

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Stabilities of Constituent Hairpins Determine Whether RNA Folds via Ordered and/or Parallel Mechanisms<sup>1</sup>** SAMUEL CHO, DEVARAJAN THIRUMALAI, University of Maryland — RNA molecules are increasingly becoming seen as a set of critical players in numerous cellular processes, and a firm understanding of their folding energy landscapes is essential for understanding how they carry out their functions. While it might seem natural to assume that the simplicity of RNA molecules, with only four possible bases, dictate that they must fold via simple mechanisms, experiments continue to point to complex folding energy landscapes involving parallel mechanisms. In our present study, we address how even simple RNA molecules can give rise to very complex folding mechanisms. We begin by making the argument that the complexity observed for RNA folding are in fact fully expected because the lack of variability of the RNA subunits leads to a lack of specificity for folding to the native basin. To illustrate our point, we performed coarse-grained simulations of three RNA pseudoknots and a tRNA molecule, which each are all relatively simple RNA molecules that contain at least two hairpins. From our simulations, we find that the main determinant for how these RNA molecules fold is largely dependent on the relative stabilities of their constituent hairpins. Ordered mechanisms arise if the stabilities of the constituent hairpins are sufficiently dissimilar and parallel folding mechanisms occur if the stabilities of the hairpins are similar.

<sup>1</sup>SSC is supported by Ruth L. Kirschstein National Research Service Awards from the National Institutes of Health.

Samuel Cho  
University of Maryland

Date submitted: 21 Nov 2008

Electronic form version 1.4