Special Issue

Application of Computer Simulation in Drug Design

Message from the Guest Editors

The growing power of computer simulations is reshaping the landscape of modern drug discovery. From early hit identification to lead optimization, in silico methods—including molecular docking, pharmacophore modeling, molecular dynamics simulations, and AI-driven algorithms—are becoming essential components in the development of novel small-molecule inhibitors (SMIs). This Special Issue aims to showcase recent advances and innovations in the application of computational simulations to drug design, with a particular emphasis on the rational discovery and optimization of SMIs. We encourage submissions of original research and comprehensive reviews exploring diverse computational techniques applied to various disease areas, including oncology, infectious diseases, and neurodegeneration.Topics of interest include, but are not limited to, the following: virtual screening, structure-based drug design, molecular dynamics, AI/ML-assisted drug discovery, binding free-energy calculations, drug repurposing, and integrative strategies.

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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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