Special Issue

Computational Analysis of Protein and Nucleic Acid Structures, Interactions, and Functions

Message from the Guest Editors

This collection of studies features pioneering integrations of AI and molecular dynamics, including neural network-enhanced force fields for accelerated conformational sampling and hybrid architectures that combine deep learning predictions with physics-based simulations. Highlighted innovations include 3D structure determination (cryo-EM and AI-based folding), molecular dynamics simulations of conformational changes in challenging biomolecules, and network-based analysis of biological macromolecule interactions. Emphasis is placed on integrative methods that combine structural biology data with multi-omics datasets to reveal mechanistic insights into cellular processes. Emerging applications in drug design (targeting protein–nucleic acid interfaces) and synthetic biology demonstrate these technologies' translational potential. Key themes include (1) next-generation prediction tools (AlphaFold3 and RoseTTA-NA), (2) AI-optimized analysis of binding thermodynamics/kinetics, (3) multi-scale modeling from the atomic level to cellular level, and (4) high-throughput screening of functional variants.

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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