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Capricious Companions: Polycations Show Sequence-Dependent DNA Affinity

DNA is a fundamental molecule of life, and its folding is critical for gene regulation, medical applications, and disease prevention. While proteins like histones are known to drive highly ordered DNA packaging, both experimental and theoretical studies have shown that DNA duplexes can also associate selectively in the absence of proteins, mediated by small molecules such as polycations.1 In this work, we use atomistic unbiased and biased molecular dynamics (MD) simulations to investigate how double-stranded DNA interacts in the presence of polycations. First, unbiased simulations without polycations are used to characterize baseline features such as average interstrand distance. We then apply biased simulations with polycations to quantify the repulsive potential between DNA helices—results that we compare to experimental measurements.2 We explore how different polycations, including polyarginine and polylysine, affect DNA condensation in AT-rich and GC-rich sequences. Our findings show that condensation behavior is both sequence- and polycation-dependent, suggesting that DNA condensation is governed by more nuanced mechanisms than previously understood. These insights highlight the potential roles of non-protein biomolecules in DNA organization, with implications for chromatin structure and gene regulation.

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