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Selecting fast folding proteins by their rate of convergence

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(Submitted on 2 Apr 2012)

We propose a general method for predicting potentially good folders from a given number of amino acid sequences. Our approach is based on the calculation of the rate of convergence of each amino acid chain towards the native structure using only the very initial parts of the dynamical trajectories. It does not require any preliminary knowledge of the native state and can be applied to different kinds of models, including atomistic descriptions. We tested the method within both the lattice and off-lattice model frameworks and obtained several so far unknown good folders. The unbiased algorithm also allows to determine the optimal folding temperature and takes by 3--4 orders of magnitude less time steps than those needed to compute folding times.

Submission history

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