

3D Printing a Model Designed in Jmol

Part of the Jmol Training Guide from the MSOE Center for BioMolecular Modeling

Interactive version available at <http://cbm.msoe.edu/teachingResources/jmol/jmolTraining/3dprinting.html>

Introduction

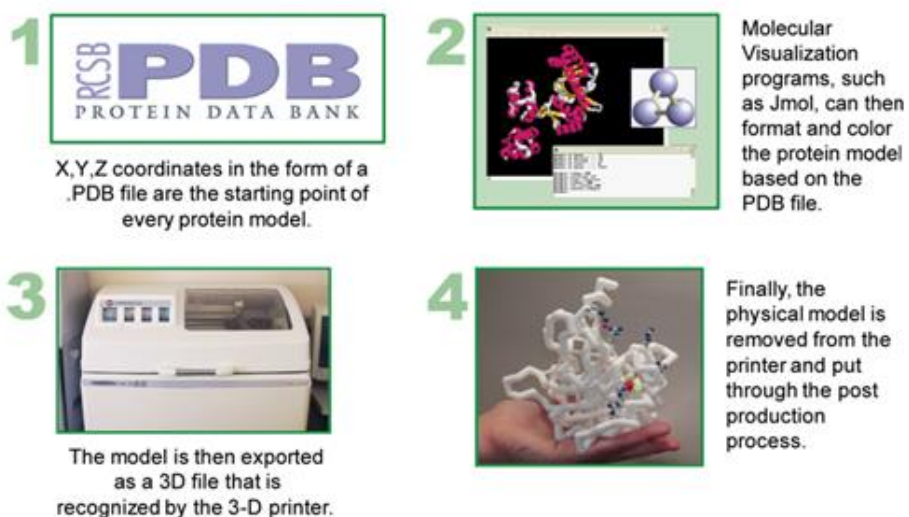
Jmol is an excellent program for designing **molecular illustrations** and is incredibly powerful even when simply generating static images. If you take Jmol further, you can also use it to make fully interactive displays and even **dynamic web pages**.

At the MSOE Center for BioMolecular Modeling, however, the most fascinating final product that Jmol can produce is a **3D printed physical model!** A physical model can make the abstract molecular world real and tangible. Proteins are complex 3-dimensional structures and so logically the most relatable way to communicate their features are with physical sculptures.

What is 3D Printing?

3D Printing is a cutting edge technology that can use stacked serial planes to build physical 3-dimensional models from any computer generated 3D file. Every physical protein model will go through four key steps:

The end result of this process is a designed and printed protein model will be an exact replica of the model created in the 3D visualization program.



At the MSOE Center for BioMolecular Modeling, we use two industrial grade **3D Systems Z-Corporation Printers**, as well as a number of lower cost tabletop printers like the **Stratysus Mojo** and **Makerbot** printers.

There are more types of 3D printers on the market than we will ever be able to discuss here, each with their own strengths and weaknesses.

It is fair to say that the technology continues to expand, improve and spread - especially in education.



Standard Sizes and Formats

There are an almost limitless variety of ways to represent a molecular structure using a molecular visualization program like Jmol. While any design would work for creating a printable image or interactive webpage, we have found that certain design specifications work better for 3d printing than others. Below are some of our suggested sizes, formats and design specifications.

Note that while these are our suggested design settings, they are by no means the only formats that may work. You should always feel free to experiment with new designs and new ideas. . . and we would love to hear from you about what worked and what new models you were able to produce!

For Printers with Support Material

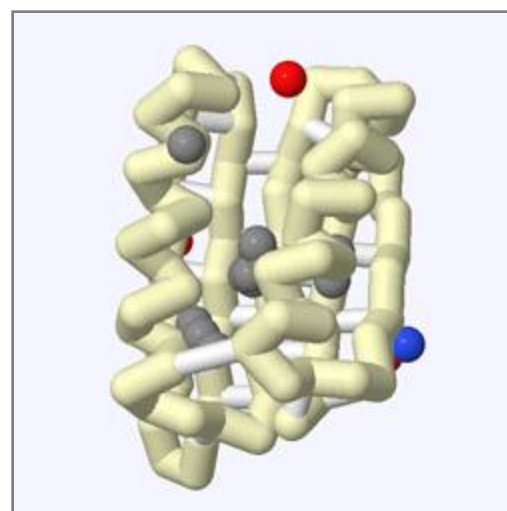
Some 3d printers, usually the higher end models, include a support material that can be used along with the modeling material to hold up all areas of a molecular structure while it is printing. For these types of printers, a model can be created in **backbone format**. It will have gaps and holes but because of the support material these holes will not prevent the model from successfully printing.

We suggest you use the following Jmol specifications for the protein backbone:

```
backbone 1.5  
strut 1.0  
hbond 1.0
```

We suggest you use the following Jmol specifications for sidechains:

```
spacefill 1.5  
wireframe 1.0
```



For Printers without Support Material

Many lower cost tabletop printers do not have the ability to print support material and therefore have a much harder time building structures with a lot of gaps or holes, such as a protein backbone with the settings backbone 1.5.

For these types of printers, we have a different set of suggested Jmol sizes and specifications. As a general rule, the more you can choose display formats and sizes that do not have gaps and holes, the more likely you will successfully build your molecular model with your printer.

We suggest you use the following Jmol specifications if you display a protein backbone:

```
backbone 3.0  
strut 2.0  
hbond 2.0
```

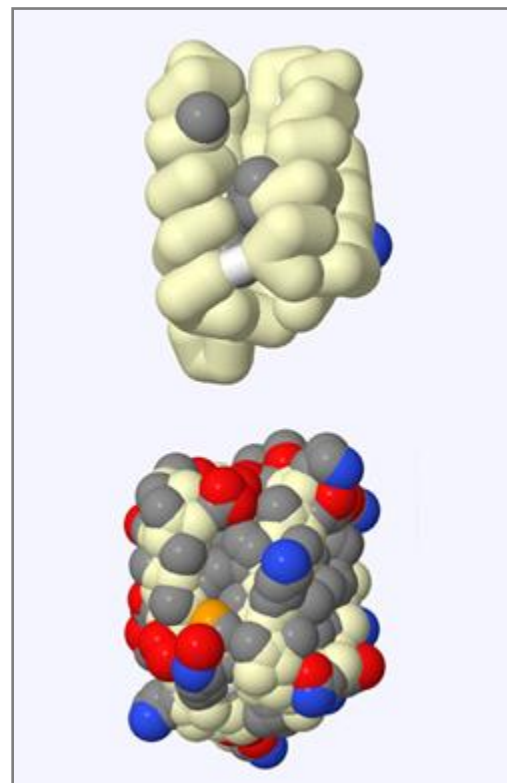
We suggest you use the following Jmol specifications if you display spacefill format:

```
spacefill 3.0  
strut 2.0  
hbond 2.0
```

We suggest you use the following Jmol specifications for sidechains in ball and stick format:

```
spacefill 3.0  
wireframe 2.0
```

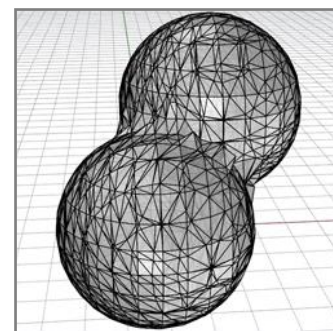
Note how much more solid and globular your design will need to be if you are using a printer without support material.



Converting Your Structure into an .stl File

We suggest you use a Jmol .jpg file or a written script text file to save your work as you design a model. However, neither of these files can be used by a 3d printer to actually print your structure. You will need to convert your Jmol design into a **Stereolithography (.stl) File**.

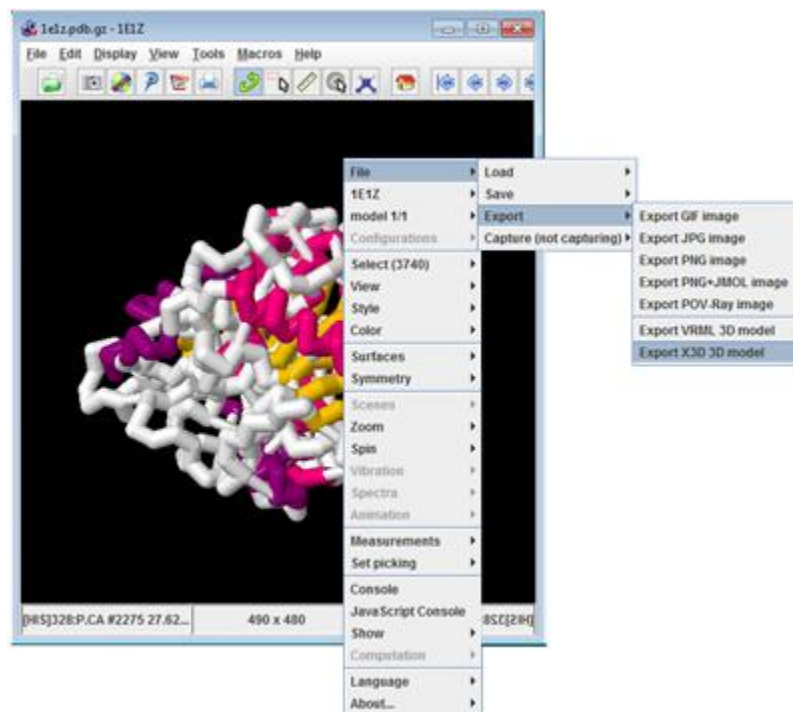
An .stl file contains the 3d mesh information used by 3d printers to produce physical models of proteins and molecular structures. A structure mesh essentially breaks complex 3-dimensional shapes down into a network of triangles. The higher the resolution and detail in a structure, the more triangles will be used to describe it.



Below are step by step instructions to create an .stl file using Jmol.

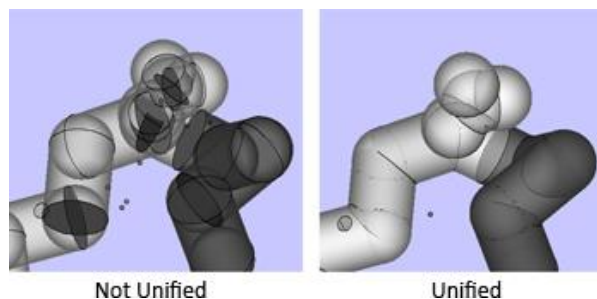
Step 1: Creating an .STL File From Jmol

1. Load the .pdb file into Jmol
2. Manipulate the .pdb file into a form that you would like to print
3. Right-click within the **display window** to bring up the **display window menu**
4. Select "**File**"
5. Select "**Export**"
6. Scroll down the menu and select "**Export STL 3D Model**"
7. In the resulting window, name your file.



Step2: Solidifying Your .STL File Using MeshMixer

When first exported from **Jmol** and converted into an .stl file using **Blender**, a molecular structure will be composed of cylinders and spheres. These basic primitive shapes will overlap with each other to create the overall shape of your molecular structure.



For some 3d printing software and settings, these overlaps can cause unpredictable problems while building.

If the model is comprised of many small individual elements it will print as a group of elements and will most likely break apart at the seams.

In order for the model to print correctly, therefore, all of the elements in the model need to be **unified** or **solidified** into a single solid element. To do this, you will need to use the freeware program **MeshMixer** (<http://www.meshmixer.com/download.html>).

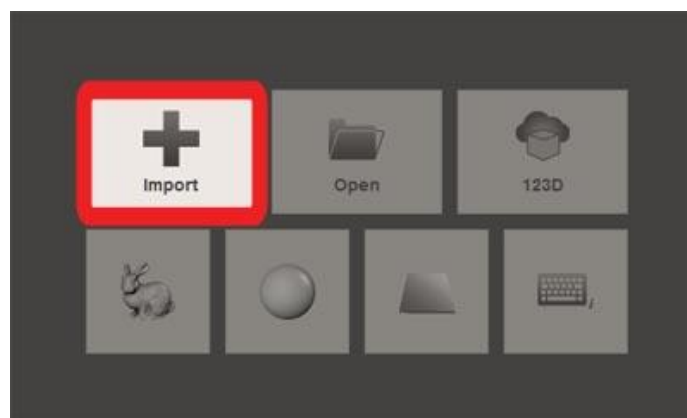
Note that many new 3d printers and slicer programs do not require a model to be **unified/solidified** in order to print properly. If this is the case with your printer, you can entirely skip these MeshMixer steps and bring your Jmol-created .STL file directly into your slicer program to 3d print.

1. MeshMixer is a simple but powerful 3d-solid modeling program made by **Autodesk**. Begin by launching the program.



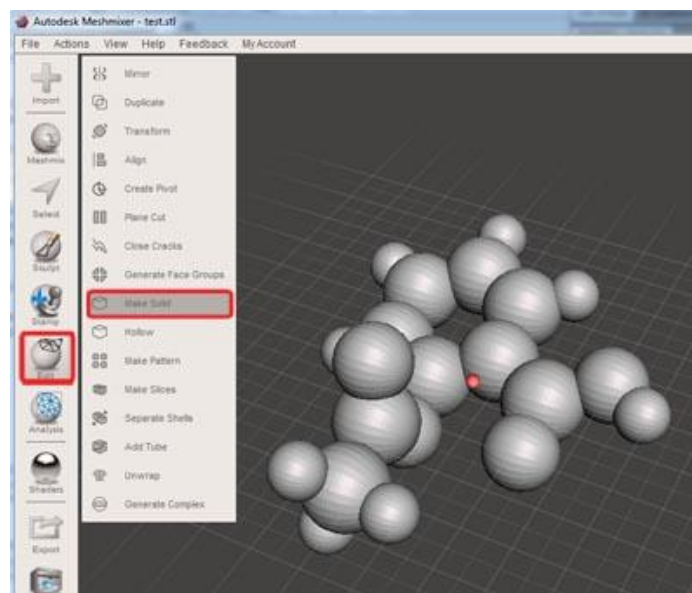
2. In the center of the opening screen there should be a button that says "**Import**". Click on this button to bring up the open dialog box and select the **.stl** file you created using Blender.

Note to make your imported molecule easier to see, we suggest you remove the **printer bed** rendering (the opaque grid). To do this, click "**View**" from the top menu and the uncheck "**show printer bed**" from the dropdown menu that appears.

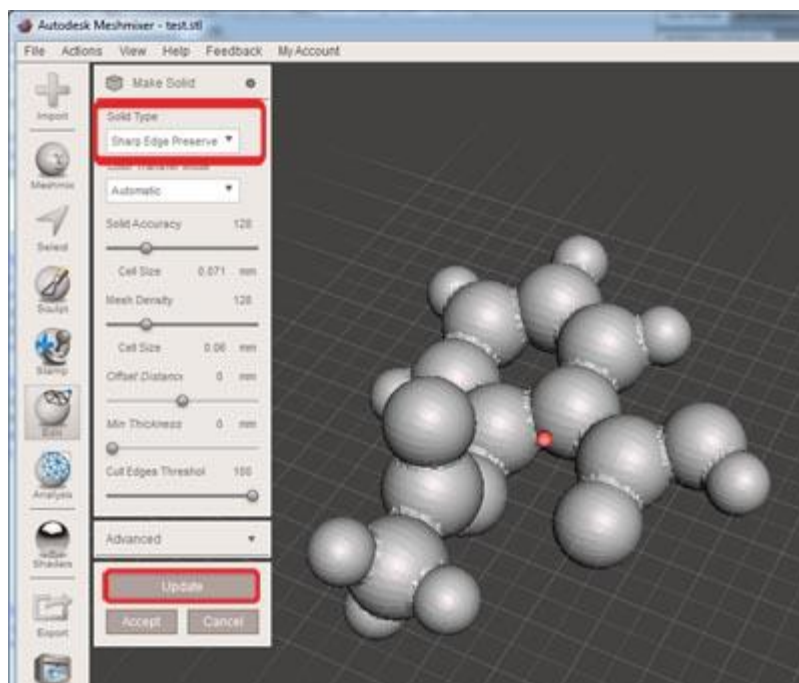


3. You should now see your molecule in the workspace window. You can **right-click** and **drag** with the mouse to rotate your view of the model.

4. To **Solidify** your structure, click the "**Edit**" button about half way down the left-side toolbar. Next, select the "**Make Solid**" button from the new menu that has opened.



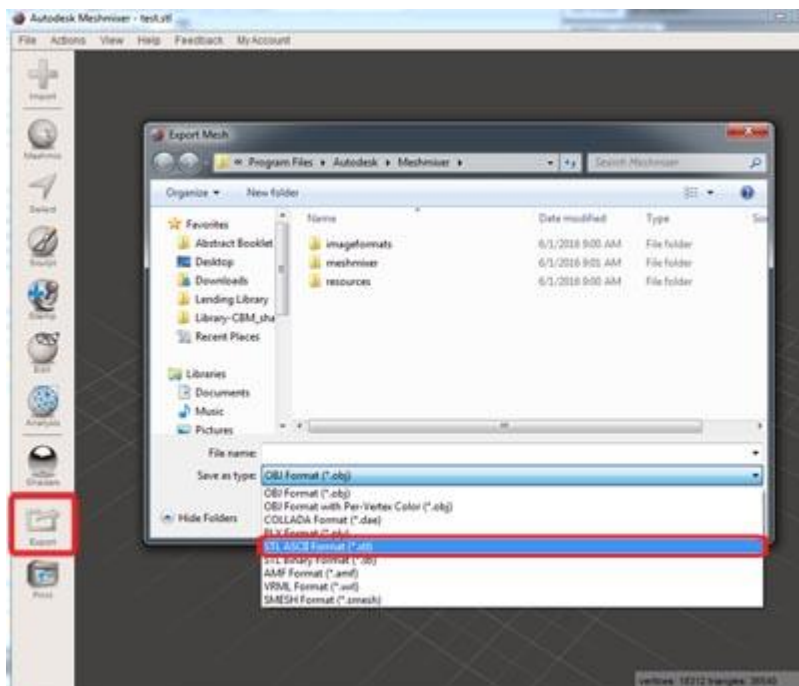
5. You will now see the expanded **Make Solid** menu, which includes a number of options to help you **solidify** your model in the best way possible. We recommend using the default settings, with the exception of changing the "Solid Type" from "Fast" to "Sharp Edge Preserve".
6. Click the "Update" button at the bottom of the **Make Solid** menu to view the results of your settings adjustment.



7. When you are happy with your **Solidify** settings, click "Accept" at the bottom of the menu to finalize the process. You now have a fully unified model that is ready to export!
8. To save your final model, click the "Export" button near the bottom of the left side-side toolbar. Make sure to select "STL ASCII Format (*.stl)" for your file-type.

Note we recommend giving this file a new name so you know it is the final and **Solidified** version of your design.

9. You're ready to bring the file in to your 3D printer/slicer software!



You will need to import your .stl file into the program, often called a slicer, that communicates with your particular 3d printer. All 3d printers we have had experience with will accept .stl files, and therefore this Blender-created .stl file should allow you to print to any 3d printer currently available!