

Special Issue

Catalytic Reaction Mechanics of Enzymatic Reactions

Message from the Guest Editors

Theoretical methods (molecular docking, molecular dynamics simulation, quantum mechanical/molecular mechanics, and so on) are a new cross-biological means with the development of biological science and computer science technology. They have been applied to the research of biological macromolecular catalytic mechanism, protein conformation change between enzyme and ligand, which can affect the catalytic efficiency of the enzyme, and rational design of enzyme. Hence, in order to better explore the catalytic reaction mechanism of many macromolecules, it is necessary to introduce relevant research into the Special Issue to promote the development of this field. In this Special Issue, original research articles and reviews are welcome. Research areas may include (but are not limited to) the following: structure–activity relationship between protein and ligand, QM/MM enzyme catalytic reaction mechanism, structural modification of enzymes, and rational design of enzymes. We look forward to receiving your contributions.

Guest Editors

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Deadline for manuscript submissions

closed (10 April 2022)



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