Evaluating RNA single bulges with a mesoscopic model

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Thermodynamic models at the mesoscopic scale such as the Peyrard-Bishop model are capable of reinterpreting experimental measurements in terms of intramolecular interactions. For instance we recently were able to obtain detailed information about hydrogen bonds for the GU wobble pair in RNA. For example the distinctive single hydrogen bond that GU may assume under certain circumstances was correctly predicted with a mesoscopic models. Here we address the far more complex situation of single bulges in RNA. In this case a single nucleotide is left unpaired which may then either flip out or interact with neighboring intrastrand bases through $\pi - \pi$ interaction. A bulge may in some cases also disrupt neighboring base pairs. Representing bulges with mesoscopic approaches represents a challenge as such models were developed for unperturbed helical structures. We adapted successfully the Peyrard-Bishop Hamiltonian to represent the perturbation induced by a single bulge, in particular we were able to treat the resulting asymmetry of the stacking interaction. We are now determining the optimal parameters for this model, for this we used from the literature 133 melting temperature sequence data of A, C, G and U bulges surrounded by AU and CG base pairs. Our first results indicate that for some sequence contexts the hydrogen bonds of neighboring base pairs tends to vanishing values indicating that a base pair rupture has occurred. However, for most contexts the flanking base pairs retain a very stable hydrogen bond. We are also addressing the problem of location of type II bulges. In this case the exact pairing of the bulge is not known. Our parametrization procedure will cover the various location possibilities and work out the most stable location for the type II bulge to reside in the sequence. We acknowledge financial support by Capes, CNPq and Fapemig.