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Macroscopic Mechanisms of DNA Flexibility

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In recent experiments Cloutier and Widom found that the cyclization efficiency of short DNA fragments, about 100 bp in length, exceeds the theoretical expectations by 3 orders of value. Is it possible to revise the theoretical model of DNA bending, based on harmonic potential for the bend angle between adjacent base pairs, to fit these unexpected results? We investigated the effect of the bend angle distribution on the cyclization efficiency. Different modifications of the angle distribution, extracted from the DNA-Protein Data Bank, were tested. We found that incorporating non-quadratic terms in the potential can provide increase of the short fragment cyclization efficiency by about one order of value. The computations showed that only incorporating a possibility of sharp kinks in the distribution is capable to provide the desired increase of the cyclization efficiency. The frequency of such kinks should be about one per thousand base pairs. The kink model does not allow, however, fitting all cyclization data for DNA fragments of different lengths. Trying to resolve this problem we reinvestigated the cyclization of 100 bp DNA fragments experimentally.