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Energy Landscape and Transition State of Protein-Protein Association RAMZI ALSALLAQ, HUAN-XIANG ZHOU, Physics Department, Institute of Molecular Biophysics, School of Computational Science, Florida State University, Tallahassee, FL — Formation of a stereospecific protein complex is favored by specific interactions between two proteins but disfavored by the loss of translational and rotational freedom. Echoing the protein folding process, we have previously proposed a transition state for protein-protein association. Here we clarify the specification of the transition state by working with two toy models for protein association. The models demonstrate that a sharp transition between the bound state with numerous short-range interactions but restricted translation and rotational freedom and the unbound state with at most a small number of interactions but expanded configurational freedom. This transition sets the outer boundary of the bound state as well as the transition state for association. The energy landscape is funnel-like, with the deep well of the bound state surrounded by a broad shallow basin. This formalism of protein-protein association is applied to four protein-protein complexes, and is found to give accurate predictions for the effects of charge mutations and ionic strength on the association rates.

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