Single stranded DNA hairpin loop kinetics: A Brownian dynamics study

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The dynamics of single stranded DNA (ssDNA) molecules play a role in a number of biological functions and have a found uses in several microfluidic applications. In particular, ssDNA having complementary sequences at their ends can form hairpin loops in which the complementary sections bind to one another. The appearance of these loops and fluctuations between open and closed states depend on a number of variables including: the degree of complementarity of the end sequences, temperature and strength of hydrogen bonding and base stacking. In this study, we present a Brownian dynamics model which is used to examine the kinetics of the hairpin loop formation. We present results for the melting behavior of hairpins as a function of temperature and other system parameters. We also present results for the kinetic rate constants \( k_- \) and \( k_+ \) corresponding to the open-closed and closed-open transitions respectively.