Molecular dynamics study of mechanically unfolding a RNA kissing complex

Hui Xiong and Adrian E. Roitberg

Department of Physics and QTP, University of Florida, Department of Chemistry and QTP, University of Florida

Abstract

Recent discoveries witness RNA's increasingly important role in biological functions such as catalyzing and regulating protein synthesis. Study of RNA molecules' structure attracts great attention as it's a key to understand their functions. Intra-molecular kissing interaction is a type of tertiary interactions, which are critical in forming RNA's functional global structures. A recent experimental study by Li and coauthors [Li PTX, Bustamante C, Tinoco I Jr (2006) *Proc Natl Acad Sci USA* 103:15847-15852] showed that the kissing interaction kinetically stabilizes folded hairpins. The system studied is a RNA complex composed of two RNA hairpins with 11 and 7 base pairs respectively. The kissing interaction in between the hairpins' loops only involves 2 base pairs. We studied this system with computer simulations, by mechanically unfolding the kissing complex using molecular dynamics. The kissing interaction is always the first to break, followed by unzipping of the 7-bp Hairpin II, and at last the 11-bp Hairpin I. This result conforms to the experiments. We observe an additional drop on the force-extension curve before breaking the kissing interaction. By examining the atomic structure, we ascribe this to the so-called "B-S" transition in Hairpin I, which is reported in RNA stretching experiments.