HOW TO MAKE YOUR WEBSITE

Use Netscape Composer to make your web page presentation of a 3D structure of your choosing. You will need to download a few template web pages from the biochemistry website, and modify these according to the structure you select and the story you want to tell. For your presentation you will need to include at least one embedded structure as well as a minimum of four buttons that modify the features of the structure, such as the active site or any other pertinent functional region of the molecule. You can work on your presentation in the LSCF or at home, but if you plan to use the LSCF computers you will need a disk (preferably a zip disk) to save your work on.

1. CREATE A FOLDER

So, to get started **create a folder** in which you will keep all of the files needed for your web page. Title this folder with your last name appended to something unique to your presentation, for example sears_snaketoxin, as other students will be also be creating folders for their webs (use lowercase letters please). Place this folder on your desktop to make it easier to find.

2. FIND AND DOWNLOAD YOUR PDB FILE

Using the pull down menu at the top of the biochemistry web pages, select "Getting PDB Files from the Internet":

This will take you to web page with links several other sites (e.g. **Brookhaven PDB** or **Molecules R US**). Search one of those sites for your desired structure. Some keywords will generate long lists of molecules, while other keywords may not.

When you've found the pdb file of interest, **download it** and **note the citation** (journal article) for that structure. **You will need to obtain this article** to help you prepare for your presentation. Save this file in your folder, and name it according to its pdb name. For example, if your protein is Fas, then you would name your pdb file 1ddf.pdb – make sure to include the .pdb extension in the file name. Specifying the pdb name will make your life much easier when you are making your buttons. Repeat this process for each pdb file you download.

3. GET YOUR WEB PAGE TEMPLATES

Go to the "Demo & Downloads" page (which can be linked to via weeks 6 through 11). <u>Right click</u> on the first link, "Frames Page", and select "Save Link As". Save this file in your folder. Do the same for the second and third links. Finally, click on the link to the "Protein Page" and right click on the protein. Select "Save Molecule As" under the File menu:
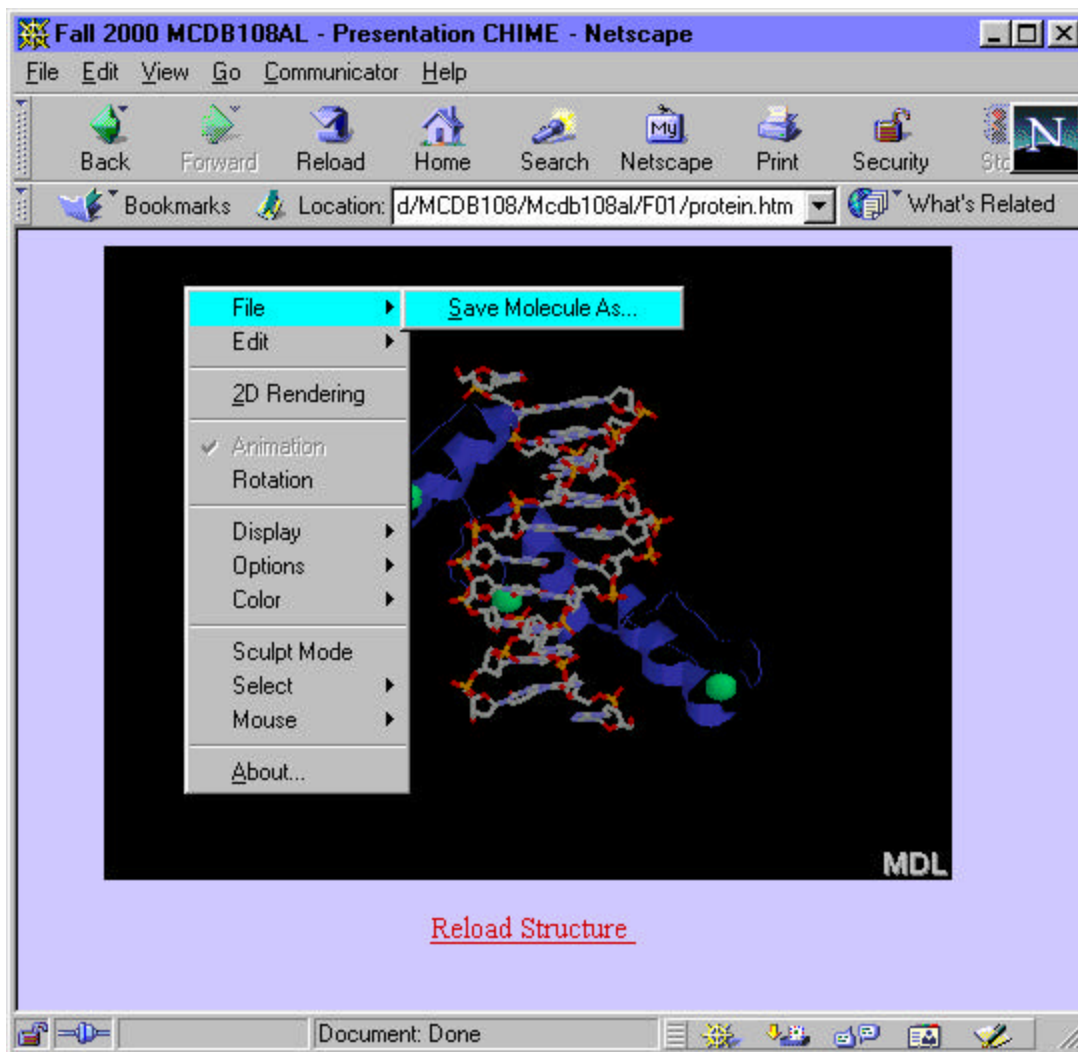

4. DO YOUR RESEARCH

Now that you have your web page templates, you need to gather information on your protein. Start by finding the citation that was listed with your pdb file. Locate the journal article and make a copy. Read through it and get a good idea of what is important and interesting about your structure. You may also want to locate other articles that give a broad background on your protein's physiological function. Are there any illnesses associated with your molecule? Why is it of interest? Ultimately you'll want to compile a few paragraphs detailing the biological importance of your molecule. Take a look at the template presentation and at examples listed in week eleven to get an idea of what students did last year.

5. PUT IT ALL TOGETHER
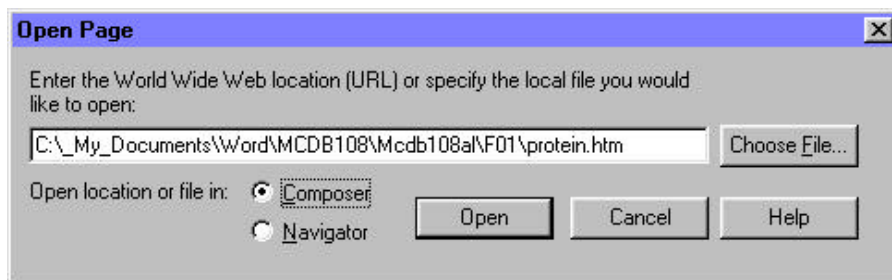### A. PROTEIN PAGE BASICS

Now that you have all of the information needed to put together your website, you can begin to piece things together. Start with the **Protein Page**. Open this page in Netscape, go to the "File" menu, and select **Open Page**…:
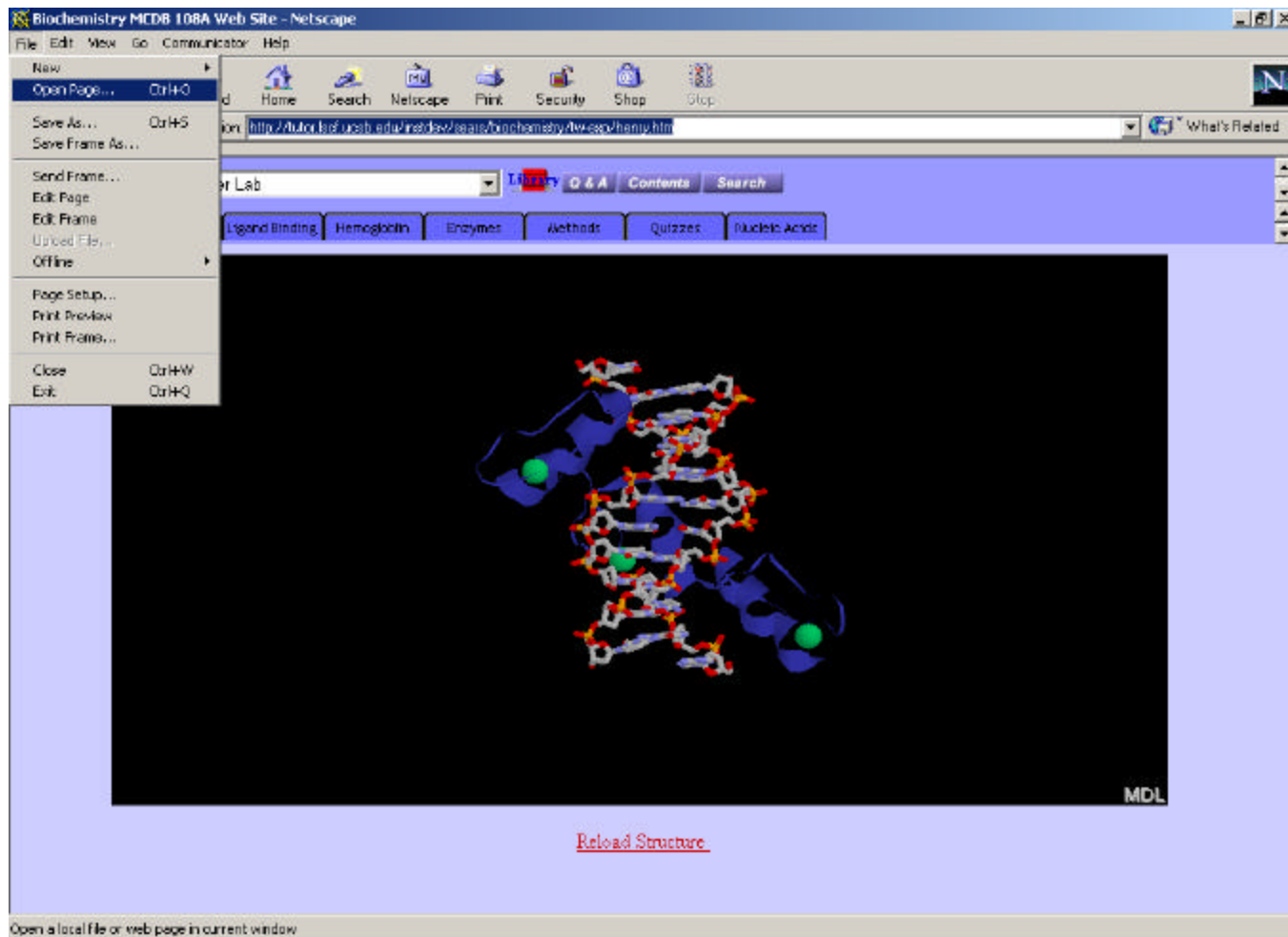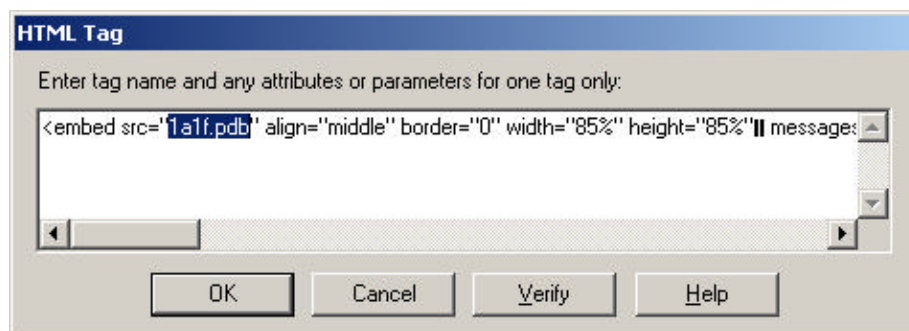

A pop-up window will then appear, choose the "**Protein Page**" from the folder that you saved it in, select **Composer** and choose **Open**:

To put your pdf file into the page instead of 1aif, right click on the embedded object, and choose **HTML Tag Properties**:
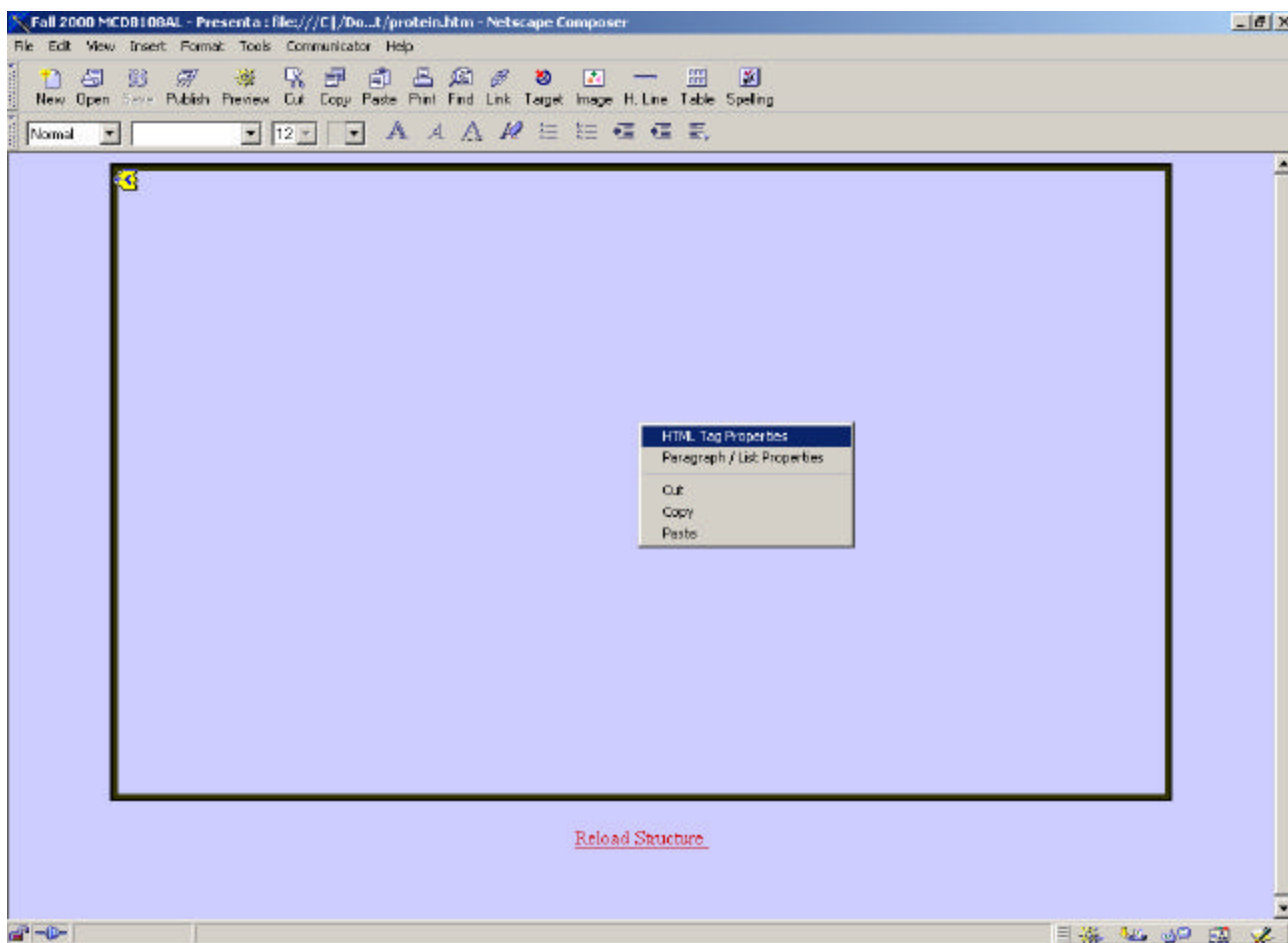
A pop-up menu that looks like this will appear:

Replace the *1a1f* in 1a1f.pdb with your pdb name so that if your pdb name were 1abc it would read src="**1abc.pdb**" for example. Next, scroll to the right and replace the *1a1f* in **name="1a1f"** with your pdb name so that for example it would read **name="1abc"**. The script appears as follows:

```
<embed src="1a1f.pdb" align="middle" border="0" width="85%" height="85%"¦¦messages3d="true"
 name="1a1f" display3d="cartoons" palette="foreground" script="rotate z -134; rotate y 64;
rotate x -174; select protein; ribbons on; color [50,50,170]; select nucleic; cartoons off;
 wireframe 100; select zinc; color [00,204,102]; spacefill 400; select within(5.0,nucleic)
and not hoh; define interacting selected; select zn202, zn203; define hiddenzincs selected;
        select 146-186; define hiddenprotein selected; select * and not hoh">
```

Click save and you are finished with this page.

B. MANIPULATING YOUR PROTEIN & MAKING BUTTONS

Next open "**Buttons Page**" in Netscape Composer, just as you did for the "**Protein Page**". You can edit its appearance, for example the text, the background color, etcetera just as you would in a Word document. (NOTE: If you are taking the creative route, it is often best to insert text into tables as shown in the template because of differences in computer monitors and browsers). To alter the buttons, right-click on the first button and select "**HTML Tag Properties**":
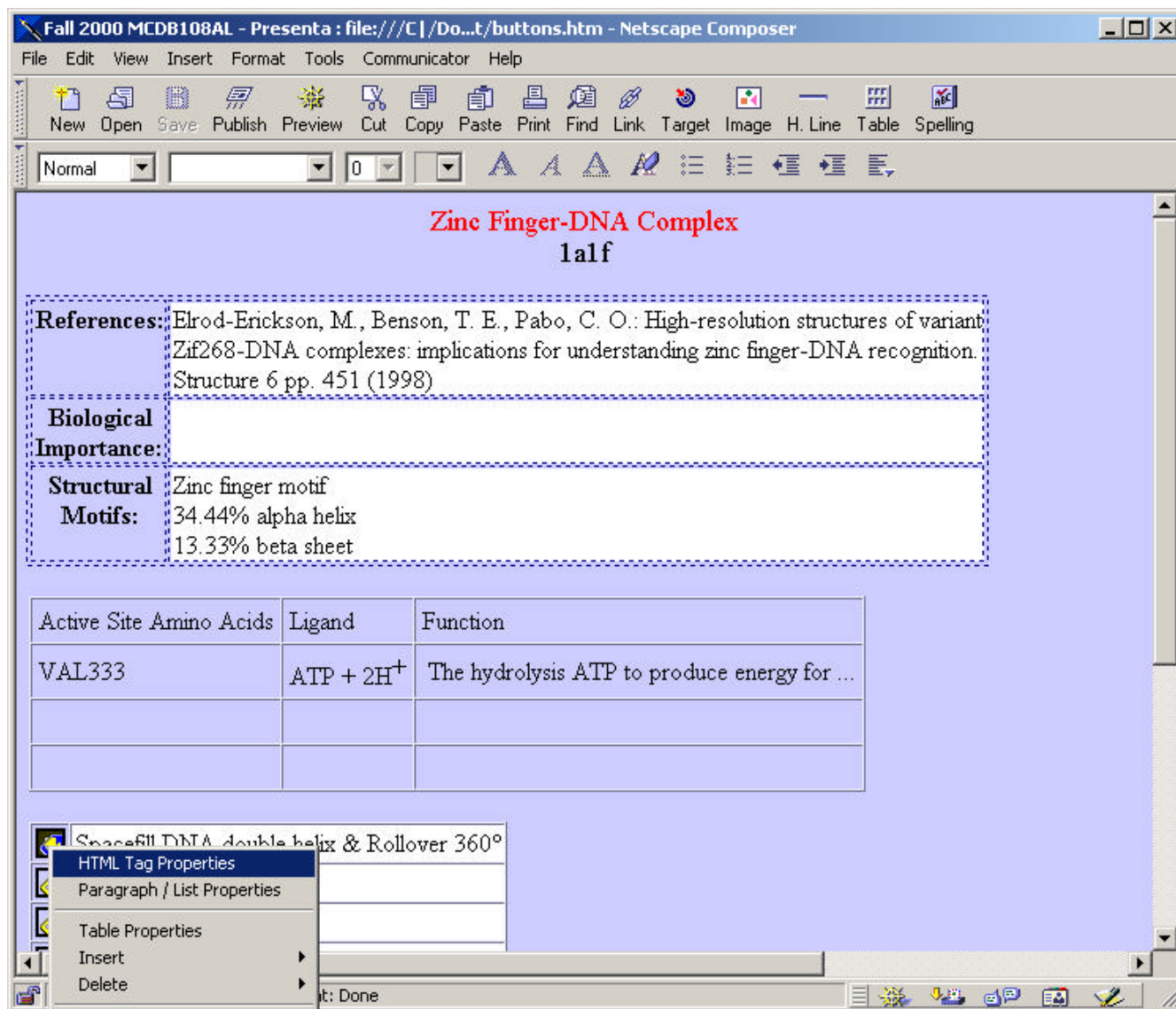
Once again, a pop-up will appear with the HTML inside. Scroll to the right until you find **target="1a1f"**:

HTML Tag

Enter tag name and any attributes or parameters for one tag only:

```
" height="15" type="application/x-spt" target="1a1f" script="select nucleic; spacefill; mov
```

OK   Cancel   Verify   Help

You must change the "**1aif**" to whatever your pdb name is for this button, and for all of the buttons that you plan to use.

Next, in order to change what the buttons do, you must change the script. It is part of the above html, and looks like this:

```
script="select nucleic; spacefill; move 360 0 0 0 0 0 0 0 3;"
```

At first glance this may seem a bit nondescript, but these commands are derived from those used for RasMol. Using the RASMOL COMMAND GUIDE found in week two should help you with your commands.

The main difference between these scripts and the commands we have used throughout the course is that a move command exists here. The nine numbers following this move command correspond to different things. The first three are rotation commands. The first dictates the degree of rotation around the X-axis. The second dictates the degree of rotation around the Y-axis. The third number dictates the degree of rotation around the Z-axis, into the plane of the page. Experiment with altering these one at a time to see how they affect your protein. The next number directs zooming. If you set this to zero, it will not zoom. If you set it to a positive number it will zoom in, but if you place a negative number before the quantity you put in, it will zoom out. Again, experiment with this parameter. The following two numbers direct translation. The first directs translation in the X direction, with positive numbers moving the protein to the right, and negative numbers to the left. The second directs translation in the Y direction, with positive values directing downwards and negative values directing upwards. The second to last number directs "slab mode". Slab mode cuts off your protein as if it were a loaf of bread so that you can view inside of it. This number dictates how deeply into your protein you would like to cut. If you don't understand what I am getting at, try it out. Finally, the last number is the load time. All of the previous values that you have entered will be implemented over a time period that is directed by this last value.

Repeat this process for all subsequent buttons.

C. DEFINING GROUPS

Knowing how to group atoms will also help you create easier scripts for buttons. To do this, open the "Protein Page" and right-click, selecting "HTML Tag Properties". Here, you may create defined groups to use later on your "Buttons Page". In order to define a group, you must place the following in the script: "select [parameter]; define [arbitraryname] selected". If you scroll to the right in the HTML Tag Properties, you will find the following three examples of defined groups:

```
script="select within(5.0,nucleic) and not hoh; define interacting selected; select zn202,
        zn203; define hiddenzincs selected; select 146-186; define hiddenprotein selected"
```

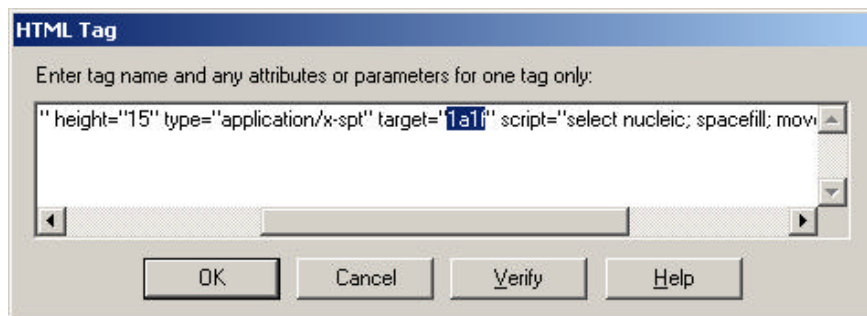The first of the three define commands above selected all atoms except for water that are within 5.0 Å of nucleic acid (in this case DNA) and defined those atoms as "interacting". So if one were to make a button that said, for instance: "select interacting; spacefill; color red" then those atoms would be spacefilled and colored red. The second defined two of the zinc molecules (selected using their atom names) as "hiddenzincs", while the third example selected a series of amino acid residues by their numbers (146-186) and defined them as "hiddenprotein". The names that you use to define the groups selected can be anything except for those that are already used in Rasmol/chime commands. Please see the RASMOL COMMAND GUIDE if you are not familiar with the commands or names used.

6. FINISHING TOUCHES

Now that you know the basics, a few hints:

?? Keep your page simple – avoid flashy colors & patterns, small or condensed fonts, & busy design.

?? Put your elements (such as text, buttons, graphics, etcetera) in tables! This assures that both viewers with regular and wide monitors will see your page properly.

?? Use lowercase letters when naming folders, documents, pdb's, etcetera.

?? For each table, *uncheck* the Table width & Table min. height boxes & **Cell width** and **Cell min**. height boxes:
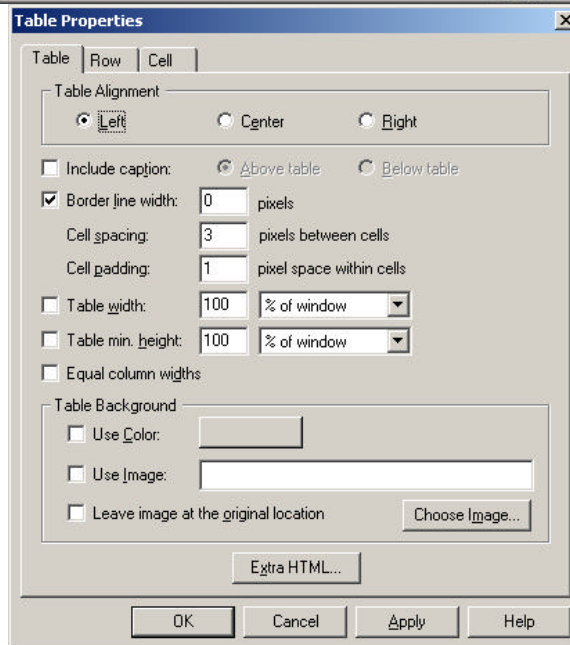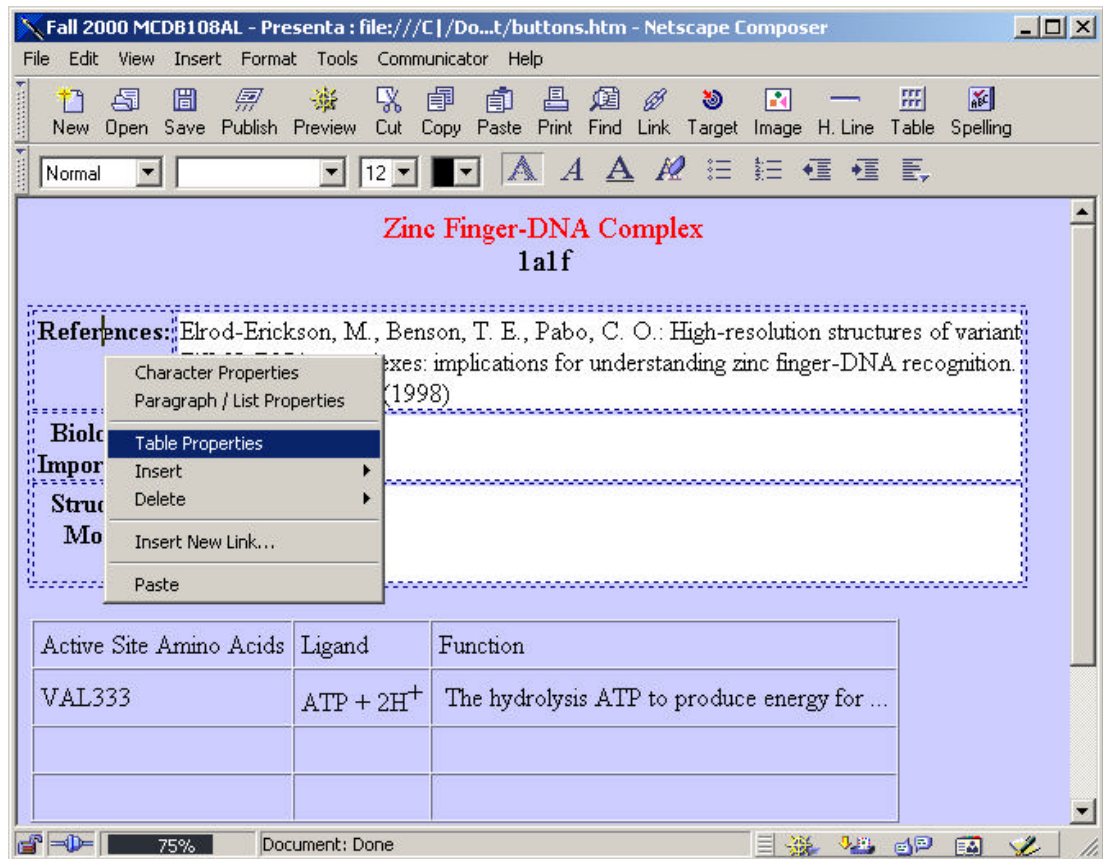
?? Start this project **EARLY!!! See your TA at office hours or contact him/her via email with any questions!**