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Modelling Ultra-fast folding proteins KINGSHUK GHOSH, S. BANU OZKAN, KEN DILL, Dept of Pharm. Chem, University of California, San Francisco — Ultrafast-folding proteins are interesting because of their complex temperature dependent rates (including negative activation barriers). We develop a simple mesoscopic model that represents protein folding as a funnel through multiple routes. We have compared the model to experiments on several ultra-fast folding proteins. The model predicts the observed temperature dependences of folding and unfolding relaxation. Our model allows us to calculate the number of routes a molecule takes as it folds. We show that number of folding routes correlates with the folding time and also with the relative contact order: faster folders have more folding routes. Our model suggests a hard speed limit of 50 ns, when every protein folds via its own private route, and this corresponds to the folding time of an alpha helix. The model also computes folding time distributions which will be of interest for single molecule experiments.

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