

Special Issue

Computation-Driven Discovery of Modern Small-Molecule Therapeutics: From Enzyme Inhibition to Targeted Protein Degradation

Message from the Guest Editor

With the rapid evolution of structural biology, artificial intelligence, and molecular simulation technologies, computational strategies have become indispensable across the modern drug discovery pipeline—from target identification and mechanistic studies (e.g., enzyme inhibition) to the rational design of emerging therapeutic modalities (e.g., PROTACs and molecular glues).

This Special Issue aims to highlight the transformative impact of computational approaches in accelerating the discovery and development of small-molecule therapeutics. We welcome contributions featuring advanced computational methodologies, including but not limited to molecular docking, free-energy calculations, machine learning-driven virtual screening, multi-scale modeling, molecular dynamic simulation, quantum chemical calculations, and AI-based drug design. Studies that integrate computational predictions with experimental validation are particularly encouraged.

The goal of this Special Issue is to provide a platform for disseminating cutting-edge research that bridges computation, chemistry, and biology, thereby fostering the development of next-generation therapeutic molecules.

Guest Editor

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Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*.

Pharmaceuticals is characterized by an active editorial board and a dynamic editorial staff. Manuscripts are peer-reviewed and a final decision is provided to authors within 4–6 weeks after submission. Papers are published on the web immediately after acceptance. For details on the submission process or any other matter, please do not hesitate to contact us.

We hope to handle your contribution to *Pharmaceuticals* soon.

Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter

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