

“Dynamic Model of DNA Structure and Function”

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Abstract

Many existing models of the DNA molecule predict equilibrium properties of its molecular structure. But the biological environment within a cell is in dynamic flux. The DNA molecule is constantly disrupted through biological events like protein binding, transcription, replication, recombination and cell division. Equilibrium-based models portray molecular properties in the thermodynamic limit and do not reflect the near-term effects of such events. Non-equilibrium dynamics are essential in predicting the length of time it will take the DNA molecule to relax to its equilibrium state. Our research has focused on developing a dynamic statistical mechanical model for predicting the mechanical behavior of DNA in a dynamic biological environment. We extend the approach taken by Professors Benham and Fye in developing the equilibrium Stress-Induced Duplex Destabilization (SIDD) model, which incorporates an Ising-like framework in modeling the DNA molecule and predicts equilibrium free energy and probability of denaturation for each base pair in the molecule. The non-equilibrium properties of the one-dimensional kinetic Ising model have been thoroughly studied, and we have leveraged these results. Our model is implemented as a time-dependent simulation using Glauber dynamics. Among the measures calculated are the time-series probability distribution, time-dependent energy of opening and probability of opening for each base pair of the DNA chain. We also calculate correlation distances for events in the DNA chain. Our dynamic model thus enables a better understanding of mechanisms in the cell and function of DNA *in vivo*.