Abstract Submitted for the MAR15 Meeting of The American Physical Society

Magnesium Dependence of the RNA Free Energy Landscape RYAN HAYES, JEFFREY NOEL, Center for Theoretical Biological Physics, Rice University, ANA MANDIC, Department of Biomedical Engineering, University of Houston, PAUL WHITFORD, Department of Physics, Northeastern University, KARISSA SANBONMATSU, Theoretic Biology and Biophysics, Los Alamos National Labs, UDAYAN MOHANTY, Department of Chemistry, Boston College, JOSÉ ONUCHIC, Center for Theoretical Biological Physics, Rice University — The RNA free energy landscape is highly sensitive to ionic concentrations, and especially to Mg^{2+} , as most RNA tertiary structure will not form in the absence of Mg^{2+} . At physiological concentrations, the energy landscape must be smooth and funneled to fold on biological time scales, but changes in ionic concentration may affect the relative stability of alternative states. We perturb a structure-based model, which captures the funneled nature of the energy landscape, to include electrostatic effects. Our model includes explicit Mg²⁺ and screening by implicit KCl. A dynamic model for the local competition between Manning condensed Mg^{2+} and KCl is introduced, which makes the model more broadly applicable and transferable than a previous static model. We use the excess Mg^{2+} ions associated with the RNA (Γ_{2+}) to test the model. Γ_{2+} is an ideal metric because it is closely related to the Mg²⁺-RNA interaction free energy, and is easily measurable in both experiment and simulation. The model captures intermediate states of a small pseudoknot missed by models without electrostatics.

> Ryan Hayes Center for Theoretical Biological Physics, Rice University

Date submitted: 14 Nov 2014

Electronic form version 1.4