International Journal of
Molecular Sciences

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Computational Simulation of Macromolecular Processes Involved in Disease

Guest Editor:

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Deadline for manuscript submissions:
closed (30 April 2024)

Message from the Guest Editor

Dear Colleagues,

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.

mdpi.com/si/188997

Special Issue

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Message from the Editor-in-Chief

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