

Contents

Dilpreet Singh, Pooja A. Chawla, Viney Chawla, and Kamal Dua

- 1 Introduction to computer simulations in drug delivery: current strategies and future prospects — 1**

Ram Babu Sharma, Sakshi Tomar, Swati Kaushal, and Amardeep Kaur

- 2 The role of multiscale approaches for the rational design of nanoparticulate drug delivery system: recent advances — 19**

Mohit Motiwale, Himanshu Verma, Om Silakari, and Bharti Sapra

- 3 The utilization of descriptors in convoluted Lipinski's rule of five — 39**

Sunil Kumar Kadiri, Dhritija Sathavalli, and Prashant Tiwari

- 4 Computer-aided pharmacokinetic functions for extravascular route for oral drug delivery system — 71**

Sarwal Amita, Bharti Sunil, and T.V.S. Padmajyoti

- 5 Computational approaches to the prediction of the blood-brain distribution and design of targeted drugs — 87**

Malti Arya, Sarita K. Yadav, Madhuri Verma, Pranay Wal, Pooja A. Chawla, and Viney Chawla

- 6 Computational methods in the pragmatic development of nanoemulsions, polymeric micelles, and dendrimers for drug delivery — 113**

Gowtham Menon, Rutuja Vilas Nikam, Sachin S. Gaikwad, and Hemant U. Chikhale

- 7 Virtual screening of mucoadhesive polymers for the development of efficient drug delivery system: current approaches — 127**

Neha Jain, Triveni, Aarushi Kaith, Aditi Sinha, Tanya Mathur, Shreya Kaul, Manisha Pandey, and Upendra Nagaich

- 8 QbD and artificial intelligence in nanoparticulate drug delivery systems: recent advances — 163**

Apporva Chawla, Prince Ahad Mir, Md Sadique Hussain, Sameena Ramzan, Tooba Dedmari, Roohi Mohi-ud-din, Pooja A. Chawla, and Reyaz Hassan Mir

9 Nanotoxicity prediction in nanotechnology-driven drugs using QSPR modeling — 183

Shivang Dhoundiyal, Md Aftab Alam, Sakshi Sagar, Shikha Yadav, Sumbul Shadab, and Niyaz Ahmad

10 Molecular simulations strategies for designing 2D nanomaterials for drug delivery applications — 221

Aditya Sharma, Sakshi Sagar, Md Aftab Alam, Manjeet Kaur, Tarique Anwer, and Pramod Kumar Sharma

11 Applications and molecular simulation strategies for excipient–excipient compatibility — 247

Abhishek Singh, Seema Yadav, Narahari Narayan Palei, and Biswa Mohan Sahoo

12 Application of simulation system for selection of nanocarrier for biopharmaceutically challenging pharmaceuticals — 269

Sankha Bhattacharya

13 Applications and challenges in molecular dynamic simulations in polymeric nanoparticle drug delivery systems — 307

Rania M. Hathout

14 Role of principal component analysis in drug formulation and delivery — 331

Vimal Arora, Payal Mittal, and Sanjay Kumar Elisetti

15 Computational approaches for predicting drug solubility and permeability in pharmaceutical formulation — 347

Neha Jain, Manisha Pandey, Unnati Garg, Triveni, Sakshi Malhotra, Jatin Rathee, Deepika, Shreya Kaul, and Upendra Nagaich

16 Molecular simulations and process modeling of tableting technology: recent advances and future insights — 369

Abhishek Singh, Seema Yadav, Narahari Narayan Palei,
and Biswa Mohan Sahoo

**17 Molecular simulation-based technology for antibody–drug conjugates for
tumor targeting: current scenario and future insights — 383**

Index — 437

