International Journal of
Molecular Sciences

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Advance in Computational Protein Structural Biology

Guest Editor:

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Deadline for manuscript submissions:
closed (31 December 2022)

Message from the Guest Editor

Dear Colleagues,

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.

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Message from the Editor-in-Chief

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