

Special Issue

Advanced Algorithms for Small-Molecule Therapeutics Development

Message from the Guest Editors

The advancement of small-molecule therapeutics is revolutionizing drug development and enhancing our understanding of pharmacokinetics and pharmacodynamics. As drug targets are becoming increasingly complex, the integration of computational methods into therapeutic development offers unprecedented precision in predicting drug behavior, efficacy, and safety. These approaches are pivotal in enhancing the development pipeline, improving therapeutic outcomes, and minimizing adverse effects. This Special Issue seeks to delve into cutting-edge computational techniques that directly address challenges in drug development, with a specific emphasis on pharmacokinetics, pharmacodynamics, and related fields. By exploring the interface between computational algorithms and therapeutic design, we aim to highlight strategies that bridge the gap between molecular innovation and clinical application. Contributions should focus on advancing algorithmic approaches that optimize drug metabolism, distribution, and efficacy, and on addressing the complexities of multi-target and patient-specific therapies.

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