Special Issue

Molecular Structure and Simulation in Biological System 2.0

Message from the Guest Editor

Structural information at the atomic scale of macromolecules allows a precise understanding of the mechanisms underlying different types of biological system, including intermolecular interactions, intracellular interactions, and so on. Knowledge of this information, as well as techniques capable of computationally simulating the movement of these macromolecules in their biological system, helps us to rationalize the mechanisms and understand how biological systems work. This Special Issue welcomes papers using 3D molecular structure and/or virtual modeling techniques in computational biology, alone or in combination with in vitro or in vivo strategies. The aim of these techniques may be the prevention, discovery, characterization or therapy of diseases, including cancers, genetic diseases, or those related to viral or bacterial infections. We also welcome 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 system.

Guest Editor

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