The simulation of enzymatic processes is a well-established field within computational chemistry, as demonstrated by the 2013 Nobel Prize in Chemistry. It has been attracting increasing attention in recent years due to the potential applications in the development of new drugs or new environmental-friendly catalysts.

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The book provides the basic knowledge for postgraduate students and researchers in chemistry, biochemistry and biophysics, who want a deeper understanding of complex biological process at the molecular level.

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Computer model showing the structure of a bacterial dihydrofolate reductase molecule (green) bound to a folic acid molecule (spheres). Dihydrofolate reductase is an enzyme that converts folic acid into a coenzyme. Enzymes and coenzymes control chemical reactions inside living cells.

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