winmostar tutorial

CNDO/S Basic

V11.5.6

12 November, 2024 X-Ability Co., Ltd.

About This Document

- 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.
- 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 from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

- After Structural Optimization of the Indigo Molecule Using MOPAC, Calculating the UV-Vis Spectrum with CNDO/S.

Procedure Overview:

A. System Modeling

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B. Execution of Calculation
MOPAC Structural Optimization → CNDO/S
UV-Vis Calculation

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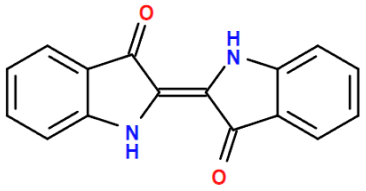
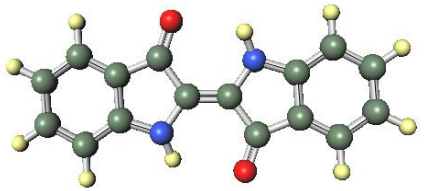
C. Results Analysis
UV-Vis Spectrum

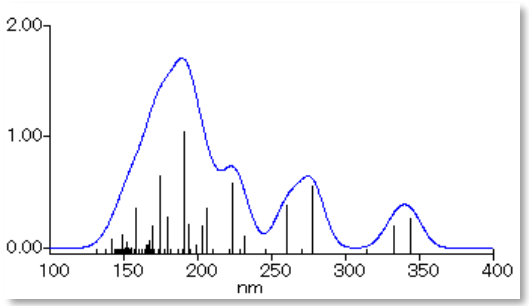


(Structural Formula)



(3D Structure)

Indigo Molecule

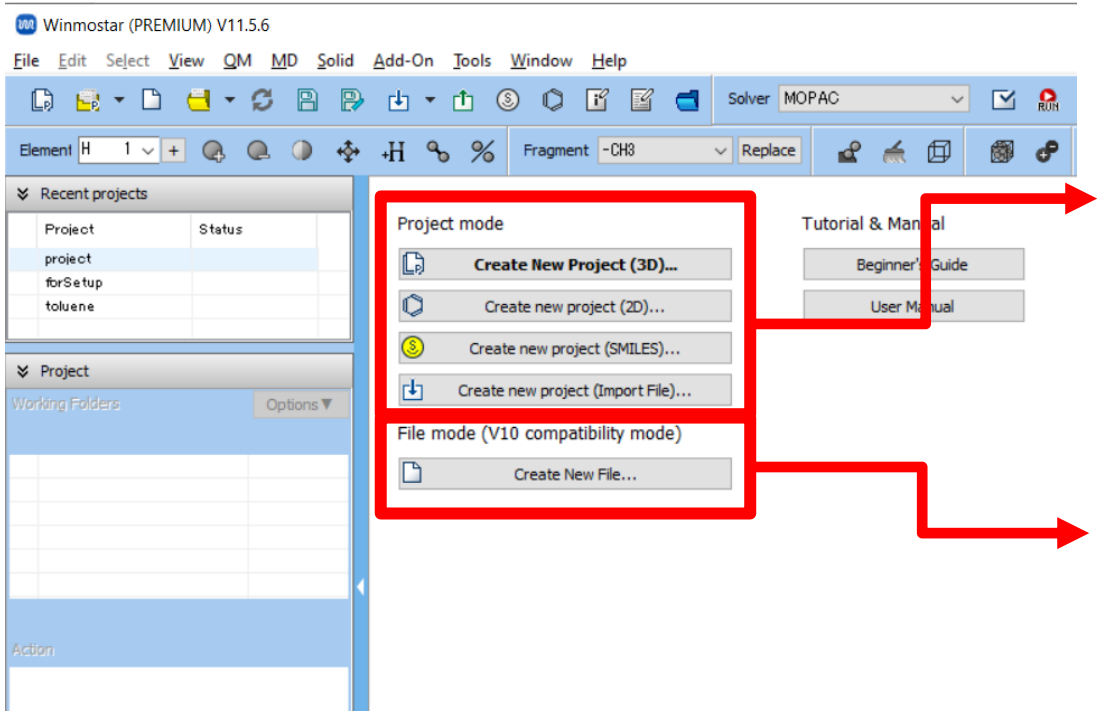


Note:

- Semi-empirical molecular orbital methods that introduce approximations to the Hartree-Fock method can be calculated rapidly, but they may differ from experimental values, both quantitatively and, in some cases, qualitatively.
- If higher accuracy calculations are desired, please refer to the introductory tutorials for GAMESS, Gaussian, and NWChem.

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 CNDO/S tutorial for V10.



Project Mode New Features in V11

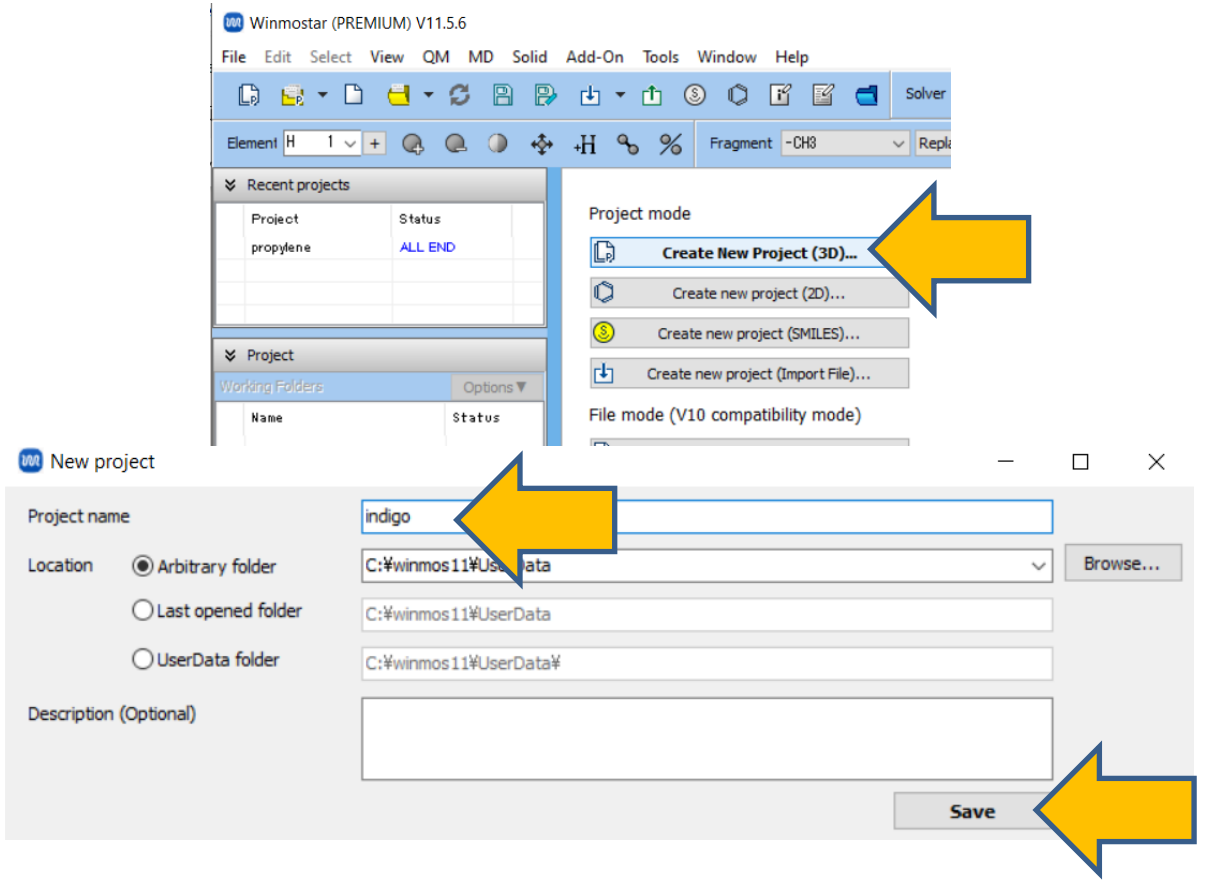
Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. System Modeling

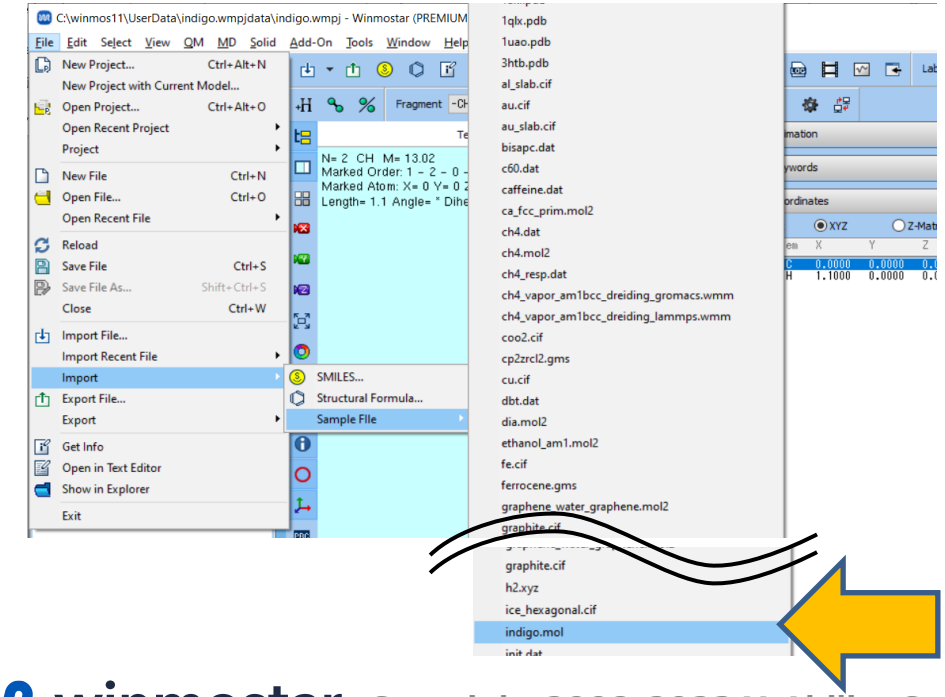
A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File** | **Close**.
B. Enter '`indigo`' for **Project name** and click **Save**.

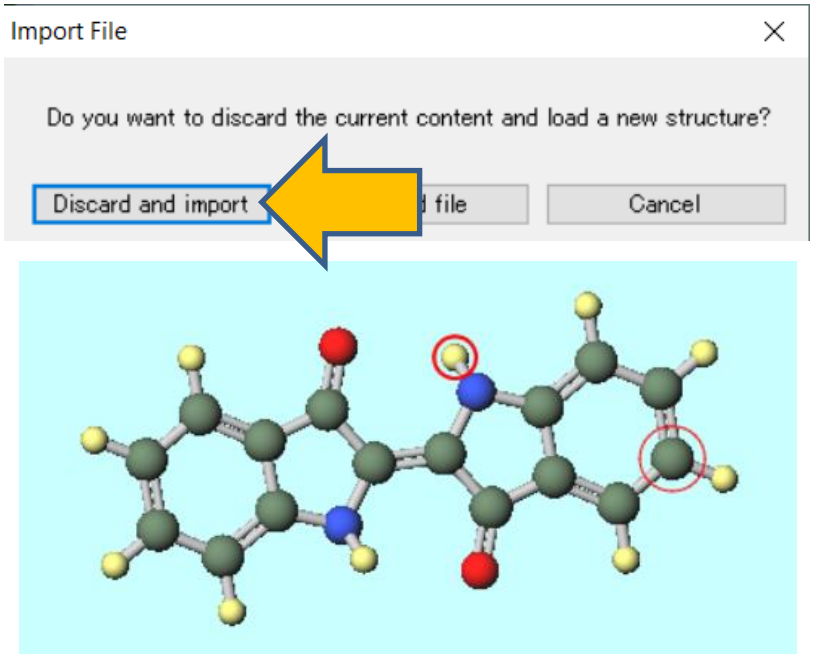


A. System Modeling

For details on creating an initial structure, please refer to Molecular Modeling Organic Molecules Tutorial.
In this section, we will load an existing molecular structure file.

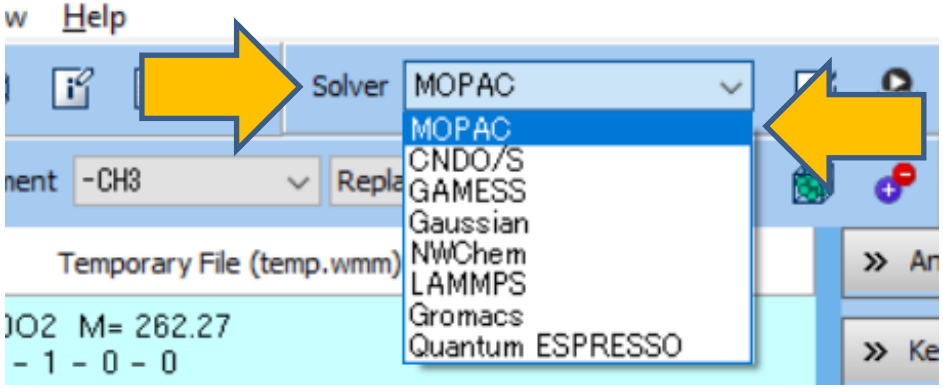
A. Click **File** | **Import** | **Sample File** |**indigo.mol**.
   -If you wish to load a different file at this stage, use **File** | **Import File** instead.
B. In **Import File** dialog, click **Discard and import**.
C. Verify that the desired molecule appears in Viewport.

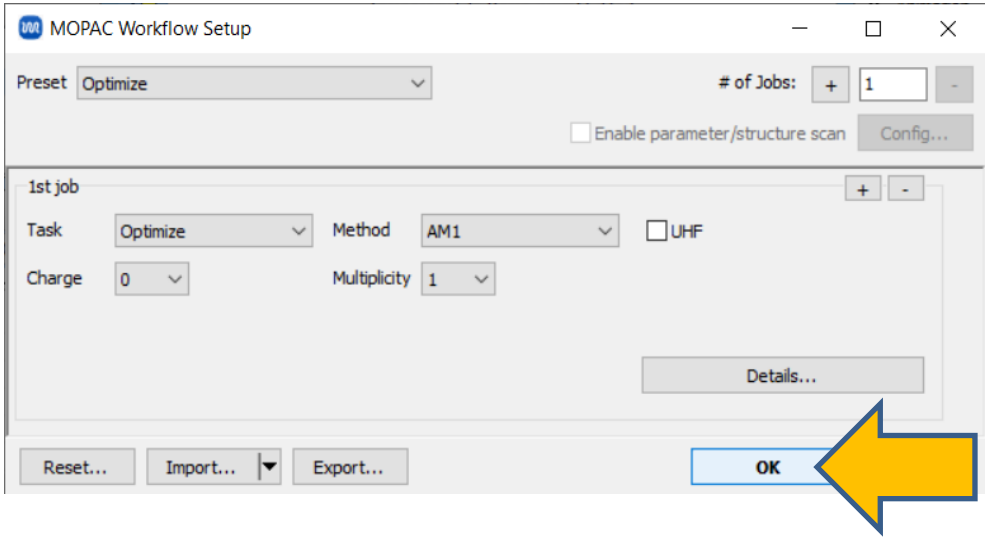




B. Execution of Calculation (MOPAC Structural Optimization Calculation)

A. Select **MOPAC** from Toolbar's **Solver**.
B. Click **Workflow Setup**.
C. Click **OK** at the bottom right of **MOPAC Workflow Setup** window.
D. In **Job Setting** window, click **Run**.

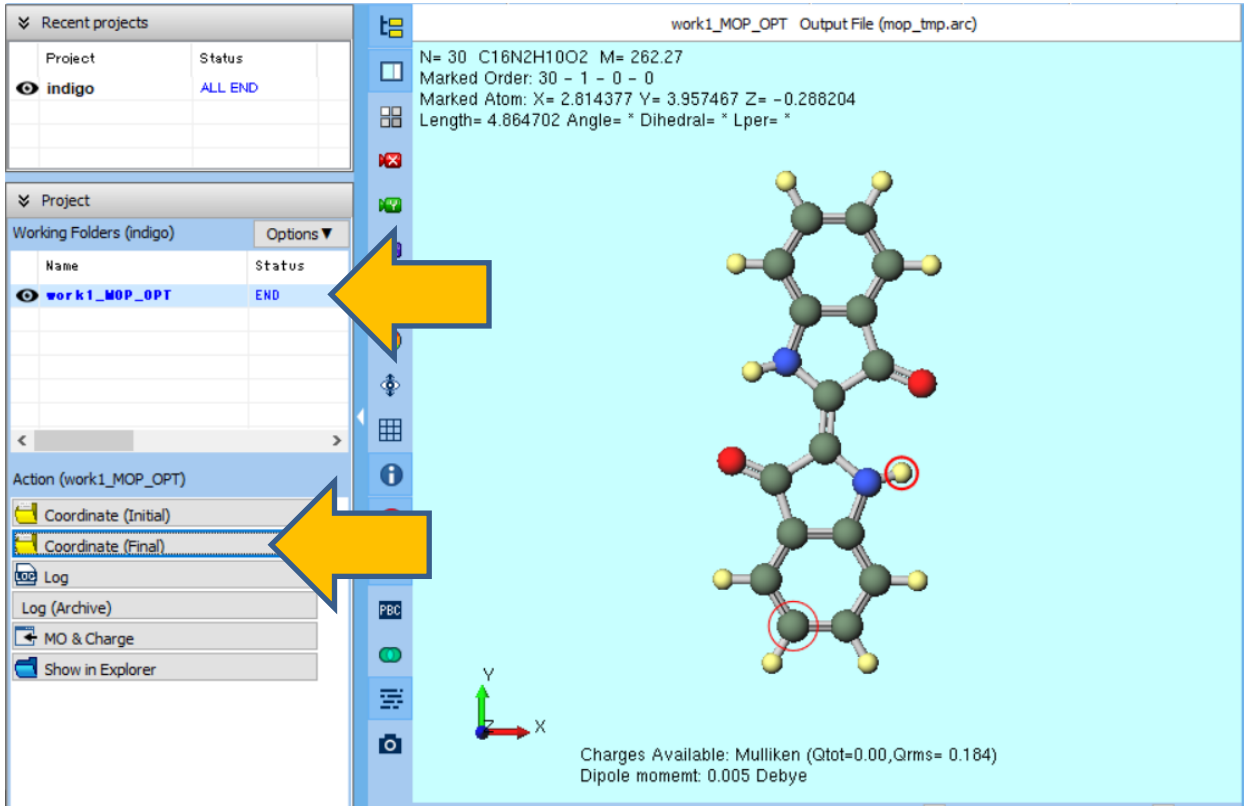




B. Execution of Calculation (MOPAC Structural Optimization Calculation)

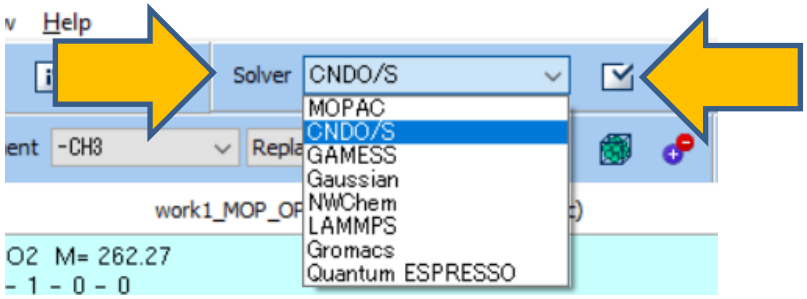
A. In Project Area, once **the status** of work1_MOP_OPT in **Working Folders** changes to **END**, click on work1_MOP_OPT in **Working Folders**, and then click on **Coordinate (Final)** under **Action**.

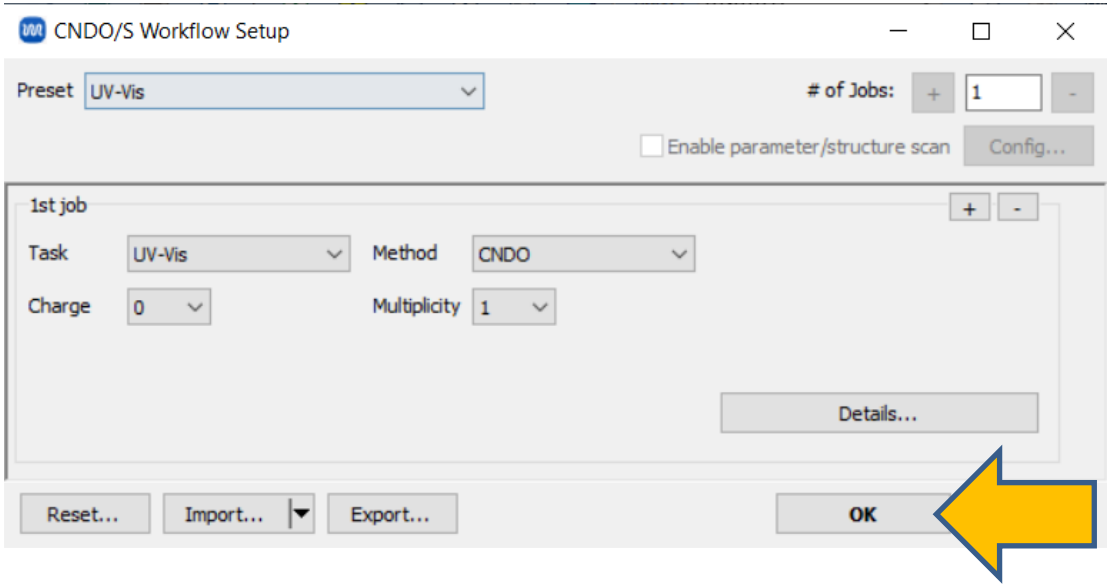
B. Verify that the structure after optimization is displayed in Viewport.



C. Execution of Calculation (CNDO/S Calculation)

A. Select **CNDO/S** from Toolbar's **Solver**.
B. Click **Workflow Setup**.
C. Click **OK** at the bottom right of **CNDO/S Workflow Setup** window.
D. In **Job Setting** window, click **Run**.

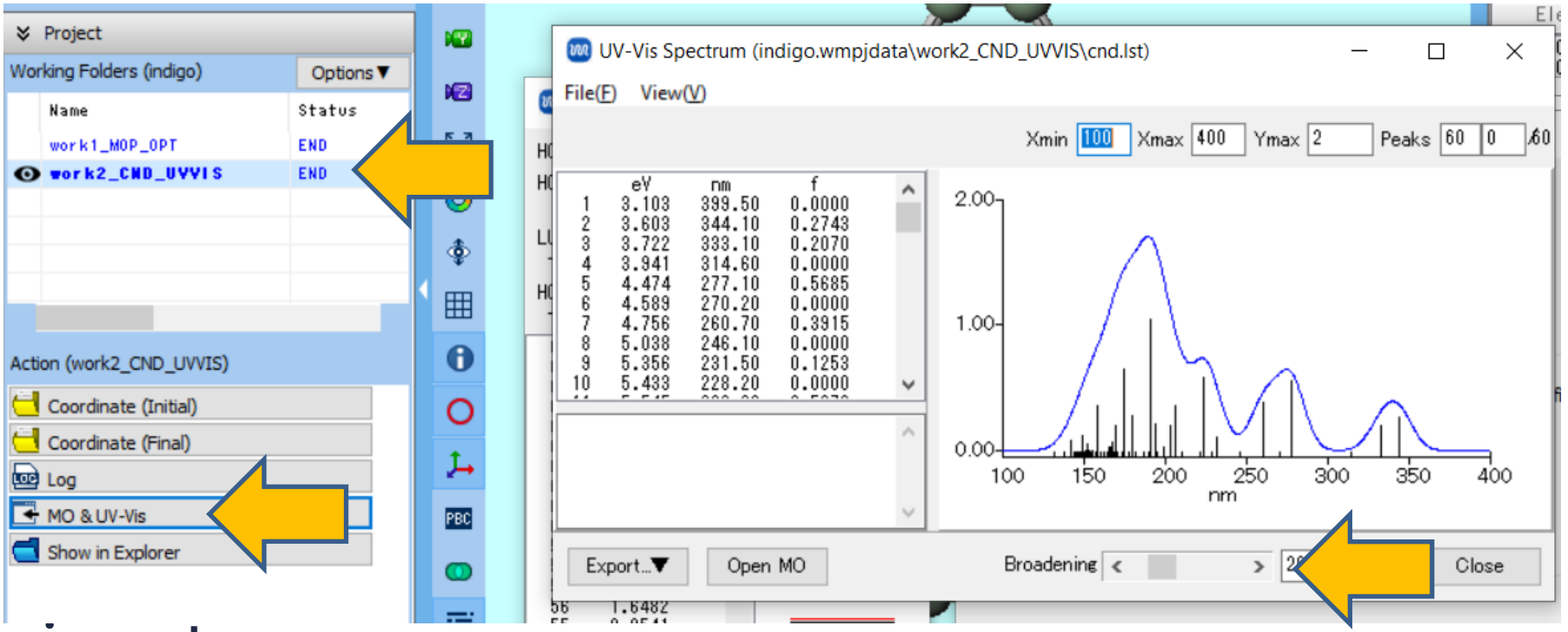




D. Results Analysis

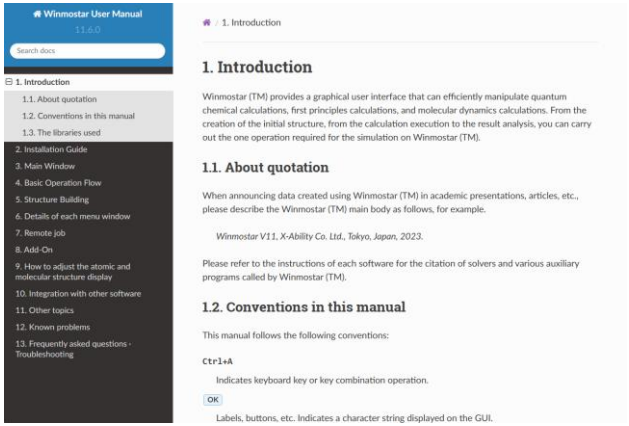
A. In Project Area, once **the status** of work2_CND_UVVIS in **Working Folders** changes to **END**, click on work2_CND_UVVIS in **Working Folders**, and then click on **MO & UV-Vis** under **Action**.

B. CNDO/S UV-Vis Spectrum window appears, displaying each peak's excitation energy (**eV**), wavelength (**nm**), and oscillator strength (**f**). You can modify the width of the blue curve spectrum by moving **Broadening** scrollbar.



Troubleshooting and Additional Resources

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



Winmostar User Manual

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