

PyMOL is a molecular visualization software widely used to create 3D representations of molecular structures, analyze protein complexes, and visualize macromolecular interactions. PyMOL was first developed in 2000 by Warren DeLano, an American scientist and entrepreneur as an open-source project. Schrodinger acquired PyMOL from Warren DeLano in 2006. Today, Schrödinger offers Educational-use-only PyMOL builds available at no cost for academics.

Installation of PyMOL

▪ **For Mac Users – Method 01**

1. Visit <https://pymol.org/2/> and download the DMG disk image file
2. Once downloaded, double-click on *.dmg file and drag PyMOL icon to Applications folder

▪ **For Mac Users – Method 02 via terminal**

1. Install Homebrew, the default package manager for MacOS : `/bin/bash -c "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/HEAD/install.sh)"`
Requires the Bourne-again (Bash) shell for installation.
To switch to Bash shell: <https://www.howtogeek.com/444596/how-to-change-the-default-shell-to-bash-in-macos-catalina>
2. Install PyMOL : `brew install pymol`

▪ **For Windows Users**

1. Visit <https://pymol.org/2/> and download the exe file for windows
2. Once downloaded, execute the .exe installer and follow the setup wizard

▪ **For Linux Users**

1. Unpack the .tar.bz2 file: `tar -jxf PyMOL-2.2.0_0-Linux-x86_64.tar.bz2`
2. Run PyMOL: `cd pymol; ./pymol`

▪ **With existing Anaconda installation**

1. Update conda package manager to the latest version:
<https://docs.anaconda.com/free/anaconda/install/update-version/>
2. Install PyMOL: `conda install -c schrodinger -c conda-forge pymol`

▪ **License Installation**

1. Visit <https://pymol.org/edu/> and fill in your details
2. An email containing the link to the license file will be sent to you shortly. Use it to register when prompted in PyMOL.

PyMOL Molecular Visualizing Tutorials

- Beginner Tutorial: <https://dasher.wustl.edu/bio5357/software/pymol/simple-tutorial.pdf>
- Visualizing: https://www.youtube.com/playlist?list=PL4eF1KHNgDfLKD96SJB_1_luSjvVr9RV1
- Manipulating a section of a protein: <https://youtu.be/wiKyOF-pGw4?si=IGRfbqjzawiZaHl>
- Mutagenesis: https://youtu.be/M-VCBz83nfs?si=U1FeMHWoyu_zSS-X