JMOL/JSMOL TUTORIAL

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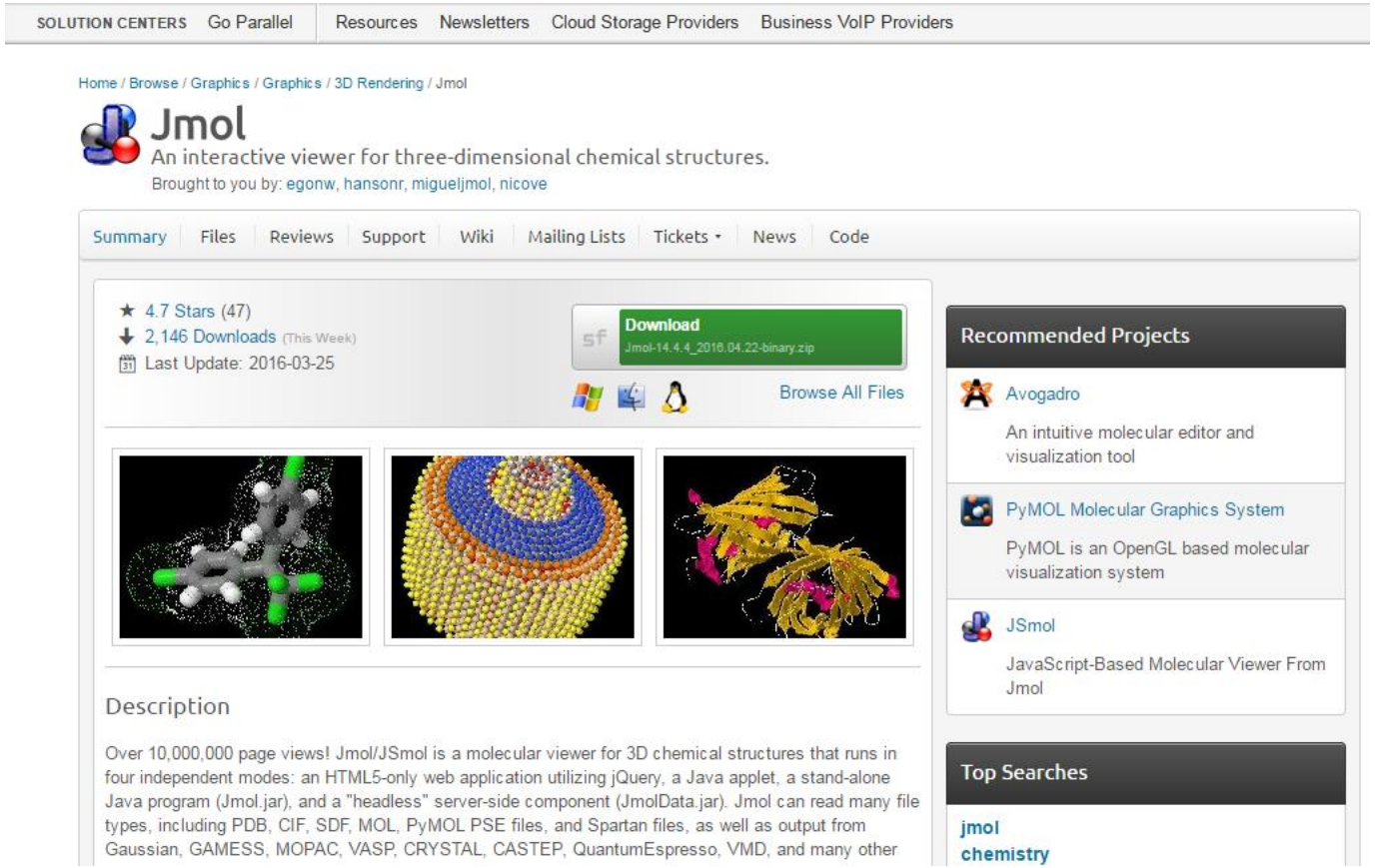
1) DOWNLOAD JMOL APP OFF OF SOURCEFORGE

https://sourceforge.net/projects/jmol/?source=typ_redirect

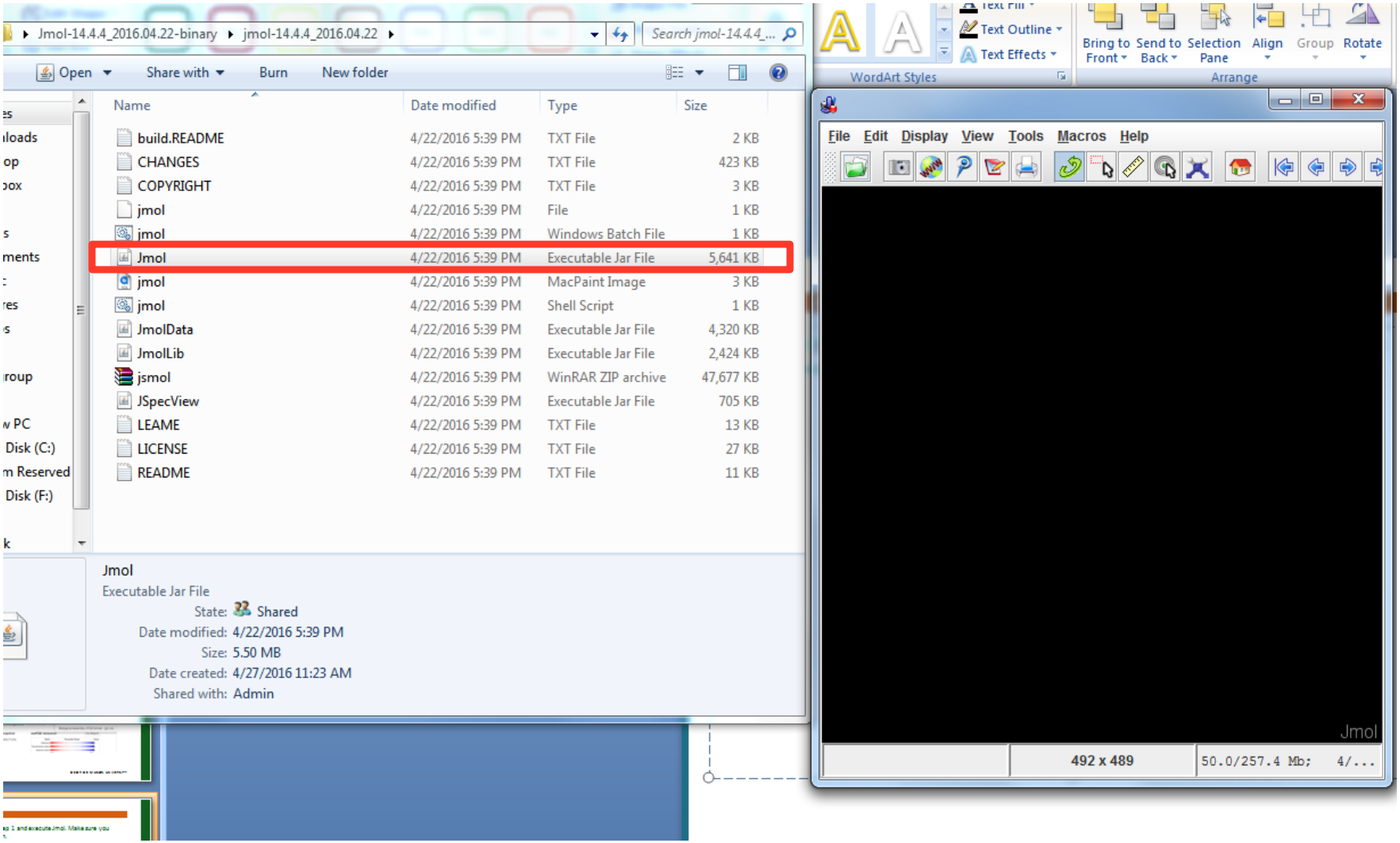


2) DOWNLOAD YOUR PROTEIN PDB FILE

- Search for it on RCSB.

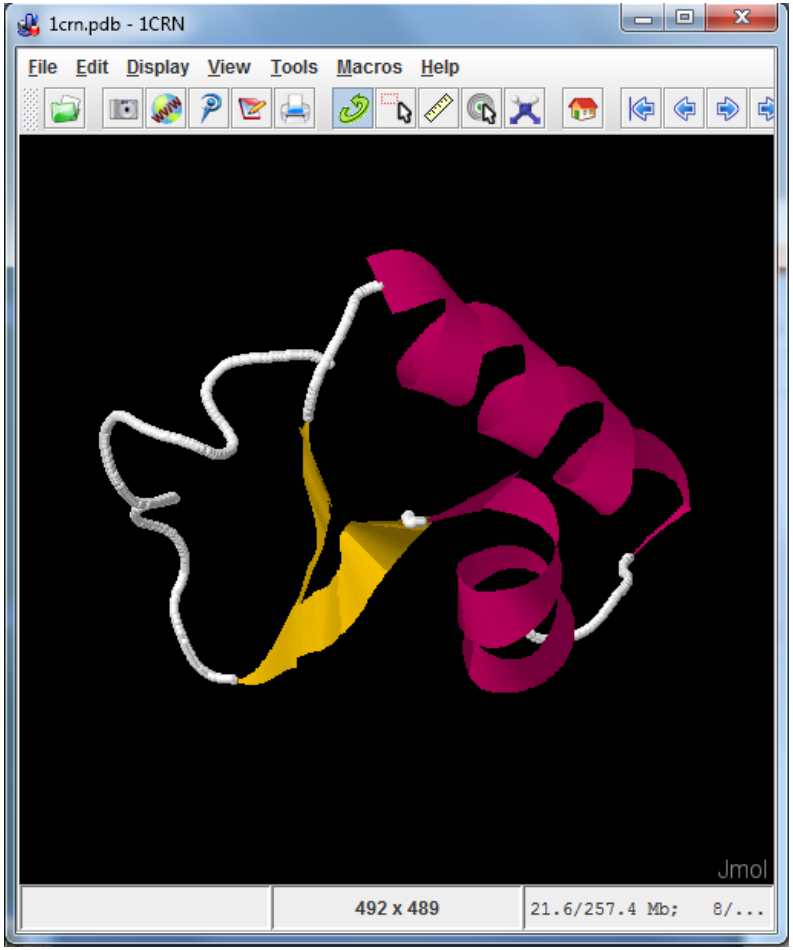
3) EXECUTE JMOL

- Unzip the jmol file you downloaded in step 1 and execute Jmol (Executable Jar File). Make sure you have Java updated to the latest version.



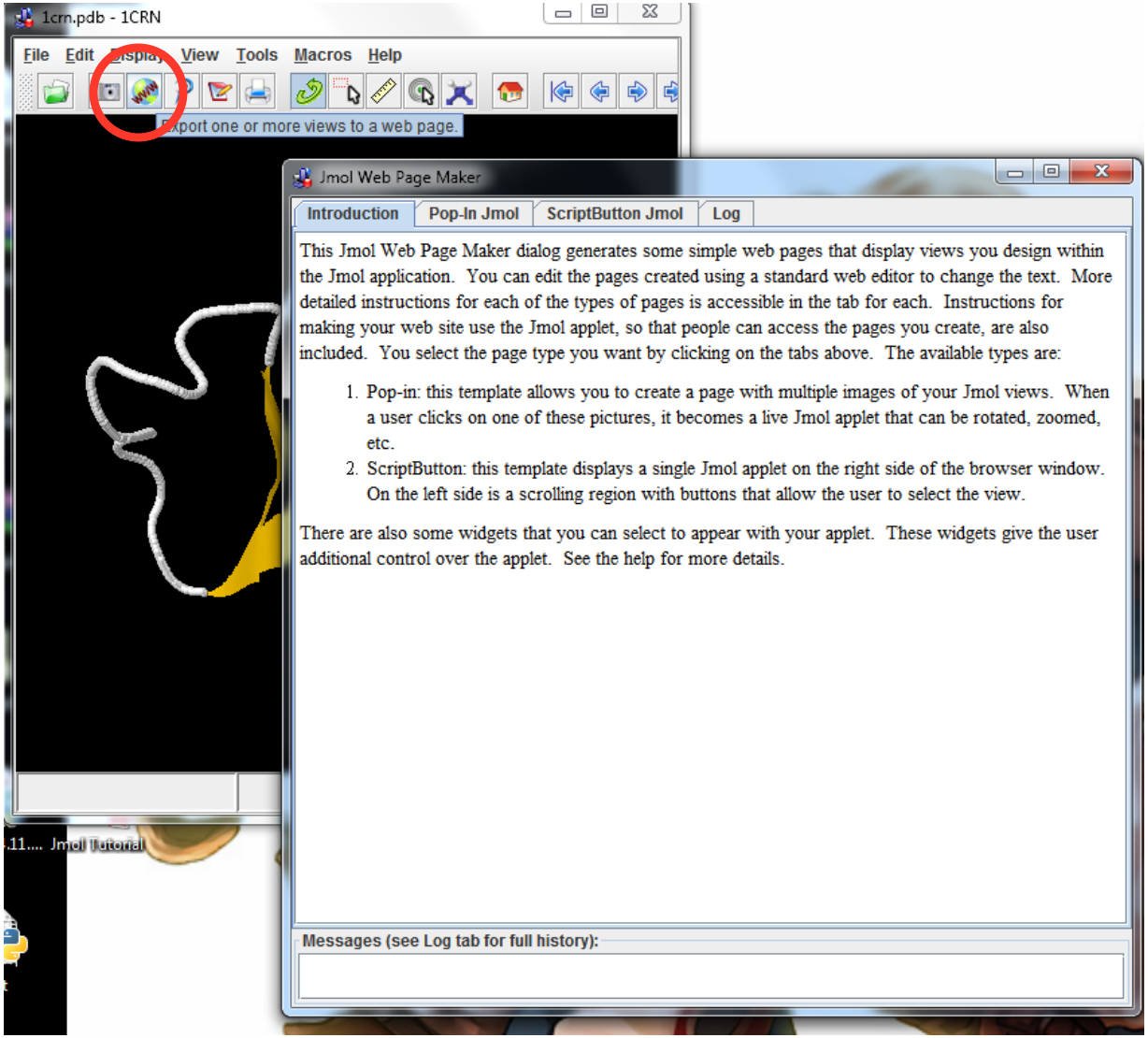
4) OPEN YOUR PDB FILE

- Select the “File” tab and click “Open”
- Navigate to where your .PDB file is saved and open it. The 3D model of the protein should appear

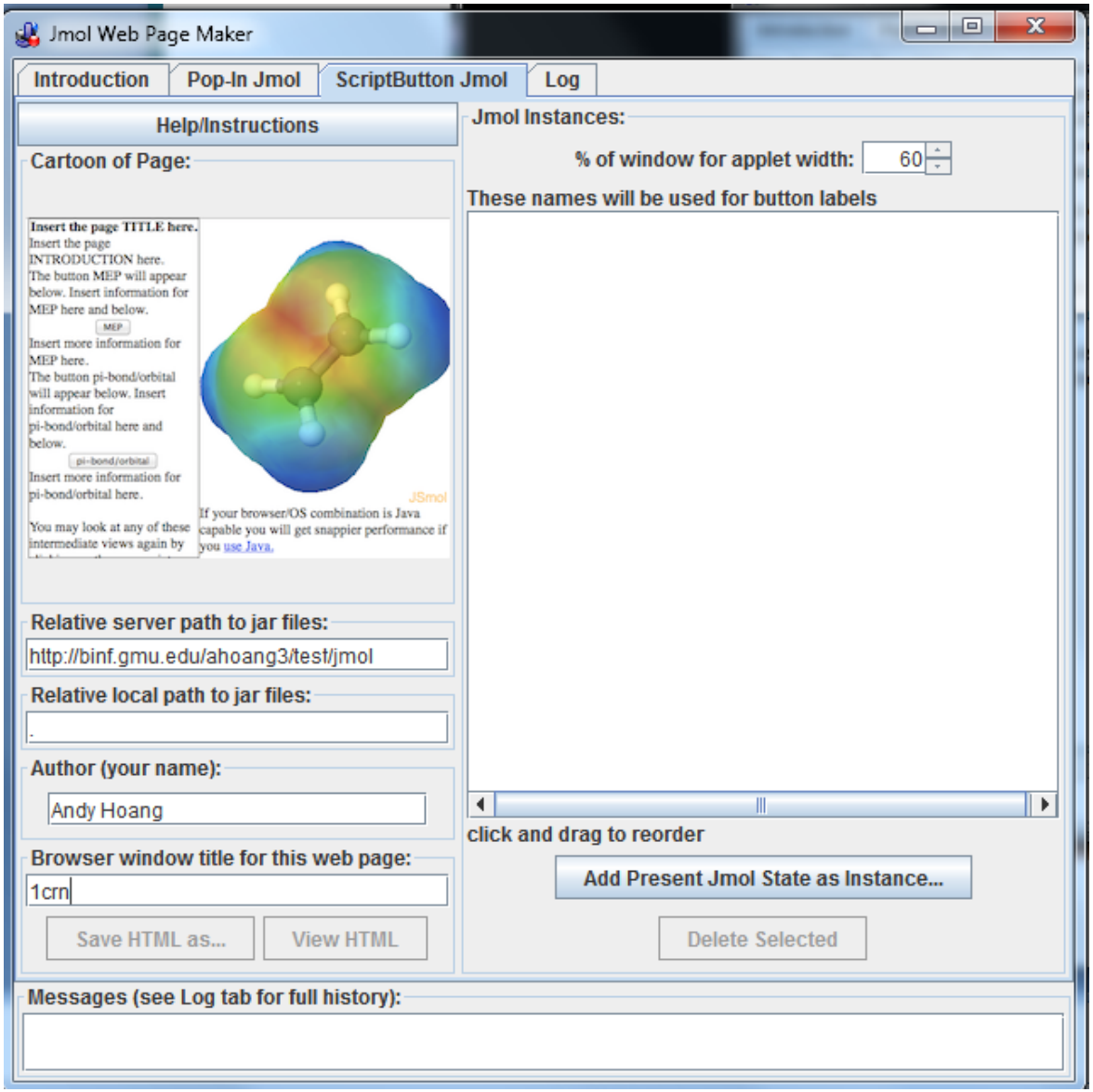


5) EXPORT PDB AS A WEBPAGE

- Click the little globe icon on the upper left hand corner

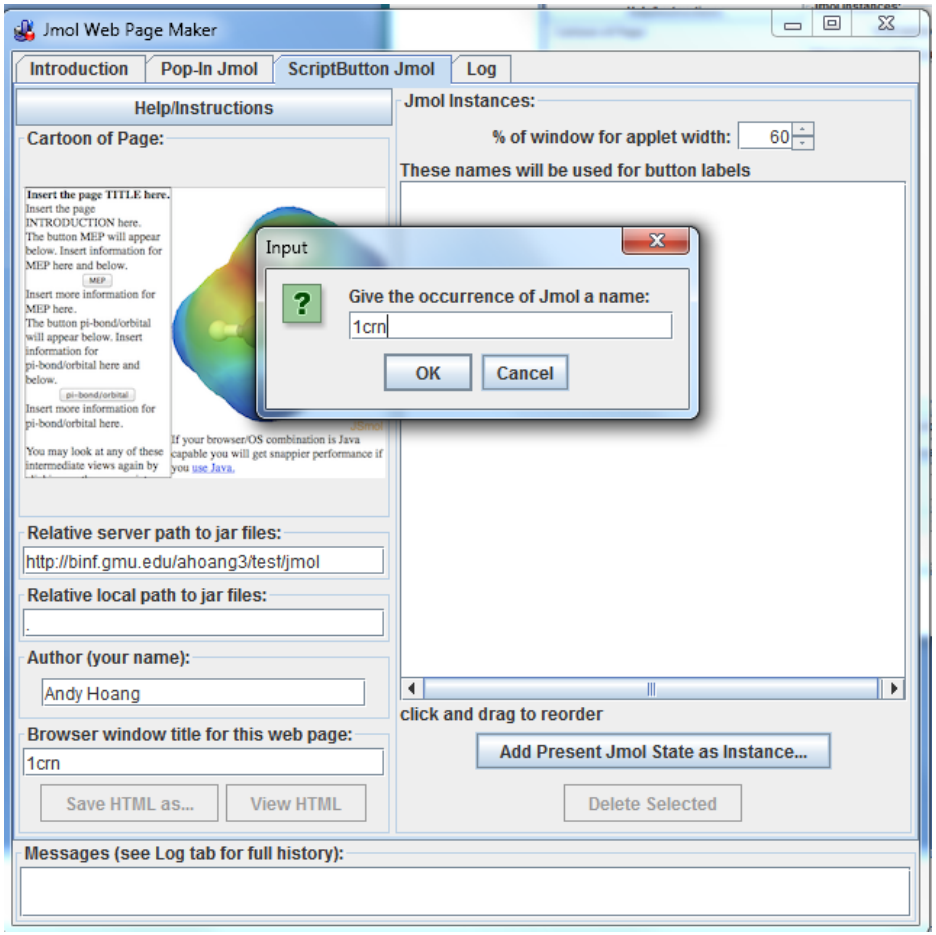


6) NAVIGATE TO SCRIPTBUTTON JMOL TAB



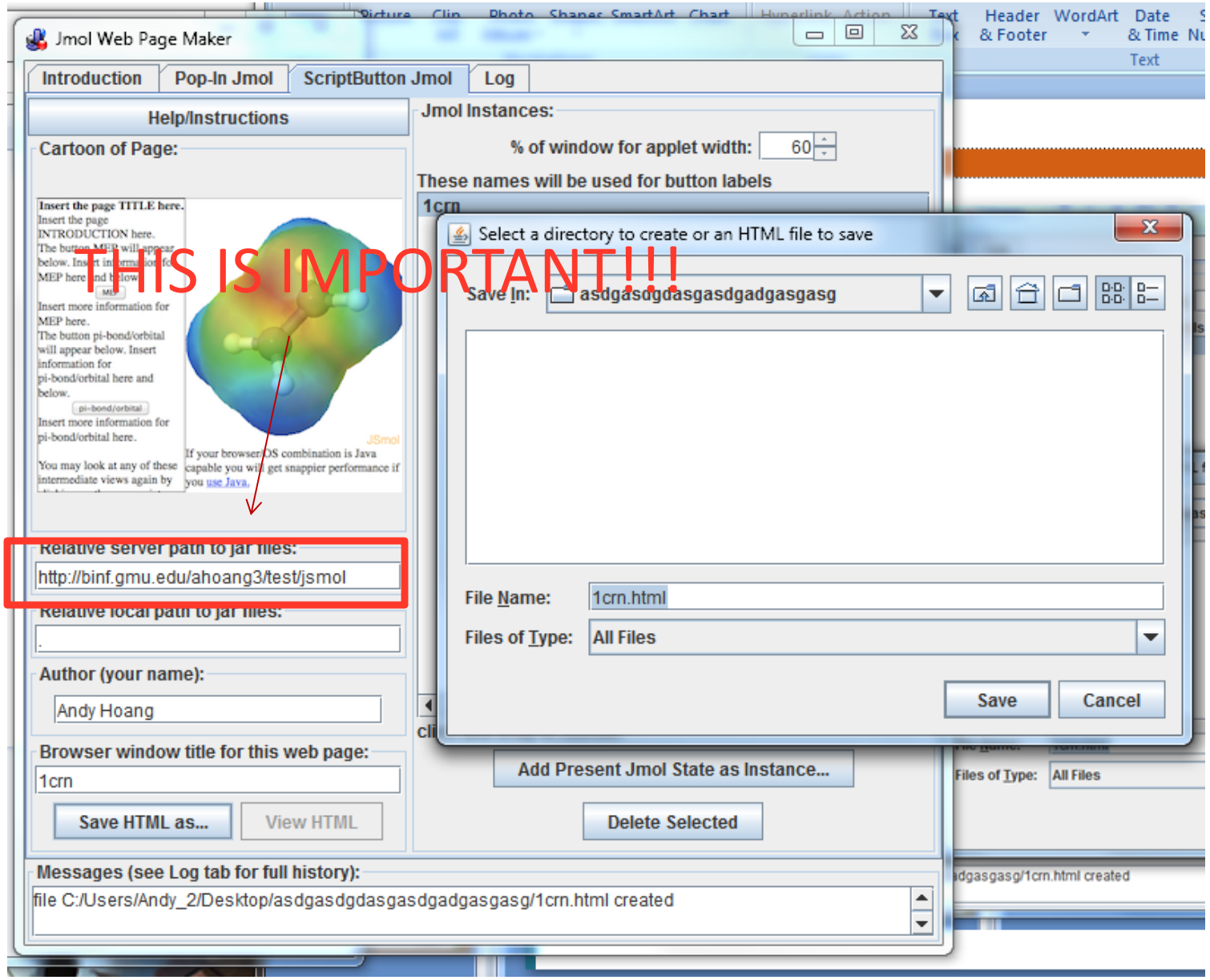
7) ADD JMOL STATE

- Click “Add Present Jmol State as Instance” to save what protein jmol window is currently viewing. Name the instance and hit “Ok”
- You can even add multiple states if you wish to have a list of PDB proteins to view on your page. Simply repeat steps 2-7 for each different PDB protein



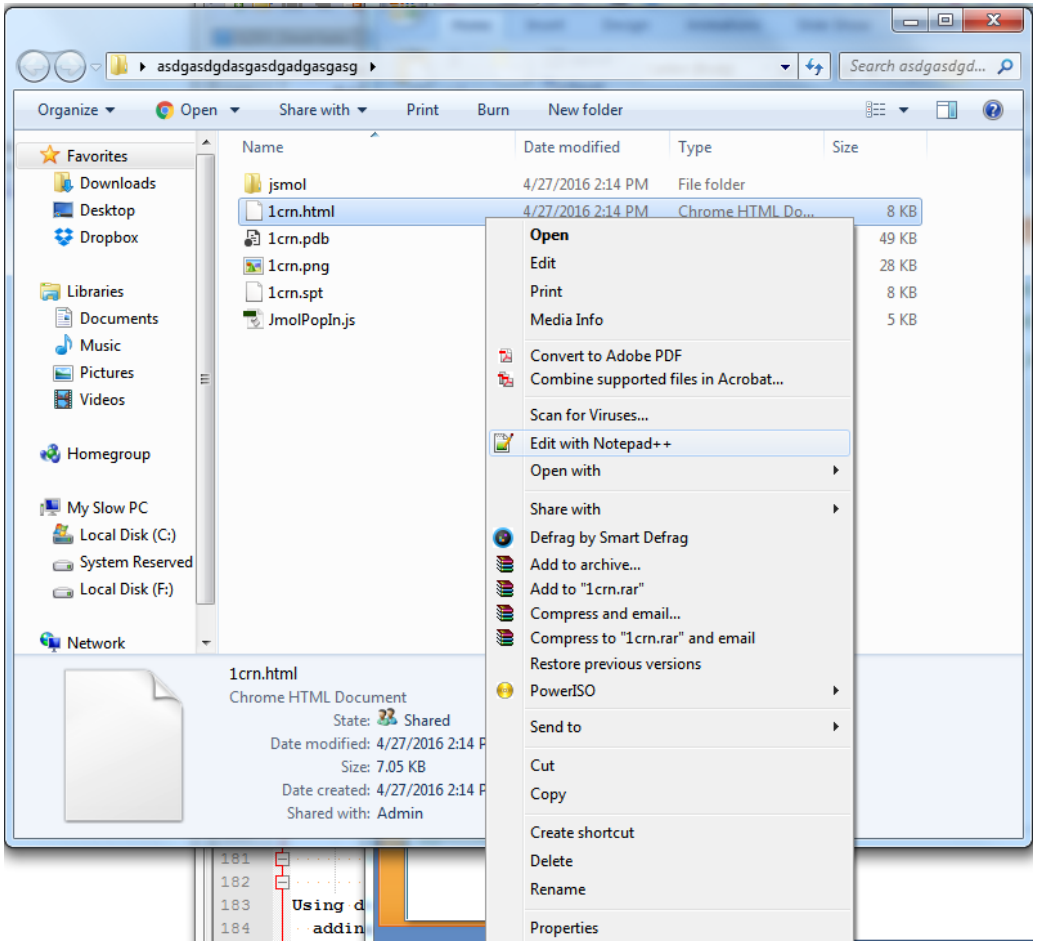
8) SAVING THE HTML (THIS IS TRICKY!!!)

- Be sure to know the URL to where your BINF files will be added for this assignment. (For example: binf.gmu.edu/ahoang3/test) Do not include "public_html"
  - If you're not sure, check using WinSCP or a similar drag and drop tool for SSH
- In the "Relative server path to jar files" text box, input the URL to your HTML pages and add "/jsmol" to the end (http://binf.gmu.edu/ahoang3/test/jsmol)
  - The "s" in jsmol is important!
- "Relative local path to jar files" can be left with a "."
- Enter the Author and Browser window title and then hit "Save HTML as…" and save it as an .html file


Jmol Web Page Maker
Introduction
Pop-In Jmol
ScriptButton Jmol
Log
Help/Instructions
Cartoon of Page:
Jmol Instances:
% of window for applet width:
60
These names will be used for button labels
1crn
THIS IS IMPORTANT!!!
Select a directory to create or an HTML file to save
Save In:
asdgasdgdasgasdgadgasgasg
File Name:
1crn.html
Files of Type:
All Files
Save
Cancel
Relative server path to jar files:
http://binf.gmu.edu/ahoang3/test/jsmol
Relative local path to jar files:
.
Author (your name):
Andy Hoang
Browser window title for this web page:
1crn
Save HTML as...
View HTML
Add Present Jmol State as Instance...
Delete Selected
Messages (see Log tab for full history):
file C:/Users/Andy_2/Desktop/asdgasdgdasgasdgadgasgasg/1crn.html created

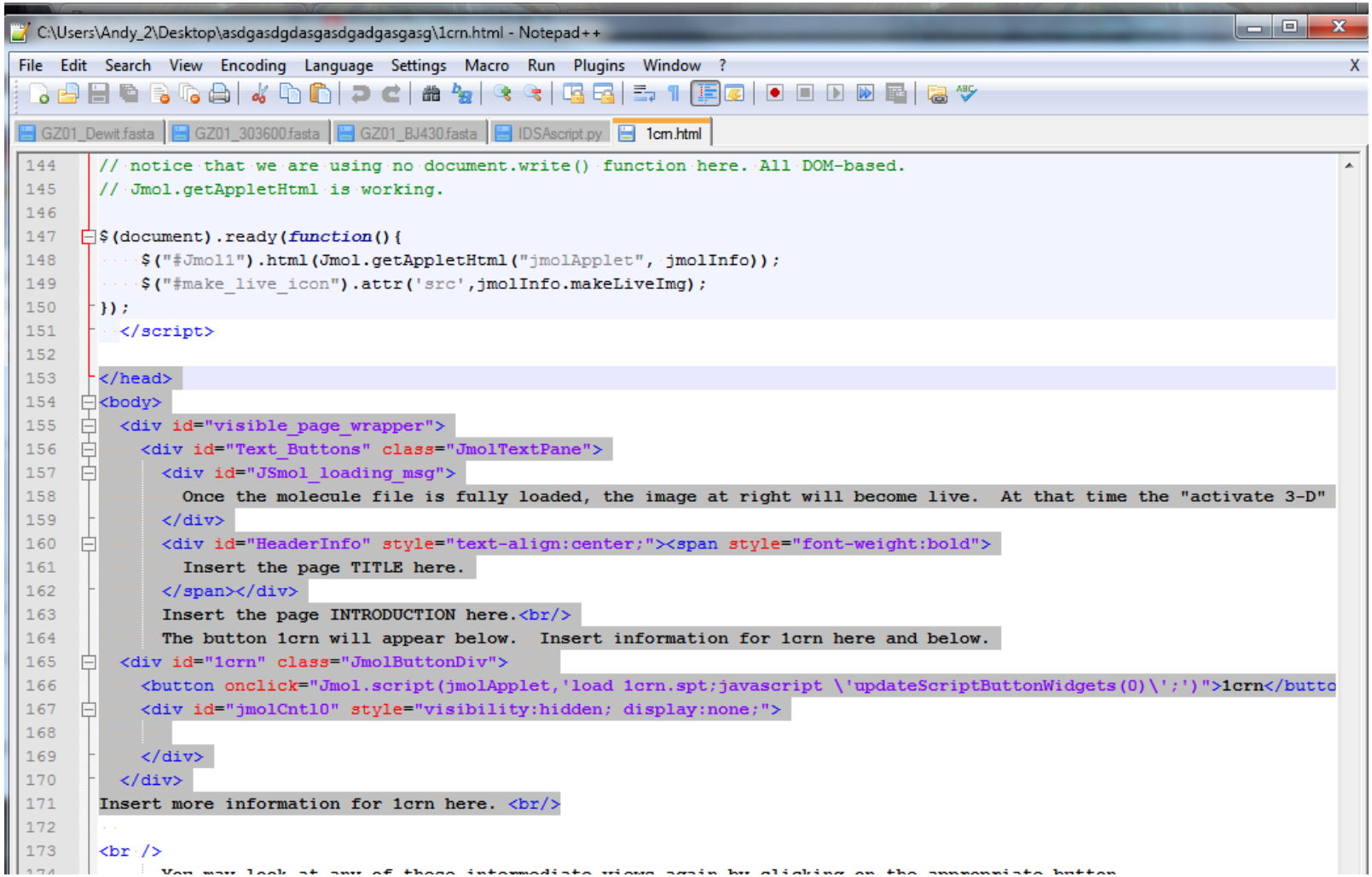
9) EDIT YOUR JMOL HTML FILE

- After you hit “Save HTML as…” an html file should generate along with the necessary jmol files to run it on your webpage.
- Manually edit the html file using a text editor, such as Notepad++ or TextWrangler.



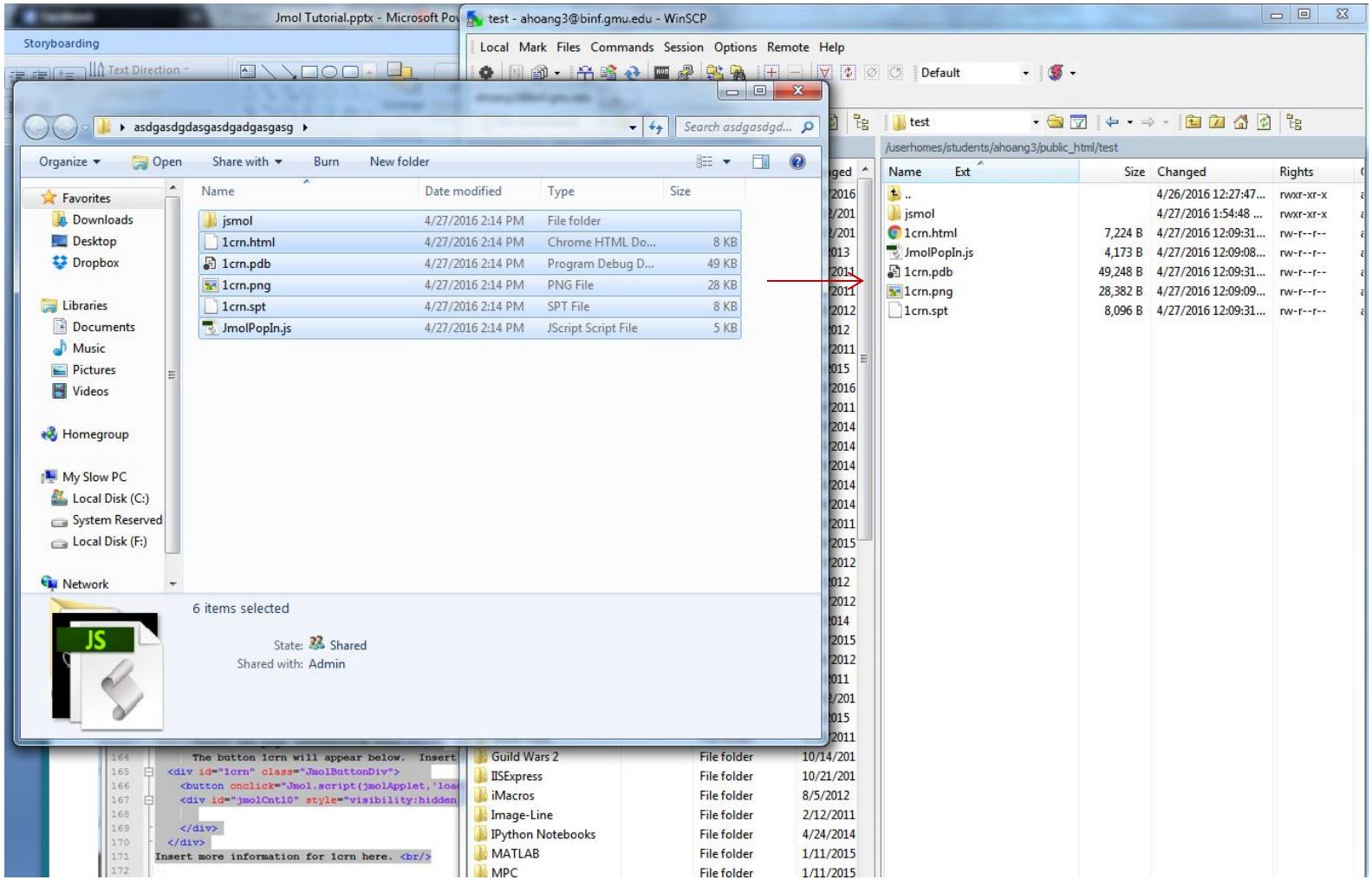
HTML EDITING CONTINUED

Scroll down and find this section of code. This is where you can edit for more details on your PDB file. Don't edit anything else unless you know what you're doing. Save when done.



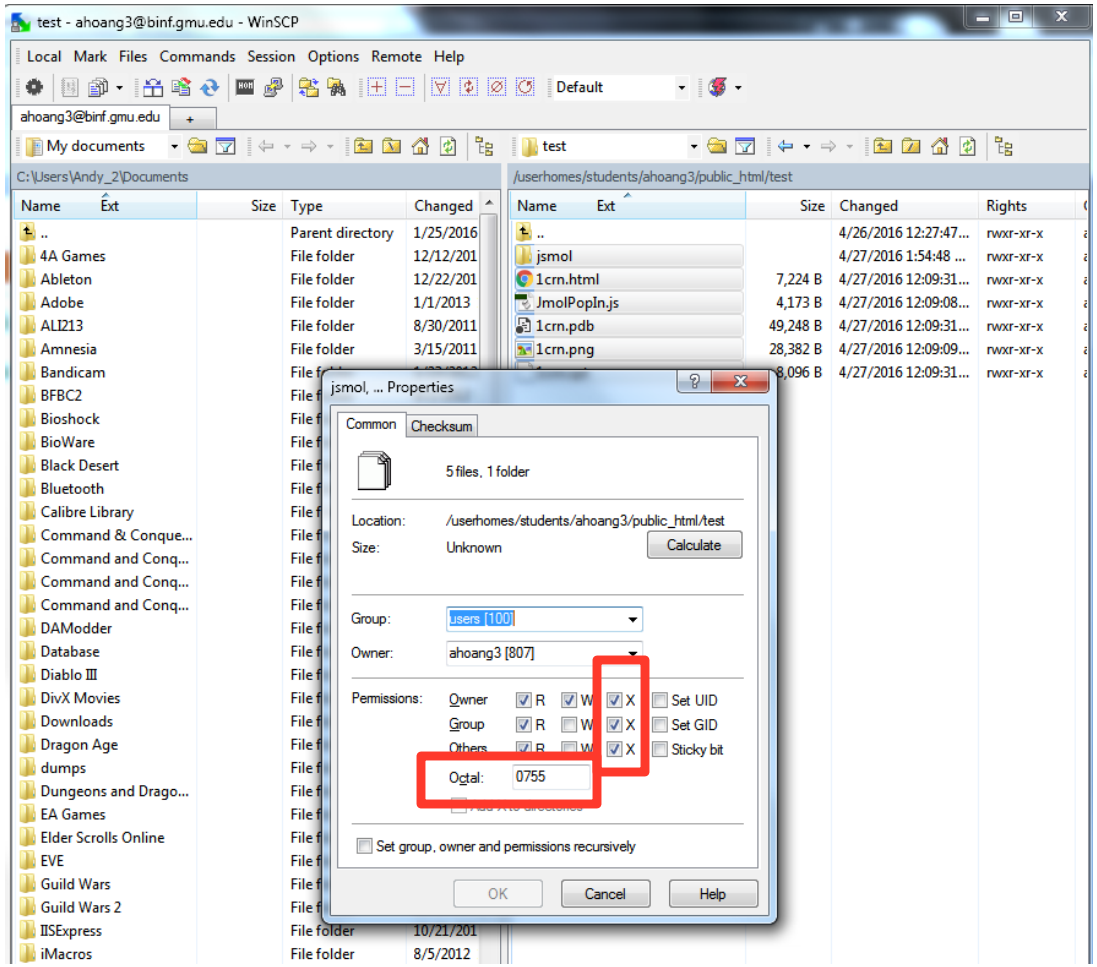
10) TRANSFER FILES TO BINF

- Transfer all your files to your binf server and where your project is stored using WinSCP or an equivalent program



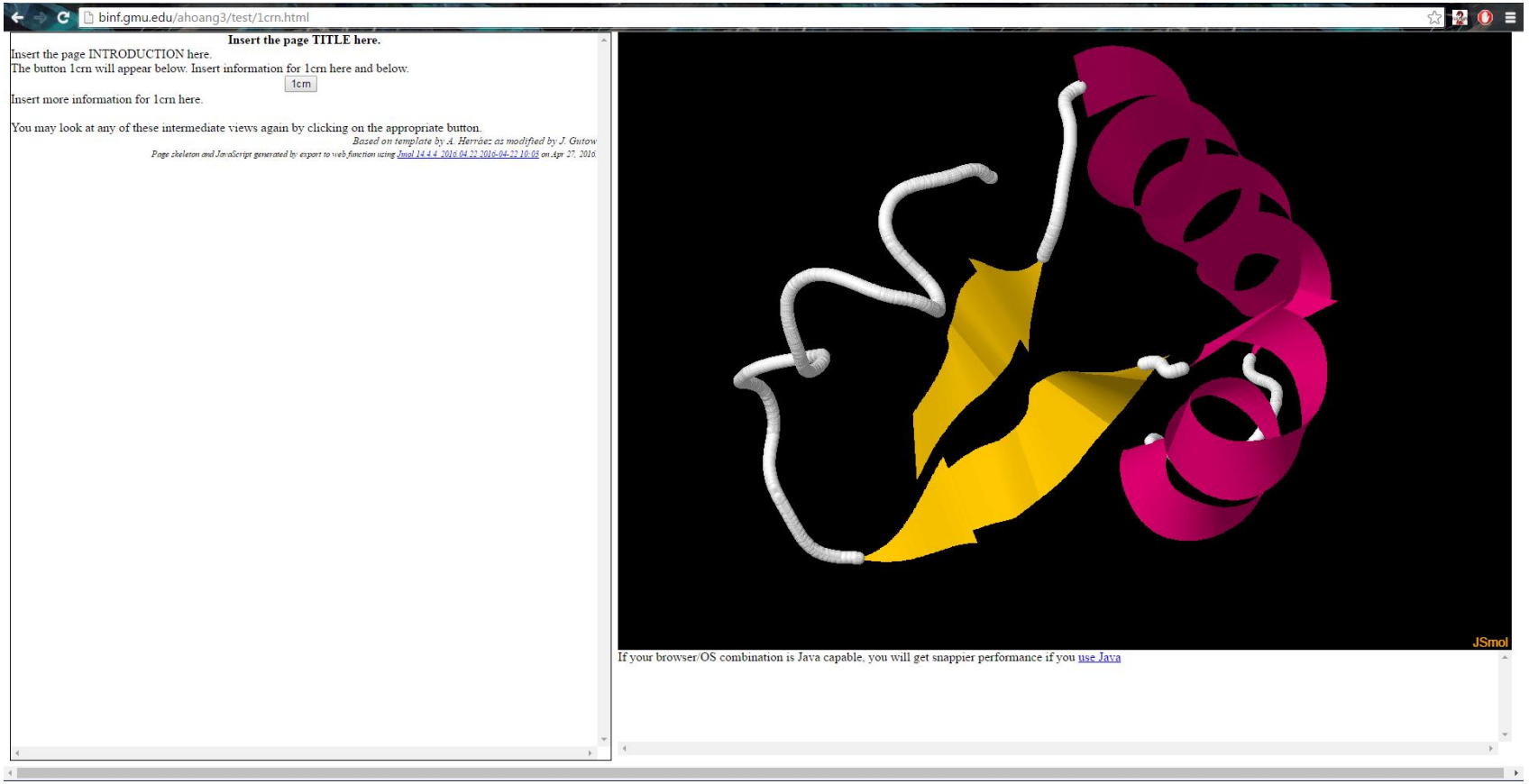
SET ALL FILES TO BE EXECUTABLE

- Highlight over all your files and click “Properties”
- Set all of the permissions to be exactly like the image below or manually type “0755” as the octal. Hit OK when finished



11) CHECK TO SEE IF THE PAGE IS WORKING

- Type the URL of where the jmol html file is stored. For my file, it was: http://binf.gmu.edu/ahoang3/test/1crn.html
- Check to see if it runs. If it does, yay! If not, double check the steps above and retry...



CONTACT

Feel free to email me any questions or concerns:

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