International Journal of
Molecular Sciences

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Molecular Simulation of Protein Structure and Interactions

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Deadline for manuscript submissions:
31 December 2024

Message from the Guest Editors

Molecular simulation methods allow the study of biomolecules in exquisite atomistic detail, enabling the characterisation of molecular mechanisms and their associated thermodynamics and kinetics properties. Developments in force fields and enhanced sampling methods, alongside the wider availability of exascale computing resources, are facilitating the investigation of much more complex systems at substantially larger time and length scales. The interface of biology and materials in molecular sciences are also being increasingly characterised by various molecular simulation and artificial intelligence approaches.

This special issue is aimed at recent research using molecular simulation approaches to study complex biomolecular systems such as intrinsically disordered proteins, protein aggregation, liquid-liquid phase separation, membrane receptor activation, peptide- and protein-membrane interactions, macrobiomolecular complex formation and interactions, protein-surface interactions, and proteins in biomaterials. New methods and force fields developed for these systems, including the use of artificial intelligence, are also of particular interest.

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Message from the Editor-in-Chief

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