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RACER a Coarse-Grained RNA Model for Capturing Folding Free Energy in Molecular Dynamics Simulations SARA CHENG, DAVID BELL, PENGYU REN, University of Texas at Austin — RACER is a coarse-grained RNA model that can be used in molecular dynamics simulations to predict native structures and sequence-specific variation of free energy of various RNA structures. RACER is capable of accurate prediction of native structures of duplexes and hairpins (average RMSD of 4.15 angstroms), and RACER can capture sequence-specific variation of free energy in excellent agreement with experimentally measured stabilities (r-squared =0.98). The RACER model implements a new effective non-bonded potential and re-parameterization of hydrogen bond and Debye-Huckel potentials. Insights from the RACER model include the importance of treating pairing and stacking interactions separately in order to distinguish folded an unfolded states and identification of hydrogen-bonding, base stacking, and electrostatic interactions as essential driving forces for RNA folding. Future applications of the RACER model include predicting free energy landscapes of more complex RNA structures and use of RACER for multiscale simulations.

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