Accelerated sampling of the conformational space in biopolymers: From small proteins to RNAs

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Recently developed free-energy methods (steered molecular dynamics, well-tempered metadynamics, parallel tempering and solute tempering) will be discussed, and their application to the accelerated sampling of small proteins and RNA molecules in the context of atomistic molecular dynamics simulations will be shown. Using these techniques, a proposed model for RNA unwinding is validated and interpreted at atomistic resolution.