

 winmostar tutorial

MOPAC

Dihedral Angle Scan Calculation

V11.6.5

11 April 2024

X-Ability Co., Ltd.

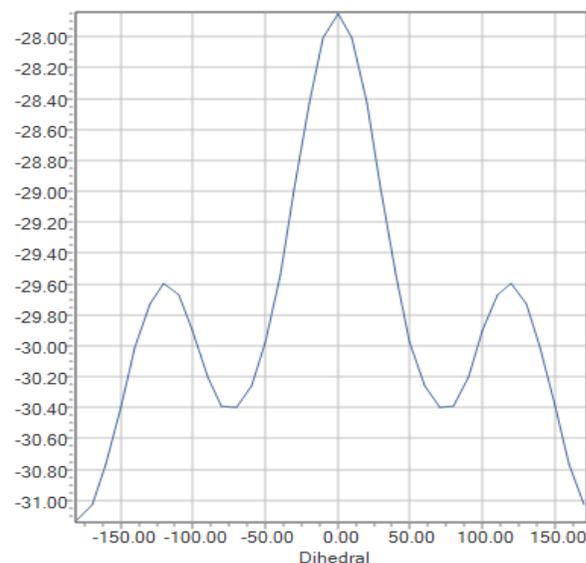
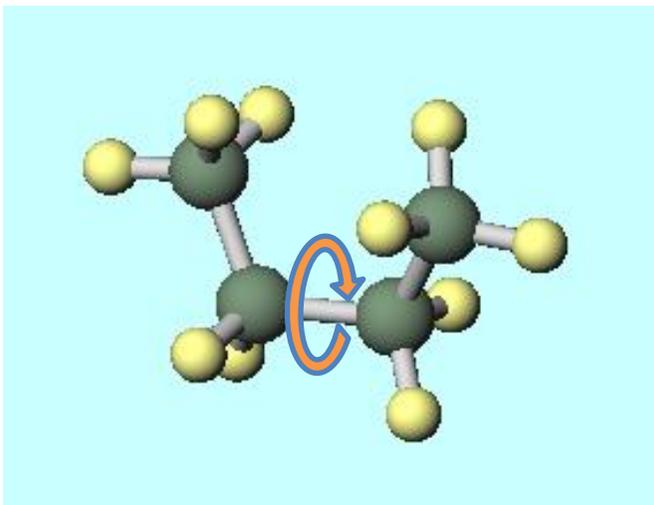
About This Manual

- 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

This tutorial demonstrates the procedure for a dihedral angle scan calculation using the AM1 method for energy (in this tutorial, the heat of formation as defined by MOPAC), using butane in vacuum as an example.

In the scan calculation, a specified internal coordinate (bond length, angle, dihedral angle) is varied incrementally to investigate how the energy changes. All other internal coordinates not specified are optimized for each structure.



Note :

- The calculations in this tutorial are semi-empirical and conducted in vacuum, so if accurate results are desired, please use GAMESS, NWChem, or Gaussian.

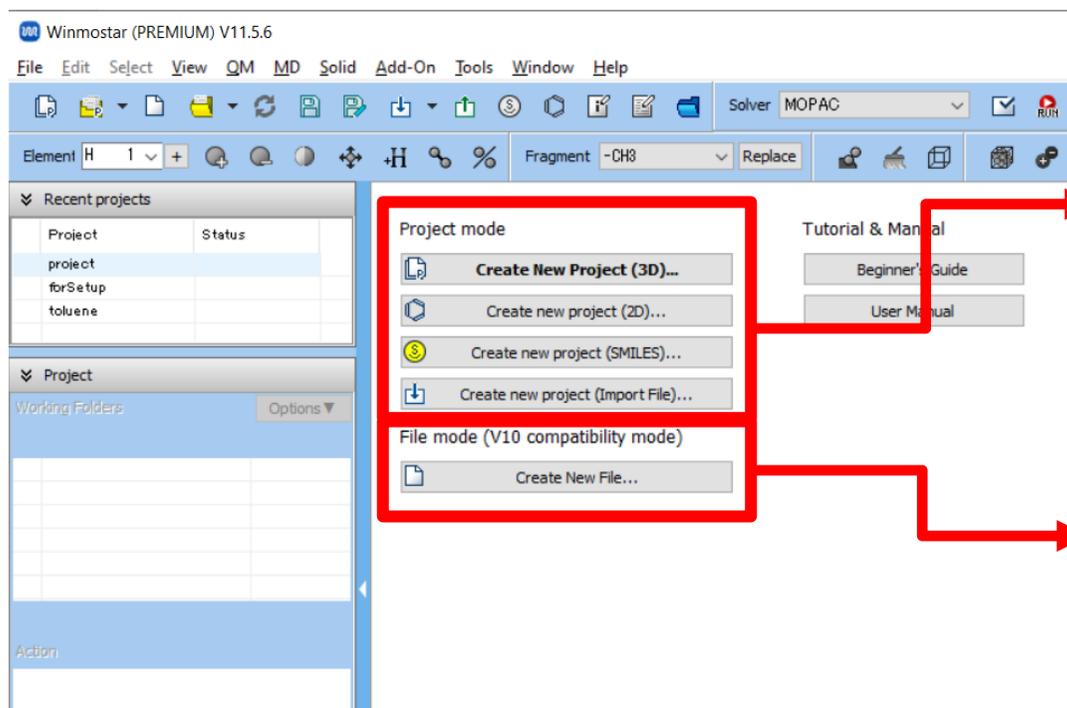
Acknowledgment: This material was created with reference to documents by Hiroshi Kihara, formerly of Toyama University.

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 [MOPAC 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.

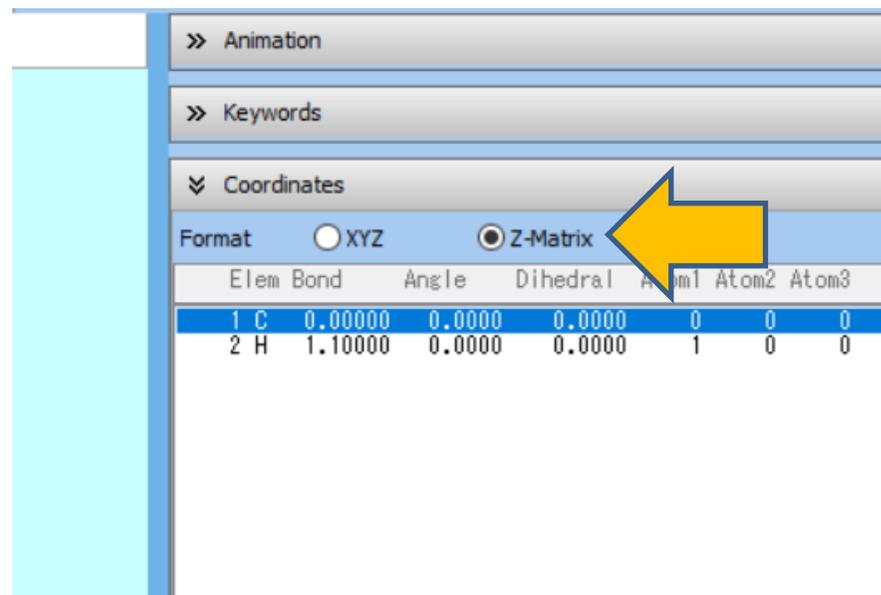
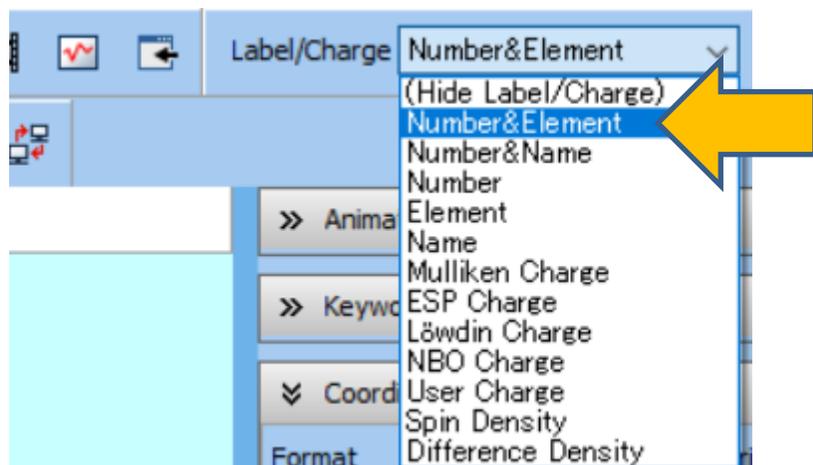
The operational procedure is the same as from V10 and earlier versions.

When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. Modeling of the System

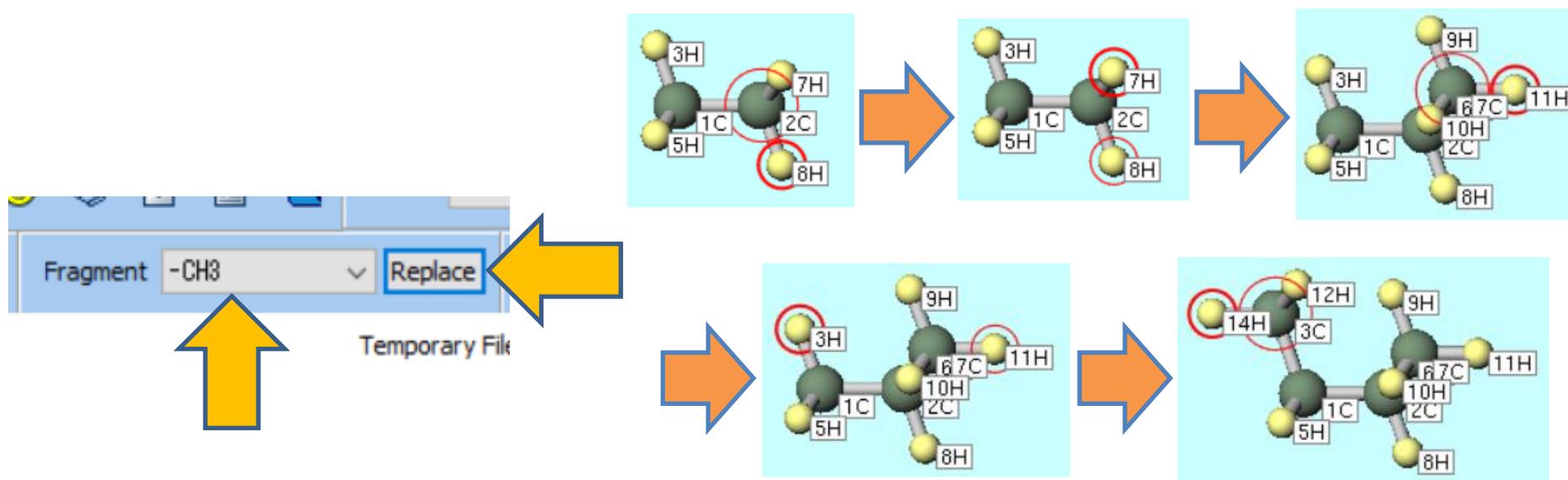
Please refer to [MOPAC Basics Tutorial](#) for basic operation methods.

- Click **File | New Project**, enter 'butane_mopac' as **Project name**, and click **Save**.
- From **Label/Charge** menu in the top right of Main Window, select 'Number&Element' to display the names of each atom in Viewport.
- Change **Format** in Coordinate Viewer to 'Z-Matrix'.



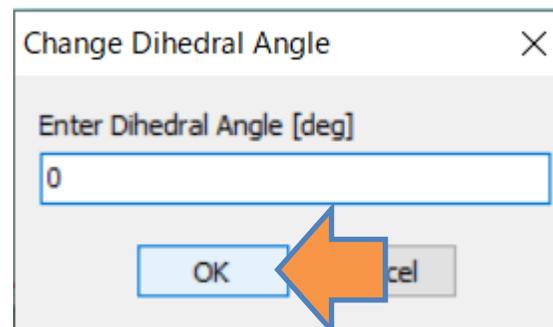
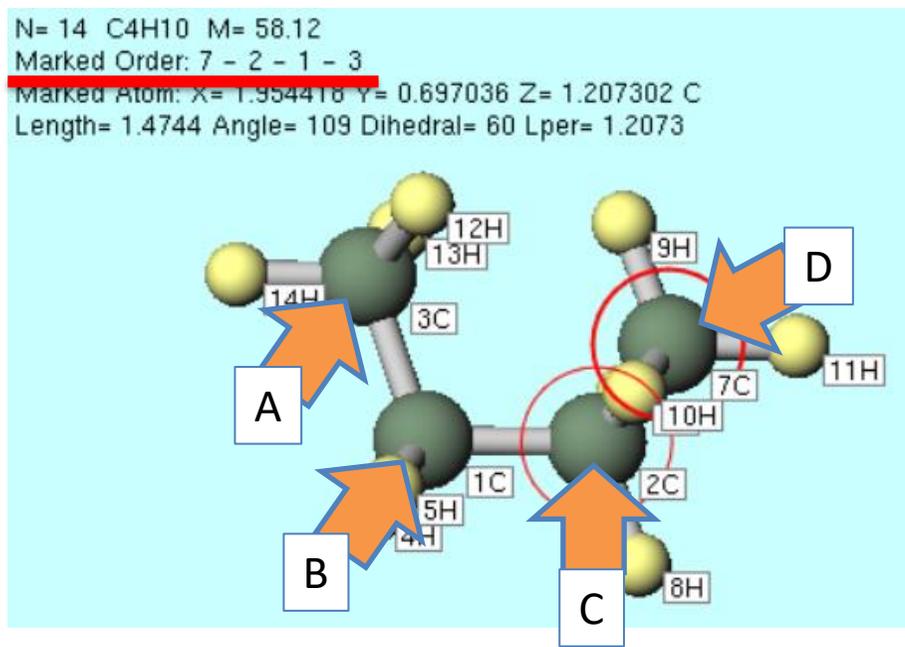
A. Modeling of the System

- Change **Fragment** to **-CH3** and then click **Replace** twice to create ethane.
- Click on the atom **7H** to highlight it with a thick red circle, and click **Replace** to convert it into propane.
- Further, click on the atom **3H** to highlight it with a thick red circle, and click **Replace** to convert it into butane.



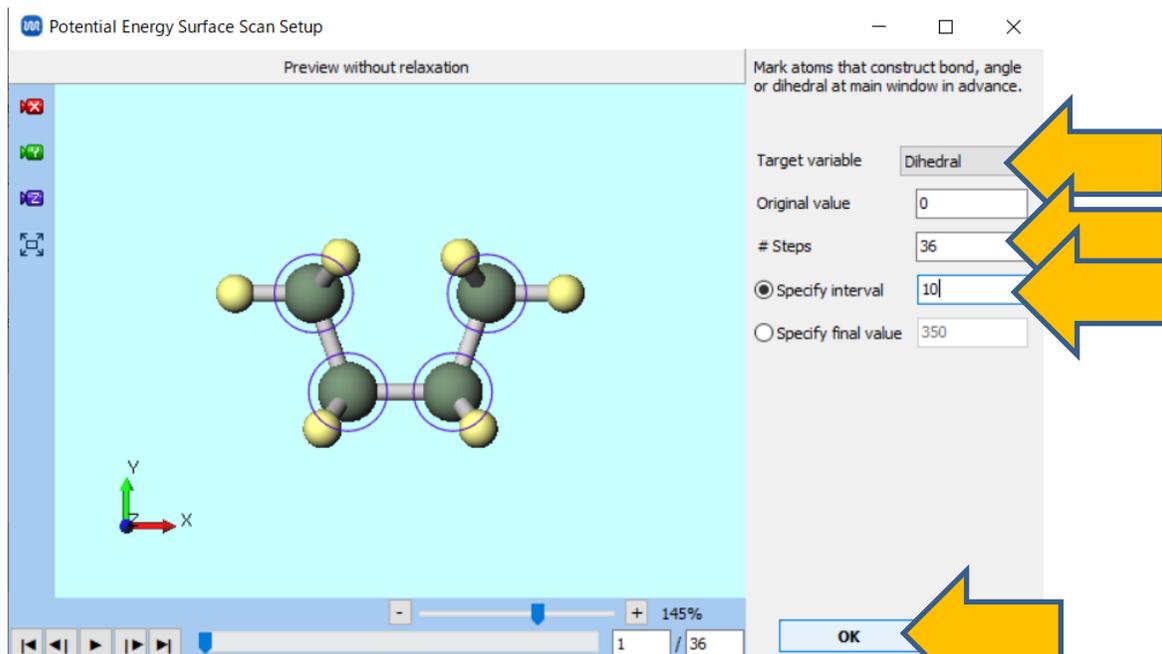
B. Execution of Calculate (Scan Calculation)

- Click on the main chain carbon atoms in the order of **3C**→**1C**→**2C**→**7C**, and verify that '7-2-1-3' is displayed in **Marked Order** at the top left of Viewport.
- Click **Edit | Change Distance/Angle of Marked Atoms | Dihedral**.
- In the dialog that appears, enter '0' and click OK. The dihedral angle of **3C-1C-2C-7C** becomes 0, and the scan will start from this position.



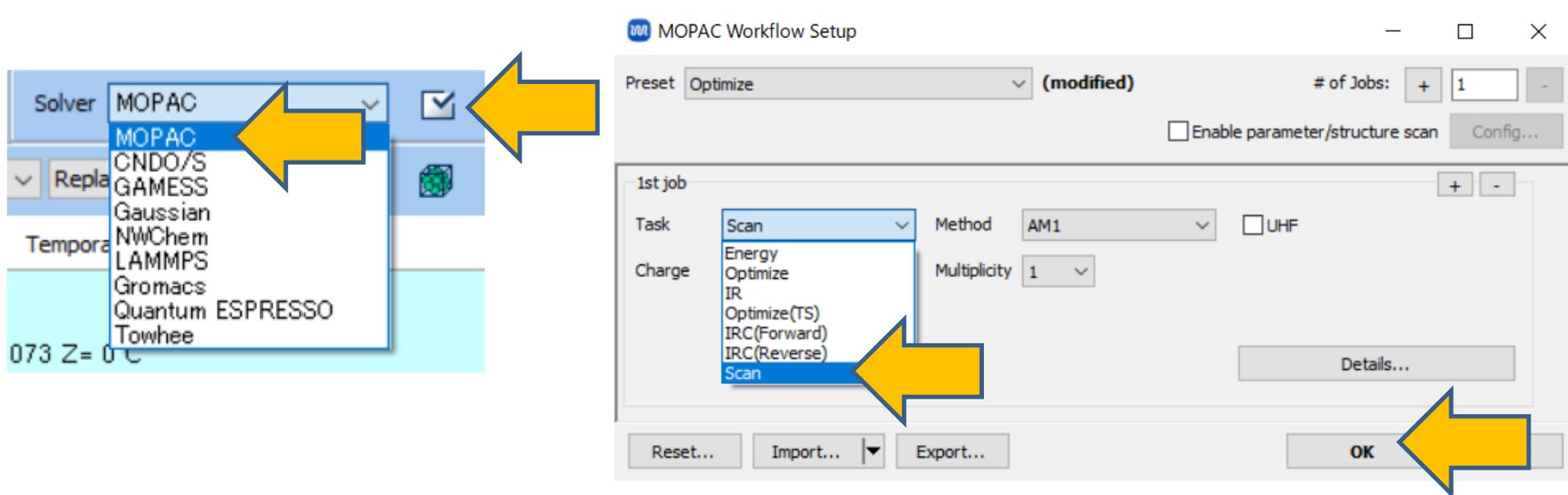
B. Execution of Calculate (Scan Calculation)

- Click **QM | MOPAC | Potential Energy Surface Scan | Setup**.
- In the window that appears, set **Target variable** to **Dihedral**, **# Steps** to **36**, **Specify interval** to **10**, and click OK. The dihedral angle of 3C-1C-2C-7C will be varied by 10° at a time, and structural optimization calculations will be performed 36 times, excluding this dihedral angle.
- Click **Yes** in the dialog that appears. Verify that '**PES Scan configured**' is displayed at the bottom of Viewport.



B. Execution of Calculate (Scan Calculation)

- Select **MOPAC** from **Solver** and click **Workflow Setup**.
- Change **Task** to 'Scan' and click **OK**.
- In **Job Setting** window, click **Run**.



C. Result Analysis (Scan Calculation)

- A. After the calculation is complete and the status of Working Folders **work1_MOP_SCAN** changes to **END**, click **work1_MOP_SCAN** folder and click **Animation** in **Action**.
- B. Verify that the energy changes from the Scan calculation are displayed in the graph in Animation Panel.

The screenshot displays the winmostar software interface. The central window shows the output file 'work1_MOP_SCAN Output File (mop_tmp.arc)' with the following details: N= 14 C4H10 M= 58.12, Marked Order: 14 - 1 - 0 - 0, Marked Atom: X= -0.380057 Y= -1.051092 Z= 0.00032 H, Length= 1.117693 Angle= * Dihedral= * Lper= *, and Constraints Found: 1 variables (Z-Matrix). A ball-and-stick model of the butane molecule is shown with atoms labeled 1C, 2C, 3C, 7C, 11H, 12H, 14H, 5H, and 8H. Two yellow arrows point to the 'work1_MOP_SCAN' folder in the 'Working Folders' panel and the 'Animation' action in the 'Action' panel.

The right-hand panel, titled 'Animation', is highlighted with a red border. It contains a list of energy values (KCAL) corresponding to different frames of the scan calculation:

Frame	Energy (KCAL)
.0000	-27.849308
10.0000	-28.010587
20.0000	-28.430344
30.0000	-28.983888

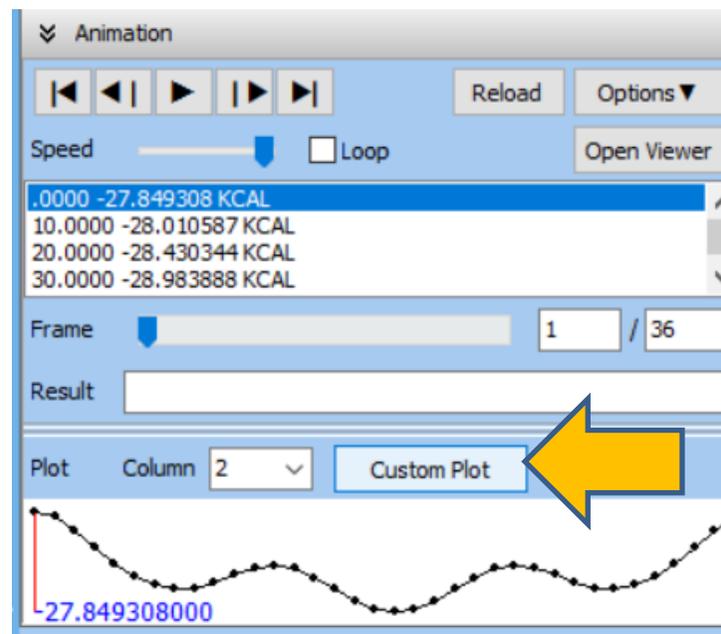
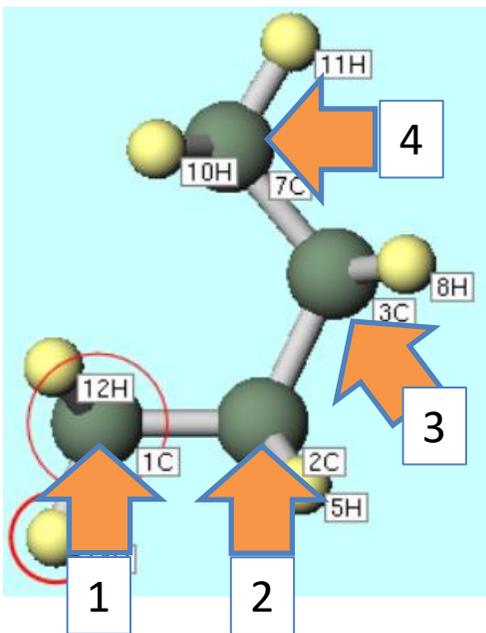
Below the list is a graph showing the energy profile over 36 frames. The energy starts at -27.849308000 and fluctuates, ending at -28.983888. The graph is labeled 'Plot Column 2' and 'Custom Plot'.

Below the graph is a table of coordinates in Z-Matrix format:

Elem	Bond	Angle	Dihedral	Atom1	Atom2	Atom3	
10	H	1.11662	111.0651	60.3261	7	3	2
11	H	1.11770	109.8767	179.9818	7	3	2
12	H	1.11662	111.0640	-60.3263	1	2	3
13	H	1.11662	111.0606	60.3643	1	2	3

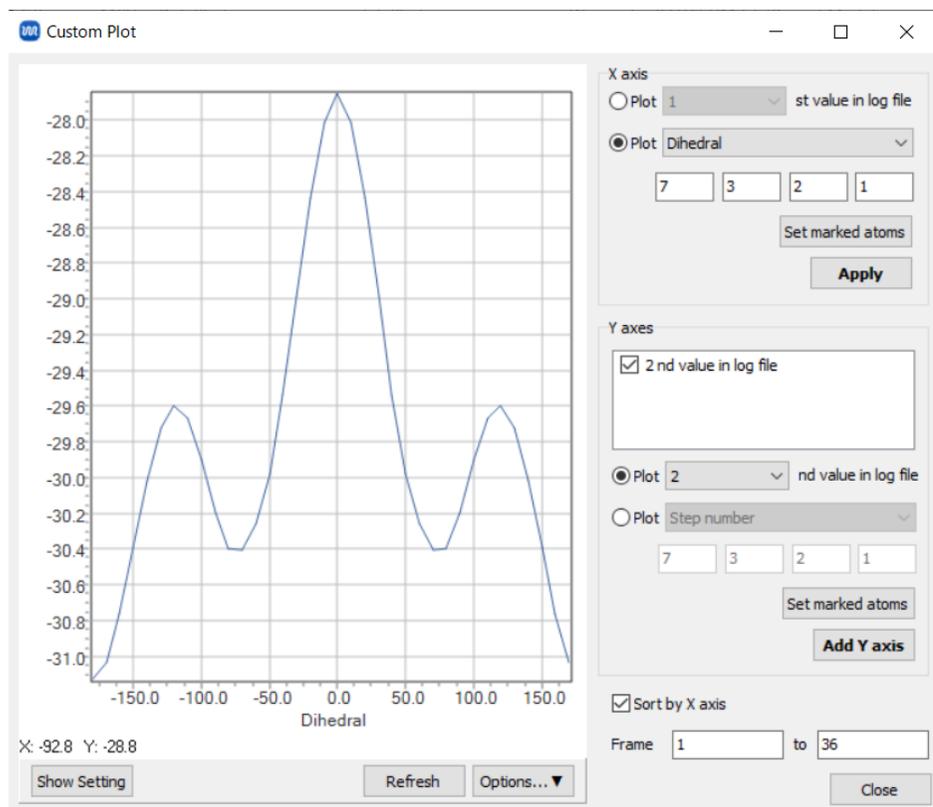
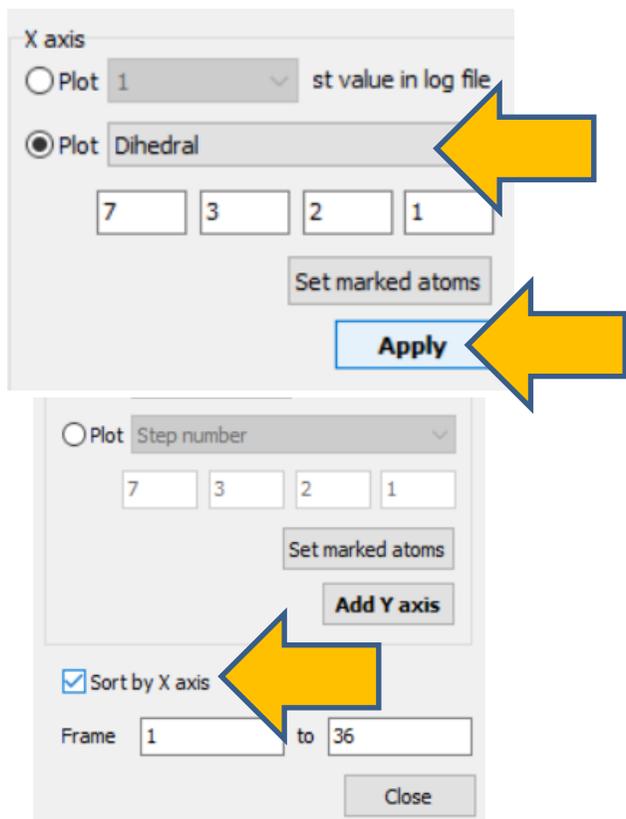
C. Result Analysis (Scan Calculation)

- Click the main chain carbon atoms in the order of **1C**→**2C**→**3C**→**7C**.
- Click on **Custom Plot** in Animation Panel.



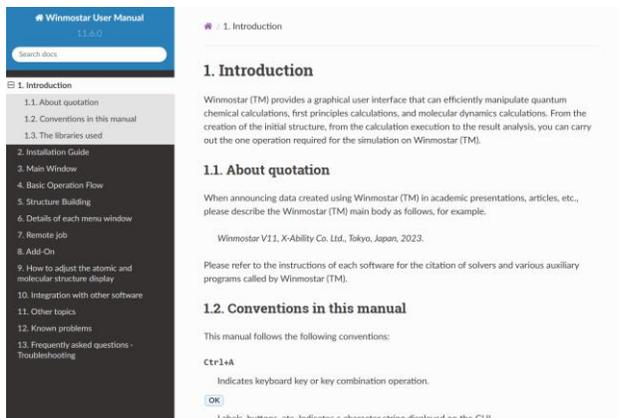
C. Result Analysis (Scan Calculation)

- In **Custom Plot** window, change **Plot** of **X axis** from **Step number** to **Dihedral** and click **Apply**.
- If **Sort by X axis** is displayed at the bottom right of the window, check it.
- A graph of energy as a function of the scanned dihedral angle 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.)
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