EDITORIAL

Advances in Drug Discovery based on Genomics, Proteomics and Bioinformatics

The process of drug discovery based on targets has brought a revolution in drug industry. The first attention in this direction was focused on enzymes responsible for various diseases and it was successfully exploited. However, human diseases are correlated with many factors, including genetic and environmental causes and so attention was diverted to gene medicine, which is at present one of the most attractive medical disciplines affecting the human health including allergies, bone growth, cell proliferation, cancer development, cardiovascular diseases, etc. This gene medicine led to the development of three most important areas in the discipline of biology and that are genomics, proteomics, and bioinformatics, where the prime function of genomics is to focus on statistical genetic information, proteomics takes into account the genetic information of DNA or mRNA, as well as events after translation such as the stability, structural modification (phosphorylation, glycosylation, nitrosation, ethylation, and methylation), and cellular location of protein. Thus, today, the discovery of drug targets for specific diseases requires the understanding and use of both genomic and proteomic information.

The genomic and proteomic technologies together have shifted remarkably to the point where the number of attractive targets available is no longer rate limiting - it has actually created the new problem of how to select the targets most likely to succeed from an embarrassment of riches. So here comes the role of bioinformatics which has been developed for target validation. The challenge of bioinformatics is to shorten the list of targets evolved by genomics and proteomics to a point where it may be most crucial to disease and least likely to fail for drug development. Thus, the impact of genomics, proteomics and bioinformatics in drug discovery has been recognized by both academia and pharmaceutical industry. The objective of this thematic issue is, therefore, to present the advances in drug discovery based on these challenging areas.

The present issue contains four excellent articles written by experts. The very first article entitled “The Role of Water Network Chemistry in Proteins: A Structural Bioinformatics Perspective in Drug Discovery and Development” [1] and written by Sobhia et al. presents the primary aspects of water molecules chemistry in drug design. Attempt has been made to glorify that water is a molecule that enables biomolecules in myriad of functions that are vital for life. In the second article entitled as “Omnics-based Strategies: Tools for Discovering Potential Targets in Breast Cancer Drug Development” [2], Scandolara et al. presented the main omics-based tools, such as Genomics, Epigenomics, Transcriptomics, and Proteomics, and discussed how such approaches have improved drug and biomarkers discovery in breast cancer research.

Briton’s tyrosine kinase plays a vital role in B-cell antigen receptor signaling transduction pathway. Thus, controlling BCR signaling by BTK inhibitors is a promising therapeutic approach for the treatment of inflammatory and autoimmune diseases. Therefore, in Chapter 3 entitled “Next Generation Bruton’s Tyrosine Kinase (BTK) Inhibitors Potentially Targeting BTK C481S Mutation- Recent Developments and Perspectives” [3] Das et al. have summarized the discovery and developments of next generation BTK inhibitors and their applications for the treatment of lymphomas and autoimmune diseases. The lengthy and complicated process involved in the development of a novel drug usually takes quite a few years and involves huge monetary costs owing to its low success rate. Thus, reducing the time and as well as the cost of development of a drug demanded discovery of some modern techniques. Consequently, attention was focused on innovative Artificial Intelligence-driven technologies that are proven to improve the efficiency and accuracy of drug discovery. Therefore, Pasrija et al. in the last Chapter, Chapter 4, entitled “Machine Learning and Artificial Intelligence: A Paradigm Shift in Big Data-Driven Drug Design and Discovery” [4] present an overview of the drug discovery and development timeline, different methods of drug designing, and the application of Artificial Intelligence (AI) in various aspects of drug discovery, followed by a brief on the fundamental concepts of AI-based technologies. Furthermore, some sophisticated algorithms involved in Machine Learning and Deep Learning are explored in detail. I have greatly enjoyed reading all these articles and hope that the readers will also find them useful for further advancement in research on drug discovery based on genomics, proteomics and bioinformatics.

REFERENCES


Satya Prakash Gupta

(Co-Editor)

Current Topics in Medicinal Chemistry
Department of Pharmaceutical Technology
Meerut Institute of Engineering and Technology (MIET)
Meerut-250005,
India

E-mail: spgbits@gmail.com

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