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Will it fold? Structural and statistical analysis of a 10mer of Fdu

RYAN MELVIN, FREDDIE SALSBURY, Wake Forest Univ — Small strands of RNA are often drawn as extended structures in both journal articles and textbooks. However, a microsecond all-atom GPU-based simulation of a 10mer therapeutic, Fdu, shows folding into stable hairpin-like structures. After a 300ns equilibration phase, this 10mer has a 90 percent probability of existing in 1 of 5 folded states. A Markov analysis shows that despite the existence of a kinetically trapped state, the dynamics among the folded state converges on the nanosecond scale and is ergodic. Knowledge of these structures and probability of their occurrence will allow for estimates of free energies for binding proteins to potentially improve the delivery and design of this therapeutic.

Ryan Melvin
Wake Forest Univ

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