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Rate Constants and Mechanisms of Protein-Ligand Binding[1]

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Whereas protein-ligand binding affinities have long established prominence, binding rate constants and binding mechanisms have continued to gain increasing attention in recently years. Both new computational methods and new experimental techniques have been developed to characterize the latter properties. It is now realized that, binding mechanisms, like binding rate constants, can and should be quantitatively determined. In this talk, I will summarize studies and synthesize ideas on several topics, in the hope of providing a coherent picture and physical insight on binding kinetics. The topics include: microscopic formulation of the kinetic problem and its reduction to simple rate equations; computation of binding rate constants; quantitative determination of binding mechanisms; and elucidation of physical factors that control binding rate constants and mechanisms.

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