

Protein Stability of a 21 Residue Alanine Based Peptide

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The central dogma of biochemistry today is to understand how proteins go from a chain of amino acids to a 3-dimensional folded structure. It is well known that the stability of proteins is strongly affected by ion interactions, hence the conformations that a protein may adopt depend on the environment. A short polyalanin 21 residue peptide, immersed in different environments, has been studied, through molecular dynamics, to understand the role ions play in peptide stability. This knowledge will be useful in understanding the folding problem for much larger proteins. Computer simulations were ran using the same peptide in Na_2SO_4 , NaCH_3COO , and Na_3PO_4 salt solutions. AMBER9 was used to perform the molecular simulations and the goal was to identify which salts would stabilize and which would destabilize the protein and why.