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Winmostar tutorial

Amber

Basics

V8.007

X-Ability Co., Ltd.

question@winmostar.com

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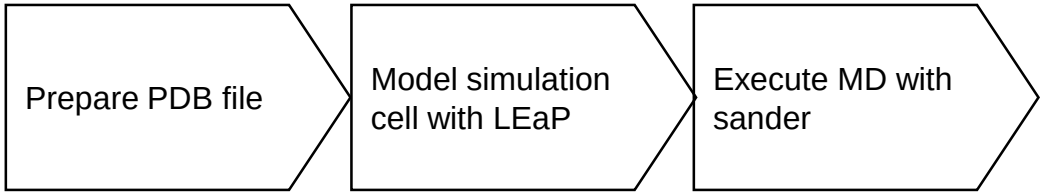
Summary

- In this tutorial, we will show the procedure to perform calculations from a PDB file of chignolin protein using Amber.



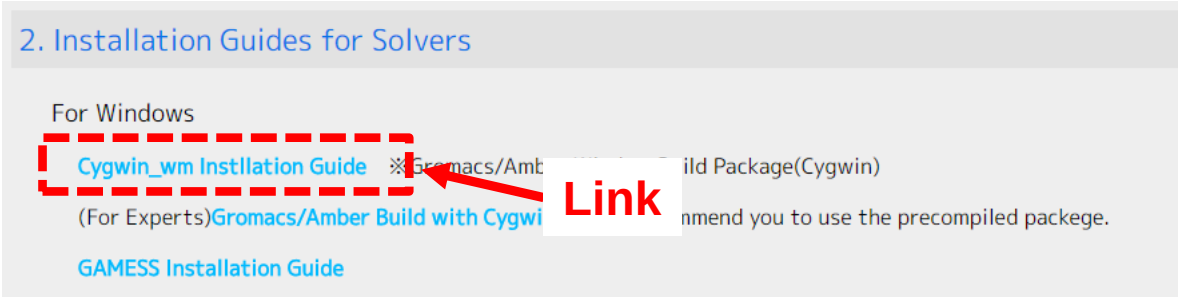
Note:

- We will only show a small part of general MD procedures.
- Na ion has been inserted in order to keep the whole system neutral.
- The size of the system also affects the behavior of the protein.
- The number of steps required for equilibration are dependent on the type of molecule and initial density and may differ from the example given in this tutorial.
- Longer simulation times will produce better reproducibility, and higher accuracy in calculation results.
- Interaction calculation methods and force field will also significantly affect calculation results.

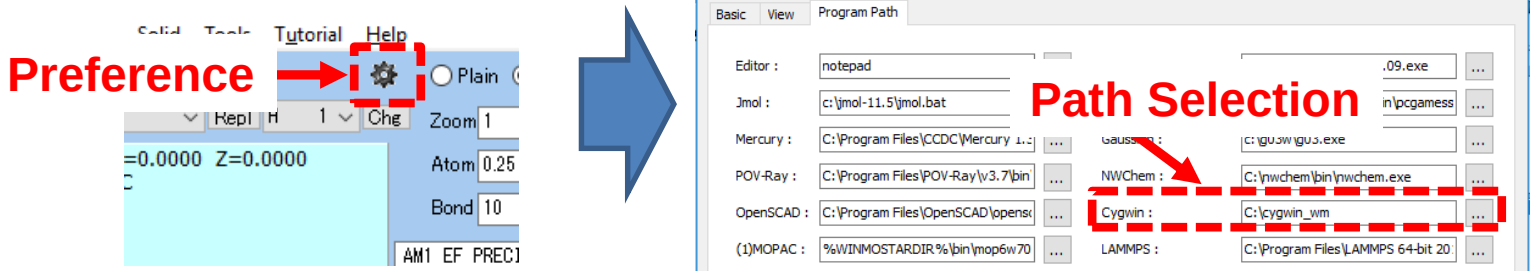
Setting Up Cygwin

Setting up Cygwin is required to use Amber on Winmostar.

- Go to https://winmostar.com/en/manual_en.html and find “2. Installation Guides for Solvers” section. Download the installer for Cygwin from the link indicated below and run installer.



- Cygwin will be installed under “C:¥” by default. To use Winmostar with Cygwin installed in a different location, open “Preference,” then “Program Path” and select the correct path for Cygwin.



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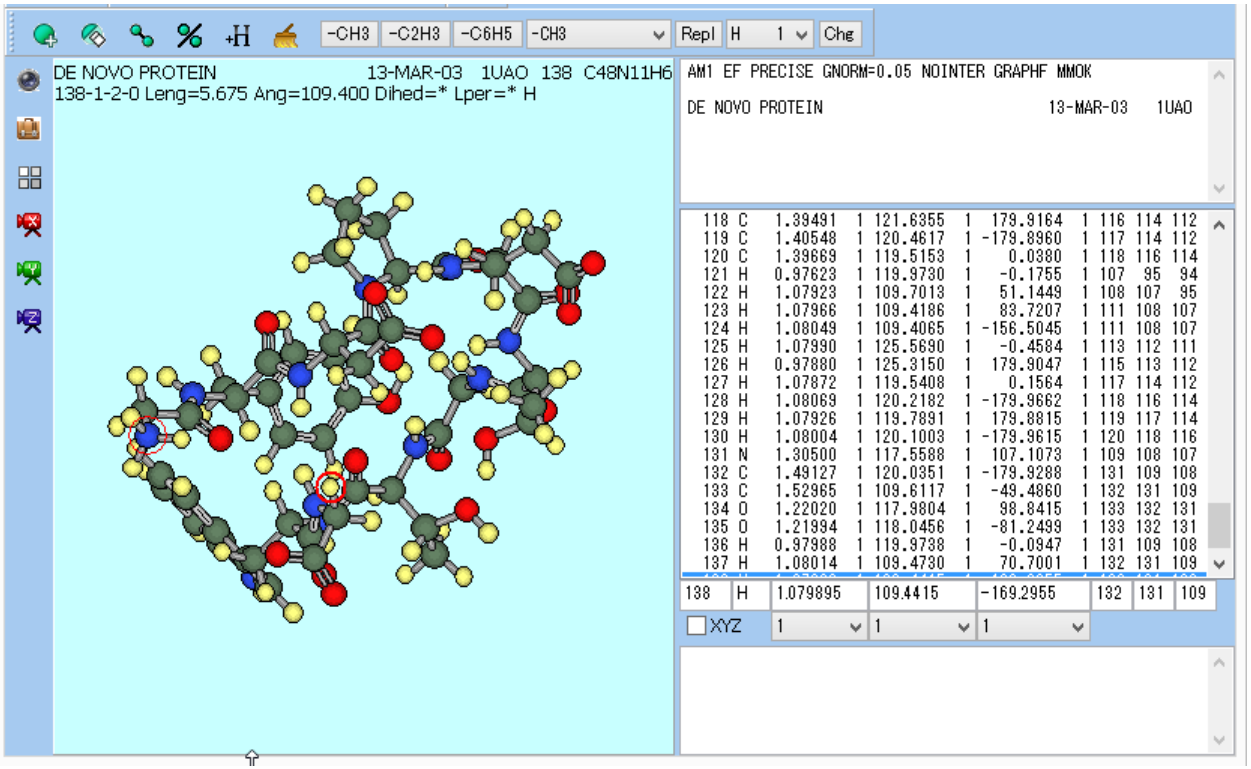
I. Build a simulation cell

1. Click **File | Open**.
2. Open 1uao.pdb in the sample directory.
   （default path; C:¥winmos8¥samples¥1uao.pdb）
3. Click **File** | **Save as**. Then save as **1uao_last.pdb**.
   (This extracts only the last record from a pdb file that includes multiple records)



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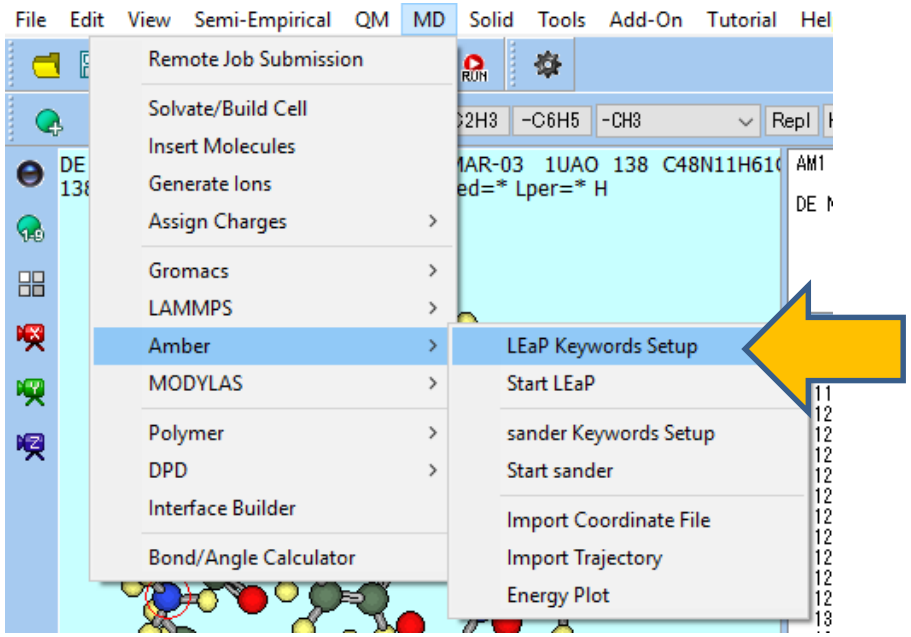
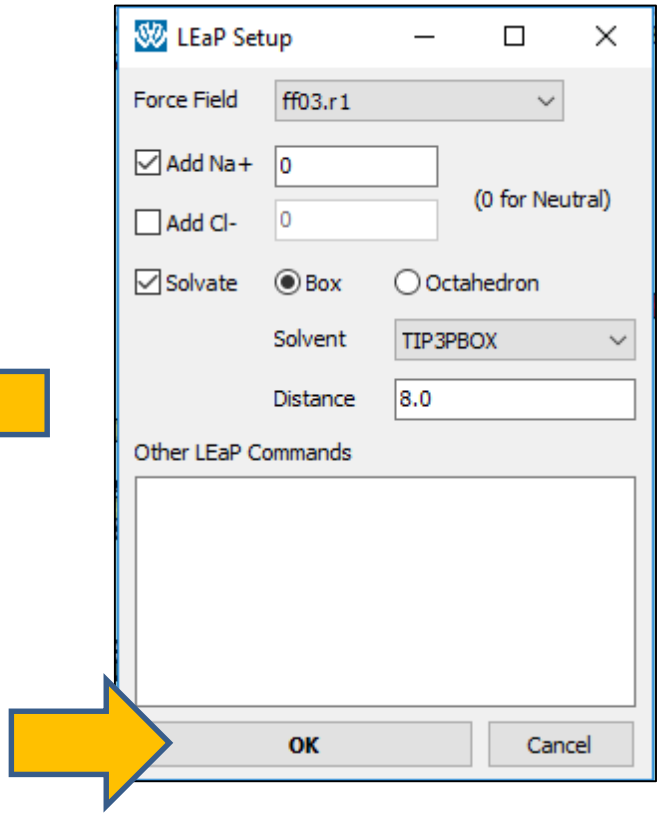
I. Build a simulation cell

1. Click **MD** | **Amber** | **LEaP Keywords Setup**.
2. Click **OK** with default setting.





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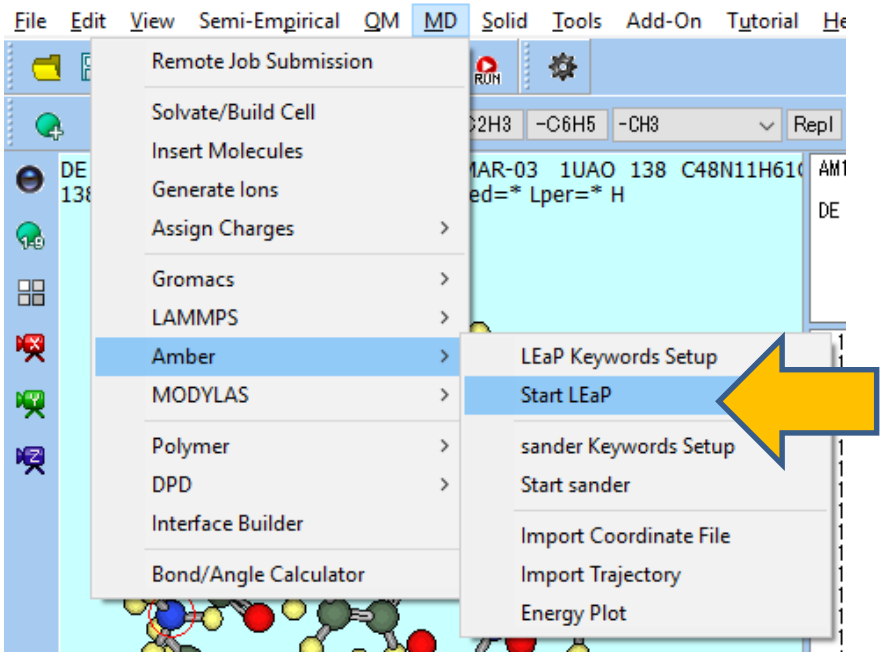
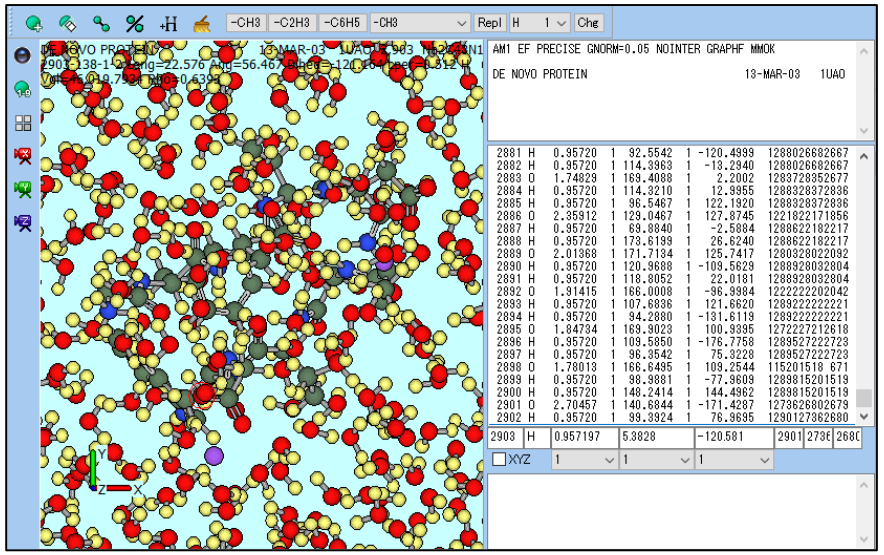
I. Build a simulation cell

1. Click **MD | Amber | Start LEaP**
2. Name and save coordinate（crd）file and topology (prmtop) file.
   Temporarily name the files “**1uao.crd**” and “**1uao.prmtop**”
3. The simulated cell will be displayed on the main window.





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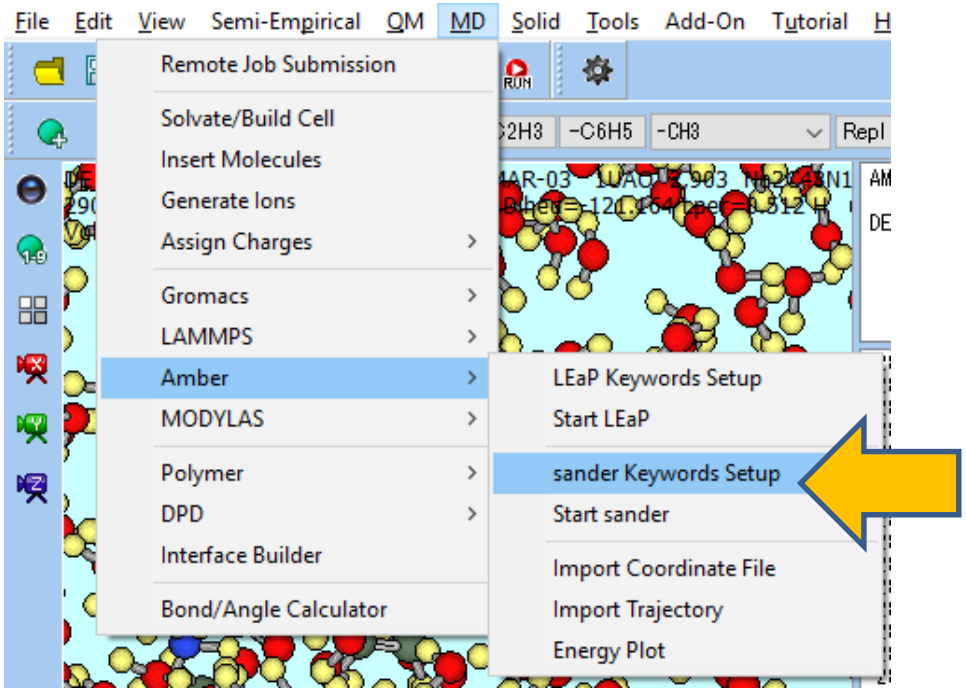
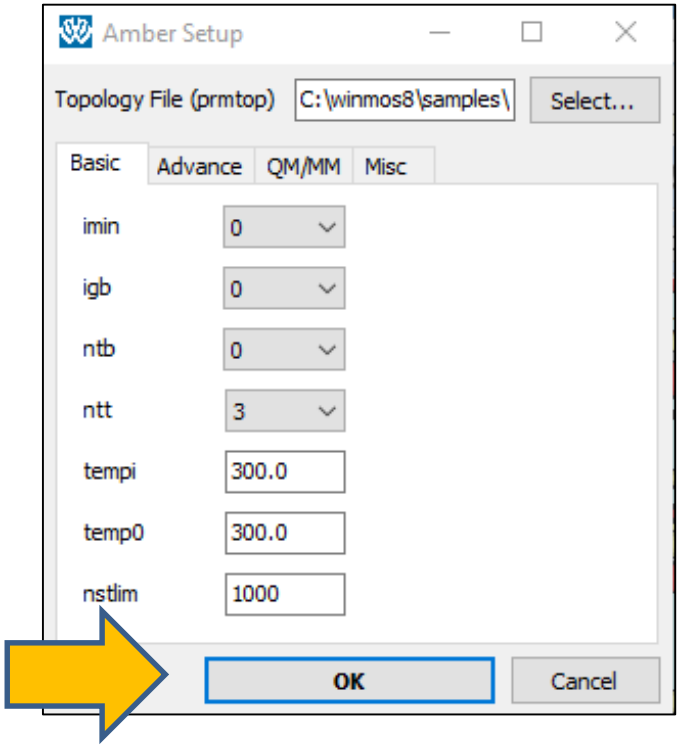
II. Execute simulations

1. Click **MD | Amber | sander Keywords Setup**.
2. Click **OK** by default setting.

In the default setting, Amber will run 1000 steps of constant temperature MD at 300K.





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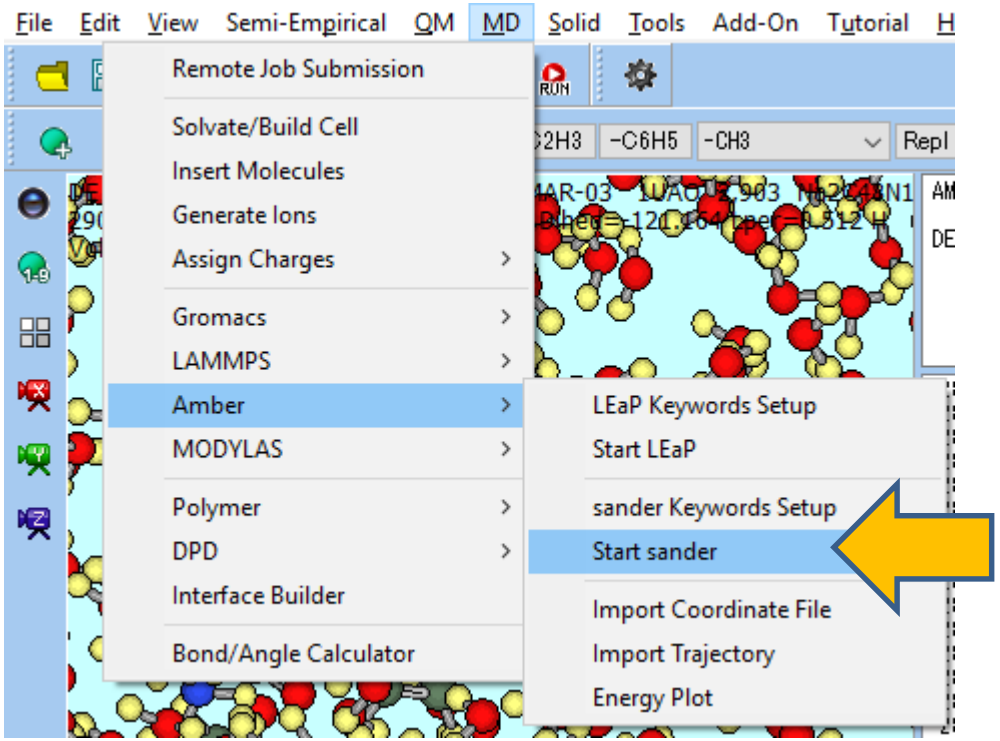
II. Execute simulations

Click **MD | Amber | Start Sander**.



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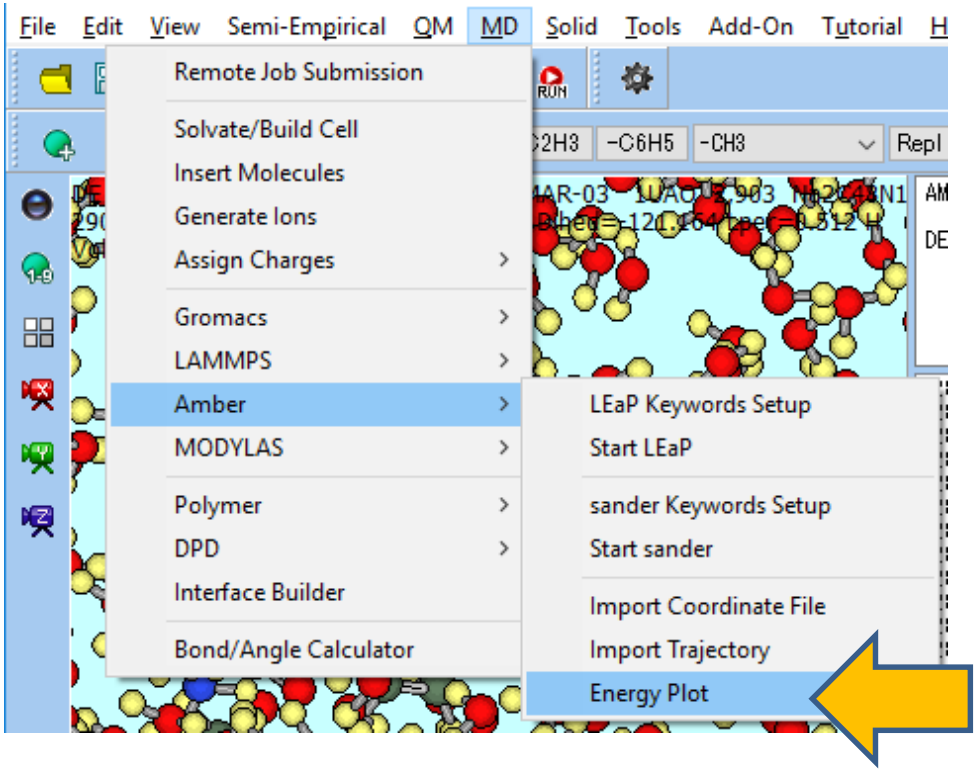
III. Analysis

1. Thermodynamic properties

1. Click **MD** | **Amber** | **Energy Plot**.
2. Open the file suggested by default.



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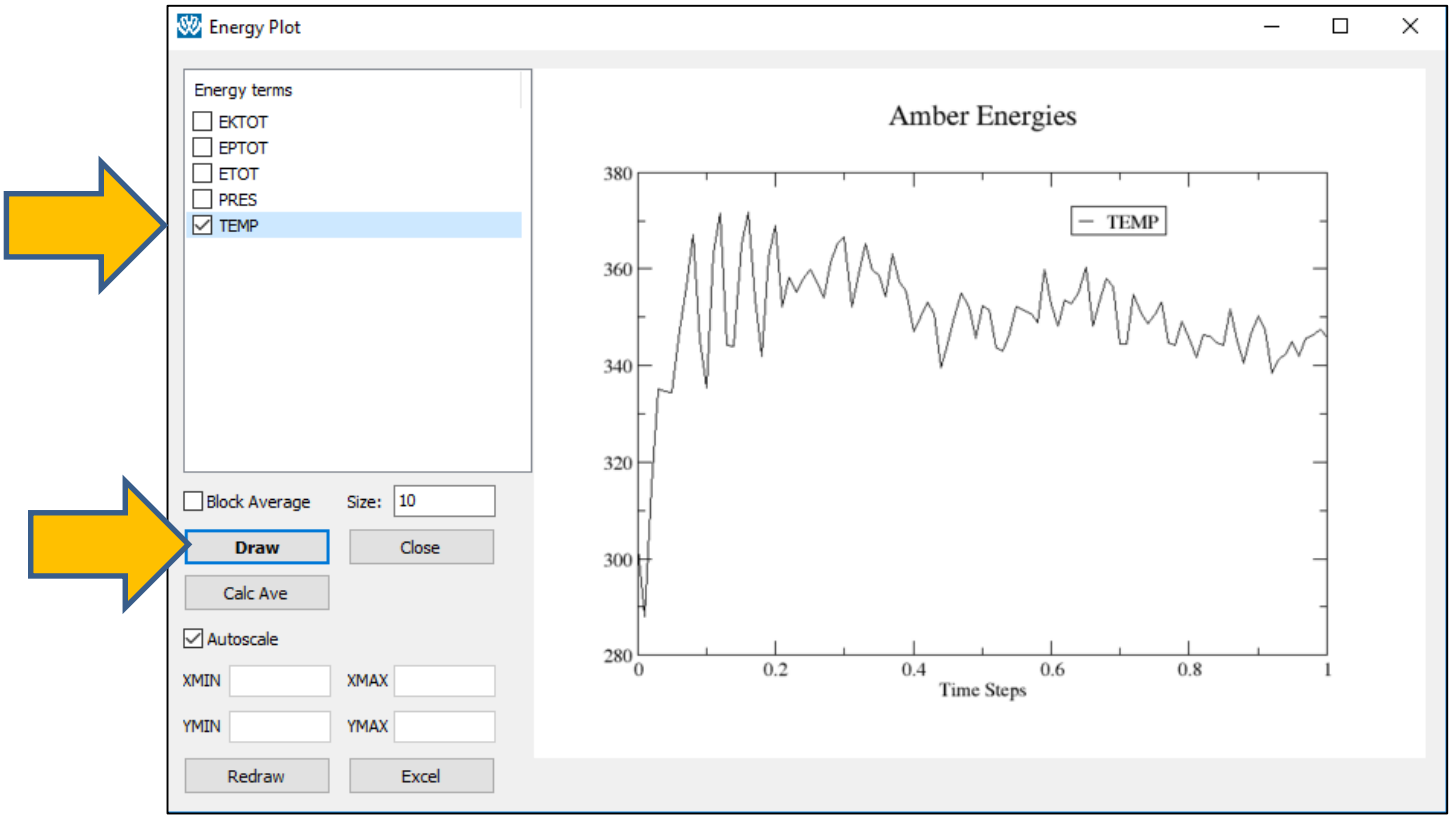
III. Analysis

1. Thermodynamic properties

1. Select a property in **Energy terms** on the window.
2. Click **Draw** to display the graph.

For example, the following graph will show after checking **TEMP**.



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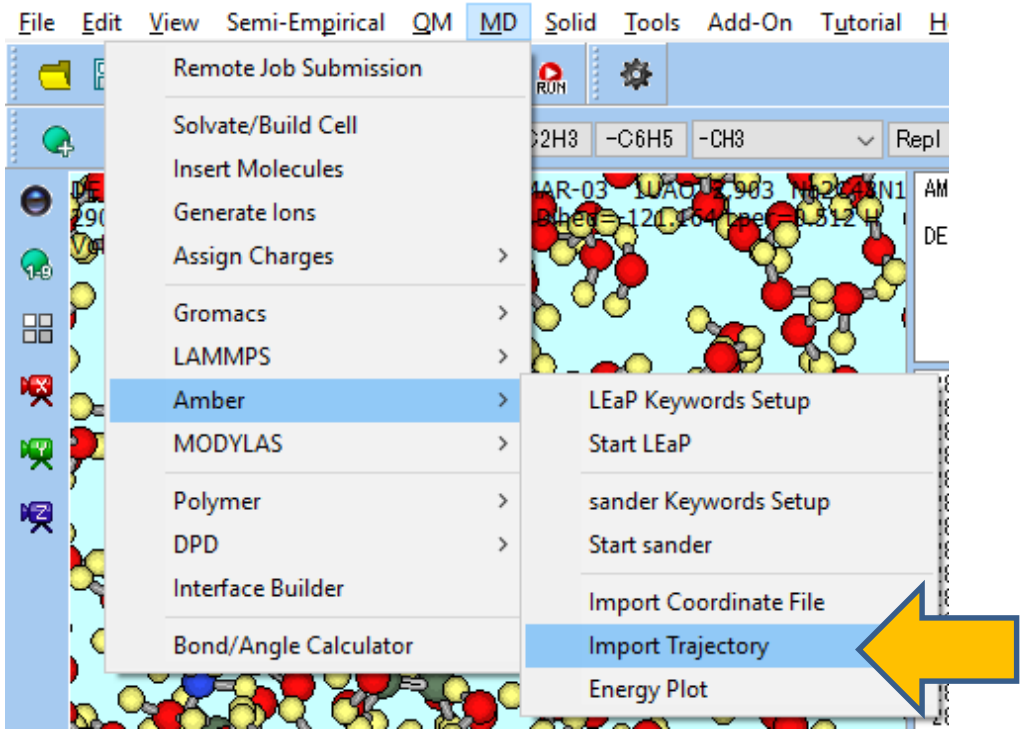
III. Analysis

1. Thermodynamic properties

1. Select **MD** | **Amber** | **Import Trajectory**.
2. Open the coordinates and topology files suggested by default.



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III. Analysis

2. Animation

1. Animation window will be appear when the file is opened.
2. On the animation window, click any frame or click |>(play) button.
   Then a snapshot will be displayed on the main window.