Loading a Macromolecule
for PACUPP

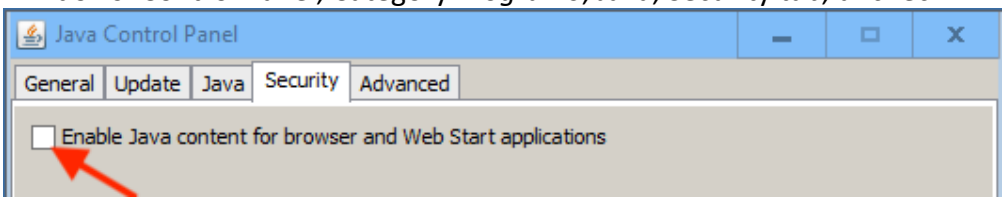
(Pockets And Cavities Using Pseudoatoms in Proteins)
molviz.org/pacupp – by Eric Martz

These instructions assume that you have already downloaded PACUPP and that you are looking at the files in the folder *Fill_Cavities_PACUPP*.

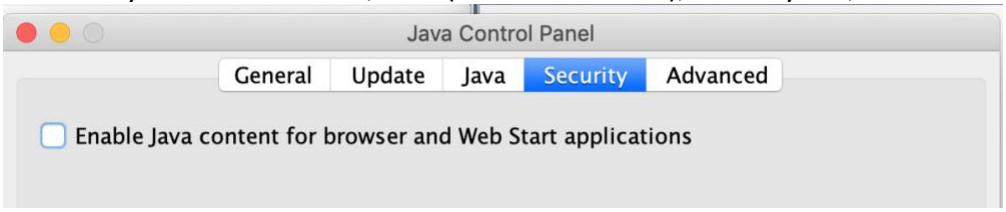
1. **Run Jmol**: double click on the file **1-Jmol.jar**. This requires that Java be installed. If any problem, go to java.com to download the latest, most secure version.

For PACUPP, you do NOT need to enable Java in your web browsers.

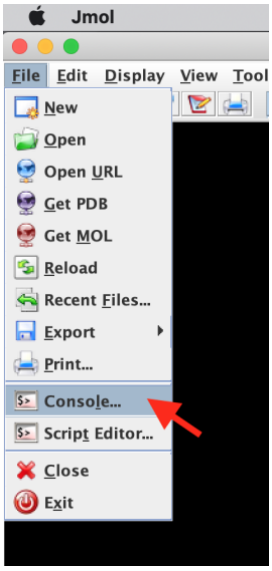
- Windows: Control Panel, Category *Programs*, Java, Security tab, uncheck:



- MacOS: System Preferences, Java (near the bottom), Security tab, uncheck:



Open the Script Console: If Jmol has only one black window, use its File menu to open the Script Console as shown to the right. A second, white window will open. This is where you enter commands, and view reports from Jmol.



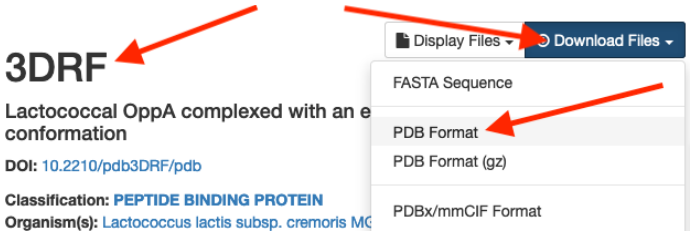
2. **Load a macromolecule**. If you know its 4-character PDB Code, and if you are online, enter the command below in the Jmol Script Console. Our example is 3DRF but substitute your own PDB Code. *No space after the equal* '='!

load =3drf

If you do not know the PDB code for the macromolecule of interest, you can search for it at UniProt or at the Protein Data Bank. Here is some guidance.

Alternatively, you can download PDB files from the Protein Data Bank. Then you can drag and drop them into Jmol (black window), even when you are offline.

Go to RCSB.Org, find the PDB code of interest, go to the page about that single entry (title is a single PDB code) and use the Download menu to download the file in PDB format. [PACUPP *requires PDB format*. PACUPP *will not work with .cif* format (PDBx/mmCIF). Approximately 1% of entries in the Protein Data Bank are too large to fit in the PDB format, and are available only in CIF format.]



Once your molecule appears in the black window of Jmol, you are ready to proceed.

In brief:

3. Drag the file **3-FILL-CAVITIES.spt** and **drop it onto the molecule** in Jmol (don't drop into the Script Console window).

See complete instructions in the PACUPP folder 0-INSTRUCTIONS. There, double-click on the file **How-To-Use-PACUPP.pdf**

For unusually large models that take many minutes for PACUPP to process, you may prefer to use PACUPP's **Batch Mode.** You can set up a batch script that will load models and process them with various settings, unattended. See example template scripts in Fill_Cavities_PACUPP/batches.