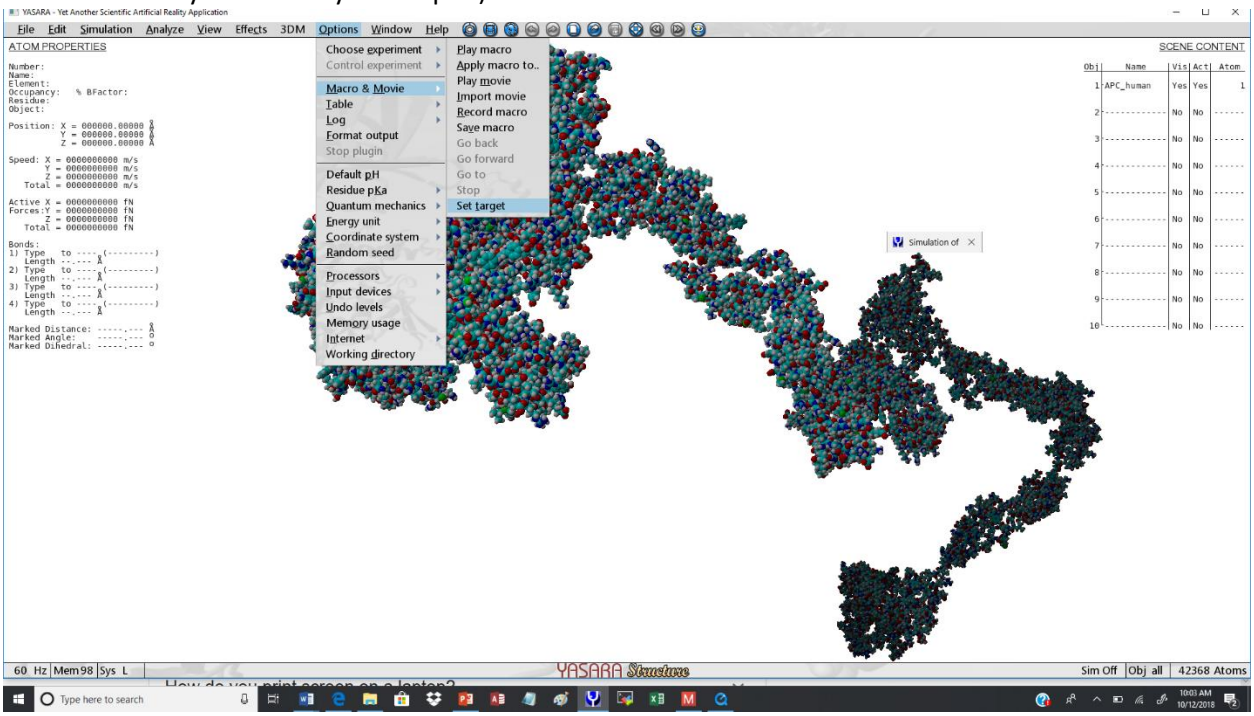
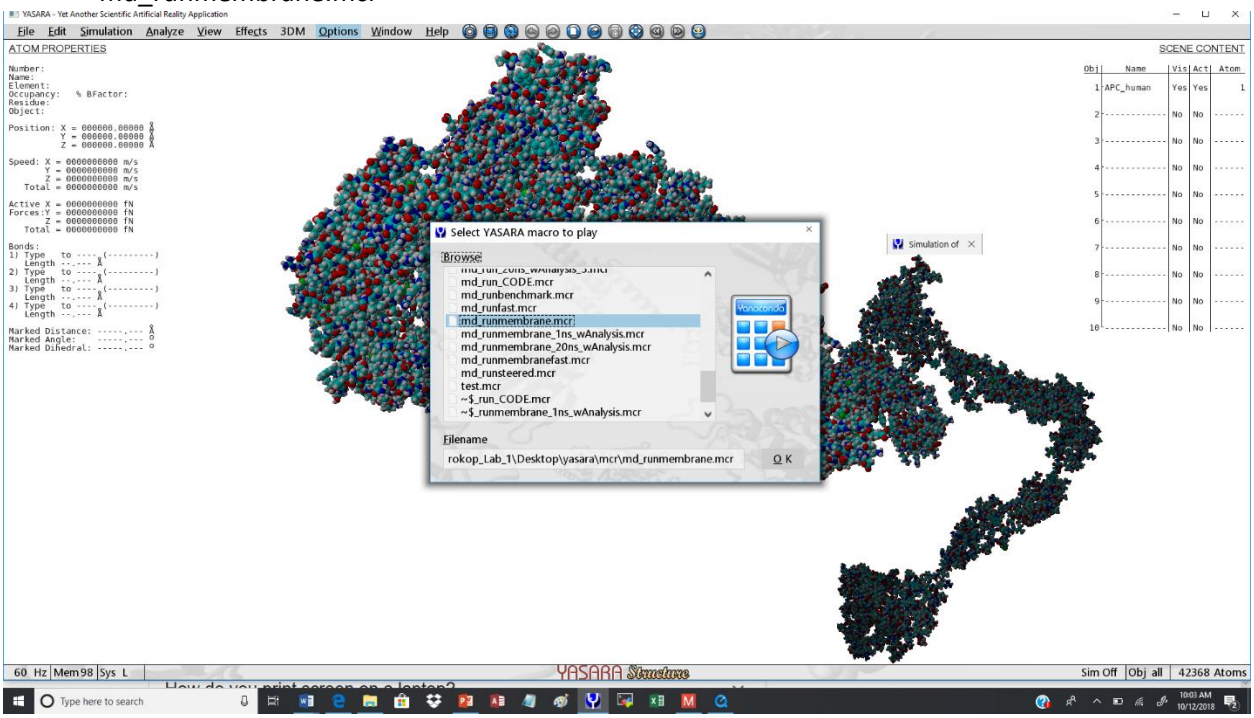
Transmembrane Protein MDS

1.) Open .pdb file inside of YASARA (.sce & .yob files will not work for this purpose)

2.) Select the target by clicking Options-> Macro & Movie-> Set Target (this is when you will select the model that you currently have open)



3.) Now tell YASARA which macro to run by clicking Options-> Macro & Movie-> Play Macro-> md_runmembrane.mcr



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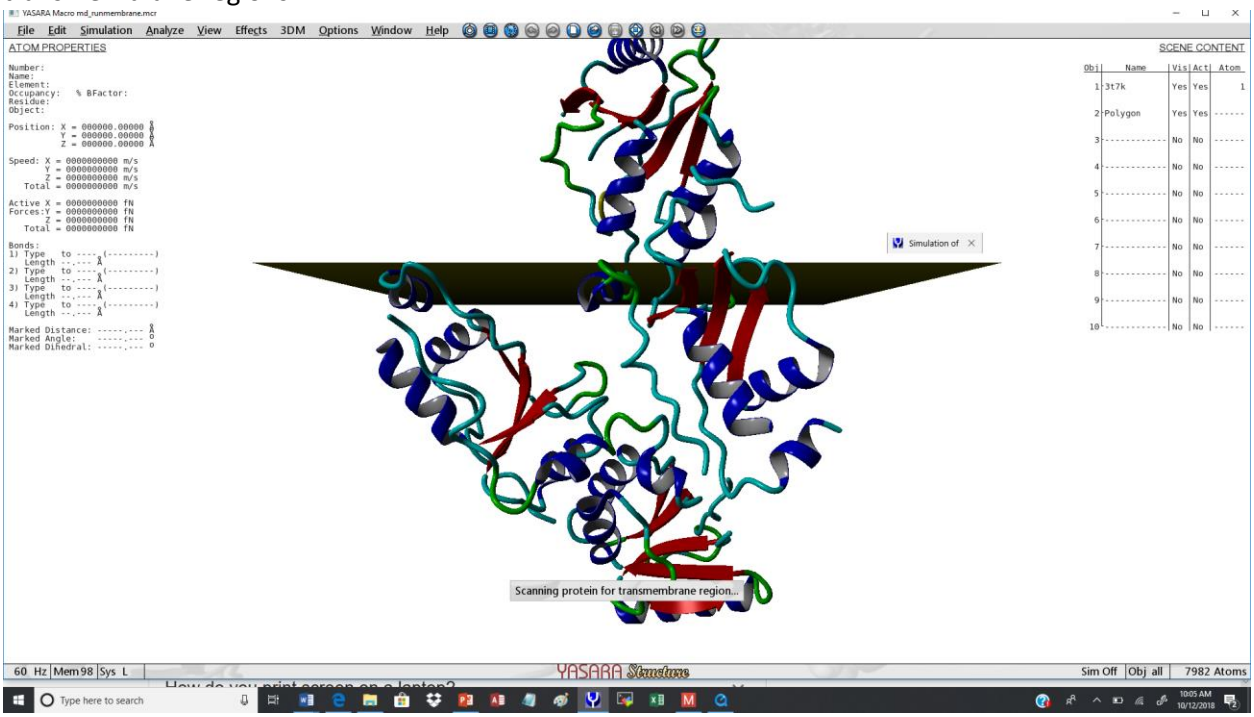
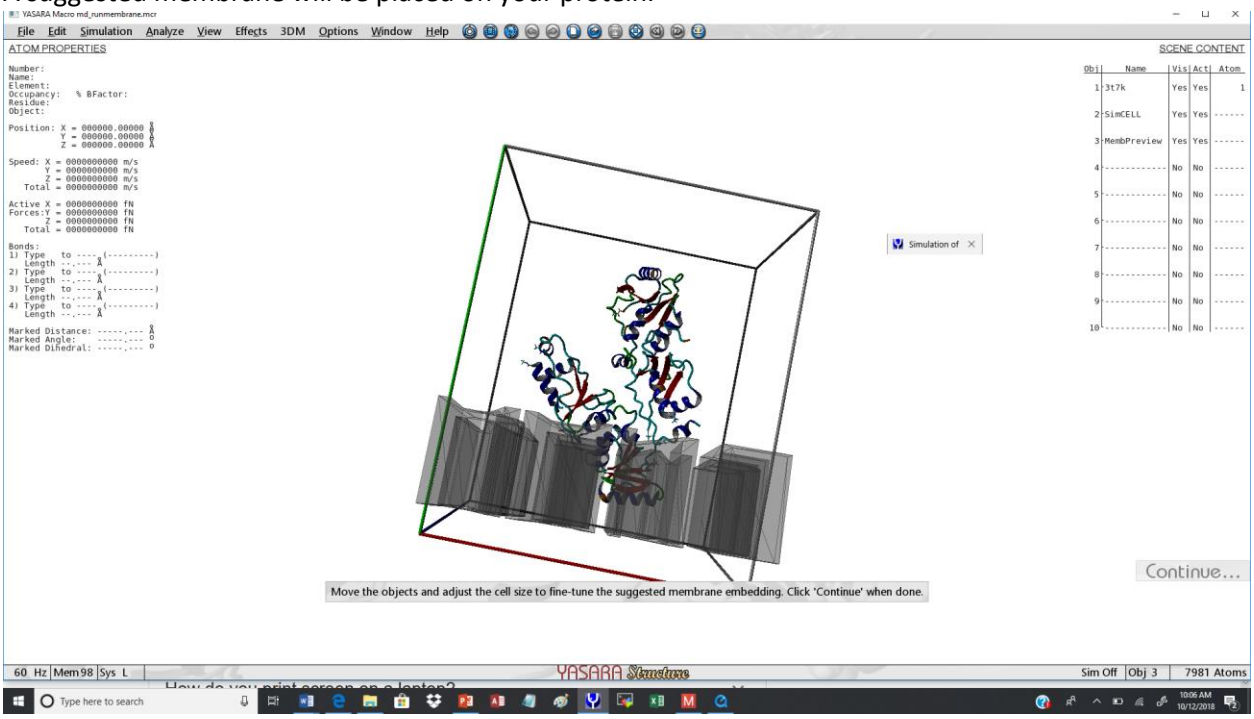
4.) YASARA will now scan your protein for exposed hydrophobic regions that suggest potential transmembrane regions



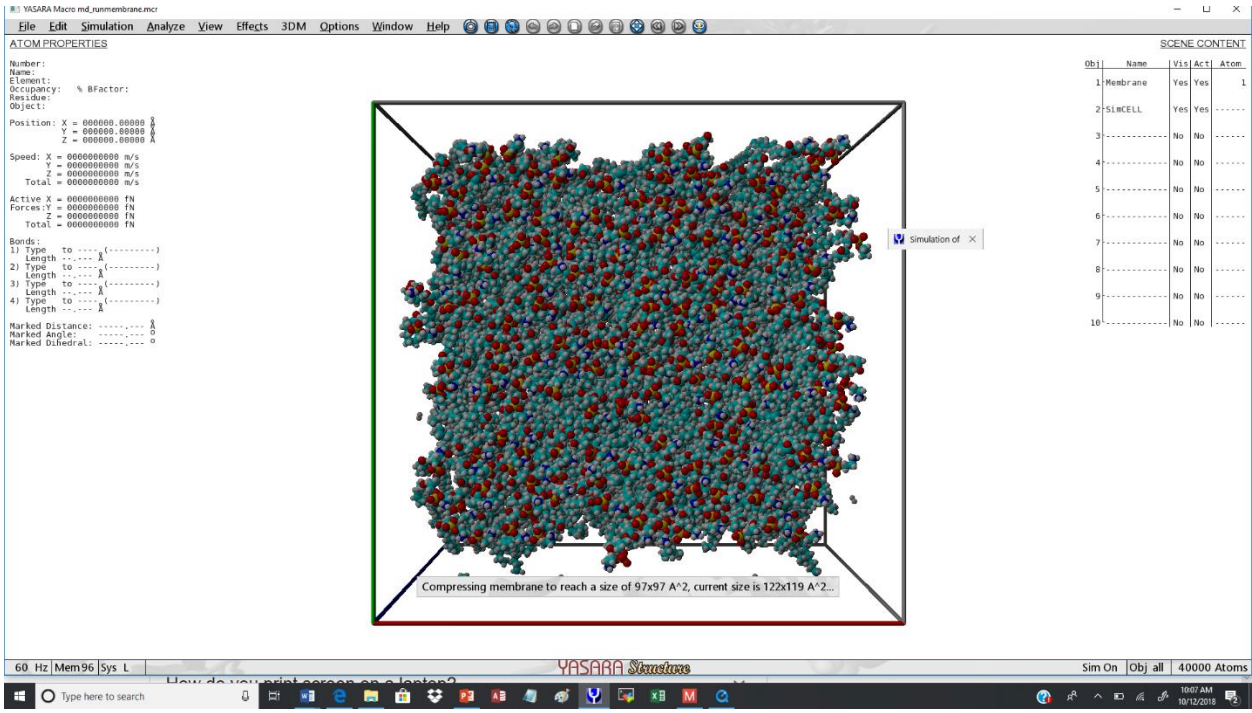
5.) A suggested membrane will be placed on your protein.



a. You can edit location and orientation of your membrane by clicking shift twice to control Object 3

Transmembrane Protein MDS

b. Select Continue when content with membrane location and orientation



c. IMPORTANT: Yasara is not always accurate. Be sure to compare predicted membrane location with outside sources.

6.) YASARA will now build the actual membrane using default conditions. These conditions can be edited in the actual macro document. (current options are phosphatidyl-ethanolamine, -choline, and -serine)

7.) YASARA will slowly build out the membrane inside of the simulation cell

8.) Occasionally there will be an error stating that the membrane exploded

a. This usually means that your membrane location was not optimal. Trial and error is the best way to fix this issue.

9.) Once the membrane has been completely built a 250 picosecond molecular dynamic simulation will occur to stabilize your protein in the membrane environment.

10.)You should now have a protein embedded in a lipid transmembrane environment.