The Sequence-Dependent Statistical Mechanics of DNA

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Abstract

The recently developed cgDNA sequence-dependent rigid-base coarse grain model of DNA is parameterised from Molecular Dynamics simulations at the scale of 20bp and less. However the cgDNA model free energy also allows numerically efficient Monte Carlo sampling of the configuration space equilibrium ensemble for DNA fragments with arbitrarily prescribed sequence at the much longer length scales of a few hundred to a few thousand bp and more. These Monte Carlo simulations reveal strong sequence dependence of the classic correlation functions of polymer physics through the effect of both intrinsic shape and differing stiffnesses. On the other hand when the ensemble includes averaging over sequence, the cgDNA Monte Carlo simulations predict the single effective persistence length of 163bp, which, given that there is no model parameter fit other than the 20bp scale MD simulation data, is in remarkably good agreement with the consensus experimental value of 150 bp or so.

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