

## 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

Dr. Paulino Gómez-Puertas

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### Deadline for manuscript submissions

closed (31 July 2023)



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### Message from the Editor-in-Chief

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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### Editor-in-Chief

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