

Next-Generation Computational Drug Discovery



Edited by **Mohammad Kalim Ahmad Khan**
and Mohammed Tarique



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Next-Generation Computational Drug Discovery

This book presents the fundamental principles, contemporary methodologies, and practical applications that define modern computer-aided drug design. It explores the integration of Cryo-EM structures, AlphaFold predictions, and homology modeling to expand structural insight into biologically relevant targets. In addition, it covers molecular docking, molecular dynamics simulations, enhanced sampling approaches, and free-energy calculations for robust hit-to-lead refinement. This book further examines in silico Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) prediction, quantitative structure–activity relationships, machine learning-based modeling, and network pharmacology frameworks applied across therapeutic areas, including oncology, infectious diseases, neurodegenerative disorders, and metabolic and cardiovascular conditions.

Key Features:

- Explores foundational and advanced Computer-Aided Drug Design (CADD) techniques, including molecular docking, molecular dynamics simulations, in silico ADMET prediction, and network pharmacology
- Integrates Cryo-EM, AlphaFold, and homology modeling to enhance structure-based drug discovery
- Details machine learning applications for pharmacokinetic profiling, toxicity prediction, and lead prioritization
- Discusses computational workflows for multi-target drug design across major therapeutic domains
- Presents systems biology perspectives and translational case examples linking computational discovery to experimental validation

This book is intended for researchers and students in pharmaceutical sciences, computational biology, bioinformatics, and related disciplines.



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Contents

<i>Preface</i>	vii
<i>About the editors</i>	ix
1 Molecular dynamics simulations in drug discovery: Integration with artificial intelligence and future viewpoints	1
SANGAVI PANDI, DAPKUPAR WANKHAR, J. H. SHAZIA FATHIMA, PRIYANKA GANAPATHY, LANGESWARAN KULANTHAIVEL, AND GOWTHAM KUMAR SUBBARAJ	
2 In silico ADMT prediction	19
MUTTHURAJ DASEGOWDA, H. D. SAHANA, MOUVANAL SAJANA, MOGANAMURTHY BRUNDA, PRASAD TEJAS, AND KANTHESH M. BASALINGAPPA	
3 Multi-target and polypharmacology-oriented drug design	70
KOUSHIK SEN, BHANUMATI SARKAR, TANMAY SANYAL, SUMAN ADHIKARI, AND NITHAR RANJAN MADHU	
4 Computational strategies for cancer drug discovery	94
SAJANA MOUVANAL, MOGANAMURTHY BRUNDA, MUTTHURAJ DASEGOWDA, KAUSTUBHA BELIYA, K. M. VARUN, M. VASUNDHARA, AND KANTHESH M. BASALINGAPPA	
5 Structure-based approaches for infectious disease therapeutics	113
KURALAYANAPALYA PUTTAHONNAPPA SURESH, VARSHA RAMESH, AND NAGARAJU CHAITHRA	

6 In silico drug design for metabolic and cardiovascular diseases	136
BHANUMATI SARKAR, SANGRAM POLLEY, SARTHAK RANJAN SARKAR, SHUBHADEEP ROYCHOUDHURY, CHANDAN ACHARYA, AND NITHAR RANJAN MADHU	
7 Computational design for neurodegenerative disease targets	165
MUTTHURAJ DASEGOWDA, H. D. SAHANA, AND KANTHESH M. BASALINGAPPA	
<i>Index</i>	209