

The following is text from the kinemage file 3Dlit4atst.kin. The purpose of the kinemage is to test the student's proficiency at visualizing 3D objects. Five kinemages are in this file:

[Kin 1:](#) Practice at the tools for the kinemage: drawline and rotation

[Kin 2:](#) Exercise at connecting the neighboring atoms

[Kin 3:](#) Exercise at labeling geometries of bond-angles

[Kin 4:](#) Exercise at determining backbone oxygen atoms

[Kin 5:](#) Exercise at determining interactions (H-bonds)

## **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. This kinemages will have the drawline function already turned on. 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. A summary of these instructions will be in the caption window, and an even briefer reminder is written at the top of the graphics screen.

If rotating the image shows you a mistake, you can use "eraselast" as an undo. [Turn on "PickEraseNew" to punch out earlier drawn lines (if several lines meet, you may end up removing an extra one and need to redraw it afterward). Remember to turn "Drawline" back on to continue the test.]

Now turn on the "DrawBall" button. Click on the last three points at the green end of the figure to decorate them with purple balls.

You will notice that each time you picked (that is, clicked on) a point, the point's identifier was shown at the lower left corner of the graphics screen. Place labels at the first 3 points on the blue end of the graphics object, by selecting the "Labels" button in the panel on the right side of the graphics screen, and picking each of those points in turn.

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, go to the "Kinemage" pulldown menu and choose "next" in order to start the 3D molecular literacy test, each part of which is timed.

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

The first thing that comes up is a dialog box requesting a unique personal identifier for you: e.g. a short form of your name. The results of this timed test will be put into a file named with some characters of the original file name, some characters of your personal identifier, a time-stamp number, and then .kin for the file type. (Some systems restrict file name length to 31 characters.)

Once you have entered your name, the timer will start counting down.

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.

This kinemage will have the drawline function already turned on. Click on two points to draw a green 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 "Eraselast" to take that last one away, or invoke "PickEraseNew" to punch out any of your drawn lines (remember to turn "Drawline" back on to continue the test).

When the timer reaches zero, a dialog box will come up to save your work (you may need to move the mouse to wake it up). Your name and a time-stamp should already be part of the output file name. Read the brief summary of the exercise to come, then click the "OK" button, which will automatically start the next part of the test (also timed).

### **KINEMAGE 3 - Label-particular-geometry exercise:**

This kinemage shows backbone in white and sidechains in cyan, from a small piece of protein structure with all of the sidechains branched.

The object of the exercise is to distinguish the type of geometry at branch points in protein sidechains. Some branch points are planar: that is, constrained to have only 3 covalently bonded neighbors all in the same plane which includes the central atom ( $sp^2$  hybridization for you chemists). Other branch points have tetrahedral geometry ( $sp^3$ ), where the 3 bonded non-H neighbors are symmetrically placed but strongly non-planar with the central atom.

The task is to label each atom that is a sidechain tetrahedral branch point. Atom types and residue names are not given, so you must distinguish tetrahedral from planar branches just from their 3D geometry. Label just one branch-point per sidechain, and do not label any backbone atoms.

Click on the atom to select and label it. Remember the "eraselast" button to remove the last one made, or "PickEraseNew" to remove any one you decide was a mistake. NOTE: the picking-point of a label is the lower-left corner of the first character (which may be a space)!

(The "w" key toggles label-character size)

The timer will show the time left; when it reaches zero, a dialog box will come up to save your work. (Your name and a time-stamp should already be part of the output file name.)

Read the brief instructions for the next part. Then click the "OK" button to accept the output, and you will start in the next timed kinemage exercise.

### **KINEMAGE 4 - Identify-particular-types-of-atoms exercise:**

This kinemage shows both backbone and sidechains in white, for a short peptide.

The task in this exercise is to identify all the backbone Oxygen atoms in this piece of structure by placing balls on them. (Do not mark any sidechain atoms.)

Click on an atom to select and place a ball on it. Remember the "eraselast" button to remove the last made one, or "PickEraseNew" to remove any one you decide was a mistake.

When the timer reaches zero, a dialog box will save your work. (Your name and a time-stamp should already be part of the output file name.)

Read the brief instructions for the next part. Then click the "OK" button to accept the output, and you will start in the next timed kinemage exercise (or exit the program after the last timed exercise).

## **KINEMAGE 5 - Find-the-interactions exercise:**

This kinemage shows the backbone (in white) and the sidechains (in cyan), for a small piece out of a protein structure. Find a good view, and choose "Set Reader's View" on the Views pulldown menu so you can get back to it.

The object of the exercise is to find the hydrogen bonds and draw them in. This kinemage has the drawline function already turned on. Click on two atoms to draw a green line between them, which will be shortened for less confusion with the covalent bonds.

(If you uncheck the drawline 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 "eraselast" button.)

Once you have drawn lines for all the backbone H-bonds, see if you can find any sidechain-to-backbone or sidechain-sidechain H-bonds and draw them in also, again checking for suitable geometry.

When the timer reaches zero, a dialog box will come up to save your work. (Your name and a time-stamp should already be part of the output file name.) Click the "OK" button to accept the output, and then you will exit the program.