



Computational Approaches to Biochemical Reactivity (Understanding Chemical Reactivity)

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A quantitative description of the action of enzymes and other biological systems is both a challenge and a fundamental requirement for further progress in our understanding of biochemical processes. This can help in practical design of new drugs and in the development of artificial enzymes as well as in fundamental understanding of the factors that control the activity of biological systems. Structural and biochemical studies have yielded major insights about the action of biological molecules and the mechanism of enzymatic reactions. However it is not entirely clear how to use this important information in a consistent and quantitative analysis of the factors that are responsible for rate acceleration in enzyme active sites. The problem is associated with the fact that reaction rates are determined by energetics (i. e. activation energies) and the available experimental methods by themselves cannot provide a correlation between structure and energy. Even mutations of specific active site residues, which are extremely useful, cannot tell us about the totality of the interaction between the active site and the substrate. In fact, short of inventing experiments that allow one to measure the forces in enzyme active sites it is hard to see how can one use a direct experimental approach to unambiguously correlate the structure and function of enzymes. In fact, in view of the complexity of biological systems it seems that only computers can handle the task of providing a quantitative structure-function correlation.

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