Plan for reproducing key results from “Conservation and Role of Electrostatics in Thymidylate Synthase”

- To reproduce the key results, we’ll need computational models of thymidylate synthase from *homo sapiens*, *E. coli*, and W.g.b.
  - For the former two, there are many structures of TS in the PDB. Garg et. al. used PDB ID 1HVY for *homo sapiens* and 2G8O for *E. coli*
  - For the latter, we will use a model from the I-TASSER web server
- Next, we’ll align the models with the MultiSeq module in VMD
- We’ll then calculate the electrostatic potential with PDB2PQR and APBS
- Finally, we’ll visualize the results in VMD

- In interest of time, I will not ask you to do every step. Instead, I will guide you through what I did and ask you to download results from previous calculations.

- Getting structures from the PDB (https://www.rcsb.org/) is pretty straightforward.
- For a particular crystal structure, you can just click on “Download Files” and select “PDB format”
- We will use the PDB files for 1HVY and 6NNR, which has superceded 2G8O.
- Next, let’s go through getting a model for W.g.b. thymidylate synthase.