Special Issue

Computational Methods in Drug Development

Message from the Guest Editor

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.

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

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