Special Issue

Computational Approaches to Understand the Mechanisms of Diseases at Molecular Level

Message from the Guest Editors

The rapid advancement of computational techniques brings computational biology to the forefront in the race to understand the mechanisms of disease at a molecular level. Cutting-edge computational tools have been widely used to solve problems in biology, including protein structure prediction, protein–protein complex structure prediction, pKa prediction, drug design, simulations of biomolecules, etc. With the structures of biomolecules in hand, atomic simulations, coarse-grained models, and other computational approaches have been successfully implemented to study health-related problems. This Special Issue shall focus on advanced computational approaches and their applications in understanding the mechanisms of disease at a molecular level. This Special Issue aims at developing and utilizing state-of-the-art computational algorithms to study a wide range of diseases.

Guest Editors

Dr. Lin Li

Department of Physics, University of Texas, 500 West University Ave, El Paso, TX 79968, USA

Dr. Yi He

Department of Chemistry & Chemical Biology, The University of New Mexico, Albuquerque, NM 87131, USA

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Pathogens
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
pathogens@mdpi.com

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Message from the Editor-in-Chief

The worldwide impact of infectious disease is incalculable. The consequences for human health in terms of morbidity and mortality are obvious and vast but, when infections of animals and plants are also taken into account, it is hard to imagine any other disease that has such a significant impact on our lives—on healthcare systems, on agriculture and on world economics. *Pathogens* is proud to continue to serve the international community by publishing high quality studies that further our understanding of infection and have meaningful consequences for disease intervention.

Editor-in-Chief

Prof. Dr. Moriya Tsuji
School of Engineering Medicine, Texas A&M University, 2121 West Holcombe Blvd., Suite 1007, Houston, TX 77030, USA

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