Table of Contents

BlendMol 1.0

BlendMol 1.0 is a Blender plugin that can easily import VMD "Visualization State" and PyMOL "Session" files. It interfaces directly with the VMD or PyMOL executable to 1) normalize the VMD/PyMOL camera position, 2) render molecular meshes to Blender-compatible files, 3) import those files into Blender, and 4) optimize mesh geometries as needed.

One can also work entirely within Blender, without ever opening a dedicated molecular-visualization program. If the user provides a PDB ID or a PDB file, the plugin uses VMD or PyMOL to automatically generate a simple, default visualization.

BlendMol empowers scientific researchers and artists by marrying molecular visualization and industry-standard rendering techniques. The plugin works seamlessly with popular analysis programs (i.e., VMD/PyMOL). Users import into Blender the very molecular representations they set up in VMD/PyMOL.

The Latest Version

To view the source code of the latest version, visit http://git.durrantlab.com/jdurrant/blendmol.

Visit http://durrantlab.com/blendmol/ to:

- read the documentation
- suggest an improvement
- point out a bug
- ask a question about usage

Authors and Contacts

BlendMol was created by Jacob Durrant (durrantj@pitt.edu).

Installation

Quick Start

BlendMol installation within Blender is the same as with any Blender plugin:

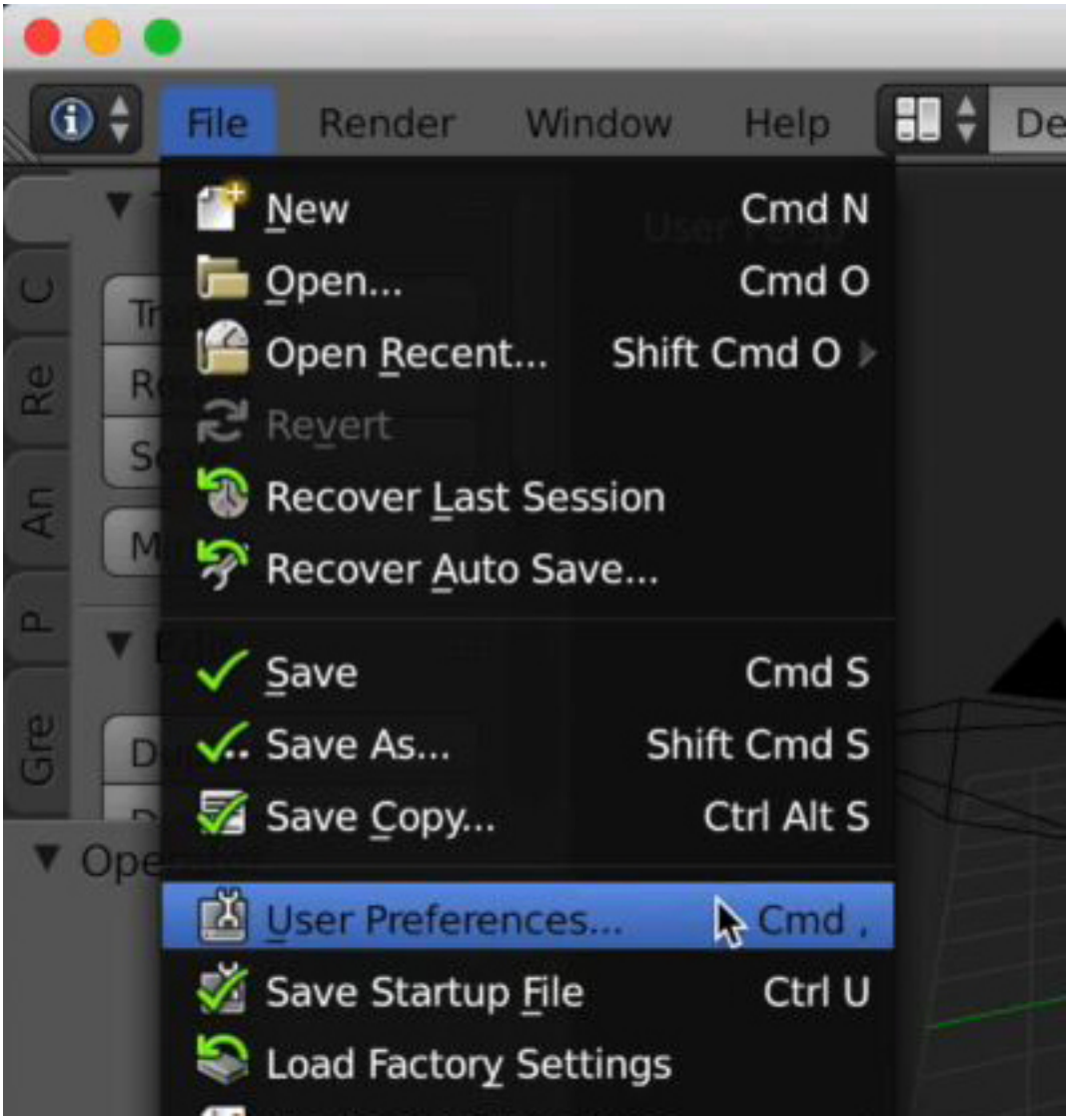
1. Visit http://durrantlab.com/blendmol/ to download the BlendMol ZIP file.
2. Within Blender, click on the `File > User Preferences...` menu item to open the `Blender User Preferences` window.
3. Click the `Add-ons` button at the top of that window to open the add-ons panel.
4. Specify the location of the downloaded ZIP file by clicking on the `Install Add-on from File...` button at the bottom of the window.
5. Once installed, click the `Import-Export: BlendMol - PDB/VMD/PyMOL` checkbox to activate the plugin.

6. To keep the plugin active after Blender restarts, click the `Save User Settings` button at the bottom of the window.
7. Critical plugin preferences can be set from the Add-ons panel by clicking the expanding carat. See the BlendMol manuscript for full details.

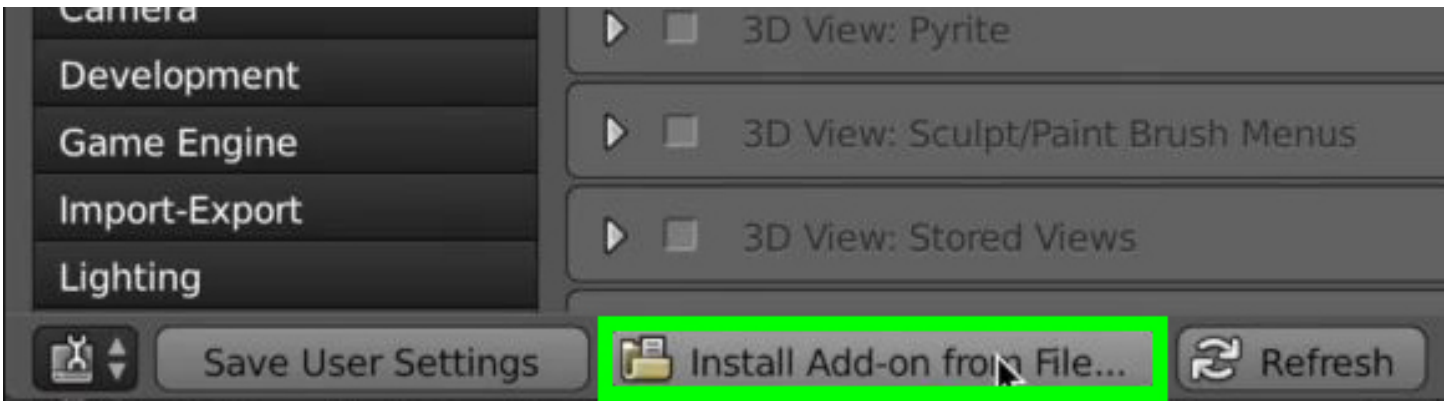
Detailed Installation Instructions

Download the BlendMol plugin.

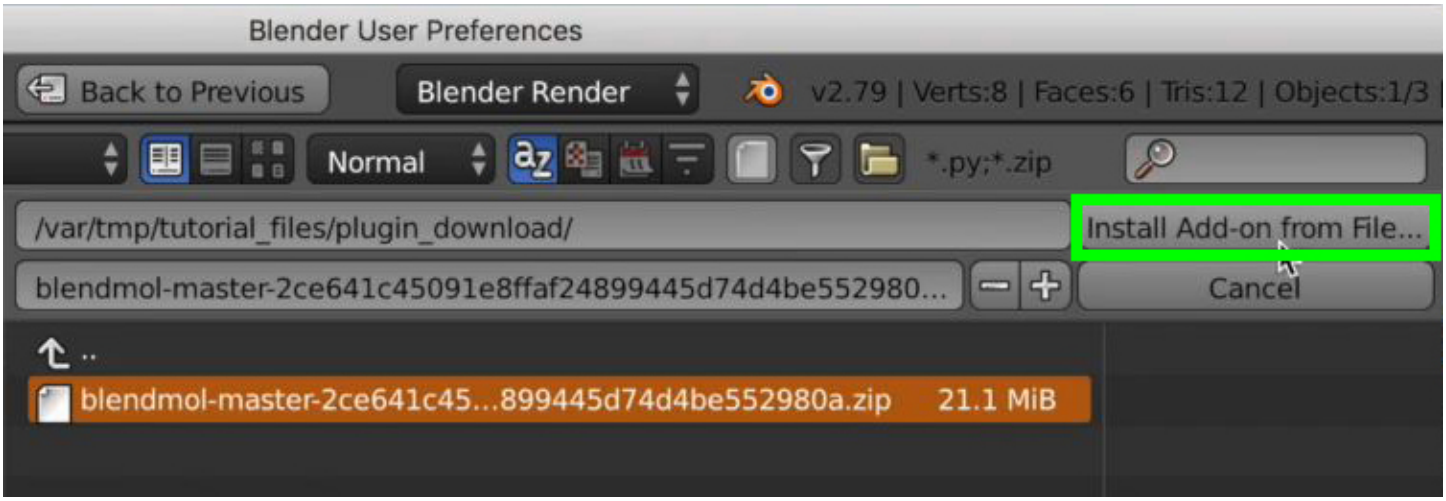
Click `File -> User Preferences...` to install the plugin.



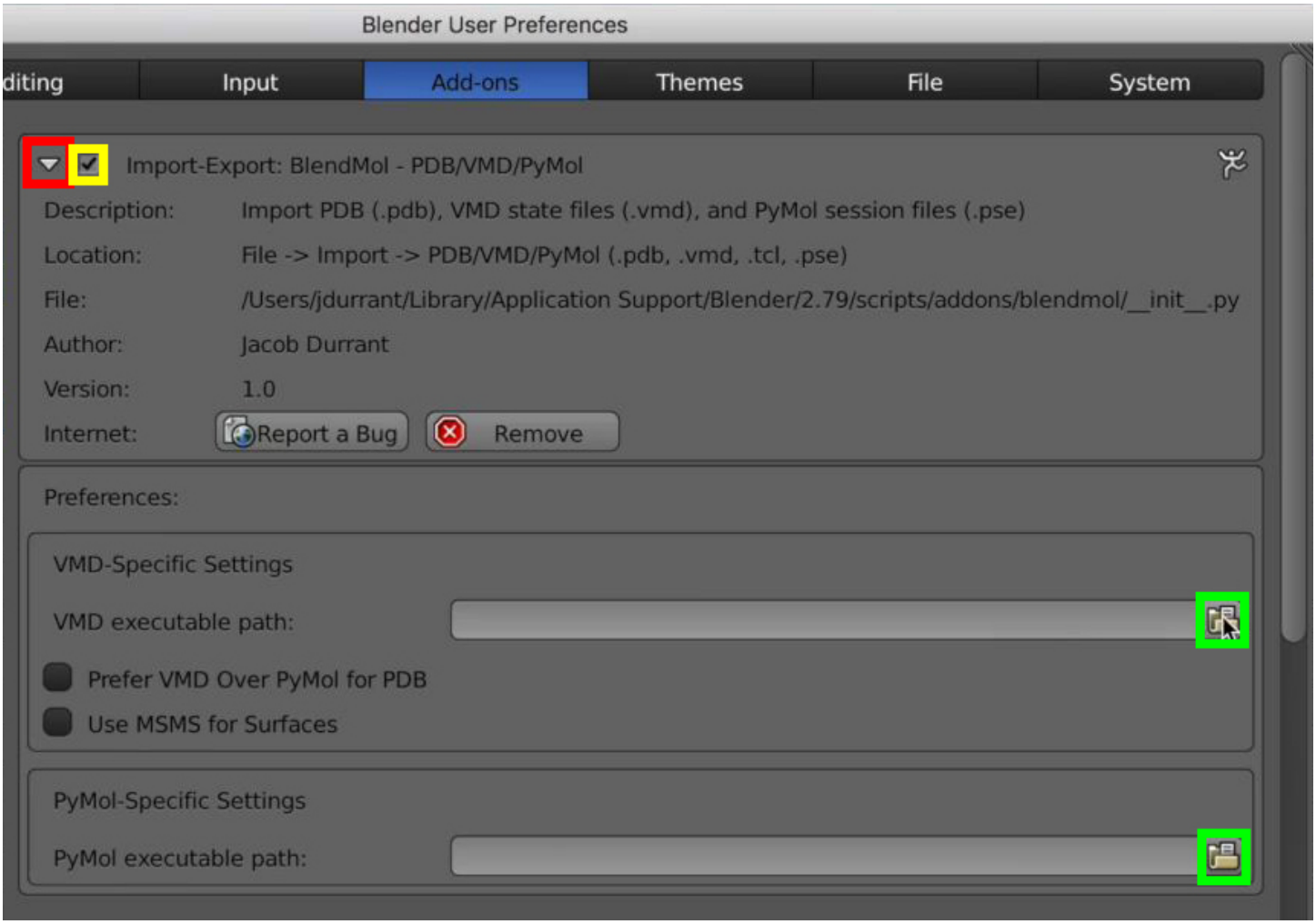
Click the `Install Add-on from File...` button.



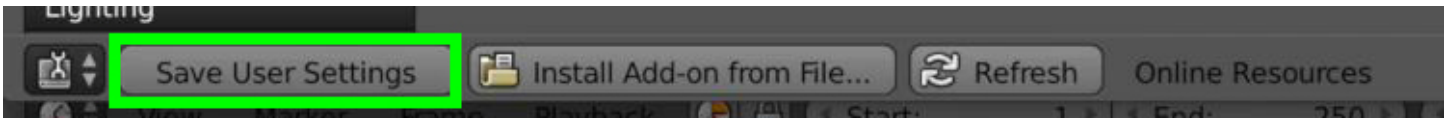
Select the BlendMol ZIP file and click the `Install Add-on from File...` button.



Tick the checkbox (yellow) to activate the plugin. Then click the down caret button (red) to show the plugin options. Specify the location of the VMD and PyMol executables using the appropriate buttons (green).



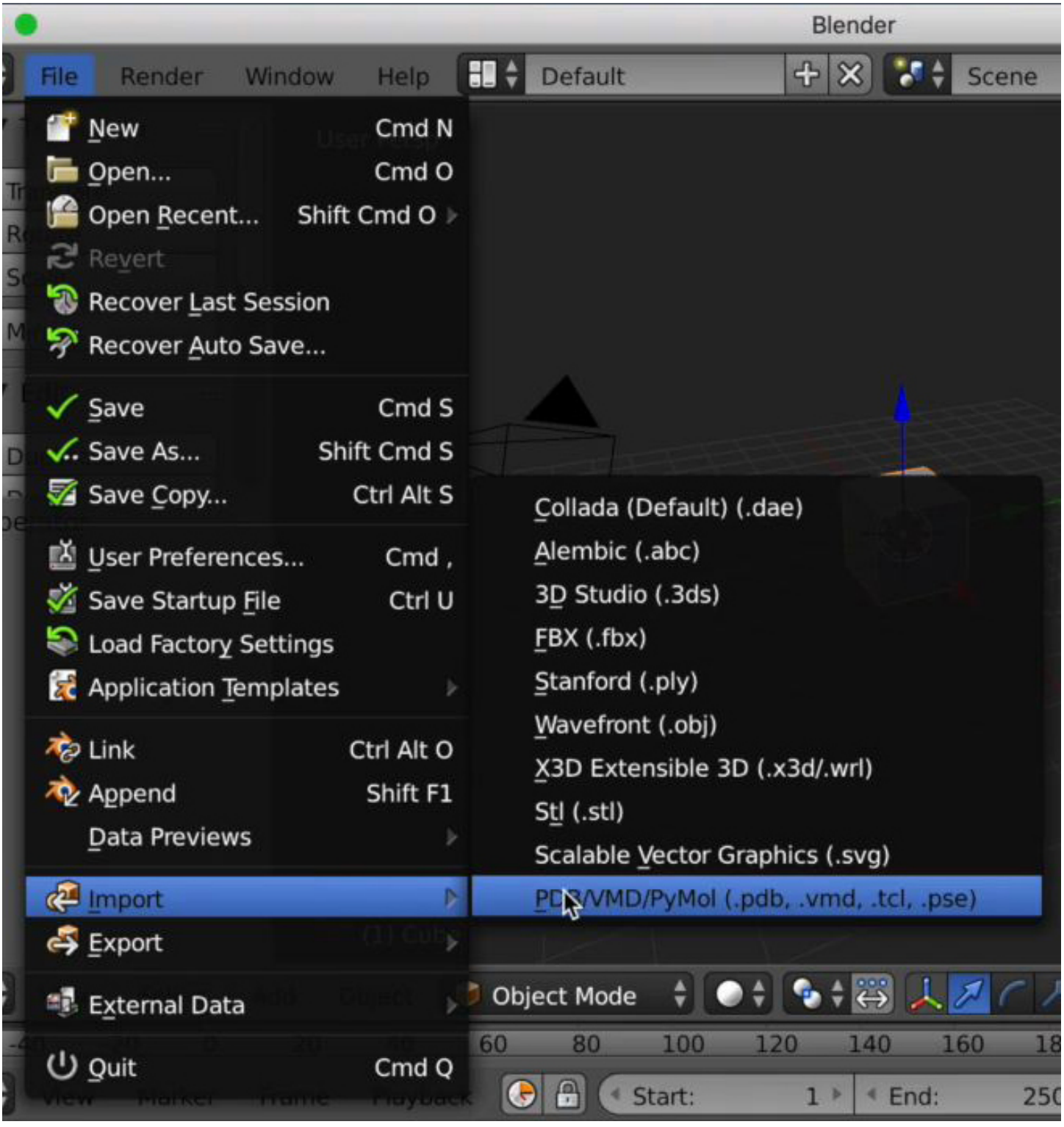
If you would like BlendMol to auto load when you restart Blender, click the `Save User Settings` button.



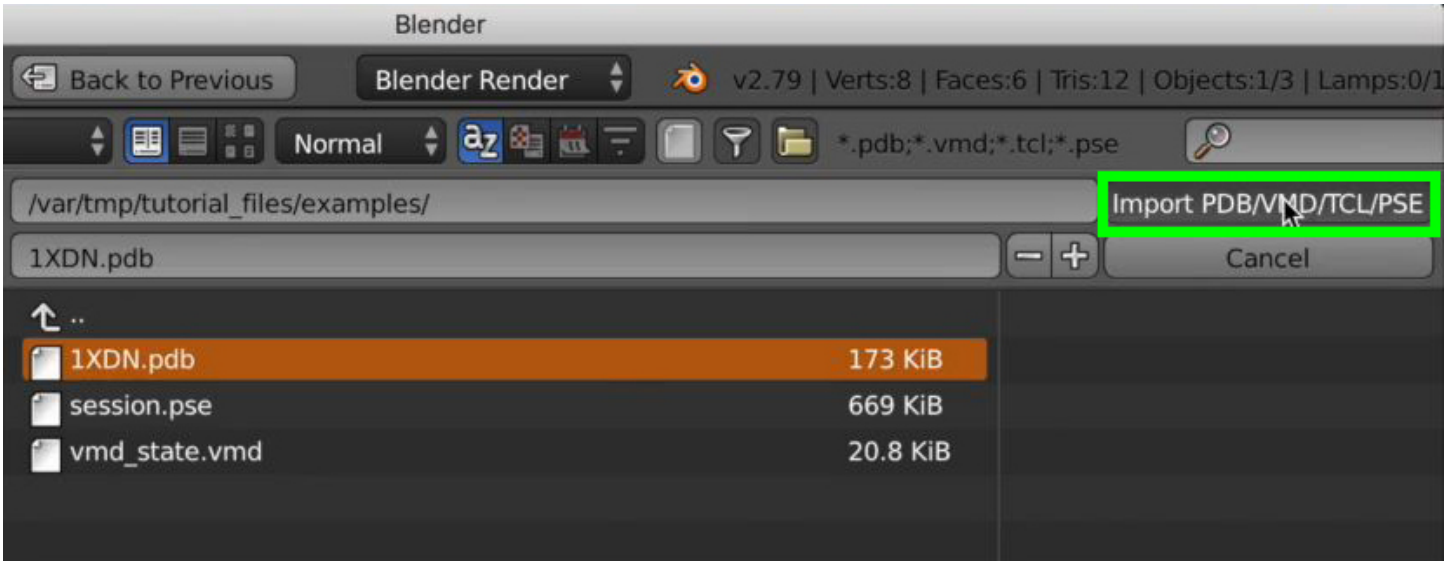
BlendMol Usage

Basic Usage

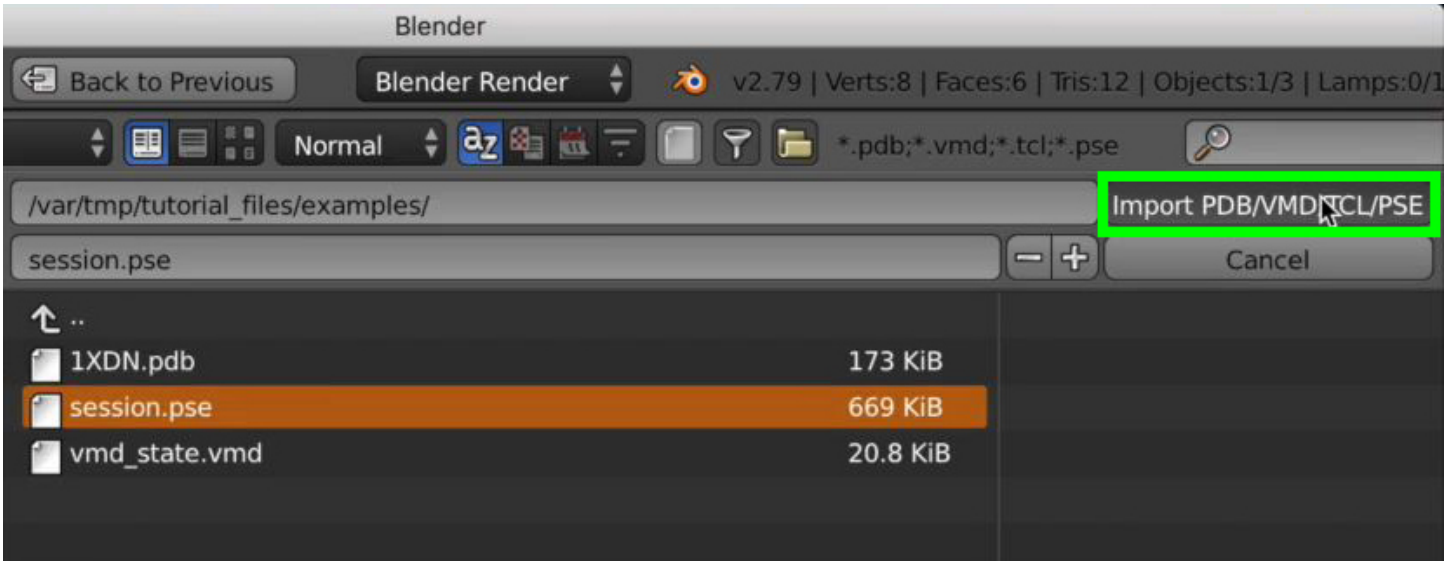
Click `File -> Import -> PDB/VMD/PyMol (.pdb, .vmd, .tcl, .pse)`.

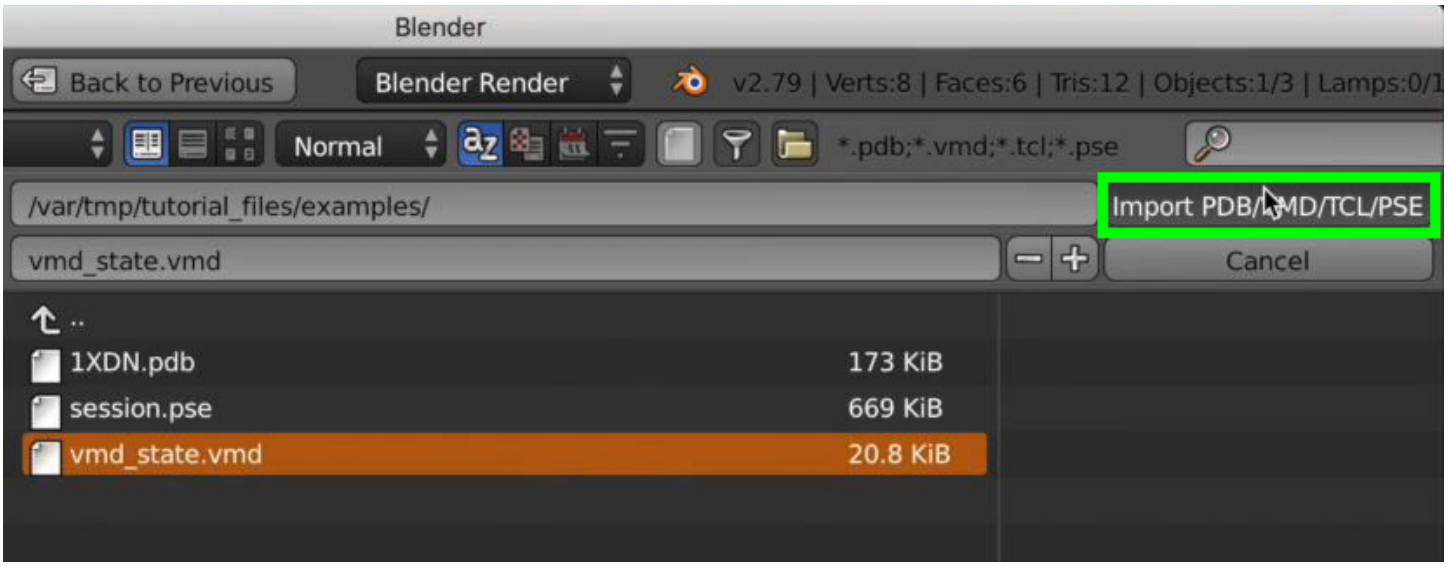


To load a PDB file, select the filename. Additional options (not shown) are given in a panel to the left. When ready, press the `Import PDB/VMD/TCL/PSE` button.

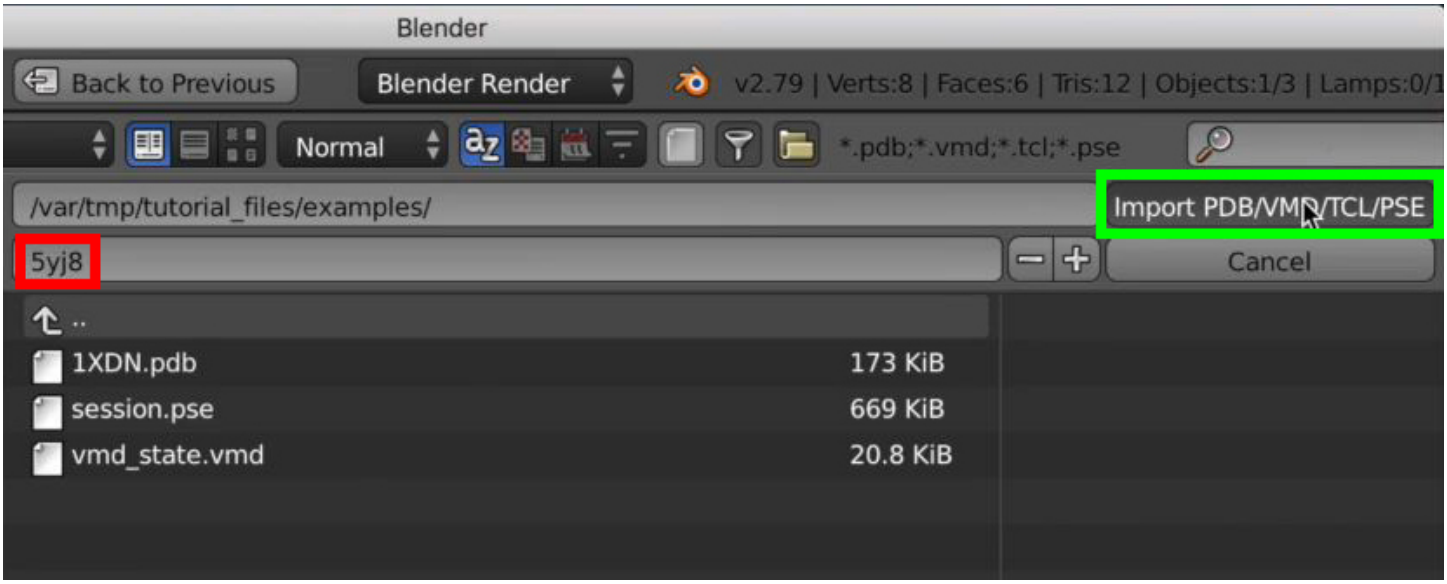


PyMol session files and VMD state files can be similarly loaded.





You can also type a PDB ID into the filename field (boxed in red). BlendMol will download the PDB model directly from the Protein Data Bank.



Advanced Usage

Video S2: Neuraminidase

Creating Video S2 required the use of many advanced Blender features that are unrelated to BlendMol's core functionality. A detailed tutorial is beyond the scope of this document, but interested users may benefit from the Blender Guru channel on YouTube, which provides many useful tutorials.

Video S3: BlendMol/Pyrite

Coupling BlendMol and Pyrite, another Durrant-lab plugin, simplifies the Blender-based visualization of molecular dynamics simulations.

Example Files

Example files can be found in `./examples/`.

- `./examples/vmd-files/` includes a PDB and VMD state file.
- `./examples/pymol-files/` includes a PyMOL session file.
- `./examples/web-files/baked-lighting-shadows/` demonstrates browser-based molecular visualization with advanced lighting and shadows.
- `./examples/web-files/virtual-reality/` demonstrates browser-based virtual-reality molecular visualization.