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Protein Folding Transition States as Eigenstates

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We are interested in the microscopic routes by which simple fast folding proteins fold, and the bottleneck steps. We model the process using a master equation. We find that folding differs from small molecule bond-formation kinetics in various ways. For example, simple mass-action miss important aspects of the heterogeneity of the routes. The energy landscape has a funnel shape. Also, the rate-limiting step is not a single microstructure; rather, the transition state can be characterized as an eigenstate. These observations may be useful for developing more efficient computational methods for conformational searching in protein structure prediction.

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