

Contents

Arshdeep Singh, Rabin Debnath, Viney Chawla, and Pooja A. Chawla

1 Historical development of computer-aided drug design — 1

Gita Chawla and Tathagata Pradhan

2 Lead-hit-based methods for drug design and ligand identification — 23

Gagandeep Kaur, Isha Rani, Prabodh Chander Sharma,
and Diksha Gulati

3 Virtual screening tools in ligand and receptor-based drug design — 51

Pawan Kumar and Ajit Kumar

**4 State-of-the-art modeling techniques in performing docking algorithms
and scoring — 65**

Yash Chauhan, Ajay Sharma, Arya Lakshmi Marisatti, Neha Singh, Sahil Kumar, and
Kalicharan Sharma

**5 Design of computational chiral compounds for drug discovery and
development — 81**

Biswa Mohan Sahoo, Pooja Chawla, Subas Chandra Dinda, Narahari Narayan Palei,
Bhupendra Singh, and Bibhas Chandra Mohanta

6 Role of integrated bioinformatics in structure-based drug design — 91

Vipul Kumar, Rakhi, Sahil Kumar, Kalicharan Sharma, and Rajesh K. Singh

**7 Molecular recognizable tools in X-ray crystallography in computer-aided
drug design — 133**

Disha Tewari, Priyanka Sharma, Shalini Mathpal, Kalpana Rawat, Tushar Joshi,
Subhash Chandra, and Veena Pande

**8 Design of target hit molecules using molecular dynamic simulations:
special key aspects of GROMACS or Role of molecular dynamic
simulations in designing a hit molecule for drug discovery — 151**

Anchal Sharma, Nitish Kumar, Jyoti, Aanchal Khanna,
and Preet Mohinder Singh Bedi

**9 Computational prediction of drug-limited solubility and
CYP450-mediated biotransformation — 175**

Abhimannu Shome, Chahat, Keshav Taruneshwar Jha, Pooja A. Chawla,
and Muralikrishnan Dhanasekaran

10 Recent advancement in binding free-energy calculation — 211

Anuradha Mehra, Vanktesh Kumar, Bhupinder Kapoor, Monica Gulati,
and Pankaj Wadhwa

11 Role of structural genomics in drug discovery — 243

Mohammad Ovais Dar, Aamir Tariq Malla, Zahid Ahmad Paul, Roohi Mohi-ud-din,
Mubashir Hussain Masoodi, Pooja A Chawla, and Reyaz Hassan Mir

**12 Unlocking therapeutic potential: computational approaches for enzyme
inhibition discovery — 295**

Bhupender Nehra, Manoj Kumar, Pooja A. Chawla, and Viney Chawla

13 Role of spectroscopy in drug discovery — 319

Kannan Sadasivam, Venkata Surya Kumar Choutipalli, and Lalitha Gummididi

14 Computer-aided design of peptidomimetic therapeutics — 351

Bhupender Nehra, Manoj Kumar, Pooja A. Chawla, Viney Chawla, Monika,
Honey Goel, and Imtiyaz Ahmed Najjar

15 Developing safer therapeutic agents through toxicity prediction — 379

Bhupender Nehra, Manoj Kumar, Pooja A. Chawla, Viney Chawla, and Sarita Pawar

**16 Identifying prominent molecular targets in the fight against drug
resistance — 403**

Index — 429