

## Jmol Workshop

*All of these web sites are best viewed with Mozilla Firefox. IE has too many problems associated with it (as do most MicroSoft apps).*

A. Molecular Visualization through the ages

B. Protein Data Base ([www.rcsb.org](http://www.rcsb.org)) or ([www.pdb.org/pdb/home/home.do](http://www.pdb.org/pdb/home/home.do))

C. National Center for Biotechnology Information ([www.ncbi.nlm.nih.gov/](http://www.ncbi.nlm.nih.gov/))

- VAST (Vector Alignment Search Tool)  
([www.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml](http://www.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml))
- Cn3D viewer download:  
([www.ncbi.nlm.nih.gov/Structure/CN3D/cn3dinstall.shtml](http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3dinstall.shtml))

C. A tour through useful websites:

1. RasMol: <http://www.umass.edu/microbio/rasmol/>

- **Select/Restrict:**  
<http://www.umass.edu/microbio/rasmol/seleccmd.htm>
- RasMol Manual:  
<http://www.umass.edu/microbio/rasmol/distrib/rasman.htm>

2. Jmol: [www.jmol.org](http://www.jmol.org)

- Jmol's Interactive scripting:  
<http://jmol.sourceforge.net/demo/#Interactive%20applet%20demonstration%20pages>
- **A much better Jmol command page:**  
<http://chemapps.stolaf.edu/jmol/docs/>

3. Online Macromolecular Museum: An outstanding collection of artful and informative Jmol routines.

- Tutorial on Jmol scripting:  
[http://www.callutheran.edu/Academic\\_Programs/Departments/BioDev/omm/gallery.htm](http://www.callutheran.edu/Academic_Programs/Departments/BioDev/omm/gallery.htm)
- Also a good link to Jmol interactive scripting on the Jmol tutorial page: <http://chemapps.stolaf.edu/jmol/docs/#top>

4. Bioc 462a Jmol routines:

<http://www.biochem.arizona.edu/classes/bioc462/462a/jmol/routines/routines.html>

5. Proteopedia (a wiki site for protein structures): [www.proteopedia.org](http://www.proteopedia.org)

6. Center for BioMolecular Modeling: <http://cbm.msoe.edu>

CBM's Jmol tutorial page: <http://cbm.msoe.edu/teachRes/jmol/index.html>

A very nicely done influenza virus hemagglutinin webpage:

<http://cbm.msoe.edu/includes/swf/HAAAnimation.swf>

## F. Tonight's introductory exercises

Background: This week we are studying ligand binding to egg white avidin, which under normal biological conditions binds extremely tightly biotin, the  $K_d$  for which is one of the lowest known in the biochemical world,  $10^{-15}$  M. The first ligand for which you will calculate a  $K_d$  is HABA (4-hydroxy azo-benzene-2-carboxylic acid). On Thursday, via a competitive ligand binding experiment you will determine the  $K_d$  for a biotin analogue, 2-iminobiotin (IMB).

Fortunately, there are high resolution structures for apo-avidin (or its bacterial counterpart streptavidin) as well as with a variety of different bound ligands. These will provide us with a good starting point for the workshop.

Avidin structures:

1ave: apo-avidin

1avd: avidin with biotin bound

1rst: streptavidin with the strept-tag bound

1sre: streptavidin with HABA bound

1nc9: streptavidin (Y43A) with iminobiotin bound

1ndj: streptavidin mutant (Y43F) with biotin bound