Special Issue

Artificial Intelligence in Structural Biology and Drug Discovery

Message from the Guest Editor

Artificial intelligence is transforming drug discovery by accelerating insights across both structure- and sequence-based approaches. This Special Issue of *Biomolecules* highlights cutting-edge AI methods for protein structure prediction, refinement, and binding site detection, as well as machine learning strategies for docking and molecular dynamics used for drug discovery. Equally emphasized are sequence-based models for predicting binding partners and designing novel therapeutics, an approach compelling for targets lacking high-resolution structural data. By showcasing hybrid frameworks and translational case studies, the Special Issue explores how integrating sequence and structural information enables scalable, rapid, and experimentally validated therapeutic development, marking an exciting frontier in biomedical innovation.

Guest Editor

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Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

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