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Computational Modeling of Kinetics in Biological Systems

Guest Editor:

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Message from the Guest Editor

Biological systems respond to changes in the environment, such as the depletion of ingredients, temperature reduction, increase in light intensity, and many other transient variations using timely molecular actions. The speed of cellular responses is critical for living systems. It depends on the rates of physical and chemical processes, making the study of the dynamics of these systems particularly relevant for life. Diffusion and searches in crowd environments, enzymatic reactions, signaling, translocation, organization, and reorganization of biological matter are a few examples of biomolecular dynamics that shape cellular life and are frequently conducted at conditions far from equilibrium. Computer simulations in molecular biophysics and biochemistry have considerable potential to shed light on these complex phenomena. Enhanced sampling techniques for molecular kinetics in biology expanded considerably in the last decade and are currently mature enough to produce useful and consistent models for atomic and molecular scale biology. Computational studies of the kinetics of biomolecular events are the focus of the current issue.

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Message from the Editor-in-Chief

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