Modeling and Simulation of Enzymatic Catalysis Processes

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Deadline for manuscript
submissions:
closed (30 June 2021)

Message from the Guest Editor

Dear Colleagues,

Enzymes play a central role in life, catalyzing many chemical and biological processes occurring in nature. Understanding how enzymes catalyze their reactions is essential, both from fundamental and practical perspectives, with application in a variety of areas, from more basic research that aims to understand how different events occur in the cell, to the development of new treatments for important diseases, and even in industrial biocatalytic applications.

Computational methods can be used to simulate and model different enzymatic reactions, circumventing some of the limitations of the experimental methodologies typically used, and providing an alternative strategy to complement the information obtained from these methods. This Special Issue focuses on the application of computational methods for modeling and simulating enzymatic reaction mechanisms, including methodological developments and computational studies addressing the activity of specific enzymes.

mdpi.com/si/41676

Special Issue

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Message from the Editor-in-Chief

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