

@text (This is the text window of kinemage: 3Dlit2a-exercise-KiNG.kin, 090823)

### 3D LITERACY EXERCISE ONLINE IN MOLPROBITY:

MolProbity is an analysis, validation, and correction web service. It can fetch certain types of files from several other resource providing web servers, and it can accept uploaded files from a user's own computer. For this exercise, you will use this upload facility with a kinemage file which you have downloaded from the bch258 website: download 3Dlit2a-exercise-KiNG.kin to your own computer, then point a web browser to:

<http://molprobity.biochem.duke.edu>

and "Browse..." to locate that file, declare it to be "type: kinemage" then "Upload" that file into MolProbity. If successful, a simple page comes up with the file name and a choice to "View in KiNG" -- click on that. KiNG comes up in a separate page showing the first kinemage.

#### KINEMAGE 1 - Practice at Drawline and rotation

In the graphics window you will see an object made of dots with the first few connected. The image is depth-cued, so dots or lines further away will look smaller and less bright. Rotate the image in 3D by dragging slowly back and forth with the mouse.

The purpose of this kinemage is for you to practice, so draw in all the rest of the lines to continue the pattern. Turn on the drawline function by selecting menu item "Tools:Edit/draw/delete". A separate small window appears that has "radio" buttons: choice of one turns off all others. So clicking "Draw line segments" sets that function, and clicking "Do nothing (navigate)" turns off drawline so you can click on a graphics point to just reveal its pointID.

Click on two points to draw a green line between them (you must pick each end of each line). Remember to frequently rotate the visual object by dragging with the mouse, starting someplace that is NOT a point. You might find it useful to turn on "Markers" at the bottom right of the window to better see that you have actually picked a point. "Show text" button at the bottom right of the window will bring up a separate text window showing on-screen what you are reading here.

If rotating the image shows you a mistake, you can use the "Undo drawing" button" at the bottom of the "Edit/draw/delete" window as an undo. This only goes back about 10 steps. KiNG's erase functions can't distinguish your newly drawn lines from the original points, so to delete one of your drawn lines, first turn off the original "object" using the button panel on the right side of the window, then select "Punch one point" and click on an end of the drawn line. (if several lines meet, you may end up removing an extra one and need to redraw it afterward). Remember to turn "Draw line segments" back on to continue the exercise.

Once you feel comfortable with the rotation and the drawing functions and have read thru at least the next section of these explanations so you know what's coming, select "Kinemage #2" at the top of the right-side panel in order to do the real 3D molecular literacy exercise. This next part can be considered a test: what you can do in 5 minutes is an interesting way to measure your current 3D molecular graphics literacy. If you are a bit slow now, doing a similar timed exercise at the end of this section of the course will show quite an improvement!

#### KINEMAGE 2 - Connect-the-atoms Exercise

KiNG does not have a way to automatically time and save your result, so if you are doing this as a test, you must time yourself. 5 minutes is suggested for Kinemage #2.

What you see is a separate white dot for each atom in this small piece of protein structure. Use Drawline to connect atoms that are covalently bonded (i.e., suitably close together in 3D) - you draw a line by clicking on each end of it.

Both backbone and sidechains are included, but not H atoms. Drag with the mouse slowly from side to side in order to see the atom dots in 3D. Turning the structure around will let you identify protruding side chains as a starting point for drawing in the bonds.

If the "Edit/draw/delete" window was invoked earlier, this kinemage will also be under its control. Click on two points to draw a colored line between them (you must pick each end of each line).

Tip: when you pick an atom its element type will be shown, and when you connect to the next atom the distance between them in Angstroms will be shown. If you make an incorrect bond, use "Undo drawing" to take that last one away, or invoke "Punch one point" to punch out any of your drawn lines (remember to turn off the "molecule" group in the right-side panel, and to select "Draw line segment" again to continue the exercise).

You can compare your drawing with the answer by turning on (and off repeatedly) the answer button in the right side panel.

### KINEMAGE 3 - Find-the-backbone-Hbonds exercise:

This kinemage shows the backbone (in white) and the sidechains (in cyan) out just to Cbeta, for a small piece out of a protein structure. 2.5 minutes is the suggested test time for Kinemage #3.

The object of the exercise is to find the backbone hydrogen bonds and draw them in. The "Edit/draw/delete" window is also needed for this exercise. However to avoid confusion with covalent lines, select "Draw dotted lines". Click on two atoms to draw a line between them. (If you select the "Do nothing (navigate)" button temporarily, you can take advantage of the atom-identity and distance displays at the bottom of the screen, without producing any new lines.)

Now start looking for possible donor-acceptor pairs on the backbone, with suitable geometry. When you find one, draw in the H-bond. (If you don't like it, once you move it around and look from all angles, then remove it with the "Undo drawing" button.)

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When finished with the whole exercise, select "close this window" at the bottom left, hit the "Continue" button on the MolProbity page, then select "Log out" on the left panel of MolProbity "Main page". Please select the "Destroy all my files and log me out" button on the "Log out & end session" page to avoid clutter on the MolProbity server. Then you are on a neutral, normal web page and can close your browser.