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INVESTIGATING COLLAGEN AS A BIO-MATERIAL BY MOLECULAR DYNAMICS SIMULATIONS

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Abstract: In this work, molecular dynamics simulation is used to describe and analyze the behavior of model collagen polymer $(Pro\text{-}Pro\text{-}Gly)_9$. This project aims to highlight the important role of molecular dynamic simulation in determining the structural stability of collagen, and establishing collagen as a hydrophobic or hydrophilic protein under different temperatures. The system was simulated at four different temperatures (300, 310, 320, and 330 K). The results indicate that the average number of hydrogen bonds within the protein and the protein backbone was similar at each temperature. The solvent-accessible surface area of hydrophobic and hydrophilic atoms for the four temperatures indicates that the collagen model peptide is mostly hydrophobic. All the results show that the structure of the studied polymer was the least stable at 320 K and the most stable at lower temperatures (300 K). The average effect across the first 100 ns was investigated. The dominant states obtained within this time interval will be explored in following studies. Researchers can use the results of this work to develop collagen with the appropriate thermal stability for biological applications.

Keywords: Collagen, polymer, hydrogen bonds, hydrophilic, hydrophobic

INTRODUCTION

Collagen is a structural protein found in abundance in all mammals. It makes up one-third of the total protein in humans, accounts for three-quarters of the dry weight of skin, and is the most widespread component of the extracellular matrix [1]. Collagen is a significant fibrous material responsible for the structural integrity of many body parts like skin, bone, tendons, and teeth. Moreover, it is a scaffold for cell cohesion as an extracellular matrix in many organs [2]. In vertebrates, there are 28 different forms of collagen, each with at least forty-six different polypeptide chains, and many other proteins have collagenous domains [3], [4]. Its

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