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The role of sequence-dependent energy landscape in the formation of nucleosome-depleted regions

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Abstract

The nucleosome-depleted region is a part of the genome that serves as a binding site for key components of the transcriptional machinery, including RNA polymerase, transcription factors, motor proteins, and other essential cellular regulators. Occupation of this region by nucleosomes can disrupt proper transcriptional function. The sequence-dependent mechanical properties of DNA strongly influence nucleosome positioning along the genome. In this study, we present a stochastic model based on the sequence-dependent energy landscape to simulate the diffusive motion of nucleosomes along DNA. Using the Gillespie algorithm, we model the dynamics of nucleosomes along a 901-base-pair DNA segment and compute the nucleosome occupancy profile. The results show that high-energy regions act as physical barriers to nucleosome formation, leading to the emergence of NDRs. Moreover, the energy landscape of the adjacent regions plays a crucial role in the formation of NDRs and the overall distribution of nucleosomes. From the simulations, we can see a natural pattern in how nucleosomes are positioned around these NDRs. This model provides a theoretical framework for improving our understanding of chromatin organization both in vitro and in vivo.

Keywords: Nucleosome, Nucleosome-Depleted region, Nucleosome positioning, Nucleosome occupancy, DNA sequence.

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