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Effect of solvent on the structure of a protein (H3.1) with a coarse-grained model with knowledge-based interactions[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Quality of solvent plays a critical role in modulating the structure of a protein along with the temperature. Using a coarse-grained Monte Carlo simulation based on three knowledge-based contact potentials (MJ[1], BT[2], BFKV[3]) we examine the structure and dynamics of a histone (H3.1). The empty lattice sites constitute the effective solvent medium in which the protein is embedded. Residue-solvent characteristic interaction is based on the hydropathy index while the residue-residue interaction is used from the knowledge-based contact matrices derived from ensembles of protein structures in the protein data bank. Large scale simulations are performed to analyze the structure of protein for a range of residue-solvent interaction strength, a measure of the solvent quality with each potential. Unlike the monotonic thermal response, the radius of gyration of the protein exhibits non-monotonic dependence of the solvent strength. Quantitative comparison of the structure and dynamics emerging from three knowledge-based potentials will be presented in this talk.

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[2] M.R. Betancourt and D. Thirumalai, Protein Sci. 2, 361 (1999).
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