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Thermodynamic Restriction on Evolutionary Optimization of Transcription Factor Proteins ALEXANDER GROSBERG, LONGHUA HU, University of Minnesota, ROBIJN BRUINSMA, University of California Los Angeles — Conformational fluctuations are believed to play an important role in the process by which transcription factor proteins locate and bind their target site on the genome of a bacterium. Using a simple model, we show that the binding time can be minimized, under selective pressure, by adjusting the spectrum of conformational states so that the fraction of time spent in more mobile conformations is matched with the target recognition rate. The associated optimal binding time is then within an order of magnitude of the limiting binding time imposed by thermodynamics, corresponding to an idealized protein with instant target recognition. Thus, we claim that it is possible for the overall binding rate of a transcription factor to approach the theoretical limiting value but only by a suitable choice of energy spectrum of conformational sub-states, and only if the dimensionless binding rate is of the order of one, or larger than one, where dimensionless binding rate is determined as the product of binding rate and the average time spent by the protein on one DNA base pair in one tour of 1D sliding along DNA. Numerical estimates suggest that typical bacteria operate in this regime of optimized conformational fluctuations.

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