

Winmostar tutorial

Amber

Basics

V8.007

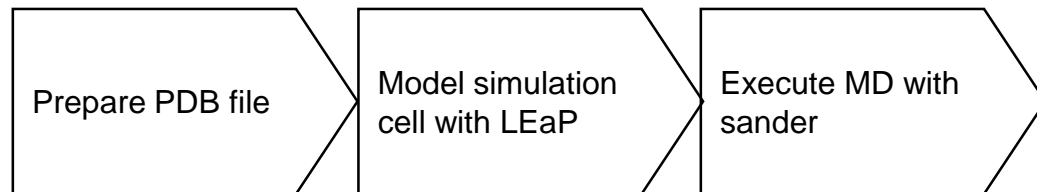
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Summary

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



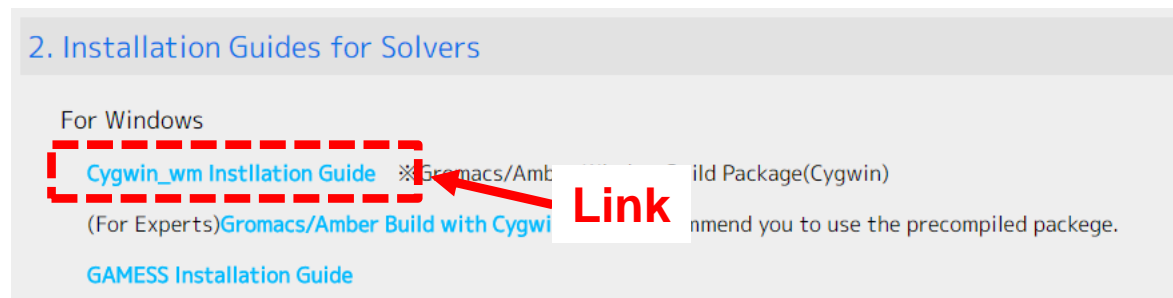
Note:

- 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.

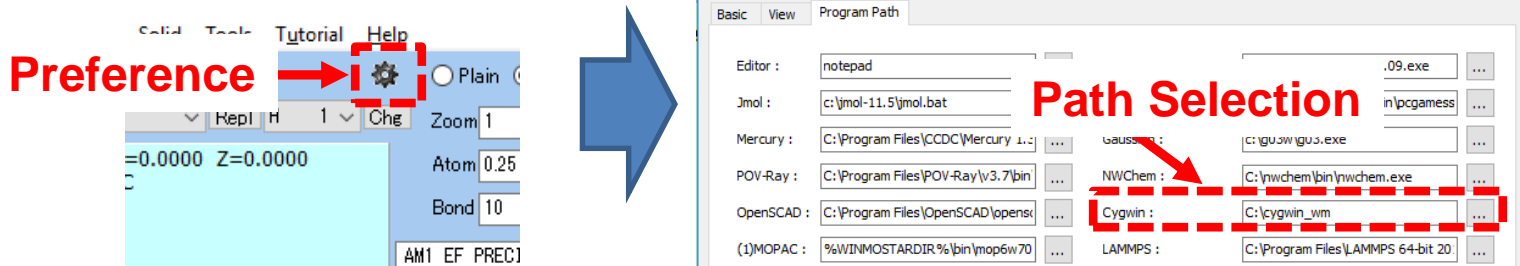
Setting Up Cygwin

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.

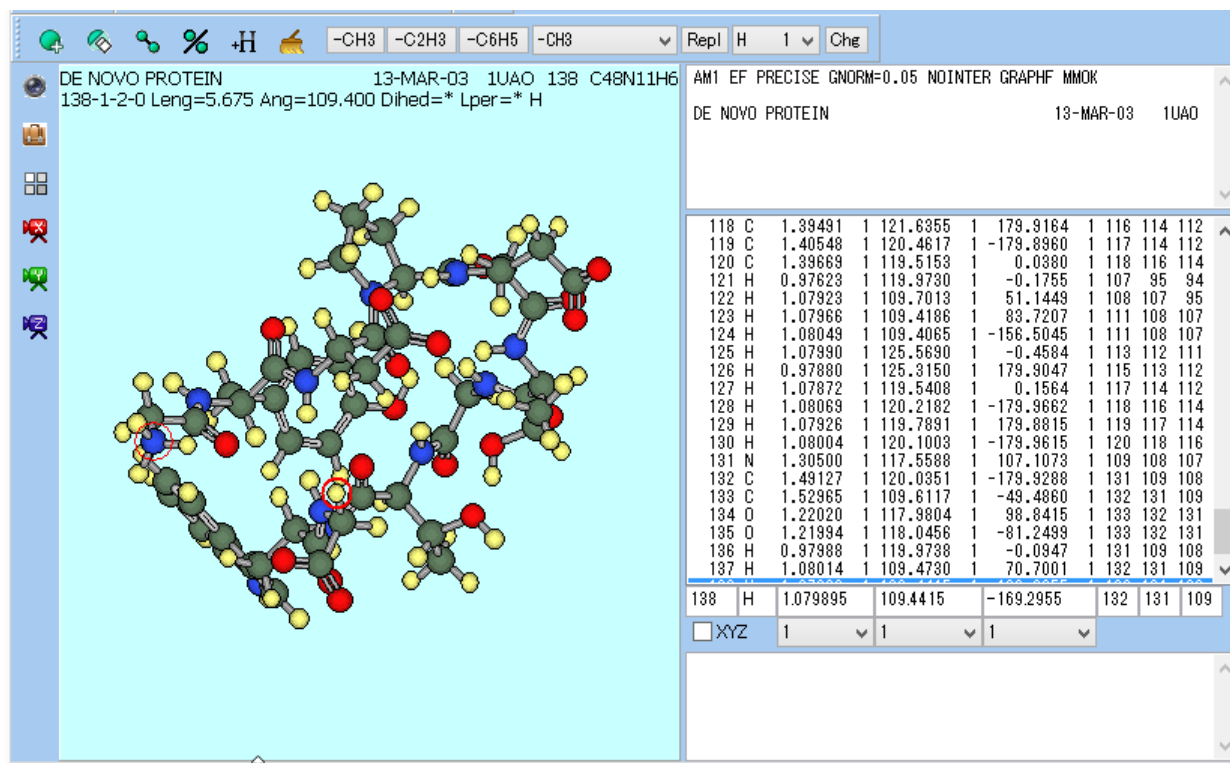


- Cygwin will be installed under “C:¥” by default. To use Winmostar with Cygwin installed in a different location, open “Preference,” then “Program Path” and select the correct path for Cygwin.



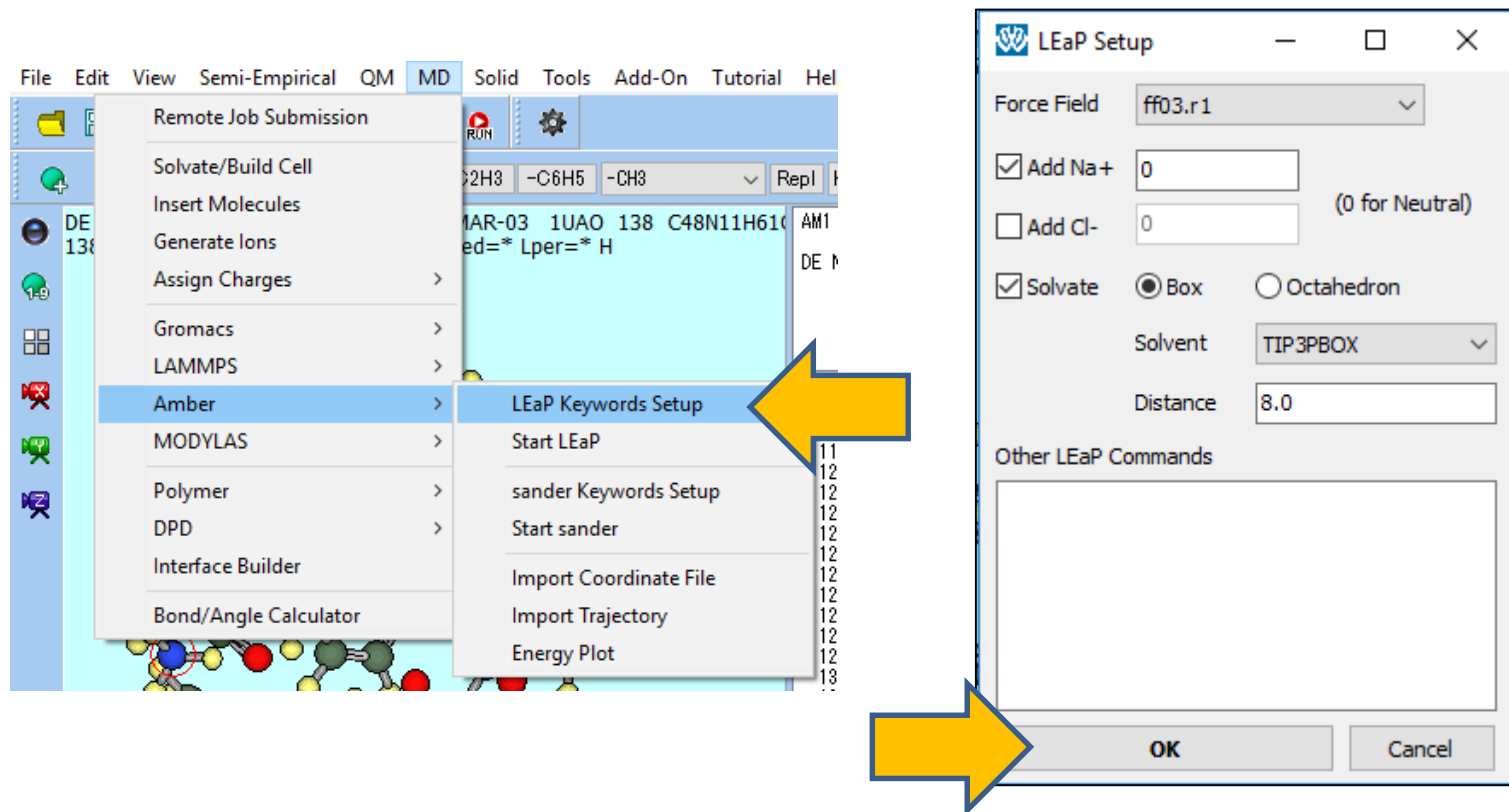
I. Build a simulation cell

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)



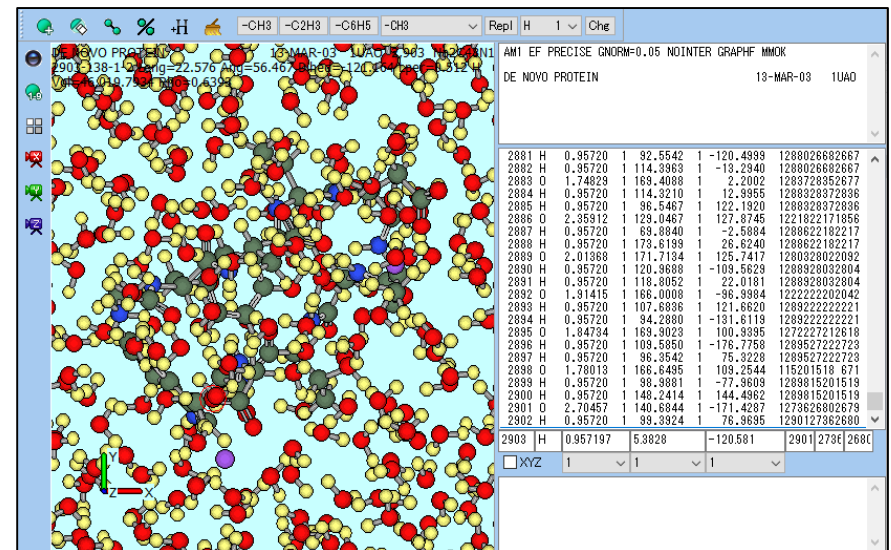
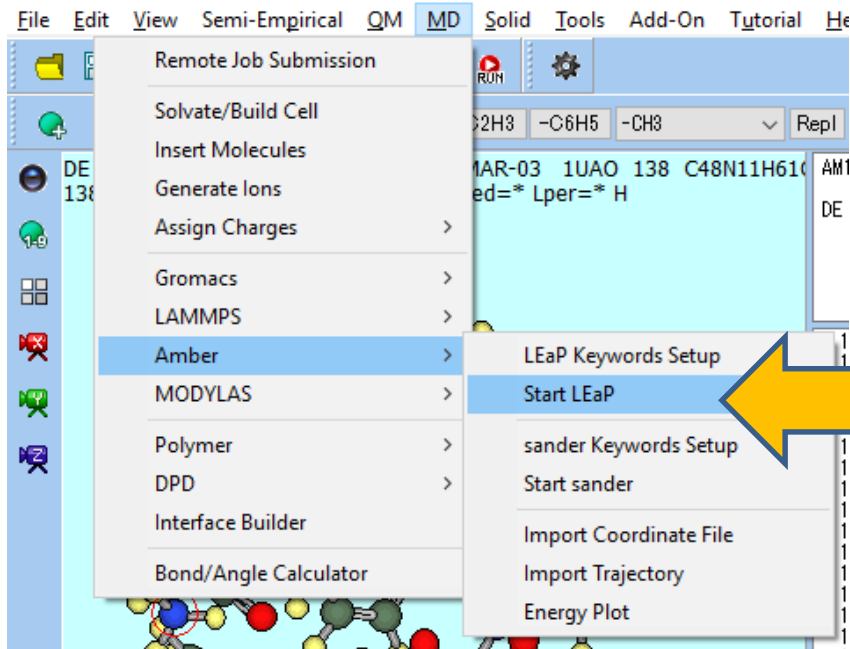
I. Build a simulation cell

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



I. Build a simulation cell

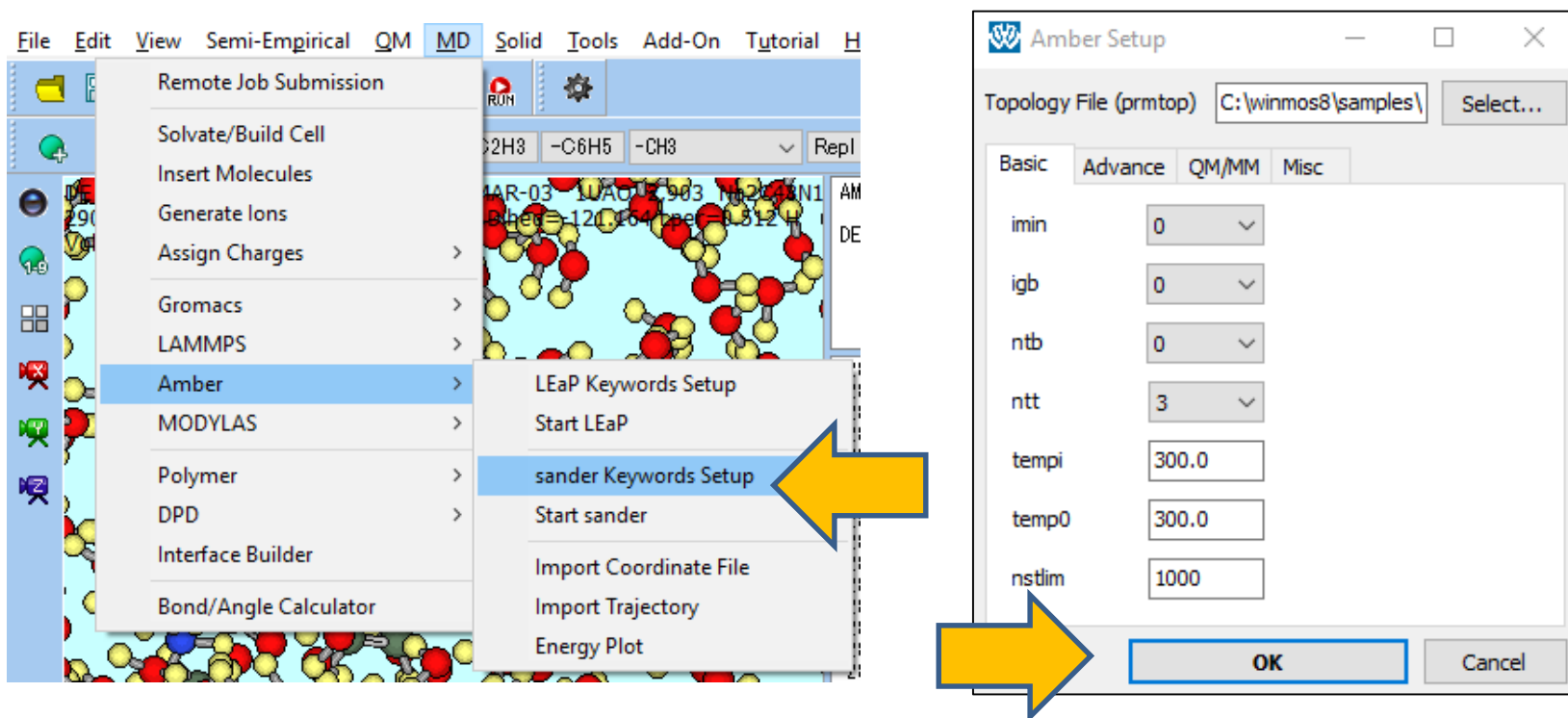
1. Click **MD | Amber | Start LEaP**
2. Name and save coordinate (crd) file and topology (prmtop) file.
Temporarily name the files “**1uao.crd**” and “**1uao.prmtop**”
3. The simulated cell will be displayed on the main window.



II. Execute simulations

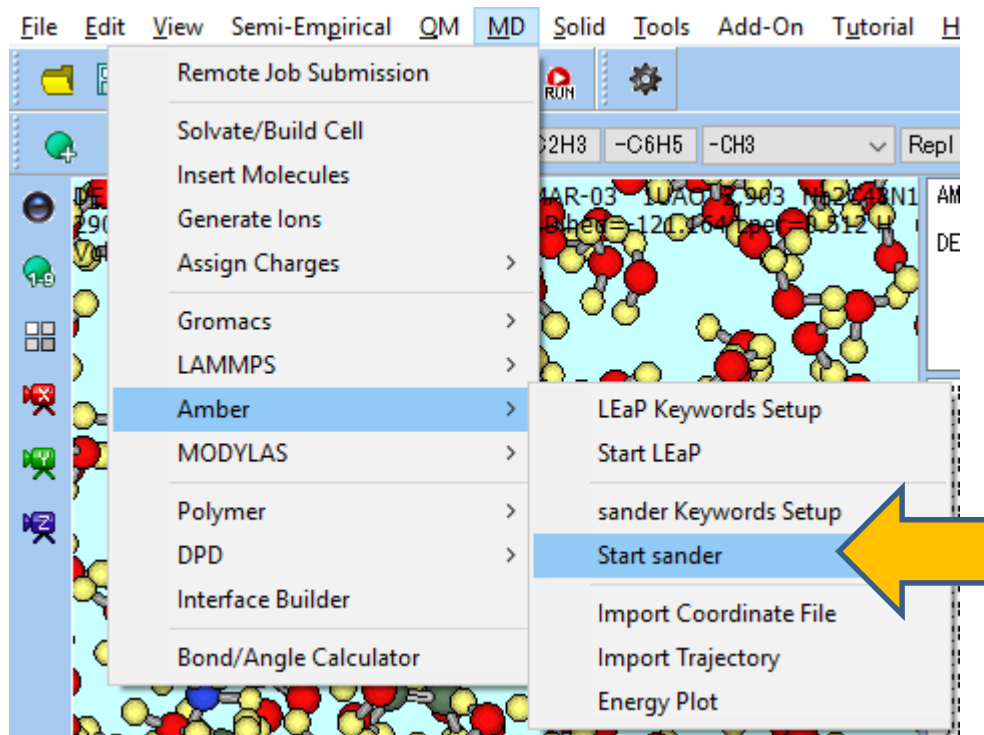
1. Click **MD | Amber | sander Keywords Setup**.
2. Click **OK** by default setting.

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



II. Execute simulations

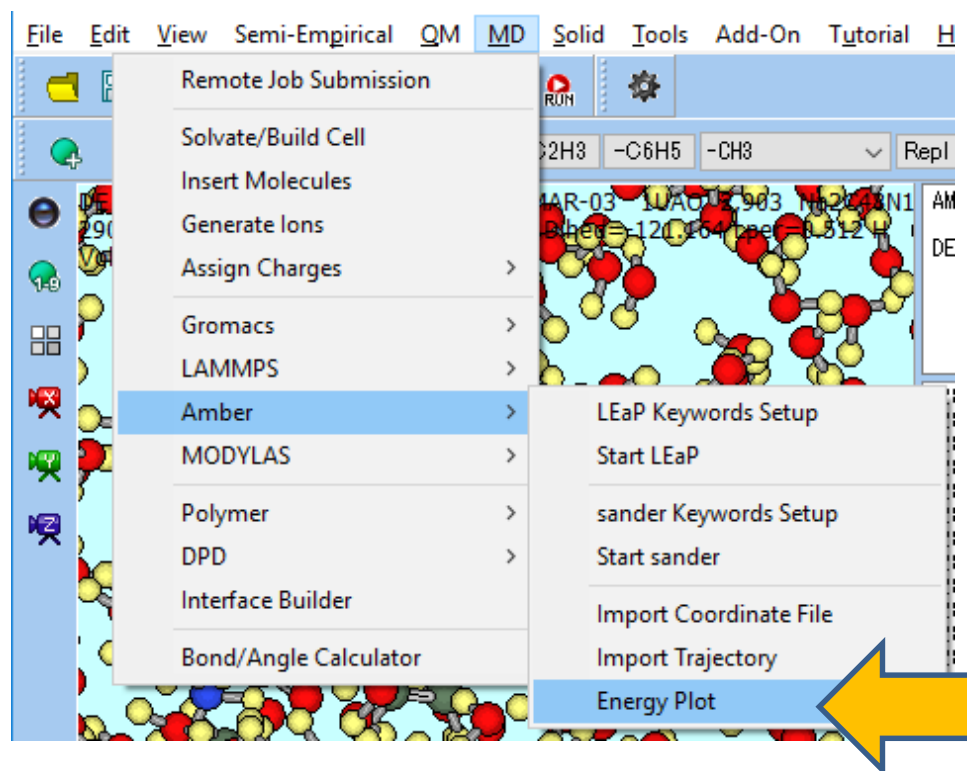
Click **MD | Amber | Start Sander**.



III. Analysis

1. Thermodynamic properties

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



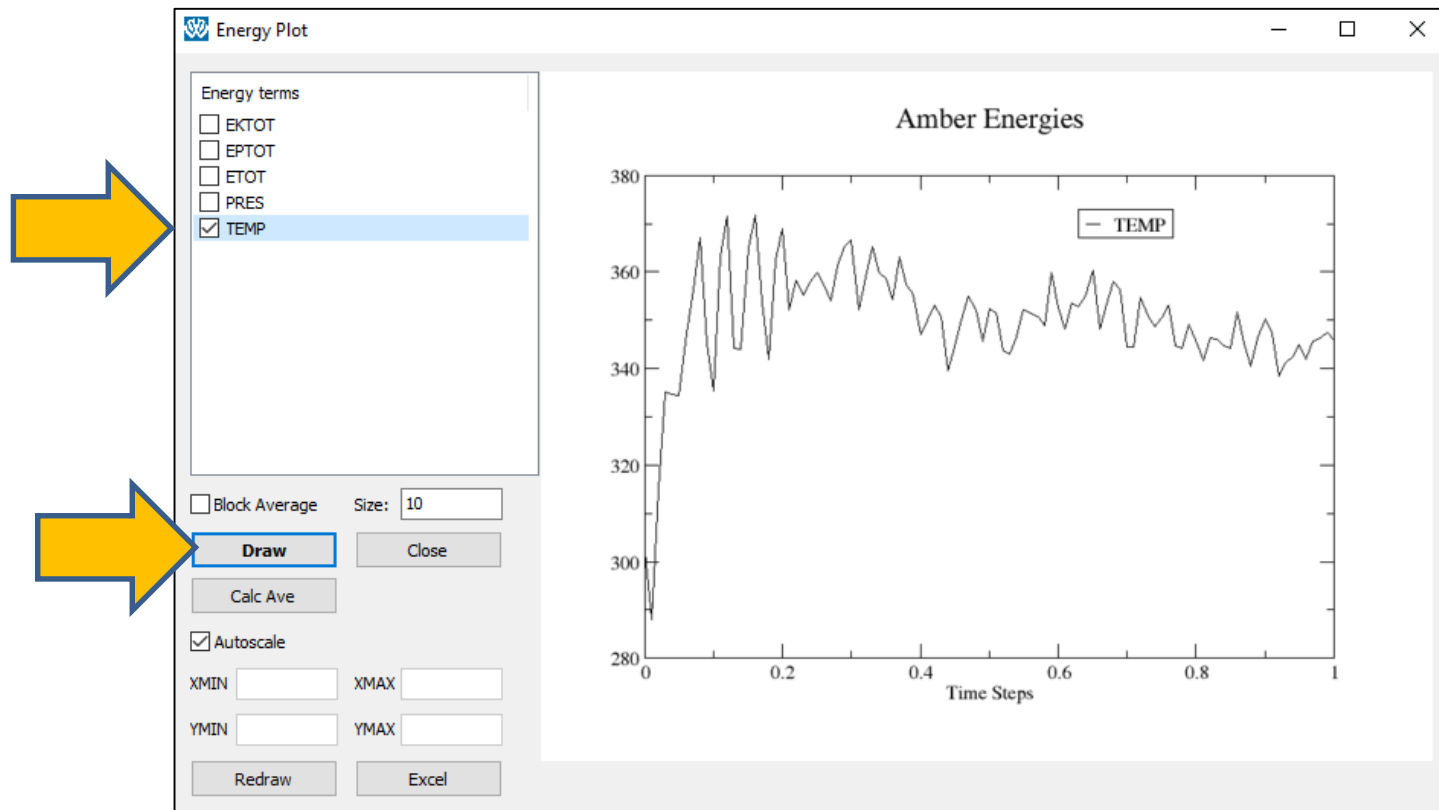
III. Analysis

1. Thermodynamic properties

1. Select a property in **Energy terms** on the window.

2. Click **Draw** to display the graph.

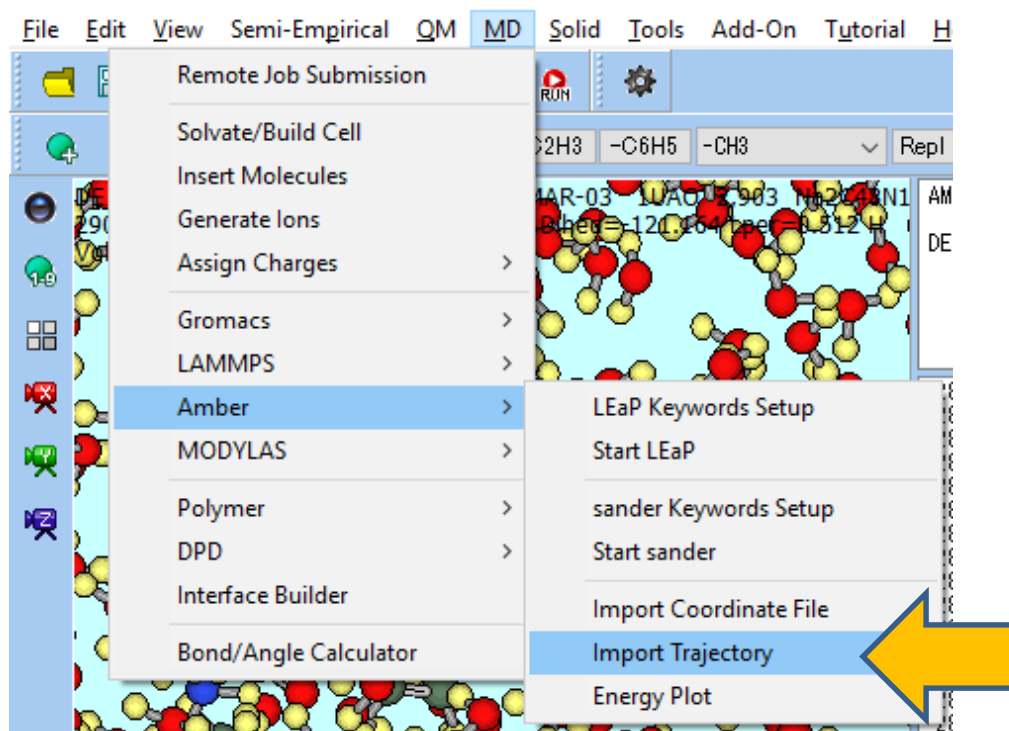
For example, the following graph will show after checking **TEMP**.



III. Analysis

1. Thermodynamic properties

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



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.

The screenshot displays the X-Ability software interface. On the left is a 3D ball-and-stick model of a protein structure. The central panel shows a table of atomic coordinates for 'DE NOVO PROTEIN'.

Atom	X	Y	Z	Occupancy	B-factor	Residue	Chain	Alt. Loc.
2881 H	0.94571	1.910544	1.74.0369	1288026352636				
2882 H	0.95308	1.159.1281	1.-159.4793	1288026352636				
2883 O	3.15347	1.90.9160	1.23.3220	1282625912589				
2884 H	0.87826	1.55.1548	1.-178.8530	1288328262591				
2885 H	0.96791	1.46.4371	1.-11.5538	1288328262591				
2886 O	2.15506	1.152.9795	1.-160.2193	1286926692685				
2887 H	0.98717	1.139.6986	1.173.6996	1288626692687				
2888 H	0.91807	1.117.6453	1.-14.1237	1288626692687				
2889 O	1.93318	1.175.2587	1.-173.9777	1280025382594				
2890 H	0.94781	1.117.0911	1.136.5893	1288926002599				
2891 H	0.94962	1.136.7238	1.-38.1288	1288926002599				
2892 O	2.10291	1.147.2519	1.-130.4555	1260626042590				
2893 H	0.94020	1.162.9395	1.-89.9102	1289226062604				
2894 H	0.96744	1.90.3128	1.101.0262	1289226062604				
2895 O	2.15942	1.176.7911	1.-81.8704	1272527242680				
2896 H	0.99284	1.82.3126	1.-145.5076	1289527252726				
2897 H	0.96001	1.156.2201	1.112.9550	1289527252726				
2898 O	1.61336	1.158.6674	1.20.2302	122282262110				
2899 H	0.97208	1.139.9707	1.121.7919	1289822822226				
2900 H	1.02124	1.100.8714	1.-0.3638	1289822822226				
2901 O	2.04112	1.154.4909	1.117.3453	1273827962686				
2902 H	0.99888	1.100.3309	1.-94.3830	1290127982796				

On the right side, there is an animation control panel. A yellow arrow points to the frame list (frames 1-24). Another yellow arrow points to the play button (|>). Below the play button are options for 'Slow' and 'Fast' animation, a 'temp' input field, and checkboxes for '3D animation', 'jpeg', 'gif', and 'autorew'. At the bottom of the panel are 'Excel' and 'Quit' buttons.