

## **SIMULATIONS OF DNA BENDING USING ADAPTIVE UMBRELLA SAMPLING ON ROLL ANGLES**

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Many proteins bend DNA significantly upon binding, and there is controversy about the extent of DNA flexibility on short length scales. To simulate this bending within the time scales accessible to molecular dynamics, we used adaptive umbrella sampling on the roll angles. We studied the inherent flexibility of bare DNA by simulating dodecamers with varying sequences and made comparisons to the worm-like chain model. Our simulations demonstrate that DNA is easier to bend through large roll angles than predicted by the worm-like chain model, but extrapolation to long length scales shows behavior consistent with the worm-like chain model. Simulations of bare DNA were also performed to assess the co-operativity of the bending of adjacent roll angles.