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| Altri autori (Persone) | Naray-SzaboGabor<br>WarshelArieh |
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| Soggetti | Biochemistry - Mathematical models<br>Enzyme kinetics<br>Quantum biochemistry<br>Ligand binding (Biochemistry) - Mathematical models |
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| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Quantum Mechanical Models for Reactions in Solution -- Free Energy Perturbation Calculations within Quantum Mechanical Methodologies -- Hybrid Potentials for Molecular Systems in the Condensed Phase -- Molecular Mechanics and Dynamics Simulations of Enzymes -- Electrostatic Interactions in Proteins -- Electrostatic Basis of Enzyme Catalysis -- On the Mechanisms of Proteinases -- Modelling of Proton Transfer Reactions in Enzymes -- Protein-Ligand Interactions. |
| Sommario/riassunto | 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 und- standing 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 st- ies 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 - portant information in a consistent and quantitative analysis of the factors that are - sponsible 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 - tween 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.