

Folding of Proteins

Simulation using Monte Carlo Approach

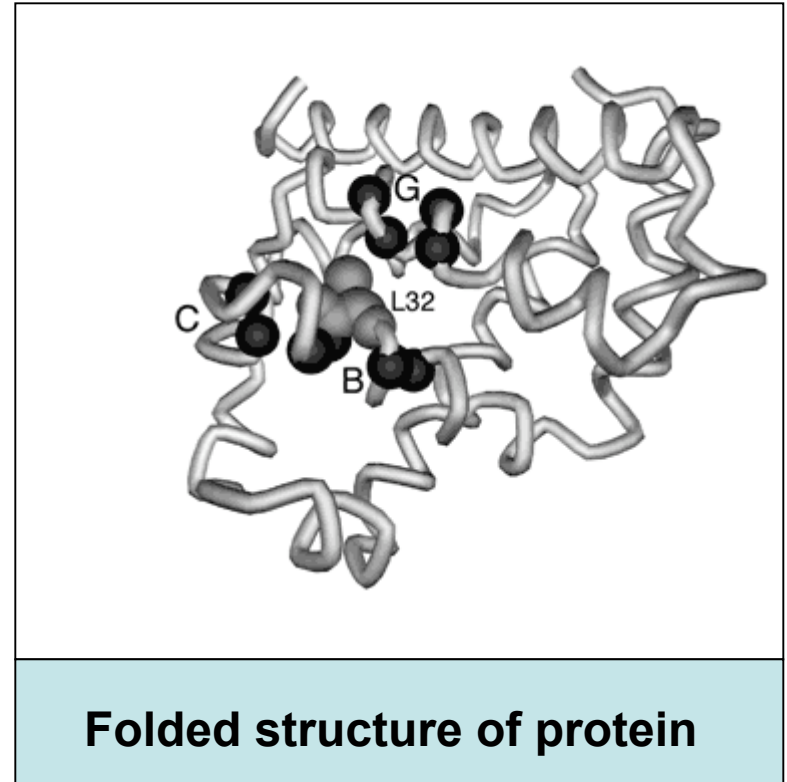
Introduction

What are proteins?

- Polymers of amino acids
- Building block of cells
 - Cellular proteins
- Important component of extra cellular matrix
 - Structural proteins (e.g. elastin, collagen)

Why is protein folding study important?

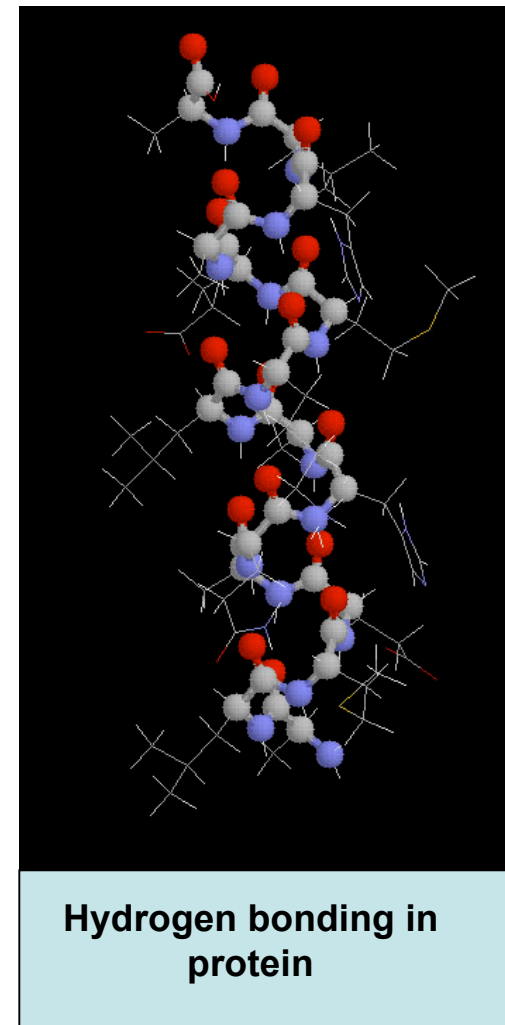
- Linking molecular changes to macro scale changes (e.g. tissue mechanical properties)



Folded structure of protein

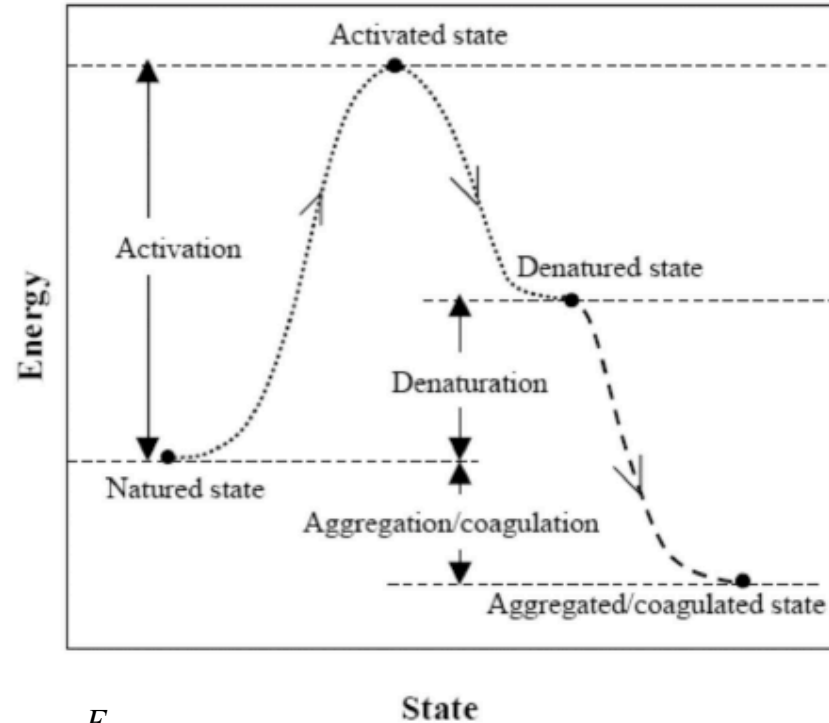
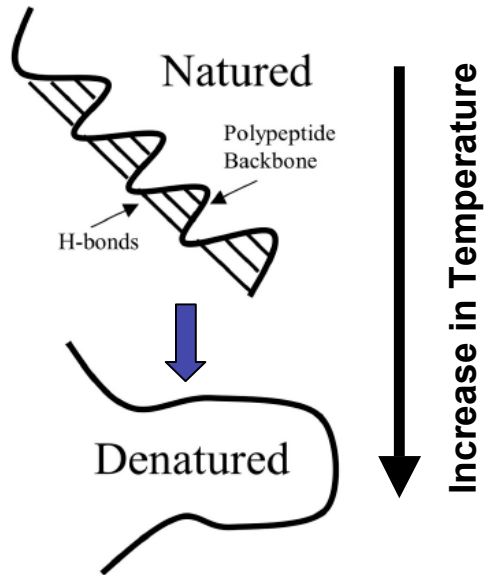
Introduction

- **Different structures of proteins**
 - **Primary**
 - **Peptide Chains**
 - **Secondary**
 - **α - helix, β -pleated**
 - **Tertiary**
 - **Higher order**
- **Bonding in proteins**
 - **Covalent bonds**
 - **Hydrogen bonds**
 - **Vander Waal's Forces**



Denaturation of Protein

- Effect of Temperature



$$\Omega(\tau) = \ln \left[\frac{C(0)}{C(\tau)} \right] \quad \Omega(\tau) = \int_0^{\tau} A e^{-\frac{E}{RT}} dt$$

* Bischof and He 2005, Ann. N.Y. Acad. Sci.

Project Goal

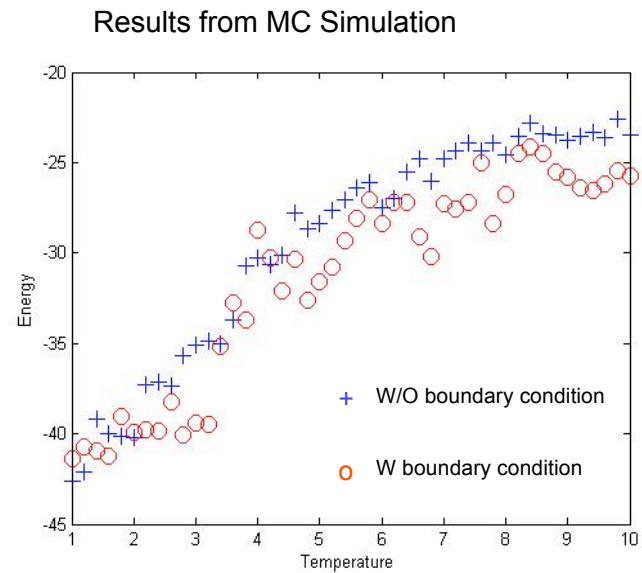
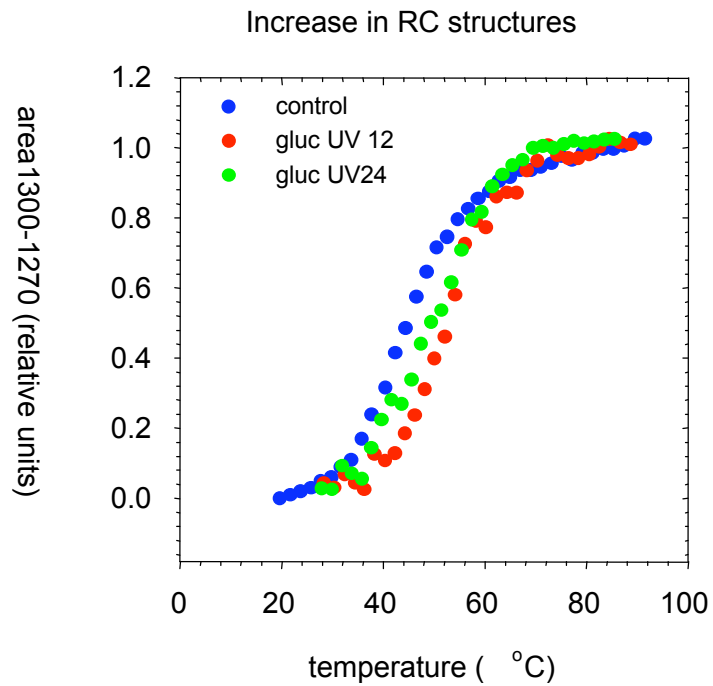
- Perform Monte Carlo simulations to predict thermodynamically favorable forms at different temperatures
 - At high temperature, denatured or unfolded or higher energy form is expected
 - At low temperature, natured or folded or lower energy form is expected
 - Parameters used to distinguish phases
 - Energy
 - End to end protein chain distance.
- Study the effect of mechanical constraints on folding of proteins (~ equivalent to application of mechanical stretch to proteins)

Preliminary results

- Energy at each temperature is the average of 50,000 MC steps

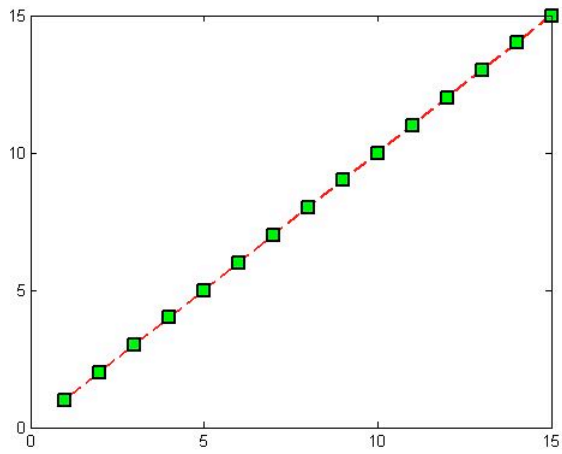
Denaturation of Protein

-Effect of chemical/mechanical modification

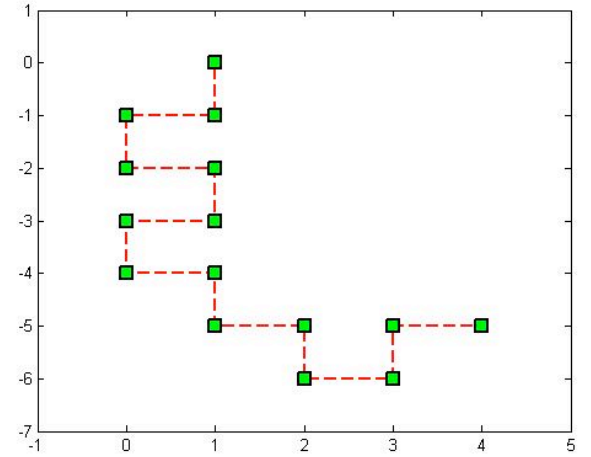


Preliminary Results

**5
Steps**



**500
Steps**



**5000
Steps**

