winmostar tutorial

Gromacs Solvation Free Energy (BAR Method)

V11.6.5

31 March 2024 X-Ability Co., Ltd.

About This Manual

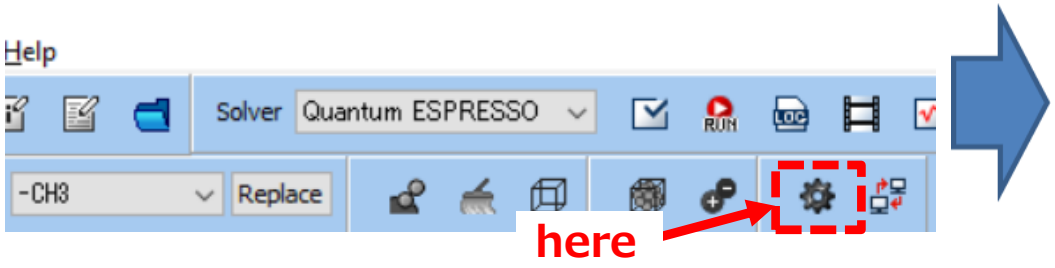
- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of 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.
-

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.

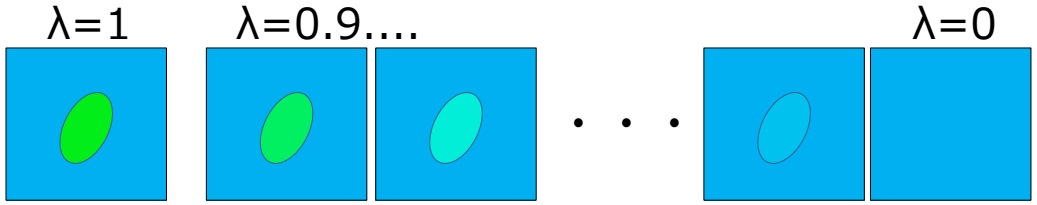
(7) Install Cygwin environment for Winmostar. ← here

- 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.



Overview

- The solvation free energy of ethanol in water is calculated using the Bennett Acceptance Ratio (BAR) method. Initially, a calculation of the actual solution state is performed, followed by calculations where the solute-solvent interactions are gradually diminished. The reaction coordinate is denoted as λ, with the initial solution calculation at λ=1, and the state with no solute-solvent interaction at λ=0.

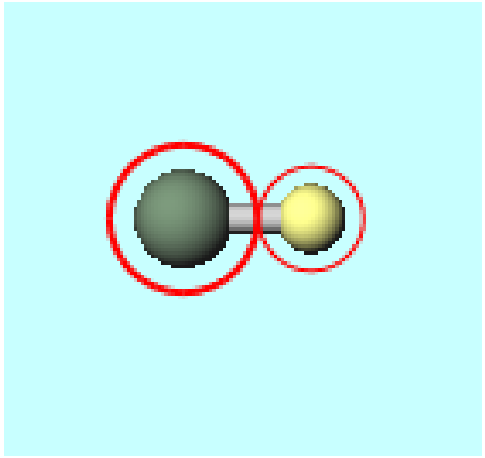


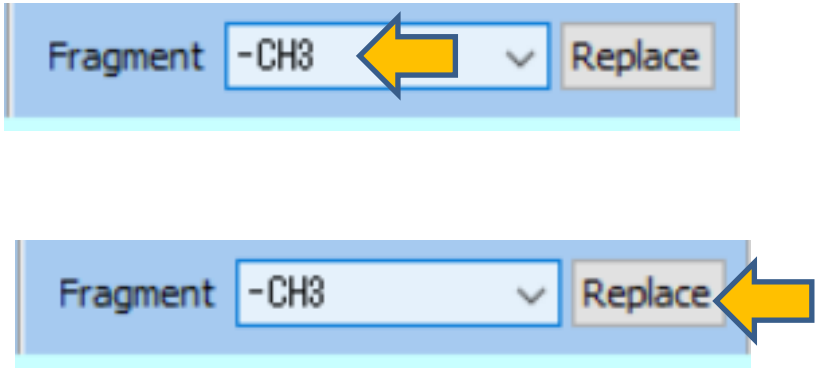
Note :

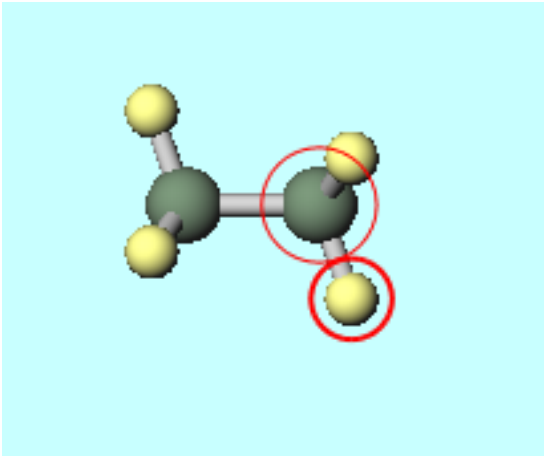
- The number of steps required for equilibration may vary depending on the type of molecules and initial density.
- Larger step numbers for the "main calculation" lead to better reproducibility and more reliable results.
- The type of force field, calculation conditions for interactions, and choices of λ can influence the calculation results.
- For full-scale operations, the use of remote job submission features is recommended.

A. MD Calculation for Solution (λ=0)

A. Click **File | New File**. Click **-CH3**, then click **Replace** twice.

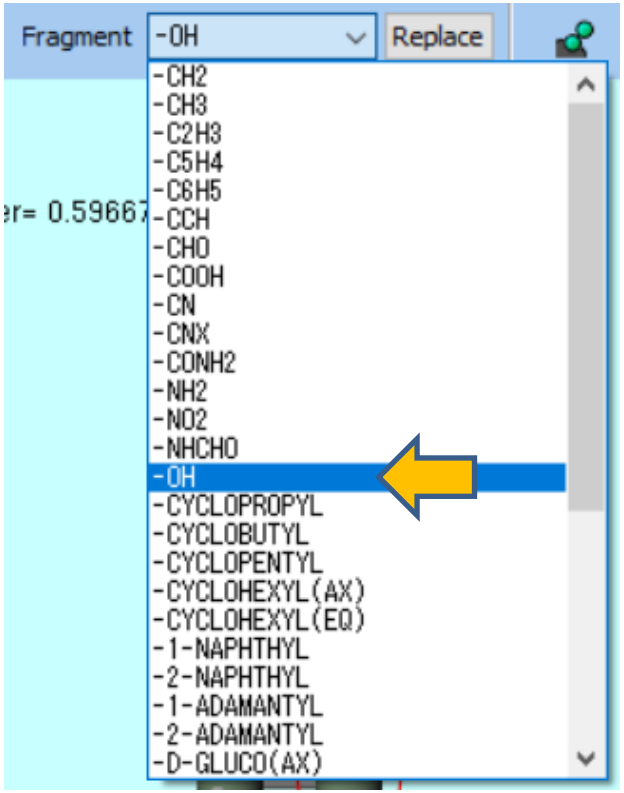


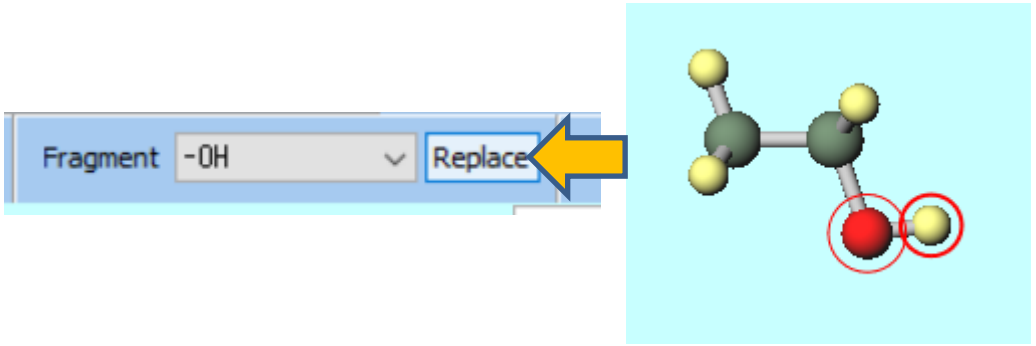




A. MD Calculation for Solution (λ=0)

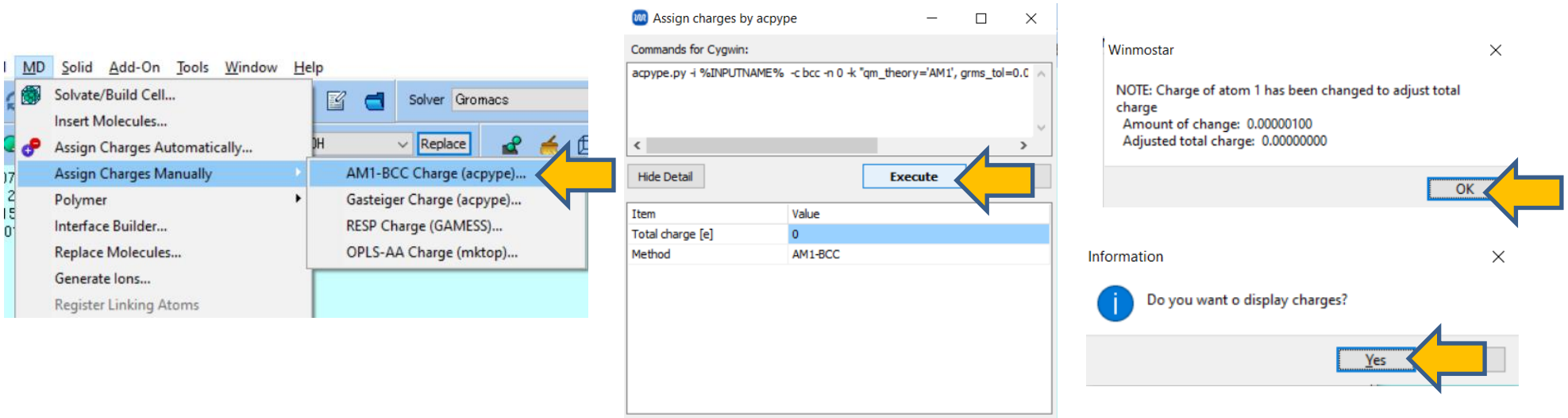
A. Select **-OH** from **Fragment** and click **Replace** once. This completes the ethanol molecule.





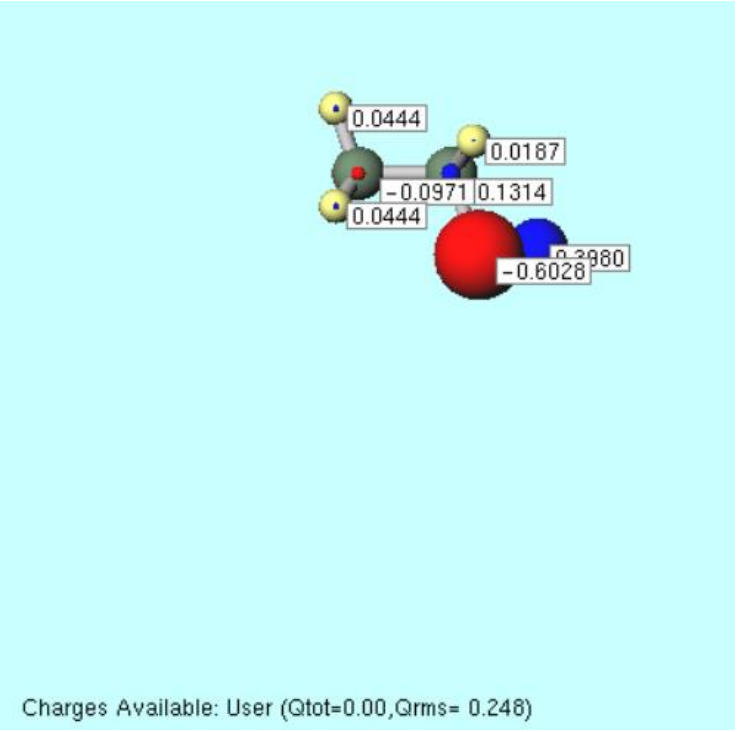
A. MD Calculation for Solution (λ=0)

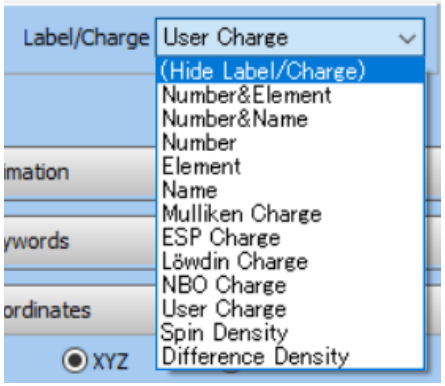
A. Click **MD | Assign Charges Manually | AM1-BCC Charge (acpype)**.
B. In **Assign charges by acpype** window, press **Execute**.
C. When the information dialog appears twice, click OK and Yes.

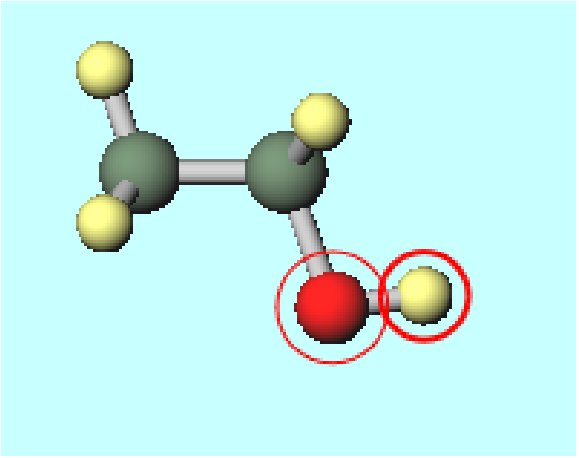


A. MD Calculation for Solution (λ=0)

A. Verify that **Charges Avail: User** is displayed below Viewport, indicating that charges have been assigned.
B. From **Labels/Charge** dropdown menu, select **(Hide Label/Charge)** to hide the charges.

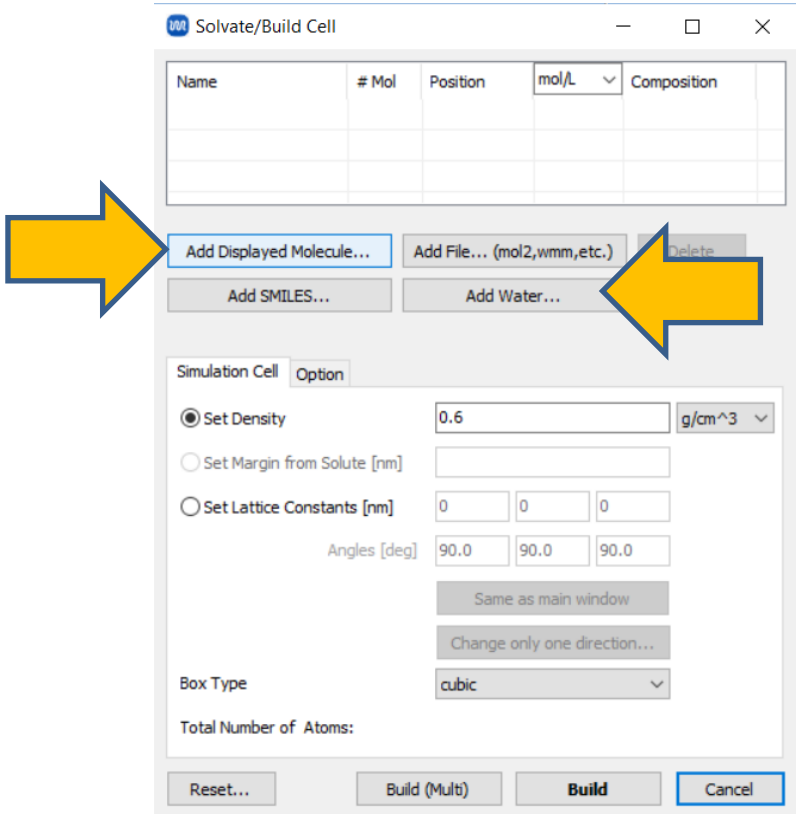


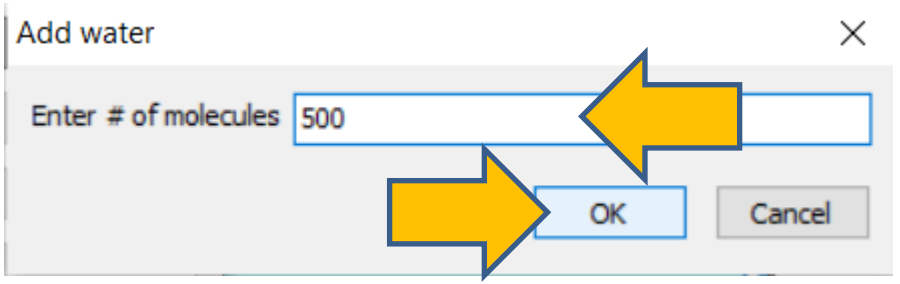




A. MD Calculation for Solution (λ=0)

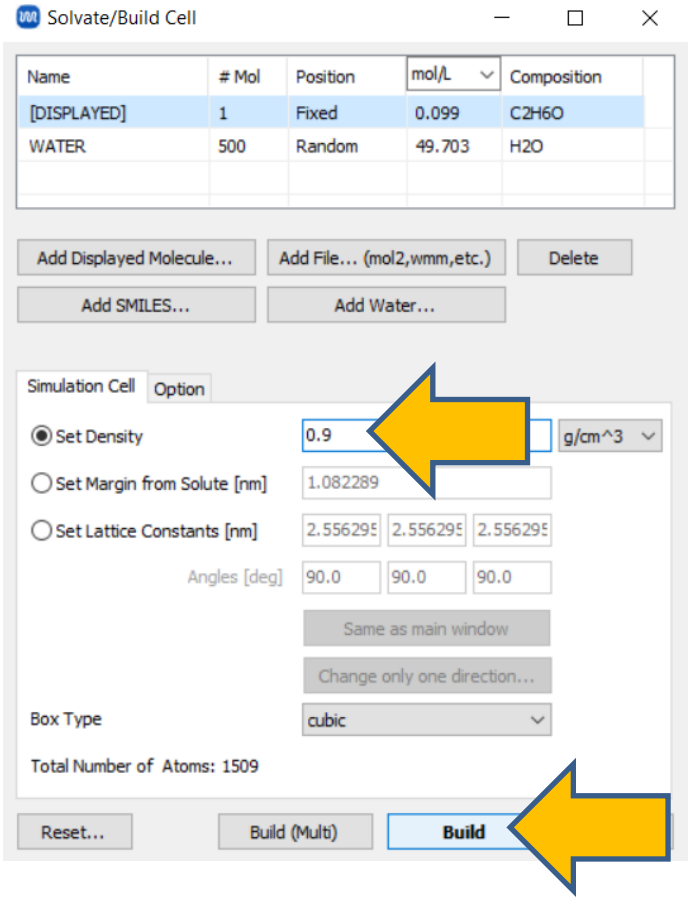
A. Click **Solvate/Build Cell**.
B. Click **Add Displayed Molecule**, enter **1** in **Enter # of molecules**, and click **OK**.
C. Click **Add Water**, enter **500** in **Enter # of molecules**, and click **OK**.

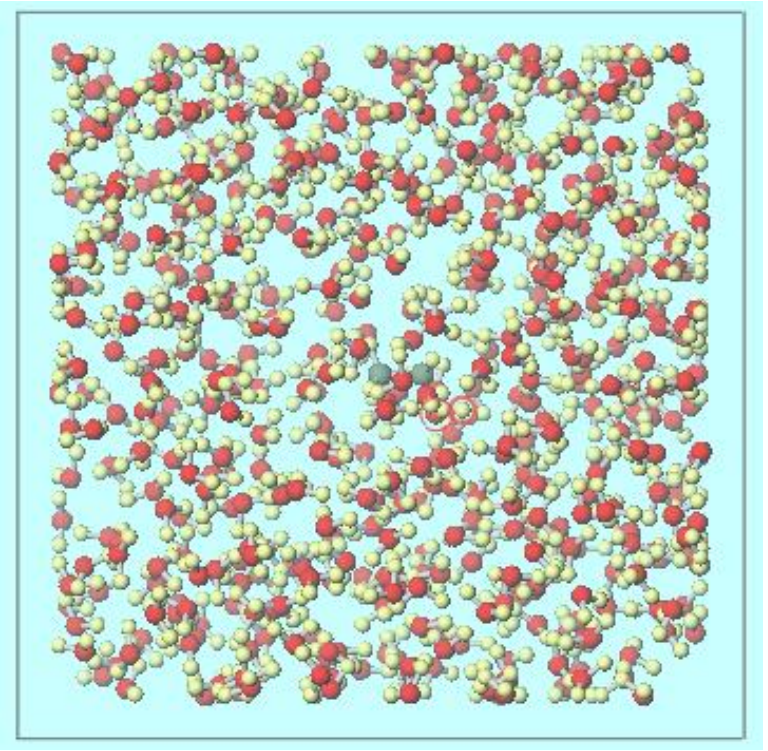




A. MD Calculation for Solution (λ=0)

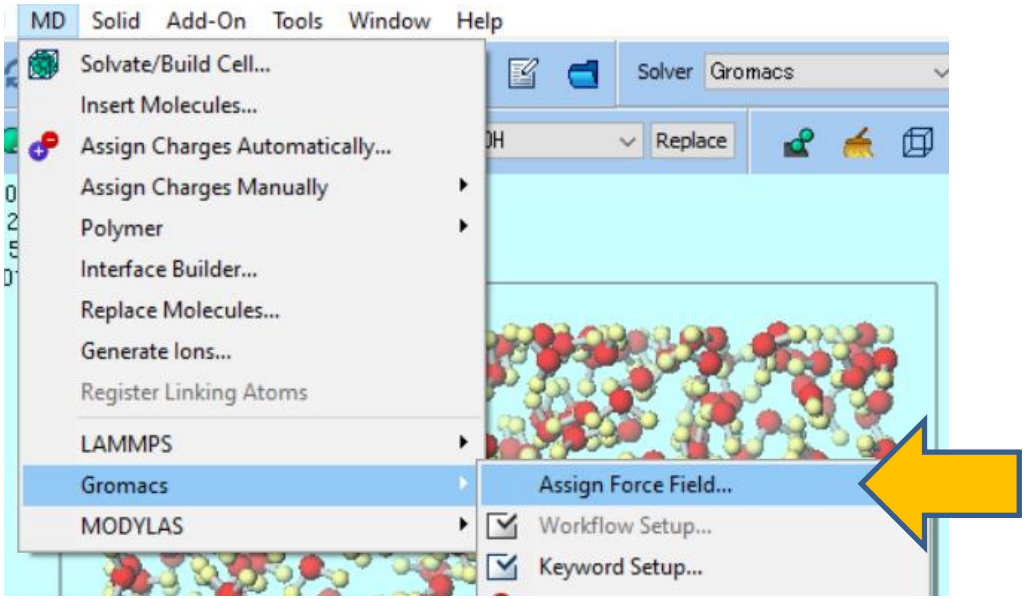
A. Enter **0.9** in **Set Density**.
B. Clicking **Build** will create a system as shown in the right figure.

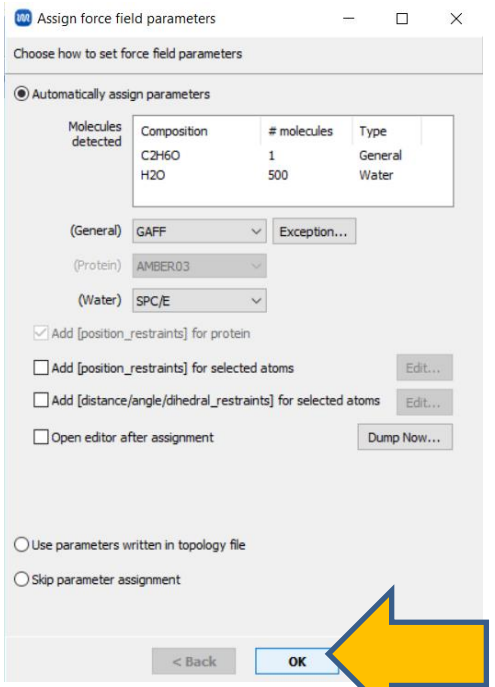


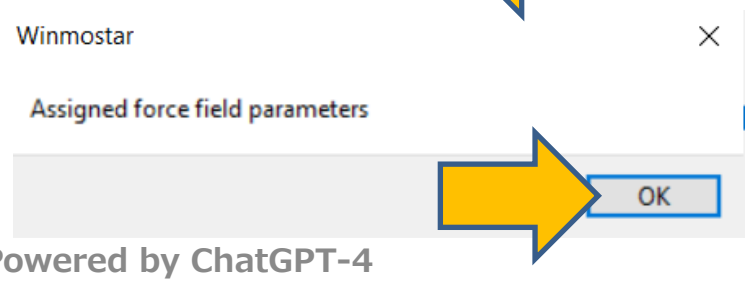


A. MD Calculation for Solution (λ=0)

A. Click **MD | Gromacs | Assign Force Field**をクリックする。
B. Clicking **OK** in **Assign force field parameters** will assign the configured force field.

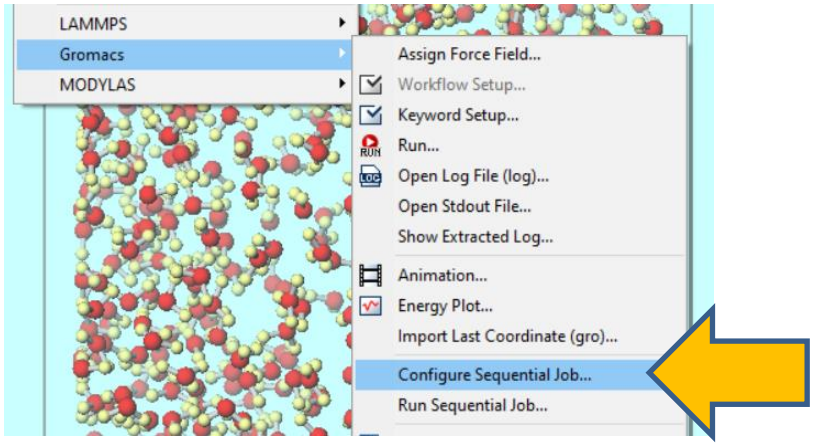


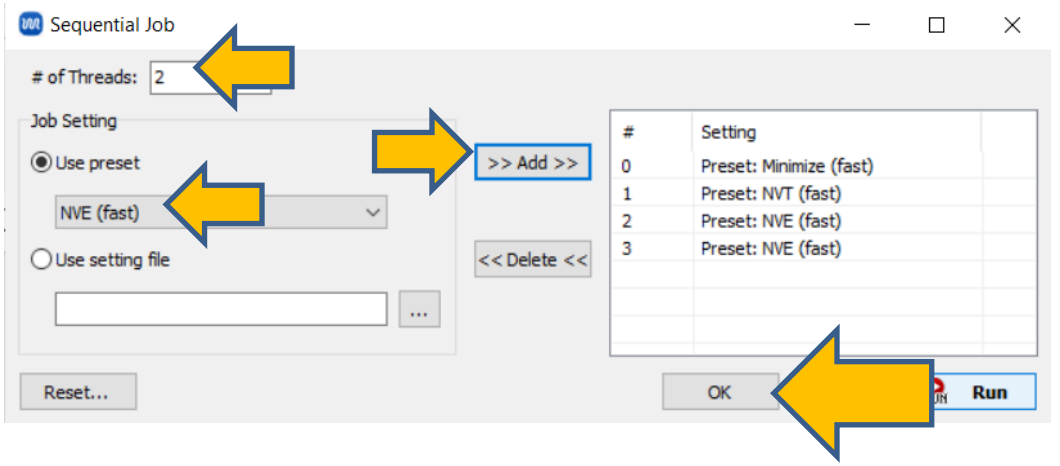




A. MD Calculation for Solution (λ=0)

A. Click **MD | Gromacs | Configure Sequential Job**.
B. Specify the number of threads in **# of Threads**.
C. Select **Minimize (fast)** in **Use preset** and click **>>> Add >>>** once.
D. Select **NVT (fast)** in **Use preset** and click **>>> Add >>>** once.
E. Select **NPT (fast)** in **Use preset** and click **>>> Add >>>** twice.
F. Click **OK**.
G. Click **MD | Gromacs | Run Sequential Job**.
H. Save the file names as **etohaq.gro**, **etohaq.top**.

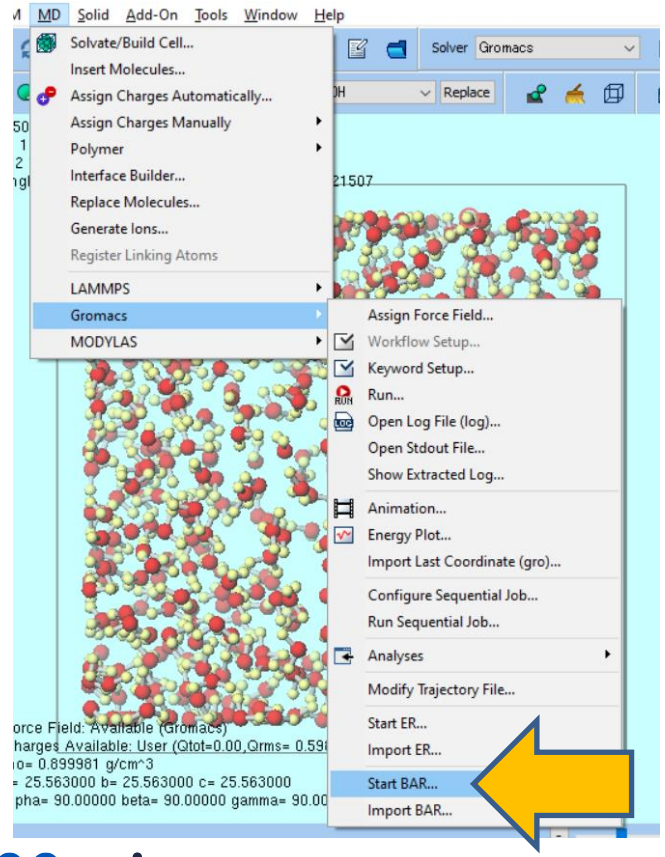


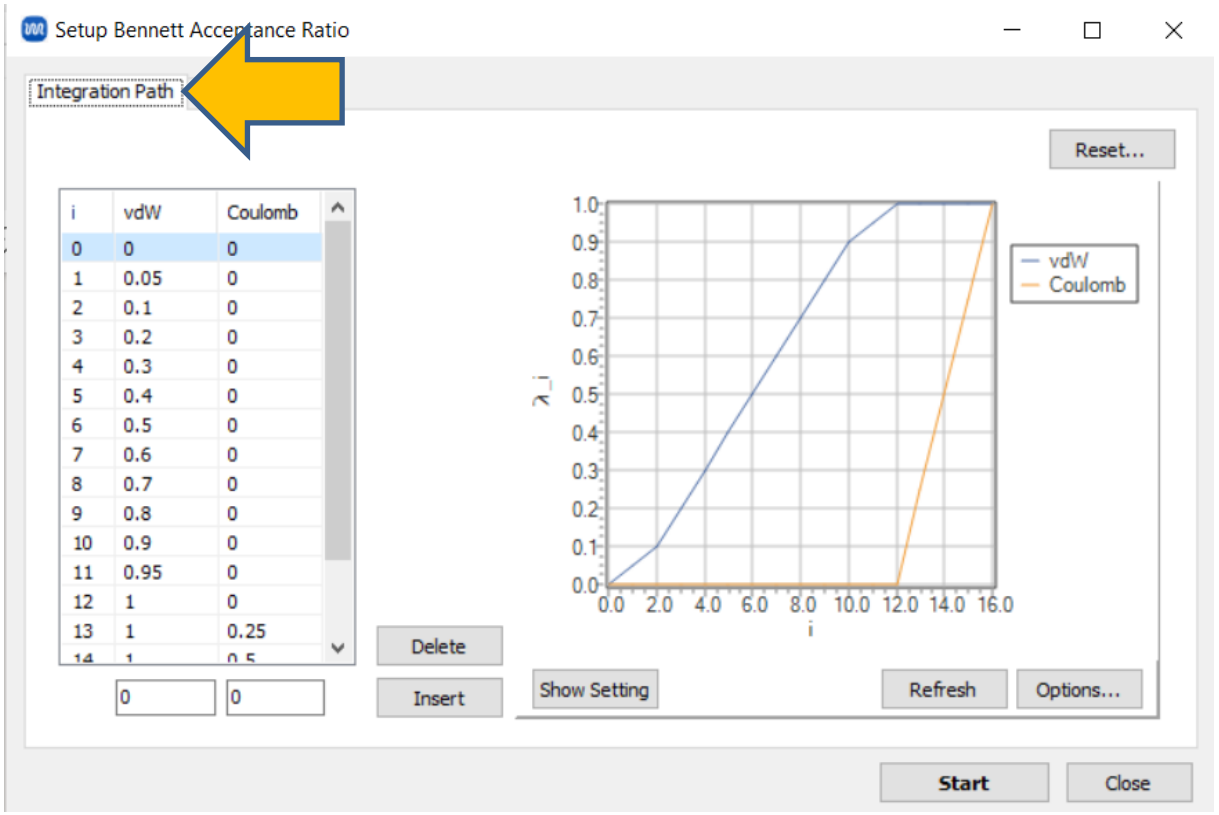


B. MD Calculation with Varying λ

A. After the calculation is completed, click **MD | Gromacs | Start BAR**.

B. In **Integration Path** tab of the displayed window, specify how to change λ.
(For this tutorial, leave it as the default.)



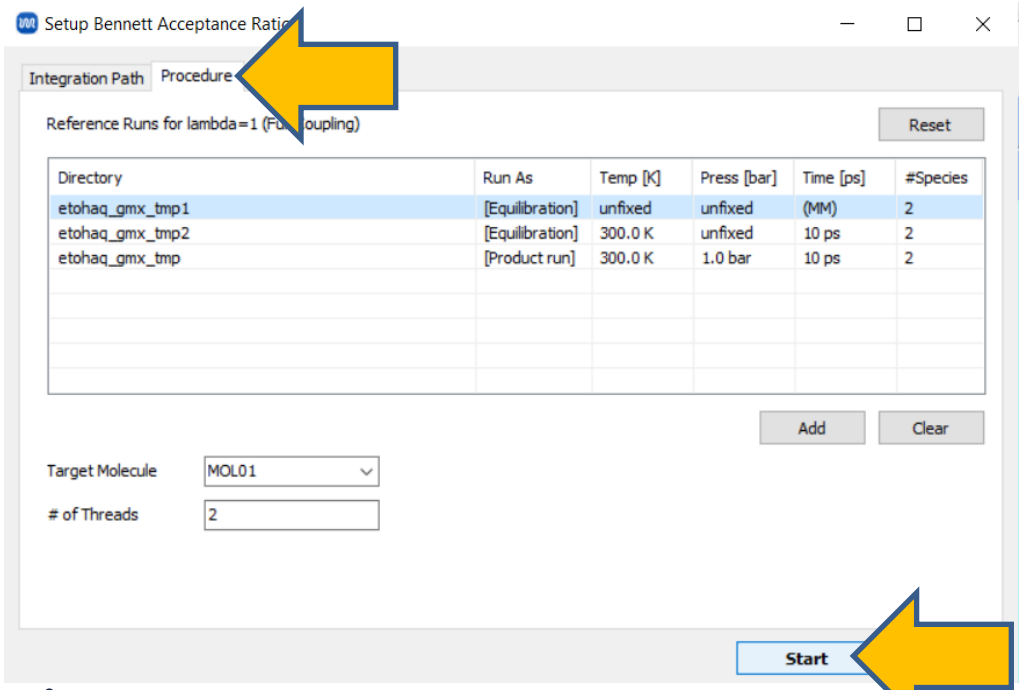


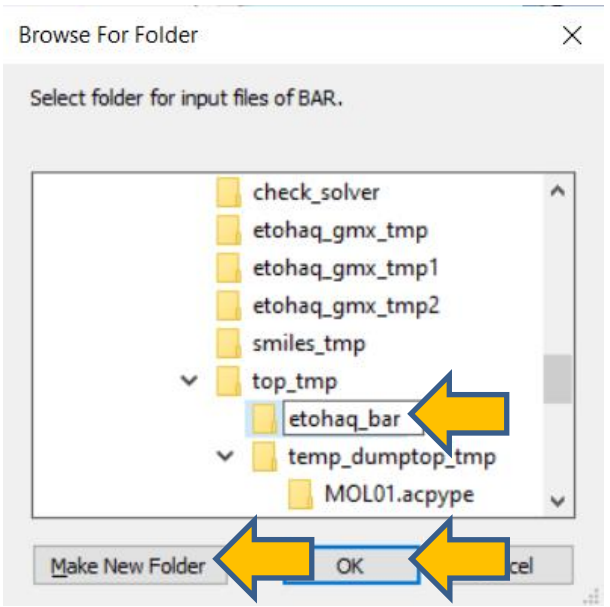
B. MD Calculation with Varying λ

A. In **Procedure tab**, specify the procedure for calculations at each λ.
   By default, the procedure from the previous calculation is loaded.
   This tutorial will use it as is.

B. Click **Start** and specify the folder for running calculations at each λ to start the calculation.

C. Create a new folder named **etohaq_bar** and specify it.

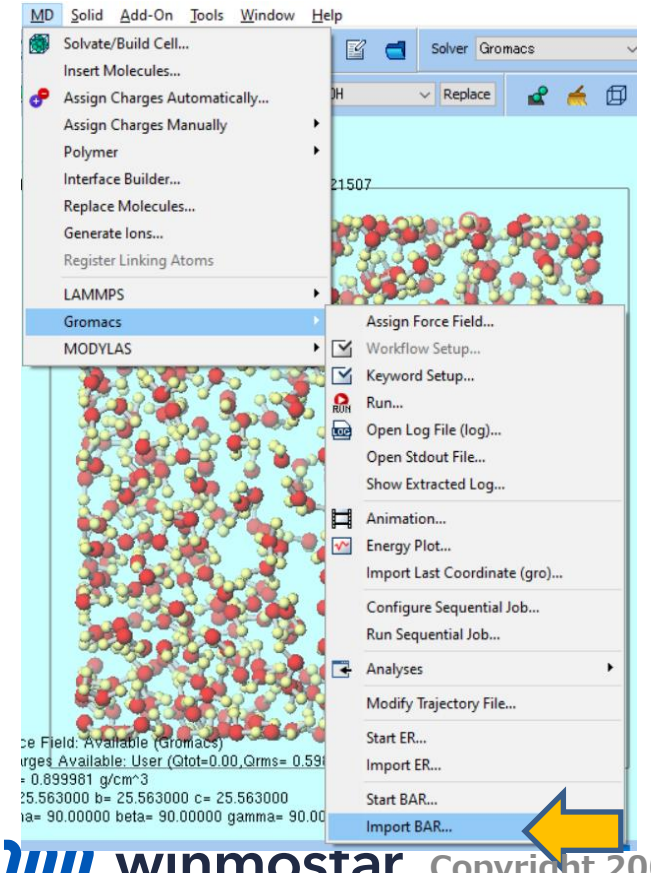


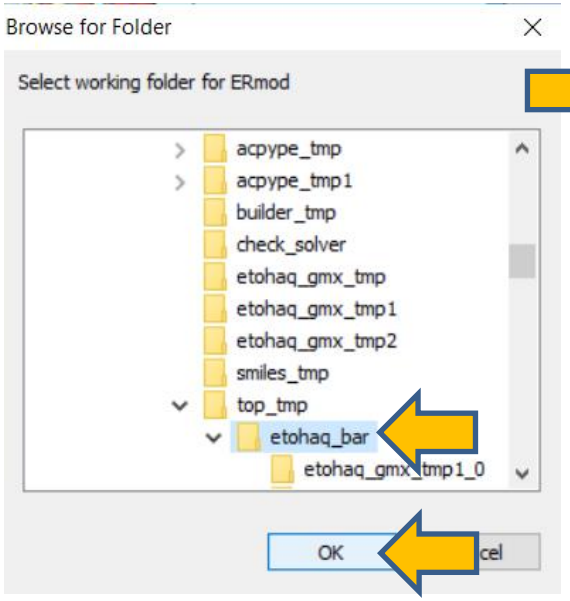


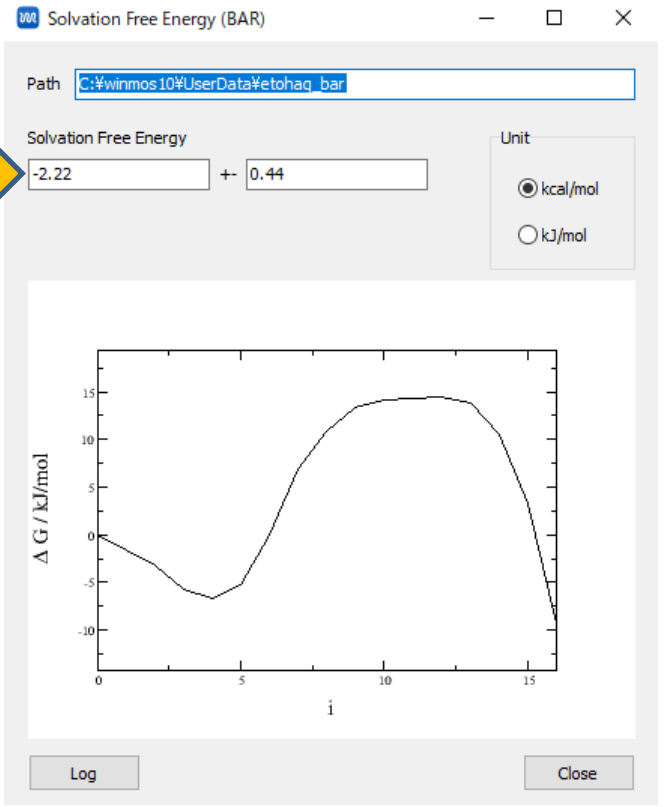
C. Displaying Results

A. After the calculations for all λ values have finished, click **MD | Gromacs | Import BAR**.

B. When asked for the location of the calculations, select the folder specified for running **Start BAR** (here, **etohaq_bar**).The solvation free energy will be displayed.

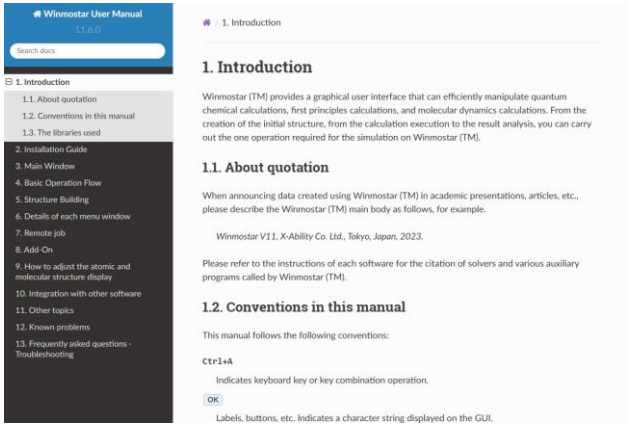






Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

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