Protein Simulation and Visualization Using Programming

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The use of programming to run simulations and visualize structures can aid in understanding the molecular functions of biomolecules. This method can be used to study biomolecular structures from a wide range of organisms. This knowledge can assist in developing breakthroughs in medicine, healthcare, and bioengineering. Chymotrypsin Inhibitor 2 (CI2) was simulated in this study to see how well simulations match experimental values established by protein folding. Near the folding temperature, there are two main conformational ensembles: folded and unfolded ensembles. The transition state, a very unstable combination of conformations with a structure between the folded and unfolded ensembles, connects these two states. Simulations were run at various temperatures to determine the temperature that populates the transition state the most. An equal population of folded and unfolded states was observed, with frequent flipping back and forth between them, confirming the ideal folding temperature. The simulations' visualization program (VMD) was used to examine CI2's real trajectory as it flipped back and forth, and data was collected to compare the structural properties of all three conformations. The data was divided into two plots, one for each structural ensemble, revealing which amino acid residues were discovered to be near together. The more connections there are, the more "native" protein structure is present. The simulated structure has a slope of +0.25 and a correlation coefficient of +0.28 when compared to experimental assessments of the transition state structure. Although the results were somewhat predictive, there is obviously space for improvement. This method can be used to anticipate the behavior of different proteins discovered in other animals under various situations.