Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Structure of a protein (H2AX): a comparative study with knowledge-based interactions[1] MIRIAM FRITSCHE, DIETER HEERMANN, University of Heidelberg, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — The structural and conformational properties of the histone protein H2AX (with143 residues) is studied by a coarse-grained model as a function of temperature (T). Three knowledge-based phenomenological interactions (MJ [1], BT [2], and BFKV [3]) are used as input to a generalized Lennard-Jones potential for residue-residue interactions. Large-scale Monte Carlo simulations are performed to identify similarity and differences in the equilibrium structures with these potentials. Multi-scale structures of the protein are examined by a detailed analysis of their structure functions. We find that the radius of gyration (R_g) of H2AX depends non-monotonically on temperature with a maximum at a characteristic value T_c, a common feature to each interaction. The characteristic temperature and the range of non-monotonic thermal response and decay pattern are, however, sensitive to interactions. A comparison of the structural properties emerging from three potentials will be presented in this talk.

[1] S. Miyazawa and R.L. Jernigan, Macromolecules 18, 534 (1985).
[2] M.R. Betancourt and D. Thirumalai, Protein Sci. 2, 361 (1999).
[3] U. Bastolla et al. Proteins 44, 79 (2001).

[1]This work is supported by Air Force Research Laboratory.

Ras Pandey
University of Southern Mississippi

Date submitted: 05 Nov 2012 Electronic form version 1.4