

Sodium acetate effects on the helical stability of a mainly-alanine peptide

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Peptide-based drugs have been developed to potentially treat various forms of cancer and HIV. Some α -helical peptides can access cells via crossing the cell's lipid bilayer. However, the environment could affect the peptide's α -helical stability making the crossing into the cell difficult. To overcome this problem, experimental and computational teams have developed techniques to stabilize the α -helix configuration of peptides. One such method is to select ions to stabilize the α -helix secondary structure in an aqueous environment. This work is part of the entire Hofmeister series investigation. We studied the stabilization effects of the acetate anion on a mainly alanine peptide. Replica Exchange Molecular Dynamics was also utilized in order to increase sampling of configurations of the system throughout the simulation. According to previous studies, the acetate ion is expected to stabilize the peptide less than perchlorate in an aqueous environment according to the Hofmeister series.