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A coarse-grained model of the 10-23 DNAzyme KEVIN DORFMAN, University of Minnesota, MARTIN KENWARD, University of California - San Diego — DNAzymes are single-stranded DNA that catalyze nucleic acid biochemistry. We have adopted a simple bead-spring model that captures, in a coarse-grained manner, the diffusive motion and self-interactions of single-stranded DNA. We used this model to investigate the structure and dynamics of the RNA cleaving 10-23 DNAzyme over long time scales via Brownian dynamics simulations. We start from an unfolded state where the DNAzyme is bound to its substrate and allow the system to relax. The structural data thus obtained agree well with FRET measurements and provide a connection between the proposed structure of the DNAzyme and chemical rate data appearing in the literature. We have also investigated the changes in the structure of the DNAzyme/substrate complex following the cleavage of the substrate. In agreement with single-molecule FRET data, we find that the DNAzyme rapidly unwinds into an extended structure.

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