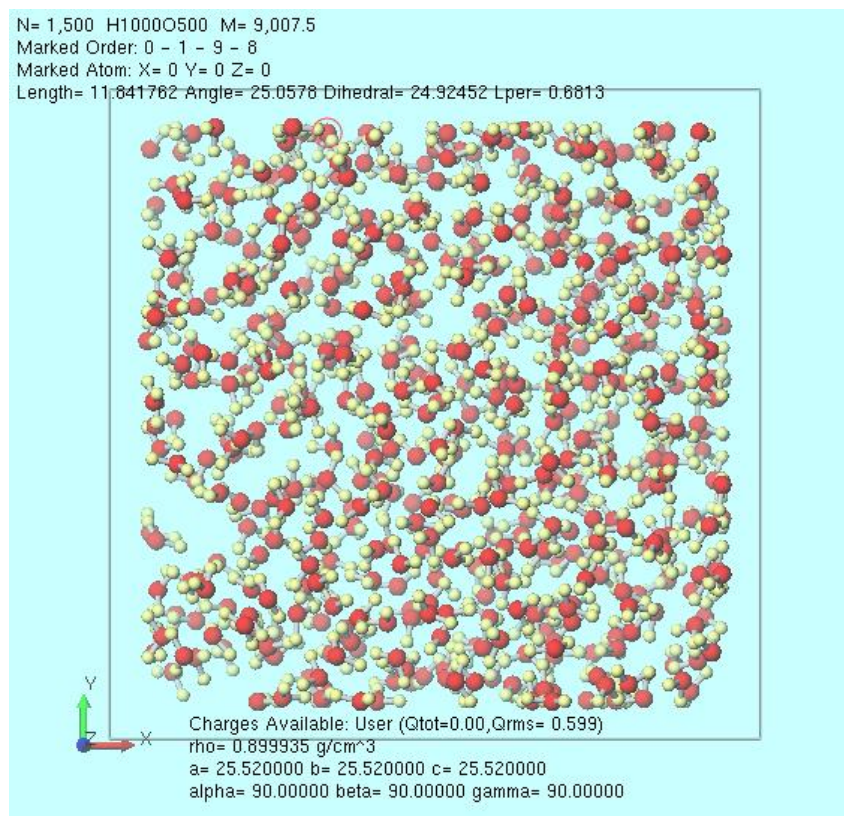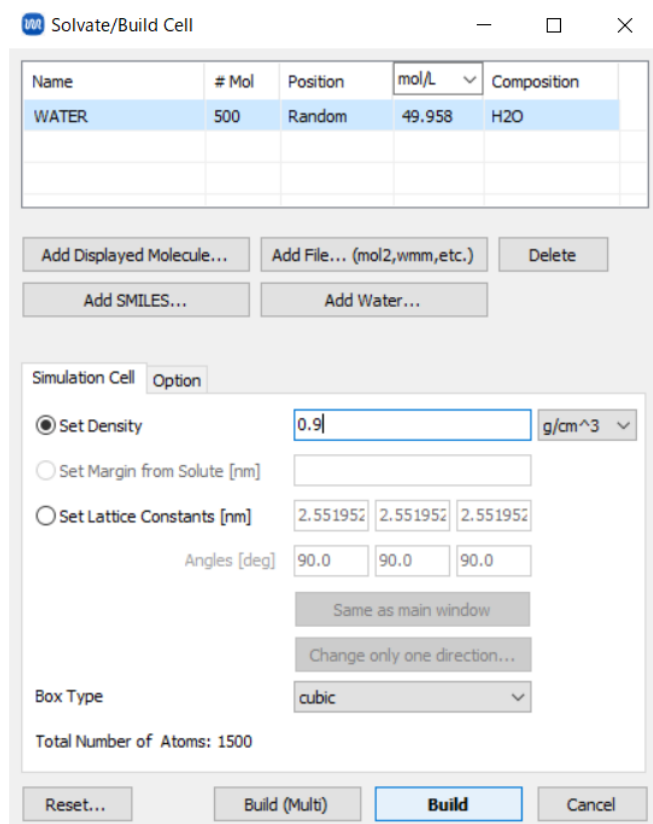
D. Execution of Calculate (Solvent System)

A. Open ☑ **(Workflow Setup)**.

B. Click **No** when prompted with 'Do you want to continue from previous run?'.

C. Click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.

D. Change **Simulation time** of **4th job** to '50'. Click **Yes** when prompted with '...Are you sure you want to continue?'.

E. Adjust **Simulation time**, **Temperature**, and **Pressure** as needed (no changes required for this tutorial).

F. If you want to finish the calculation faster by reducing the accuracy, change all **Precision** settings from **1st job** to **3rd job** to 'Low'.

G. Click **Details** for **4th job**, make the following changes, then click **OK**:

   – In **Output** tab, change **nstxout-compressed** to '100'.

H. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

E. Modeling of the System (Solute System)

A. Click ⬇ **Import File** and open `etoh_am1bcc.mol2` file saved on page 6.
B. In **Import File** dialog, click **Discard and import**.

F. Execution of Calculate (Solute System)

A. Open ☑️ **(Workflow Setup)**.

B. Click **No** when prompted with 'Do you want to continue from previous run?'.

C. Click **OK** when prompted with 'Enter margin [Å]'.

D. In **Assign Force Field Parameters** window, click **OK**, and if 'Assigned force field parameters' is displayed, click **OK** again.

E. Change **Preset** to 'Isolated system NVT Equilibration'.

F. Click **+** once under **# of jobs**.

G. Change **Simulation time** of **3rd job** to '25000' and **Initial velocity** to 'From parent'.

H. Adjust **Simulation time**, **Temperature**, and **Pressure** as needed (no changes required for this tutorial).

I. Click **Details** for **3rd job**, make the following changes, then click **OK**:

   – In **Output** tab, change **nstenergy** to '10000' and **nstxout-compressed** to '100'.

J. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

G. Result Analysis

A. After all calculations are completed, click **MD | Gromacs | Start ER**.
B. Return to Main Window and click **File | Project | Show in Explorer**.
C. In Explorer, find work4_GMX_NPT folder and drag and drop it into **Summary** section of **Setup Energy Representation Method** window.
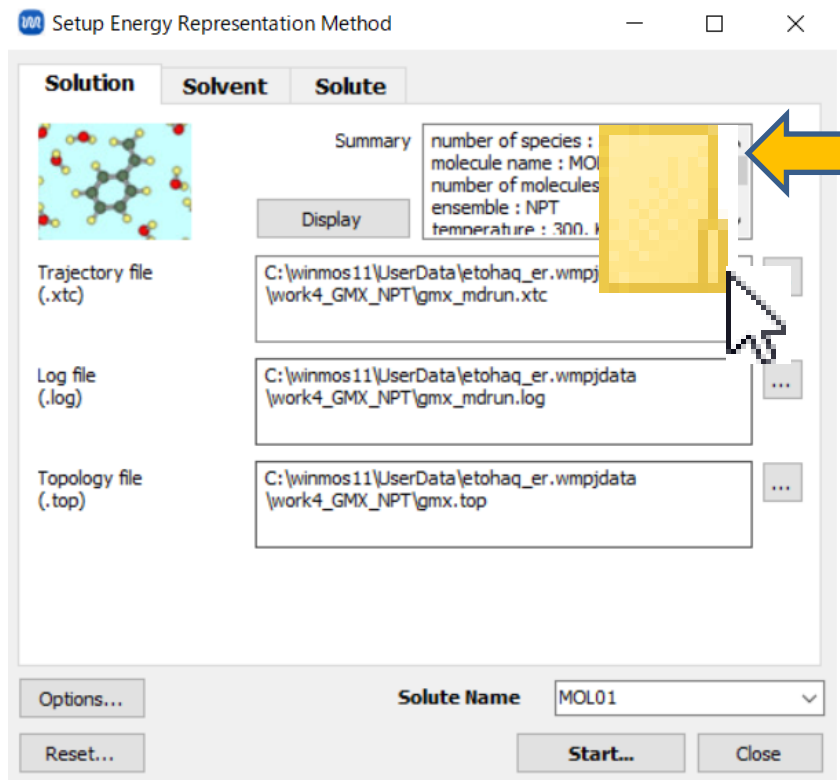
G. Result Analysis

A. Similarly, open **Solvent** tab and drag and drop work8_GMX_NPT folder, then open **Solute** tab and drag and drop work11_GMX_NVT folder.

B. Click **Start**, create a new folder (for this book, tentatively create a folder named `ertest` under `etohaq_eq.wmpjdata`), and click **OK**. A console window will open, and the ERmod process will run for a while.
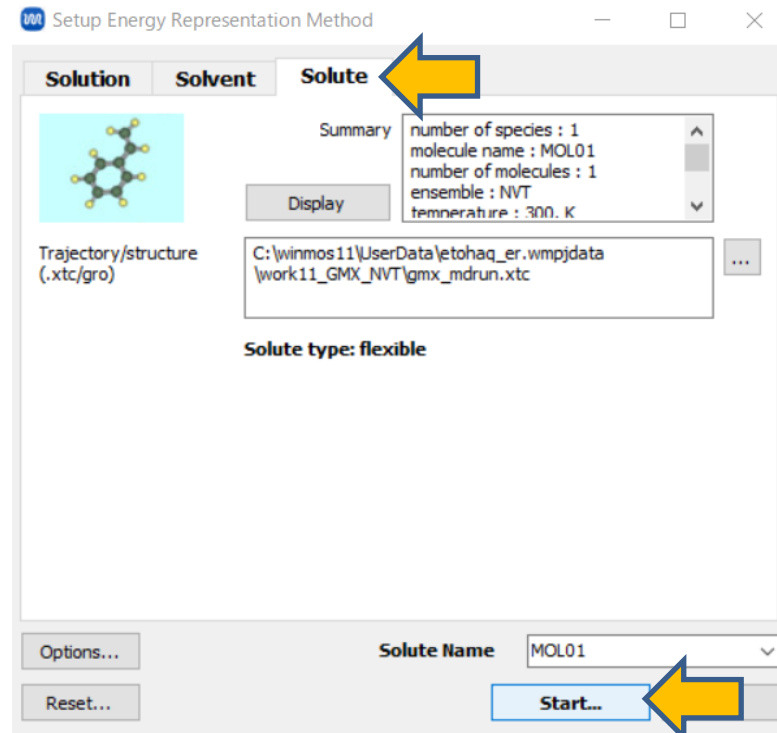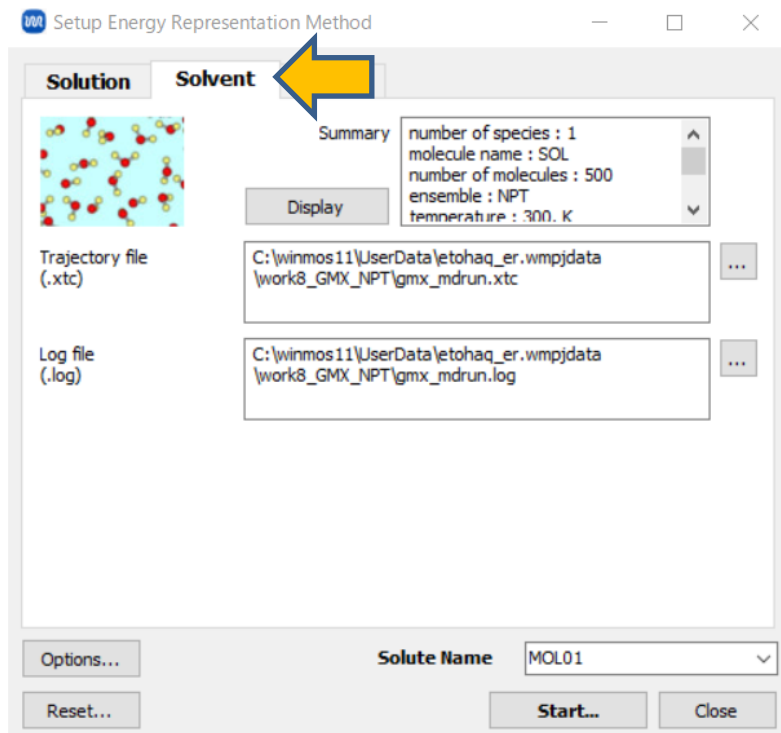
G. Result Analysis

A. After the ERmod process completes and the console window closes, click **MD | Gromacs | Import ER**. Select the folder where the calculation was performed on p. 14 (in this tutorial, `ertest`) and click OK. The graph of the interaction energy distribution and the calculated Solvation Free Energy will be displayed.
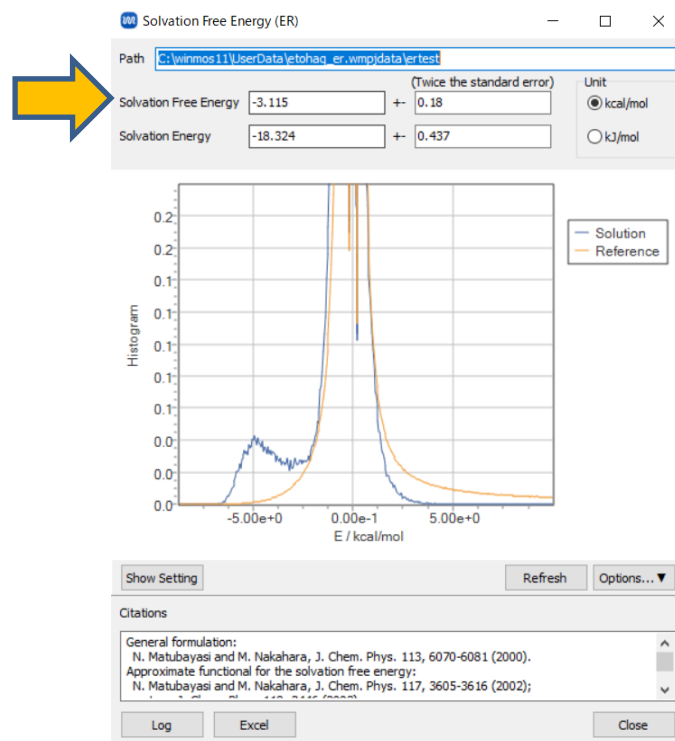
Finally

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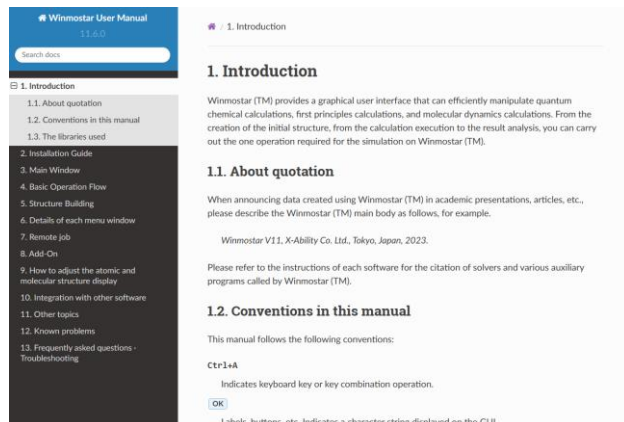
Winmostar User Manual

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.

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