## Special Issue

# Recent Advances in Structure-Based Inhibitor/Drug Design

## Message from the Guest Editor

This Special Issue aims to report recent progress in the field of structure-based inhibitor and drug design, a pivotal approach that relies on the precise threedimensional structures of therapeutic targets to rationally develop potent and selective compounds. By elucidating biomolecular interactions and the structures and functions of biomolecules through techniques such as X-ray crystallography, NMR, and molecular dynamics simulations, this strategy enables the rational design of molecules that selectively bind and modulate target functions. Additionally, the integration of bioinformatics, Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) is accelerating the prediction and optimization of drug candidates. This Special Issue will collect the latest research and review papers focused on these advances, providing valuable insights to promote future drug discovery and development. Submissions may include original research, comprehensive reviews, or perspectives.

### **Guest Editor**

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#### Deadline for manuscript submissions

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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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