



Catalytic Reaction Mechanics of Enzymatic Reactions

Guest Editors:

Prof. Dr. Weiwei Han

Key Laboratory for Molecular Enzymology and Engineering of Ministry of Education, Jilin University, Changchun 130012, China

Prof. Dr. Minghui Li

Department of Bioinformatics, School of Biology and Basic Medical Sciences, Soochow University, Suzhou 215123, China

Prof. Dr. Lihong Hu

School of Information Science and Technology, Northeast Normal University, Changchun 130117, China

Deadline for manuscript submissions:

closed (10 April 2022)

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.

