

Name: _____



Worksheet 1: 3D Molecular Literacy & Getting Started in KiNG

course website -- <http://kinemage.biochem.duke.edu/teaching/bch258/>

MolProbit website -- [http://molprobit.biochem.duke.edu/...](http://molprobit.biochem.duke.edu/)

software website -- [http://kinemage.biochem.duke.edu/software/...](http://kinemage.biochem.duke.edu/software/)

Your Contact Info

Please give us your full name:

your class, department and/or program:

your email address:

Reading Assignment

Read (or review) chapter 1 in Branden & Tooze "Introduction to Protein Structure"

Graphics Assignment -

to be done before the next class, and this worksheet handed in then

The course will use kinemages, viewed with the KiNG display program, both for homework exercises and also as the medium for individual projects. The [QuickStartKing.pdf](#) file summarizes the basic operations. You will start out (below) directly on-line by uploading a kinemage file onto the MolProbit web site and viewing it there in KiNG (thus independent of hardware, OS, or installation). Later it will often be necessary to work off-line on your own computer, so the second half of this assignment leads you into trying that method.

3D molecular literacy exercise

From the course web site (see above) download the file 3Dlit2a-exercise-KiNG.kin to your computer. Go to the MolProbit site (see above, or navigate from the main kinemage site). In the file upload section, set file type to kinemage, browse to find the 3Dlit file, and upload it. Choose the "View in KiNG" option, which will start KiNG with this kinemage in the graphics window. Click the "Show text" button at lower right or use the printed handout, and follow the instructions, answering as much of the following questions as you can.

In kinemage 2 (connect-the-dots), how many amino-acid residues (that is, how many Calphas) did you find in this piece of structure? _____ What is the sequence (remember that each atom dot is labeled as C, O, N, or S) _____

In kinemage 3, how many backbone H-bonds did you find? _____ What type of secondary structure is this? _____

Installing KiNG stand-alone

Go to the software web page (see url above). Find and download the appropriate KiNG install package for your computer/operating system. Instructions are on that web page and in the document called QuickStartKiNG.pdf. Make a working folder for these class exercises (on MSWindows, it's advisable to put KiNG in that same folder). From the course website, download the Demo5_4a-KiNG.kin kinemage file. Launch KiNG and open the demo kinemage from the file menu.

Which operating system are you using (MacOSX, MSWindows, or Linux)? _____

Did the installation procedure work? _____

Did KiNG come up when launched? _____

Did the demo kinemage file open successfully, showing the carboxypeptidase active site in the black-background graphics window? _____

If the above steps worked, proceed. If they did not, please see one of us for help as soon as feasible, but proceed with the exercise using the MolProbity-upload method as in the previous section.

Demo5_4a-KiNG.kin

Go to the file Demo5_4a-KiNG.kin on your computer (downloaded above), and open it in the local KiNG application you installed above. [If that was not successful, proceed with this exercise by uploading and viewing in MolProbity, and be sure to consult one of us for help.]

Did you do the demo on your computer, or in MolProbity? _____

In kinemage 6, what is the distance between the N-cap sidechain O (red ball) and the backbone N (skyblue ball)? _____ Å