We are IntechOpen,
the world's leading publisher of
Open Access books
Built by scientists, for scientists

6,900
Open access books available

186,000
International authors and editors

200M
Downloads

Our authors are among the

154
Countries delivered to

TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities

CLARIVATE ANALYTICS
BOOK CITATION INDEX
INDEXED

WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Prologue: Cheminformatics and Its Applications

Azhar Rasul

1. Introduction

Cheminformatics is a field of information technology that uses informational and computational techniques to provide a deeper understanding and solutions of problems of chemistry. Cheminformatics strategies originally emerged as vehicle in drug discovery where large libraries of compounds are evaluated for specific functionality or therapeutic effects [1].

Drug discovery is a highly systematic multistep procedure for the identification of new medicines [2]. Chemical toolsets including chemical probes, RNAi, and chemoproteomics have helped scientists to identify and validate novel druggable targets for therapeutic interventions [3–6]. Target validation is of pivotal importance in determining the suitability of a new target for further clinical evaluation. Following the process of target validation, hit identification and lead discovery process involves establishment of high throughput screening (HTS) systems as well as development of chemical tool compound libraries [2]. The next critical phase of the drug discovery process is pharmacokinetics and pharmacodynamic profiling of lead compounds [7] and investigation of Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties [8]. Various critical steps in drug discovery involve the applications of cheminformatics such as compound selection, virtual library generation, in silico-based screening, HTS, HTS data mining, and in silico ADMET profiling [9].

In addition, cheminformatics have also helped the scientists to develop and optimize delivery of molecules to intracellular targets for therapeutic implications [10], thus, provided solutions for various unmet medical needs.

Conjugation of therapeutic entities with peptide delivery molecules, especially cell-penetrating peptides (CPPs), has the potential to increase the therapeutic efficacy by enhancing the ability of therapeutics to reach specific intracellular targets [11]. Preclinical evaluations of CPP-mediated therapeutics have shown promising results in disease models that also prompted clinical trials in some cases. These outcomes have, thus, opened new perspectives for CPPs in the development of well-tolerated and specifically targeted human therapies [12]. Thus, insights into current approaches and potential of CPP-based drug delivery systems are presented for greater understanding of readers about powerful promises and clinical efficacy of CPP-based therapeutics.

Cheminformatics and its applications presents the applications of two fields, chemical biology and bioinformatics, in drug discovery, thus, providing comprehensive description of modern technologies such as structure-based drug design, molecular docking, high throughput screening, and pharmaceutical profiling, which are all critical steps for the development of successful marketable drugs. With the invention of advanced and modern techniques in bioinformatics, the process of drug discovery has become faster and economical. Bioinformatics-based

computational techniques have provided platform for large-scale screening of small molecules and chemical biology has served pharmaceutics for the validation of obtained data from computer-aided techniques, thus, both of the fields go hand in hand to revolutionize the field of drug discovery. Keeping in view of the emerging trends on cheminformatics in drug discovery, this book is designed to enable scientists to understand the fundamentals of drug discovery. Beginning with the highlights of the historical timeline of drug discovery, this book simply and succinctly educates its readers about screening methods, medicinal chemistry strategies in drug design, lead generation, testing the bioactivity of leads, lead optimization, clinical trial basics, as well as challenges of drug discovery such as cell-penetrating peptides and acceleration of chemical tool discovery by academic collaborations. This book will provide a clearer picture of cheminformatics and its applications and will be useful for scientific community working in the arena of drug discovery. Several recent developments are also overviewed, which will make it valuable for academicians and scientists.

Author details

Azhar Rasul
Department of Zoology, Government College University Faisalabad, Pakistan

*Address all correspondence to: drazharrasul@gmail.com

IntechOpen

References

[1] Wishart DS. Introduction to cheminformatics. Current Protocols in Bioinformatics. 2016;**53**:14 11 11-14 11 21

[2] Hughes JP, Rees S, Kalindjian SB, Philpott KL. Principles of early drug discovery. British Journal of Pharmacology. 2011;**162**:1239-1249

[3] Kurreck J. Expediting target identification and validation through RNAi. Expert Opinion on Biological Therapy. 2004;**4**:427-429

[4] Bantscheff M, Drewes G. Chemoproteomic approaches to drug target identification and drug profiling. Bioorganic & Medicinal Chemistry. 2012;**20**:1973-1978

[5] Bunnage ME, Chekler EL, Jones LH. Target validation using chemical probes. Nature Chemical Biology. 2013;**9**:195-199

[6] Moustakim M, Felce SL, Zaarour N, Farnie G, McCann FE, Brennan PE. Target identification using chemical probes. Methods in Enzymology. 2018;**610**:27-58

[7] Tuntland T, Ethell B, Kosaka T, Blasco F, Zang RX, Jain M, et al. Implementation of pharmacokinetic and pharmacodynamic strategies in early research phases of drug discovery and development at Novartis Institute of Biomedical Research. Frontiers in Pharmacology. 2014;**5**:174

[8] Wang J, Skolnik S. Recent advances in physicochemical and ADMET profiling in drug discovery. Chemistry & Biodiversity. 2009;**6**:1887-1899

[9] Xu J, Hagler A. Chemoinformatics and drug discovery. Molecules. 2002;**7**:566-600

[10] Gautam A, Chaudhary K, Kumar R, Sharma A, Kapoor P, Tyagi A, et al. In silico approaches for designing highly effective cell penetrating peptides. Journal of Translational Medicine. 2013;**11**:74

[11] Derakhshankhah H, Jafari S. Cell penetrating peptides: A concise review with emphasis on biomedical applications. Biomedicine & Pharmacotherapy. 2018;**108**:1090-1096

[12] Guidotti G, Brambilla L, Rossi D. Cell-penetrating peptides: From basic research to clinics. Trends in Pharmacological Sciences. 2017;**38**:406-424