Special Issue

Computational Simulation of Macromolecular Processes Involved in Disease

Message from the Guest Editor

The structural information of macromolecules is of great importance for understanding the mechanisms underlying various types of diseases. This atomic-scale information allows a precise understanding of the mechanisms underlying different types of biological systems, as well as techniques capable of computationally simulating the movement of these macromolecules in their biological environment, helping us to rationalize mechanisms and understand how biological systems operate. In addition, computational drug design relies on knowledge of the active sites or allosteric sites of enzymes to find chemical compounds that can stably bind to the amino acids present in them, thus inhibiting or modulating their activity. This Special Issue welcomes contributions that use three-dimensional molecular structure techniques and/or virtual modeling in computational biology, alone or in combination with in vitro or in vivo strategies. Papers addressing 3D screening strategies, the design of new drugs and therapies, and any original articles or comprehensive reviews related to molecular structure and simulation in biological systems are also welcome.

Guest Editor

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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