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Mini Review

Drug discovery using Translational Bioinformatics

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Abstract

The use of bioinformatics methods in translational drug discovery is becoming increasingly important in both academia and the pharmaceutical industry. Key difficulties in the process can now be solved by computational exploitation of the growing volumes of data produced across all stages of the drug discovery process. Here, we highlight a few of the areas where bioinformatics tools and techniques are being created to aid the pipeline for discovering new drugs (Ebeye OA et al., 2007). These include the development of sizable data warehouses, the use of bioinformatics algorithms to analyse "big data" in order to find new drug targets and/or biomarkers, programmes to evaluate the tractability of targets, and the forecasting of repositioning opportunities for the use of approved medications to treat additional indications (Friday U et al., 2015).

Keywords: Computational biochemistry, Drug discovery and design, Genomics

INTRODUCTION

Bioinformatics analysis can speed up the identification of therapeutic targets, the screening of drug candidates, and the refinement of those candidates. It can also make it easier to characterise side effects and anticipate drug resistance. Genomic, epigenetic, genome architecture, cistronic, transcriptomic, proteomic, and ribosome profiling data, among other high-throughput data, have all contributed significantly to mechanism-based drug discovery and medication repurposing. Large structure databases of small molecules and metabolites, along with the accumulation of protein and RNA structures, homology modelling, and protein structure simulation, paved the way for more accurate protein-ligand docking experiments and more insightful virtual screening (Ogori AF et al., 2016). I outline the conceptual framework that underpins the collection of these high-throughput data, summarise the benefits and potential of mining them for drugs, point out some inherent drawbacks of the software and data mining processes, suggest novel approaches to improve the analysis of these various types of data, and highlight frequently used databases and software that are pertinent to drug discovery (Ashaye OA et al., 2006).

Drug development begins with the identification of an illness

with well-defined symptoms that lower quality of life. A desirable medicine is typically defined as a chemical (which could be a simple molecule or a sophisticated protein) or chemical combination that lessens symptoms without having a significant negative impact on the patient (Banjo AD et al., 2010). Other desirable drug characteristics include low likelihood of drug resistance, which would dramatically reduce the medicine's commercial value, and low negative environmental effects, such as no reactivation of bacterial species after human usage. Consequently, a desirable medicine is one that not only works well and causes few side effects, but also has low long-term harm to the patient, society, and environment (Yusuf SR et al., 2017).

DISCUSSION

The study of biological data analysis through computer programming, mathematics, and statistics is known as bioinformatics. The 2001 completion of the human genome project is considered to be the most significant bioinformatics accomplishment. The majority of the work done in this subject is supported by research. To analyse various gene expressions, scientists create databases and create various methods (Ajiboso SO et al., 2012). Bioinformatics has effectively investigated the information of the activities of the genes which was impossible to extract by other ways

because biological data of an organism is in the raw form and it is highly time consuming to know the genes whose function needs to be identified. Other subjects, including biotechnology, the environment, medicine, agriculture, and human health, are greatly influenced by this one. When John Langley put up the hypothesis of distinct substances in 1905, the process of discovering new drugs was under way. The methodical process through which new candidate medications are found is known as drug discovery. The exponential expansion and development of primary and secondary databases, such as those containing nucleic acid sequences, protein sequences, and structures, is the subject of bioinformatics. Drugs are typically only created when the specific pharmacological target responsible for their activities has been found and researched. Validating drug targets enables us to assess the likelihood of failure during the clinical testing and approval processes. Target identification through preclinical development is only a few of the processes involved in drug discovery. This research aims to create lead molecules or new analogues with increased potency (Mohamed SA 2017).

According to recent estimates, it takes roughly 13 years and US\$1.8 billion in "capitalised" costs to introduce a new medication to the market. This price includes the development of the approved medicine as well as the price of the compounds that were developed but never brought to market. All of the stages of the drug discovery process, but especially the later stages of development, might result in projects failing. The type of disease under consideration determines the disease-based bioinformatics methodologies used in translational drug discovery, with several methods used to examine cancer, genetic, and viral disorders. A wide range of genetic and epigenetic alterations, as well as chromosomal instability, are present in cancer cells. Approaches in bioinformatics can be used to pinpoint the main causes of cancer in a given patient (Nwangwa JN et al., 2016). They therefore have the potential to facilitate a more individualised approach to cancer therapy, opening the door for innovative and repurposed medications that target certain proteins, killing or incapacitating only the diseased cells. Our genetic make-up influences how likely we are to contract a wide range of illnesses, how we react to various pharmacological treatments, and how quickly many infectious diseases spread. Bioinformatics techniques frequently focus on finding prospects for gene therapies as well as noninvasive diagnostic and prognostic tools for genetic illnesses (Obembe AO et al., 2015).

CONCLUSION

Since the beginning of time, people have acknowledged that plants have healing properties. Plant-derived medicines have been used to treat a variety of medical disorders. Without isolating the active ingredients, these medications are utilised as concentrated plant extracts or mixtures. However, the isolation and purification of one or two active molecules is necessary in modern medicine. However, there

are many worldwide health issues, including diseases like cancer, degenerative diseases, HIV/AIDS, and diabetes, for which contemporary medicine is unable to offer treatments. The isolation of the "active compound" has frequently rendered the chemical useless. therapeutic development is a multifaceted problem that necessitates consideration of a number of natural and synthetic molecule factors during the selection of therapeutic candidates, including safety, pharmacokinetics, and efficacy. Automation is now a part of drug research thanks to the development of cutting-edge technologies like artificial intelligence, "organs-on-chip," and microfluidics that improve drug design ideas. The examination of prospective compounds' safety, pharmacokinetics, and efficacy has progressed more quickly as a result, and new approaches to drug design and manufacturing based on natural molecules have been made possible. Recent improvements in computational and analytical methods have created new opportunities for processing complicated natural products and using their structures to create novel medications. Indeed, computational molecular design as it relates to natural products is in its infancy. The identification of molecular targets for natural compounds and their derivatives has been made possible in part by predictive computational software. There will be fewer false positive leads in drug development in the future because to the use of quantum computing, computer software, and databases in simulating molecular interactions and forecasting features and parameters required for drug development, such as pharmacokinetic and pharmacodynamics. This paper examines the development of drugs from plant-based natural products as well as the role that cutting-edge technology play in the creation of new drugs.

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