Taft / Lazaro

Computational Intelligence in Drug Development

This book offers a comprehensive overview of cutting-edge computational strategies in drug discovery, with a focus on in silico approaches that accelerate the identification and optimization of therapeutic candidates. Readers will find detailed insights into molecular docking, molecular dynamics simulations, and structure-based drug design, alongside predictive models for toxicity, pharmacokinetics (ADMET), and enzyme inhibition. By combining theoretical foundations with practical applications, the volume highlights how artificial intelligence and computational chemistry are reshaping modern pharmaceutical research and enabling the development of safer, more effective drugs.

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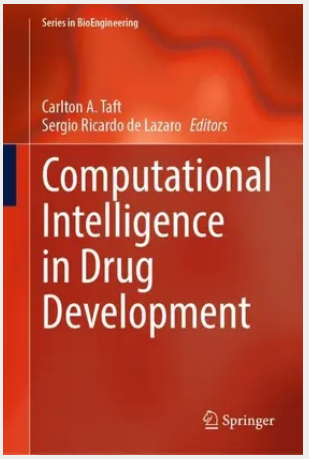

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