

Identification of Networks of Coupled Promoting Motion in Enzymatic Reactions via INM Analysis

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Abstract

Instantaneous normal mode (INM) analysis is used to identify, within the enzyme dihydrofolate reductase (DHFR), a set of delocalized modes which may be important for catalyzing the hydride transfer reaction. Both the time dependence of INMs as well as the thermally averaged nature of INMs characterizing reactant and transition state configurations are analyzed. A comparison of the modes within wild-type DHFR with the mode within mutant forms of DHFR explores the correspondence between catalysis and protein structure. How structural alterations affect the network of motions, and thus, the catalytic rate, is a fundamental issue in protein engineering.