Special Issue

Advance in Computational Protein Structural Biology

Message from the Guest Editor

One of the most fruitful combinations of experimental and computational methods is that of nuclear magnetic resonance (NMR) spectroscopy and molecular dynamics (MD) simulations, which has been successfully applied to obtain molecular information in many research areas, ranging from materials to biological systems.

Both NMR and MD simulations are used to study molecular structures, dynamics and protein interactions at the atomic level. NMR is unique in its ability to provide information on the three-dimensional structure and on the amplitude and rate of structure variations at the atomic level. MD has the unique ability to correlate different molecular states and mechanisms in time.

This Special Issue is focused on the symbiosis of these two techniques used to understand, in detail, the key molecular mechanisms that cause infectious or transmissible diseases, impact of computational structural biology on protein structure prediction methods, macromolecular function and protein design, and key methods in drug discovery.

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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