

DNA mechanics and protein-DNA recognition

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Molecular simulations make it possible to look at DNA structure and mechanics as a function of base sequence at both local and more global levels. Understanding this sequence-induced heterogeneity is a necessary step to understanding the indirect aspects of DNA recognition which play a major role in the formation of many protein-DNA complexes including multi-macromolecular assemblies such as the nucleosome. I will describe some recent work in this area based on large-scale molecular dynamics and molecular mechanics studies, notably involving our present interest in understanding how nucleosomes position themselves on genomic DNA.