# Protein Knotting Opens Multiple Opportunities

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## SIGNIFICANCE

Programming was employed to carry out simulations and visual representations of protein structures, which aid in comprehending the functions of biomolecules at a molecular scale. The insights gained through this process have the potential to drive progress in the fields of medicine, healthcare, and bio-engineering.

## OBJECTIVES

1. Configure proteins that have low energy in the folding stage.
2. Determine the temperature for each transition state
3. Compare temperatures of each transition state with experimental assessments.

## BACKGROUND INFORMATION

Chymotrypsin Inhibitor 2 (CI2) stands out as a unique protein folding model due to its simplicity. It primarily exists in three significant conformational states: (1) Folded states, (2) Unfolded states, and (3) Transition states that lie between the Folded and Unfolded states. Among these, the transition states pose the greatest challenge for comprehension and investigation because it is unstable.

Questions:

1. What is the configuration of the simulated transition states within a native topology model?
2. How does the structure obtained from the simulations compare with the results of experimental assessments?

## METHODS

### The Approach:

All-Atom structure $C_\alpha$, Model

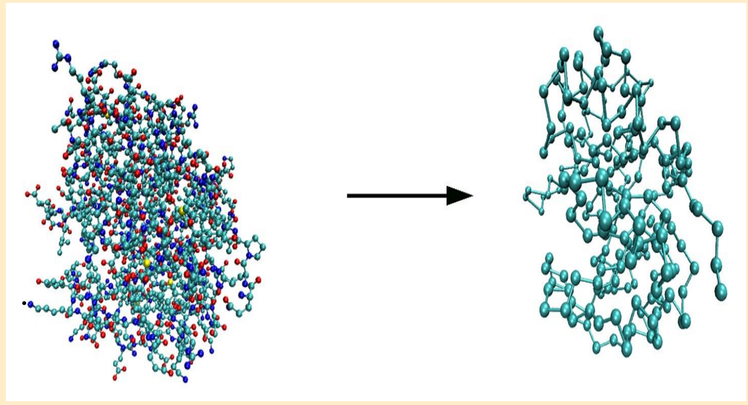

Figure 1: In this figure, the all-atom structure of Chymotrypsin Inhibitor 2 has been stripped toto $C_\alpha$, which is also known as the "Skeleton Model", which enables the process of protein folding

### Energy Terms: "Force Field" or " Rules of the Universe"

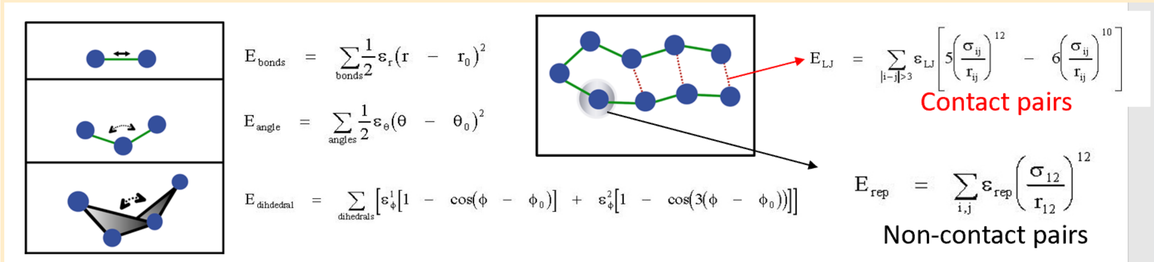


Figure 2: Native Topology Model (Figure 1) generates force field where the Protein Data Bank structure is the lowest energy state. Contact pairs have direct energy with one another and non-contact pairs do not.

### Kinetic Refolding Molecular Dynamics (MD) Simulations:

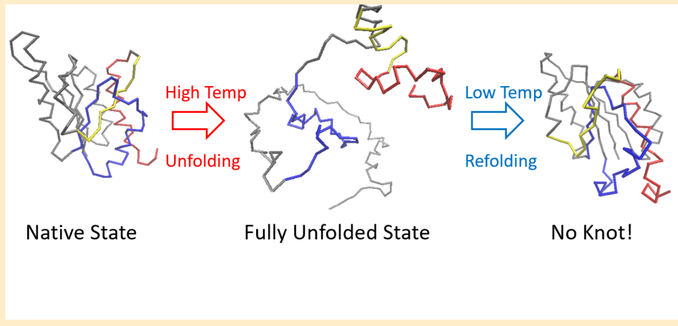


Figure 3: The different stages of kinetic refolding.

## MATERIALS

Items required:

1. laptop
2. Oracle Virtual Box
3. Ubuntu
4. Gromacs Molecular Dynamics Protein Folding Software ( MD )
5. Model Building Software.

## RESULTS AND CONCLUSION

Due to circumstance, Dr. Finke and I were not able to interpret the data. Since the system ended up crashing, all data was lost so results are inconclusive.

## REFERENCES

1. Images from Dr. John Finke's Knotting Protein PowerPoint
2. Knotting Protein PowerPoint made by Dr. John Finke

## ACKNOWLEDGEMENTS

I would like to thank Dr. Finke for giving me an opportunity to do something that was out of my comfort zone, which was coding. I have gained a skill because of him. May he rest in peace.