



Name: _____

Structural Biochemistry I

WorkSheet 1: Interactive Molecular Graphics *Rev 20110829*

course website -- <http://kinemage.biochem.duke.edu/teaching/bch258/>
MolProbity website -- [http://molprobity.biochem.duke.edu/...](http://molprobity.biochem.duke.edu/)
software website -- [http://kinemage.biochem.duke.edu/software/...](http://kinemage.biochem.duke.edu/software/)

Your Contact Info:

Full Name: _____

Your class, department and/or program: _____

Your preferred email address: _____

Do you have a laptop with wireless internet, that you could bring in for several of the class sessions? _____
What operating system (e.g. MacOSX, MSWindows, or Linux, etc.)? _____

Graphics Assignment;

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

(NOTE: If you have reason to fill out worksheets electronically and submit as uploads, please talk to Dave about how we can work together to accomplish that.)

This course will use kinemages, viewed in the KiNG display program, for homework exercises. Kinemage graphics were developed in the early 1990's initially to provide interactive 3D graphics illustrations for articles in the (then) new journal Protein Science. They proved a powerful teaching tool because as authored illustrations there is almost no learning curve for the reader to gain access and understanding. The display programs Mage and KiNG are optimized to convey 3D information interactively, designed to tell a story, but deliberately denigrate rendering slick 2D pictures. Enhancements of added research tools have not interfered with this designed ease-of-entry to learn from authored illustrations.

QuickStartKing.pdf file summarizes the basic operations. You will start out (below) directly on-line by uploading a kinemage file onto the MolProbity web site and viewing it there in KiNG (thus independent of hardware, OS, or installation - except for a browser, and Java). 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.

Viewing kinemages on-line

From the course web site (see above) download the files 3Dlit2a-exercise-KiNG.kin and Demo5_4a-KiNG.kin to your computer. Go to the MolProbity site (see above, or navigate from the main kinemage site). If it says you need a current Java, follow its instructions. In the file upload section of the MolProbity main page, set file type to kinemage, browse to find the demo 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 and go through the text following along in the graphics.

Name: _____

Doing 3Dlit2a-exercise-KiNG.kin on-line

(see 3Dlit2a-exercise-KiNG.pdf) Please affirm (i.e. check off) that you did try:
Connect-the-atoms exercise _____ and Find-the-backbone-Hbonds exercise _____

Viewing Demo5_4a-KiNG.kin on-line

Be sure to do kins 1,2,3, & 6; (4 & 5 are fun but optional).

In kinemage 3, which 6 sidechains make direct H-bonds to the biotin?

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

On the tools pulldown menu, what is the one choice under “Structural biology” ?

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). Launch KiNG and open the Demo5_4a-KiNG.kin 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? _____

On the Tools pulldown menu, how many choices show now under “Structural biology”? _____

What is one of the new ones? _____

If the above steps did not work, please see Vincent or Bryan for help as soon as feasible.