INTRODUCTION - Understanding and portraying how proteins fold into their different biological states is important in understanding how proteins act and for the design of new proteins. Folding is a vital process because proteins must be folded into specific three dimensional shapes in order to function correctly. Unfolded or misfolded proteins contribute to many diseases and disorders.

OBJECTIVES -
1. make protein models and topology models of the different energy states using computer programs like gromacs and VMD.
2. Altering the simulation parameters using VMD and gromacs will increase or decrease rates of folding.

All of this was done in a series of different tasks.

METHODS AND MATERIALS
VMD and SMOG simulations -

Energy Rules Followed -

Skills Learned -
1. Typing code in a terminal
2. Utilize gromacs to follow biological rules to build protein models.
3. Use VMD to visualize the model created
4. Distinguish folding energy states on a graph

RESULTS
Task 4 - generate model of the C-alpha protein

Task 5 - Graph of C-alpha protein and its folding energy states. Using this graph, we concluded that the optimal folding temperature is 138K.