Name:_____

CMB BCH 258 SBB MCB UPC IMM

Worksheet 1:
Interactive Molecular Graphics

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

MolProbity website -- http://molprobity.biochem.duke.edu/...

software website -- http://kinemage.biochem.duke.edu/software/...

Your Contact Info

Please give us your full name:

your class, department and/or program:

your email address:

Do you have a laptop with wireless internet, that you could bring in for several of the class sessions?

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 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.

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 _____

Name:_____

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, hoow many choices show now under "Structural biology"?_____
What is one of the new ones? _____

If the above steps did not work, please see one of us for help as soon as feasible.