

Protein Folding and Flexible Binding

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Transition state theory has been often used in protein folding. We study the effect of diffusion in protein folding dynamics. We found configurational dependent diffusion can have significant effects on the kinetics. It can shift the transition state and therefore the kinetic route or path as well as change the thermodynamic barrier height and therefore the kinetic rate. For fast folding, the effect of configurational dependent diffusion is expected to play an important role and the transition state theory should be significantly modified accordingly. Flexible molecular recognition can be very important in realizing the function and specificity in the cell. We study the flexible binding when folding and recognition are intimately coupled. We found for a particular protein interaction complex, the flexible recognition proceeds as first binding and then folding in contrast with the conventional wisdom of first folding and then binding, revealing the important underlying nature.