Visualization with VMD

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WORKSHOP ON MACROMOLECULAR MODELING

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Download pdb file (experimental structure of macromolecule)

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Saving as an image file for importing into another program

Tips for making effective images

Download pdb file

Go to: http://www.rcsb.org/

Search for macromolecule by name, pdb ID, …

- Type “triose phosphate isomerase”
- Click on structure 4ZVJ (human triose phosphate isomomerase)
- Under Download Files, choose pdb format (NOT the .gz option)
- Save to convenient location (e.g. create folder on desktop & save there)

Examine pdb file

Open file with text editor

Do NOT try to understand everything

Scan for particular information, e.g.:

Original paper	Experimental conditions
Crystallization conditions: 277 K, 35% PEG etc.	Missing residues: Gly A -5, Asp A -4 etc.
Sequence [2 chains: A and B]	List of helices and sheets
List of x,y,z coordinates	Note: 2 Na^+, 2K^+, waters at end

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Open VMD

3 Panels appear:

- Main
- Display
- Command (for typing in commands by hand: ignore)

Import pdb file

Main:File: choose New Molecule
In new window: click Browse and navigate to pdb file
Click Load: image appears.

- Play with it using the mouse
- Rotate, zoom in and out (may need to go choose Main:Mouse:Scale)

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Representations

Main:Graphics: choose Representations

In new window:

- Play with Drawing Method menu (New Ribbons, Cartoon, New Cartoon, Licorice …)
- Play with Coloring method (try Element, Chain, Secondary Structure …)

Representations (2)

Focus on one monomer (chain):

- Graphical Representations: click Create Rep
- Graphical Representations:Selected Atoms window: enter “chain A” (do not type the quotes)
- Graphical Representations: double click the top entry in the big window (it will turn red)
- Main:Display: click Reset View (image moves to center of display)
- Graphical Representations: choose
  - Drawing Method: New Cartoon
  - Coloring Method: Secondary Structure
- Play around with the image. Identify the β-barrel.

Highlighting a structural element

Loop 166-176 is said to form a hydrogen bond with the substrate's phosphate. To show the loop:

- Create another representation
- For Selected Atoms, type "chain A and resid 166 to 176"
- Choose Drawing Method: NewCartoon and Coloring Method: ColorID and, just to the right, choose "1 Red"
- Rotate and zoom until the loop is clearly visible

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Creating an image to make a point: an example

Create another representation. Make these choices:

- Selected Atoms window: chain A and resid 95 165
- Drawing Method: Licorice
- Coloring Method: Element

Orient and zoom so that His 95 and Glu 165 are large and central, with their relationship to the TIM barrel clear.

Delete the representation for loop 166-176. We do not need it now.

Show key interatomic distances (angles …)

Choose Main:Mouse:Label:Bonds

Click atom His 95 H bonded to the ring N and the nearest Glu 165 carboxylic O. The interatomic distance (Angstroms) and atom labels should appear.

Choose Main:Graphics:Labels and delete the atom labels from the window. Those labels just distract; the image is better without them.

Effective image

You have now shown secondary structure (the TIM barrel) with ribbons, key residues atomistically, and an important geometric parameter quantitatively. This layering of information at useful levels of detail, using color wisely, is the key to making effective images.

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Improve the Image for Exporting

First, change the background to white. Black is good for the monitor, but white is almost universally used for papers, reports, and presentations. To do this:

Choose Main:Graphics:Colors. Then in the new window choose Categories:Display, Names:Background, Colors: 8 white

Improving Image (2)

If the axes are still showing (depends how much you have zoomed), remove them: Main:Display:Axes:Off

Unless you really want to show how much the original crystal structure has been rotated for this view, the axes are only a distraction.

Improving Image (3)

Notice that the interatomic distance is no longer visible (because it is white). To fix:

In the Color Controls panel (Main:Graphics:Colors), choose Categories:Labels, Names:Bonds, Colors:16 black.

To adjust size of distance label, return to the Graphics:Labels window and choose Bonds in upper left, then Global Properties. Change Text Size and Thickness.

Improving Image (4)

Increase the resolution (otherwise edges will appear jagged when image is saved)

In Main:Graphics:Representations, click on the Licorice representation, and increase the Bond Resolution (as high as you can go and not create to large a file).

Next, click on the NewCartoon representation and increase the resolution as far as it will go.

Saving an Image File

Now save the image:

Choose Main:File:Render. Choose Browse to set location and name of file. Then click Start Rendering.

Go to the image file's location and click on the file. It is not yet in a format you can important into a document. You need to save it in another format. Therefore:

Choose File:Export. In window that pops up, choose format (e.g. PNG or JPEG). You will be able to import this into a document.

Use PyMOL for even better images for publications & reports

PyMOL

- Less intuitive (uses scripts)
- More flexibility
- High resolution
- Cumbersome for understanding research results
- Great for publication-quality graphics

VMD

- More intuitive (point and click)
- Less flexibility
- Moderate resolution
- Great for understanding research results
- OK for publication-quality graphics

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Creating Effective Images

Before you begin, decide on the point you want to make with the image.

Let the point guide your decisions about image composition.

Consider your audience early on. What do they need to know?

Combine representations, carefully choosing the level of detail for each.

Use color, and wisely.

Eliminate unnecessary detail: less is often more.

Every component of the image should have a purpose.

Thanks for your attention!

Questions?