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DNA flexibility and bending: Results from Brownian dynamics simulations and single-molecule experiments

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Abstract

We are investigating intrinsic and protein-induced DNA flexibility, bending, and looping by experimental and simulation methods. We are developing a Brownian dynamics simulator to model the results of single molecule tethered particle motion analysis (Sutin, et al., Biophys. J. 74: A71 (1998)) and fluctuation correlation spectroscopy (FCS) experiments. We are simulating the trajectories of DNA fragments of lengths from 10's to 100’s of base pairs on the micro to millisecond time scales. The boundary conditions of the simulations are for both a DNA fragment alone in solution and for a DNA fragment tethering a microsphere to a surface. The resulting DNA trajectories are transformed to the corresponding measured experimental parameters. For tethered particle motion analysis, the distribution of displacements of the microsphere attached to the free end of the DNA fragment will be related to the underlying DNA conformation. We will also consider the information obtainable in a scanning FCS experiment from a DNA fragment with dye bound continuously along the length of the fragment. In addition to native DNA, we will examine DNA bound and bent by the TATA binding protein (TBP). We will compare the models to the results of these experiments.