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Expert Review

A Short Note on Drug Design and Discovery: Past and Present

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Abstract

Using a combination of computational, experimental, translational, and clinical models, drug discovery identifies potential new therapeutic entities. Drug discovery is still a lengthy, expensive, difficult, and inefficient process with a high rate of new therapeutic discovery attrition, despite advancements in biotechnology and comprehension of biological systems. The creative process of developing new medications based on knowledge of a biological target is known as drug design. In the past, drugs were discovered by randomly screening higher plants. Opium, senna, belladonna, reserpine, ephedrine, and other crude plant drugs, were used for hundreds of years. The screening of microorganisms that followed the accidental discovery of penicillin led to the development of a large number of antibiotics derived from bacterial and fungal sources. Medical chemists were able to modify these antibiotic prototypes to produce better antibacterial with enhanced therapeutic profiles.

The most fundamental aspect of drug design is the creation of molecules that are similar in charge and shape to the molecular target they bind to. In the age of big data, computer modeling and bioinformatics approaches are used in drug design frequently but not always. In addition to small molecules, computational methods for enhancing the affinity, selectivity, and stability of protein-based therapeutics have also made significant progress. Biopharmaceuticals, particularly therapeutic antibodies, are a class of drugs that are becoming increasingly important. Preclinical research on cell-based and animal models, clinical trials on humans, and regulatory approval for the drug's marketing are all components of drug discovery and development. The identification of screening hits, medicinal chemistry, and optimization of those hits to improve their affinity, selectivity, efficacy/potency, metabolic stability, and oral bioavailability are all components of modern drug discovery. Prior to conducting clinical trials, the process of drug development will begin on a compound that meets all of these requirements once it has been identified.

Keywords: Drug discovery, Translational and clinical models, Biological systems, Experimental, Clinical trial

INTRODUCTION

The correlation of certain physicochemical properties of organic molecules with biological potency led to the development of rational drug design. Better molecules that resemble drugs were produced when the compounds were optimized by including the advantageous substituent. NMR and X-ray crystallography have made it possible to learn about the structure of enzymes and other drug receptors. From such information, numerous drugs, such as ACE inhibitors, have entered clinical practice. As a result, it was discovered that inhibiting strategic enzymes would halt the growth of cancer cells, viruses, and bacteria (Arreguin AMG et al., 2011).

DISCUSSION

The topic of this special issue, "Drug Design and Discovery: The topic of "Principles and Applications" was the fundamental principles and potential applications of contemporary drug design and discovery. As detailed below, it included seventeen research articles and one communication from experts from around the world (Barkley EF et al., 2005). More

than 11,000 people are believed to have perished in West Africa during the 2014 Ebola pandemic. In the fight against future outbreaks, the need for novel drug development and effective drug discovery pathways will be critical. A Computational Analysis of Novel Drug Opportunities (CANDO) platform based on the hypothesis that drugs function by interacting with multiple protein targets to create a molecular interaction signature that can be exploited for rapid therapeutic repurposing and discovery is developed by Gaurav Chopra, Ram Samudrala, and coauthors in the article titled Combating Ebola with Repurposed Therapeutic Using the CANDO Platform. They used the CANDO platform to generate the best drug candidates for the treatment of the Ebola virus and compared them to those that were found in in vitro studies. They discovered that compounds can be chosen and prioritized for further in vivo and clinical testing by combining the results of in vitro screening studies with computational docking predictions made on a proteomic scale (Block CC et al., 2002). The amount of time, money, risk, and resources required to find effective treatments for upcoming outbreaks of the Ebola virus will all be significantly cut down using this strategy. In the article titled "Boronic Acid Group:" Dimitra Hadjipavlou-Litina and colleagues presented an extensive docking analysis of the case of autotaxin. A Weighty False Negative Case in the Drug Design Process They discovered that large libraries of boronic acid derivatives failed to dock naturally during virtual screening (Duffy GG et al., 1986). Their binding poses and scoring function values are left out because they are false negatives. Based on natural bond orbital calculations, the authors more precisely characterized the formed bond between Ser/Thr residues as a polar covalent bond rather than a straightforward nonpolar covalent bond to address the issues that had arisen. When large libraries of boron compounds are virtually screened to identify novel hits in drug design, the findings presented in this article highlight the general options that must be taken into consideration (Duke NK et al., 2002) .

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To fully comprehend the networks in living cells, one needs to be familiar with protein-protein interactions and their binding sites. Because the information gleaned through this method can be used for both biomedical research and drug development, it is essential to develop computational methods for quickly identifying the protein-protein binding sites (PPBSs) based solely on sequence information in light of the avalanche of protein sequences produced in the post-genomic era. A new predictor called iPPBS-Opt has been proposed by Jianhua Jia, Bingxiang Liu, and colleagues to address this problem. In it, they used the idea of pseudo amino acid composition (PseAAC) to create intricate protein sequences. This is the first time the stationary wavelet transform approach has been used to reflect the functions of low-frequency phonons in proteins as deduced some 40 years ago, despite the fact that many researchers have also used the PseAAC to create protein sequences. They have also provided a step-by-step guide on how to use the predictor's web server to get the results you want without having to deal with the complicated mathematical equations. This was done to make it as easy as possible for the majority of experimental scientists (Ketch A et al., 2005) (Walker CA et al., 2005).

The process of discovering new drugs has been transformed by biotechnology (Lai MK et al., 2004). The drug discovery process based on recombinant DNA is beginning to open up new possibilities for some old drugs. At first, genetic engineering was only thought to be useful for making therapeutic proteins. For instance, insulin can now be produced using biotechnology in a manner that is identical to that of human insulin. Previously, insulin was made by isolating pancreatic tissue from bovine or porcine species. This was the only reason Biogen and Genentech were established. Proteins, on the other hand, are not ideal drugs due to their difficulty in administration, quick elimination, and potential immunogenicity.

CONCLUSION

For the purpose of locating pyrazole amide compounds with high levels of activity. Using DFT calculations, they investigated the structure-activity relationships of the title compounds and characterized their structures as well as their antifungal properties. According to their findings, "Design, Synthesis, DFT Study and Antifungal Activity of Pyrazolecarboxamide Derivatives," some of the title compounds had moderate antifungal activity. The 18 articles in this special issue on "Drug Design and Discovery: Computer-aided drug discovery and development, drug design and synthesis approaches, in vitro and in vivo pharmacological and toxicological evaluations, and others are all highlighted in "Principles and Applications." In addition to providing crucial information, these articles produced numerous useful tools for drug discovery and development. These studies demonstrated that computational methods, in conjunction with in vitro and in vivo experiments, continuously enhance the efficacy and efficiency of drug discovery processes for selecting lead candidates with more favourable pharmacological, pharmacokinetic, and toxicological profiles.

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None

CONFLICT OF INTEREST

None

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