Understanding Protein Folding Mechanisms through Molecular Dynamics Simulations

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Abstract. Protein folding is a critical process that determines the functional conformation of proteins. This research utilizes molecular dynamics simulations to investigate the folding pathways of various proteins. By analyzing the dynamics of folding intermediates and transition states, we provide insights into the factors that drive the folding process. Our findings contribute to a better understanding of protein misfolding diseases and the development of therapeutic interventions.

Keywords: Protein folding, Molecular dynamics, Folding pathways, Protein misfolding, Therapeutic interventions

Introduction

The process of protein folding is essential for achieving the correct three-dimensional structure necessary for protein functionality. Despite extensive research, the mechanisms underlying protein folding remain a subject of intense study. Molecular dynamics simulations have emerged as a powerful tool for exploring the complex landscape of protein folding pathways. In this study, we apply these simulations to elucidate the dynamics of folding intermediates and transition states across different proteins. Our research sheds light on the physicochemical factors influencing folding and highlights the implications for understanding protein misfolding diseases such as Alzheimer's and Parkinson's. These insights are crucial for developing therapeutic strategies aimed at correcting misfolding and restoring normal protein function.

References

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