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Ion concentration dependent tRNA folding energy landscapes RONGZHONG LI, Department of Physics, Wake Forest University, SAMUEL CHO, Departments of Physics and Computer Science, Wake Forest University — The RNA folding is highly dependent on the ionic conditions of its environment in the cell because the surrounding ions electrostatically screen the charged phosphates that line the RNA backbone. Recent studies (Cho, Pincus, and Thirumalai, PNAS, 2007; Biyun, Cho, and Thirumalai, JACS, 2011) demonstrated that the coarse-grained model we use accurately captures the RNA folding mechanisms by incorporating a Debye-Huckel potential to screen the electrostatics. We compare the ion-concentration dependent tRNA folding mechanism to the classical thermodynamic melting profiles of Crothers and co-workers, and we observe excellent agreement. We also supported our findings by performing empirical force field MD simulations with CHARMM and AMBER, and we observe remarkably comparable qualitative similarities between the average base-base distances from simulations and the empirically measured base-stacking potentials from the well-known Turner's Rules.

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