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Dynamics of Polyalanine in Water and in Glycerol ALPER BULDUM, Department of Physics, The University of Akron, Akron, OH, 44325, SHARON R. STEFANOVIC, Department of Physics, The University of Akron, Akron, OH, 44325 — Organic solvents such as glycerol and trehalose protect many organisms from dehydration and freezing. In an attempt to utilize this natural effect, solvents like these would be useful in the pharmaceutical industry. Here we present molecular dynamics simulations of a polyalanine polypeptide solvated in water and in glycerol. Many aspects of the dynamics of the polyalanine α -helix are investigated and important viscosity and hydrogen bond effects on the fluctuations are discussed. Also considered are the effects on diffusion and radial distribution of a solvent upon addition of a polyalanine α -helix. The understanding of the helix dynamics in different solvents may assist the understanding of the dynamics of entire proteins and their preservation in organic solvents.

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