

**Modeling DNA Interactions in Nucleosome Particles**  
**(A Computational Study of DNA Interactions in Nucleosome Particles)**

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Central to eukaryotic cellular support such as transcription regulation and chromatin structure are DNA interactions with the nucleosome histone core. The interactions of the histone core with DNA is understood partially at best. In this poster we present work on a refined model toward predicting DNA-histone core interactions. We are developing a DNA-histone interaction model through selected substitutions of nucleotides on the *Xenopus laevis* nucleosome x-ray crystal structure, our model system. In this poster, we present results from an all-atom molecular-dynamics trajectory of the nucleosome particle. We characterize global motions of the histone-DNA complex with respect to energy fluctuations in an assessment of the simulation length required for adequate sampling of the configuration space. Such trajectories will be used as a reference for subsequent nucleotide substitutions in our parameterized histone-DNA model. The magnitude of energy differences resulting from the nucleotide substitutions will be presented in the context of sequence-dependent DNA-nucleosome binding and our modeling capabilities. The remarkable homology of the nucleosome core proteins across eukaryotes, among the most highly conserved proteins known, will facilitate extrapolating our model from *Xenopus laevis* to other eukaryotes.