

Special Issue

Molecular Structure and Simulation: Unraveling the Basis of Disease

Message from the Guest Editor

Structural information at the atomic scale of macromolecules allows a precise understanding of the mechanisms underlying different types of diseases, including infectious diseases (viral, bacterial, or parasitic), disorders such as cancer, and others of genetic origin (e.g., rare diseases). Knowledge of this information, as well as techniques capable of computationally simulating the movement of these macromolecules in their cellular environment, helps us to rationalize the causes of diseases and to design possible treatments. In the case of diseases caused by pathogens, the structural information of key enzymes in the functioning of these viruses, bacteria, or eukaryotic parasites allows us to know how these pathogens function, and to design specific ligands that can later give rise to new drugs. 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. We also welcome papers addressing 3D screening strategies and the design of new drugs and therapies.

Guest Editor

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Message from the Editor-in-Chief

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