Computational Methods in Drug Development

Guest Editor:

Dr. Yunjie Zhao
Department of Physics, Institute of Biophysics, Central China Normal University, Wuhan 430079, China

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Message from the Guest Editor

Dear Colleagues,

Advancements in computational methods have significantly changed the drug development process, offering new solutions to speed up the discovery and improvement in therapeutic agents. These methods cover various technologies, from molecular modeling to artificial intelligence, and contribute to different stages of the process.

This Special Issue aims to gather the latest research and reviews on computational strategies in drug development. We encourage submissions that demonstrate innovative computational techniques, including computer-aided drug design, molecular docking and scoring, virtual screening, and the application of various machine learning approaches in drug discovery. By highlighting these advances, we aim to show the transformative potential of computational methods in developing new and efficacious therapeutics.

We welcome submissions discussing the challenges and opportunities in this rapidly evolving field, particularly interdisciplinary studies that combine computational methods with experimental validation. This Special Issue will provide an up-to-date overview of computational drug development and set the stage for future research directions.

Special Issue

Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter
Departamento de Química e Bioquímica (DQB) e Centro de Química Estrutural (CQE), Institute of Molecular Sciences, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

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*.

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

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