Supporting Information

Automated RNA Tertiary Structure Prediction from Secondary Structure and Low-Resolution Restraints
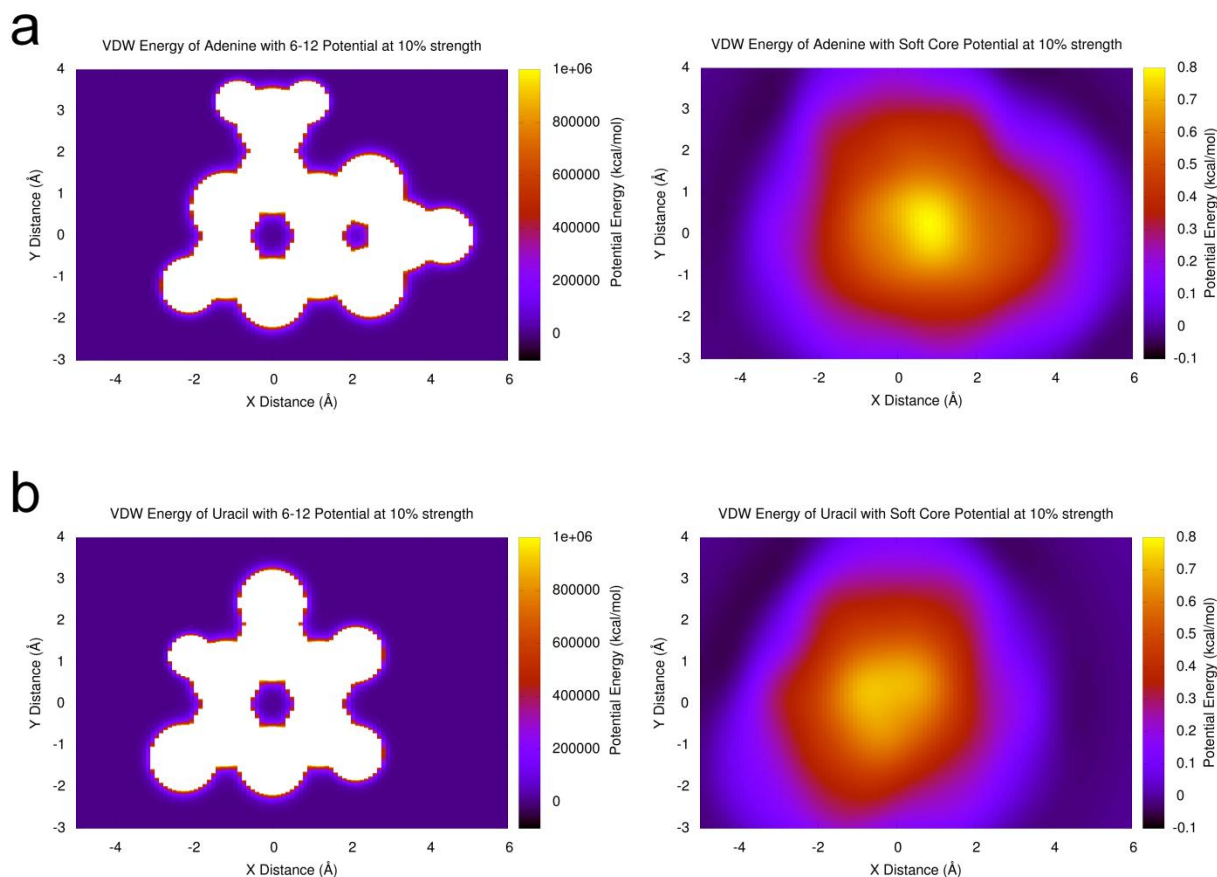
Matthew G. Seetin and David H. Mathews

Department of Biochemistry and Biophysics

and Center for RNA Biology

University of Rochester Medical Center

601 Elmwood Ave, Box 712, Rochester, NY 14624

Correspondence to: David H. Mathews; e-mail: David_Mathews@urmc.rochester.edu

Supporting Figure 1. Plots comparing the van der Waals potential energy for the usual 6-12 Lennard-Jones potential at 10% strength (left) and the soft core potential with $\lambda = 0.1$ (right) for (a) Adenine, and (b) Uracil. Parameters are taken from the AMBER ff99 force field relative to an aromatic carbon probe atom like the ones that make up nucleobases. In all cases, the Lennard-Jones potential has a local minimum at the center of each ring with barriers of escape in excess of 1 million kcal/mol, leaving the chance that two rings could interlock inseparably in an unphysical conformation when the potential is first restored. In contrast, the soft core potential has a local maximum at the center of the bases with no local energy minima inside any rings, and the energies inside each are about six orders of magnitude lower. Bases that were overlapping or interlocked during the stage of the run without VDW or electrostatic forces will smoothly slide apart.