Current Topics in Biophysics (Zagadnienia Biofizyki Współczesnej) vol. 21 (2), 1997, 103-112

Protein dynamics and microscopic theory of enzymatic reactions Michał Kurzyński

Formation of a contemporary statistical theory of biochemical processes needs simple but adequate models of phenomena underlying microscopic dynamics of biomolecules, in particular enzymatic proteins. An intentionally simplified, for this purpose, picture of protein dynamics emerging from the recent studies is outlined and two classes of theoretical models of slow activated dynamics of conformational transitions in the native phase are described. The rule seems to be that it is this dynamics, and not the very chemical mechanism, that controls the rate of protein involving reactions. In such cases, the short initial-condition dependent stage of reaction can dominate over its main stage described by standard kinetics. A simple statistical theory of a complete enzymatic reaction is proposed. The overall reaction is assumed to involve three steps (a single covalent transformation of substrate preceded and followed by association-dissociation reactions of the substrate or the product with the enzyme), each step being gated by enzyme intramolecular dynamics. The important result obtained is that the kinetics mechanisms of the transient and steady-state stages of reaction differ. It is the same nonequilibrium microscopic dynamics that affects both the coupling of component reactions in the steady-state stage and a possible initial-condition dependent pretransient stage of the enzymatic reaction. The microscopic dynamics and not that in the stage described by the standard kinetics is expected also as responsible for the coupling of component reactions in more complex processes of biological free energy transduction taking place at multienzyme protein complexes.