

## Instructor Supplement

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### Suggested Progression for Kinemage Authorship Over the Course of the Semester in a Majors-level Biochemistry Lecture Course

Full semester kinemage authorship is a concurrent "dual track" process. One track deals with learning the software and becoming familiar with working with graphics. The second track deals with selecting and researching a topic to explore with kinemages.

#### TRACK ONE

- Illustrate secondary structure in class with MAGE. Show how program works and simple things you can do with it. I have done this with DNA structure even before I get to proteins (following the chapter order of Voet, Voet, and Pratt).
- Assign premade kinemages as homework. If your text does not have a kinemage supplement, use some of the kinemages from the Branden and Tooze supplement or make some of your own. Homework should be turned in and a grade assigned to help push many students over the energy barrier of engaging the software.
- The first time I assign kinemages as homework, I simply want them to get acquainted with the program and comfortable exploring the graphics image so I ask them to come up with five questions about a particular structure (or series of structures). Again, this could be done with any structure (protein, DNA, RNA, etc).
- The second homework assignment with premade kinemages requires some analysis. One assignment I have given is to have the students measure the dihedral angles in pieces of secondary structure, then generate their own Ramachandran plot from the data. They can compare their plot to the one in the textbook and discuss any discrepancies. Other

example assignments could include finding the sidechain ligands around a metal or suggesting a position to insert a disulfide bond.

- At some point before midsemester I suggest you demonstrate to the class how to use Prekin. You can use a ricin pdb file as in the tutorial or any other pdb file of a structure that may be of topical or current interest. Using a laptop computer and data projector, run through how to make a default backbone kinemage, a helix/sheet ribbon kinemage, and a "lots" kinemage. These should only take a few minutes since they are available as built-in scripts. Explore these very briefly, then demonstrate how to use the "ranges" mode to make a kinemage of specific sidechains that are important to your structure. Then show the students how to append this kinemage to either your backbone or ribbon kinemage you just made. This will give them a jump start on the tutorial.
- Immediately after you do the Prekin demonstration in class, I suggest you ask the students to work through the ricin kinemage authorship tutorial. Many students will not work through it simply because they don't want to take the time (~2-3 hrs) to do it, but they should at least read through it to get an idea of what the tutorial contains. At this point I like to employ a paid tutor, an upper level undergraduate who is very familiar with Mage and Prekin, to assist your students in working the tutorial and with their projects. This type of peer-tutoring is very effective with kinemage authorship and undergraduates on wages don't cost very much. This will also save you personally a lot of time on trivial things that don't really need your attention like where the student saved their file or how to download the software.

## TRACK TWO

- Students should be told at the first of the semester, including in the syllabus of the course, that they will need to select a topic for their personal kinemage authorship project. If you have them work as teams, I suggest no more than two students (absolute max of three) per team. The students are prone to divide the labor in a way that reduces the benefit of the project.
- Topic selection can be done in several different ways. You can offer them a list of possible topics, and the less creative students may need such structure. You can also assign them topics based on a biochemical pathway or process, so that there is some "theme" to the class. Decide before the semester starts so that the students are not confused about how their topic will be selected/assigned.

- You should take a few minutes in class to talk about how to find literature articles. I always discuss online databases such as PubMed and talk about the holdings in our particular library. The students should be very clear about how to obtain articles that your library does not hold.
- I also hand out an example article on a structure-based topic, such as the crystal structure of glucose oxidase, ask the students to read it as best they can on their own, then go over the pertinent points in class the next period. They don't need to know the nitty gritty of X-ray crystallography, but they do need to understand the concepts of resolution and B factors, and why some pieces seem to be missing from X ray structures. In sum, they need to be able to judge the quality of the structure and what information about the molecule(s) they should be able to get from it.
- About a quarter to a third of the way through the semester have the students turn in a brief paragraph of their topic, along with one or two PDB file references and several key literature references. This should total no more than one page, but gets the students thinking about their project.
- A little over halfway through the semester, after the students have been exposed to Prekin in class and started on the tutorial, I ask them to give me a detailed written outline (~ 2 pages) of what they will do with their kinemage authorship project. This is basically the same procedure one would use to organize a standard term paper. It forces the students to think about their project at a crucial time in the semester. At this point I like to have the students turn in the face page of one or two key references to show that they have been able to find them, and they aren't just ad libbing from the popular literature.
- At the time of the outline, it is probably a good idea to have the students also submit an alpha carbon backbone and a ribbon structure of their topic just to show that they have the software and the PDB files in place.
- Between one and two weeks from the last day of class I have students turn in a draft of their kinemage project. They can email it to me, bring me a disk in class, or come by my office to show me. This gives me an opportunity to go over their project and make suggestions to improve the final kinemage. I suggest that students NOT combine their kinemages into one file for this draft, since this is a problem for many of them.
- I ask students to turn in their final project by the last regular day of class. In theory they can send it as an email attachment, but this can easily overwhelm your mailbox so I suggest you just get it on a disk from them.

Early in term	Students select topics	
Whole term	Kinemages in homework & lecture	
1/4-1/3 into term	Students turn in topic summary	
Before midterm	Demonstrate how to use Prekin	Demonstrate how to use library
By midterm	Assign tutorial	Demonstrate how to read article
~ midterm	Students turn in written outline of kinemage project	
~ 1 week to go	Students turn in draft of kinemage project	
Last class day	Students turn in final kinemage project	

### *Alternative Approaches to Kinemage Authorship*

As you can surmise from the above section, a kinemage authorship project involves a good deal of work, mostly outside the class, over the course of a semester. One must remember, however, that much of this involves learning to find and read the scientific literature, and organize it into a logical story. The software offers a vehicle to tell that story in three dimensions, a process which informs the viewer and deepens the understanding of the author.

Another approach is to use an abbreviated version of the full semester project. Several PDB files of proteins (or nucleic acid) structures that have been reviewed in the lecture, or discussed with individual students, be made available to students so that they can select a structure and construct their own kinemage as an independent assignment. This bypasses the literature dimension of the project and gives the students very specific instructions on what to portray in their kinemages.

An even more abbreviated project can be fit into a laboratory setup and assumes you have a fixed block of time for the students to work. I suggest using a computer lab with MAGE, PREKIN, and the needed Protein Databank files (in this case 2AAI.pdb) already installed on each computer (no server!). This setup works well for nonmajors because of their need for more supervision. Assuming that the students have been exposed to kinemages previously in class and hopefully have done one homework problem with Mage, you can give them a very abbreviated version of the ricin tutorial to work through. I have posted such a version on the instructor's page of the kinemage authorship website. I also pick a protein that they are working with in the lab and construct a kinemage illustrating pertinent points. I then set up a brief series of questions that guide them in exploring the kinemage.

Students can complete a group authorship project where they work in pairs. As in lab work, however, these can be problematic if the students are of unequal abilities or interest in the project.

### *Grading Kinemage Authorship Projects*

In the manual I have set up a grading rubric which hopefully will be clear to both students and instructor alike. It is important that the kinemage authorship project count for a substantial amount of credit or the students will not take it seriously. Of course, the project as I have described for a majors biochemistry course is much more substantial than that during a lab session of a nonmajors course, and so the amount of credit allotted should be adjusted accordingly. For the majors course, I suggest the project count the equivalent of a regular examination. This includes all kinemage-related homework assignments along the way.

### *Other Visualization Tools*

Many instructors will also use Chime (or Rasmol) as a companion program. Chime is a better database-browsing tool and is the preferred structure viewer, particularly for small molecules like amino acids and lipids. Since many textbooks use Chime on their accompanying website or CD, you should deliberately introduce Chime to the class and make sure they understand that Chime and Mage are different programs. Chime/Rasmol do not have the versatility of kinemages in communicating 3D concepts. Also, my experience is that most biochemistry students are not interested in writing scripts or HTML, or dealing with a command line. A web-based derivative of Chime is Protein Explorer. Many people like this viewing program, so you may want to have a look at it if you haven't already. Finally, you may also want to introduce Deep View to students planning a career as a researcher in biochemistry or biophysics. Deep View has a steep learning curve but is capable of much more than the other programs mentioned here.

### *Instructor Preparation*

The most work for you as the instructor will be learning kinemage authorship yourself. By completing Demo5\_4a.kin, Demo5\_4b.kin, and the full tutorial you will be well prepared to assist the students. You may also want to refer to KinFmtAuthors.txt as a reference for kinemage text editing.

*Final tips for instructors using kinemage authorship (or other molecular constructions).*

Please pardon some repetition with the preceding text.

- Tell students about the authorship project at the first of the semester. Make sure it carries a substantial amount of credit or they simply won't take it seriously. I give the same amount of credit as a regular exam.
- Help the students understand how the project fits into the "big picture", ie how important the understanding of macromolecular structure is to modern medicine, material science, etc.
- Encourage the students to print out the manual or print it for them. It is easier for them to follow in hand than online.
- Encourage exploration of the structure. Much can be learned from a combination of literature information and just poking about.
- Consider hiring a tutor for the project. This could be a senior undergraduate that has learned the procedures, a graduate student, or some other arrangement. Some students, particularly the weaker ones, will need a lot of handholding and this is very time consuming.
- Do what you can to encourage students to interact and work in groups. Although they have individual projects, they get ideas from each other and help each other solve problems.
- Consider kinemage authorship as part of the laboratory component of the course. There is more in-class time in the lab and the molecular construction can be tied directly to the ongoing wet experiments.
- The project works best as a progression over the course of the semester. Be sure to give homework with premade kinemages and to use them in class as a part of your lecture. This helps in teaching and gives you a chance to introduce students to a variety of kinemage features in context.
- Make an effort to put the authorship project in context of a larger study of biomacromolecules, ie physical properties, function, genomic sequence & regulation, cellular location, role in disease, etc.
- For large, nonmajor classes kinemage authorship becomes very difficult for the students. If it is done at all, you will have to not only have to assign topics but also directly give the students PDB files and specific directions on what you want them to build. It is unlikely they will be able to read a journal article. Nonmajors do benefit from simply working with premade kinemages, particularly those made by the instructor to fit with the class.

- Set up an outline or flow chart of how the project will proceed over the course of the semester. Put this in the overall context of your class exam and homework schedule.
- You yourself should be as familiar as possible with MAGE and PREKIN. This will help you answer questions and make your own kinemages for teaching or research. It will also help you understand what the programs can and cannot do.
- Consider giving a kinemage with associated questions as a take-home portion of an exam. You could make the kinemage yourself or use an available one.
- Consider giving a portion of your final exam in a computer lab using kinemages. I will be glad to help with this and have such an exam already made up that you can use.
- As soon in the semester as it will fit you should introduce your student to electronic databases such as Pubmed and the PDB. Also teach them BLAST so they can find homologs and conserved regions of macromolecules.
- Teach students how to find hydrogen bonds in a binding site and how to find ligands around a metal by noticing functional groups and measuring distances.