Introduction

Biomolecules at a molecular level can often be hard to understand and visualize through physical experiments. Simulations allow scientists to model, replicate, and explore biomolecules in an innovative and insightful approach. By using molecular dynamics, a method used in simulating molecules through technology, researchers can study the interactions between particles in different contexts.

Particularly, simulations can help explore the field of proteins and protein folding. By manipulating the environment around a molecule or protein within a simulation, scientist can analyze what changes are made and how this affects protein folding.

This project used molecular dynamics to study the affects of temperature on protein folding for Chymotrypsin Inhibitor 2 (CI2).

Methods

In this study, the following software programs were used to simulate and assess protein folding and the interactions within protein residues.

Software Used
- Ubuntu
- SMOG
- Gromacs
- VMD - Visual Molecular Dynamics

Results

![Unfolded State -20 kJ/mol](image1.png)

![Folded State at -120 kJ/mol](image2.png)

GROMACS Energies

**Protein Folding Done Using Ubuntu**

Simulations and tasks were ran through Ubuntu. The terminal was used to run programs for simulation.

![Figure 1. After exposing our CI2 molecule to temperatures of 140K we found that the protein was mainly unfolded and folded once.](image3.png)

![Figure 2. After exposing our CI2 molecule to different temperatures, we found that CI2 continuously folds and unfolds at 138K](image4.png)

**Structure of CI2**

**Chymotrypsin Inhibitor 2 (CI2) Visualized through VMD**

A. CI2 visualized as molecules
B. CI2 visualized as a tubular ribbon

**Conclusion**

- We were able to successfully simulate protein folding for Chymotrypsin Inhibitor 2
- Chymotrypsin Inhibitor 2 experiences repeated folding and unfolding at 138K.

**References**