Molecular Driving Forces for Cosolvent-induced Conformational Changes of Water-soluble Macromolecules and Proteins

(Talk #16)

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We will present our recent work on computer simulations of the coil-globule transition of poly-n-isopropylacrylamide (PNIPAM) in dilute solution driven by variations in solvent composition. In water, PNIPAM undergoes a coil-to-globule transition upon heating, resembling cold renaturation of globular proteins. We will discuss the role of Van der Waals forces and hydrogen bonds in the cosolvent-induced collapse of PNIPAM in aqueous solution with urea or methanol. The relation to cosolvent effects on protein stability will be discussed.