Research Article

BIOINFORMATICS TOOLS: ESSENTIAL FOR THE DEVELOPMENT AND DISCOVERY OF MEDICINES.

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Abstract: Pharmaceutical research and development is a difficult, high-risk, time-consuming, and potentially lucrative process. Pharmaceutical corporations invest millions of dollars to get a medicine to market. A novel medication demands technical competence, human resources, and a large capital commitment. It also requires stringent adherence to laws on testing and manufacturing standards before a new medicine may be used in the general public; in fact, some drugs fail to enter the market. All of these considerations simply raise the expense of researching and developing a novel chemical entity. Bioinformatics/Tools in the drug design process has a favorable impact on the whole process and may speed up different processes of drug design while lowering costs and total time. The current note focuses on bioinformatics' importance in the drug development and research method.

Keywords: Bioinformatics; Drug; New Chemical Entity

I. INTRODUCTION

Drug discovery is the systematic process by which novel potential medications are identified. Pharmaceutical firms often adhere to known methods of drug discovery that rely on pharmacology and chemistry. However, they encounter several challenges in their quest to develop novel medications [1]. In the fiercely competitive pharmaceutical sector, the firm that obtains the first patent for a new chemical entity (NCE), which is a novel medication candidate for a certain therapy, receives all the benefits. Other rivals are left waiting for the expiry of patents in order to share in the rewards. In the present day, pharmaceutical corporations allocate significant resources towards strategies that have the potential to expedite any stage of the drug development process [2]. The growing need to produce a greater number of medications within a limited timeframe and with little risk has led to a significant surge in interest in bioinformatics [3]. Currently, there is a distinct and emerging area called computer assisted drug design (CADD) [4].

II. DRUG TARGET IDENTIFICATION

A primary focus of contemporary bioinformatics methodologies is the anticipation and recognition of physiologically potent candidates [2], as well as the extraction and retention of associated data (Table 1). Drug development often occurs after the identification and thorough study of the specific drug target for which the medications are intended to work upon. The number of possible targets for the drug development process is growing at an exponential rate. The use of bioinformatics in mining and storing the human genome sequence has facilitated the determination and categorization of the nucleotide compositions of genes that encode target proteins. Additionally, it has enabled the identification of novel targets that have greater promise for the development of new medications [5, 6]. The human genome information is anticipated to have a significant impact in this field [7]. As more genes are discovered and the process of developing drugs becomes increasingly reliant on data, drug developers now have a greater range of options to choose from, which is a new and advantageous situation for them [8]. Bioinformatics enables the discovery and examination of an increasing number of biological therapeutic targets, hence projected to significantly expand the range of prospective medications in the development stages of pharmaceutical businesses [2, 3].

Table 1: Drug Target Database.

S. No	Database	Information
1	Drug bank Wishart, et al.[9]	The Drug Bank database is a comprehensive resource that integrates specific information on drugs, including their chemical, pharmacological, and medicinal properties, with extensive data on drug targets, including their sequence, structure, and pathway information. It combines bioinformatics and chemoinformatics to provide a full understanding of drugs and their targets.

2	Therapeutic target DB Zhu, et al. [10]	The Therapeutic Target Database (TTD) is a comprehensive drug database specifically created to offer detailed information on therapeutic protein and nucleic acid targets mentioned in scientific literature. It includes data on the associated disease conditions, pathway information, and the specific drugs or ligands that target each of these identified targets.
3	STITCH Kuhn, et al. [11]	STITCH, also known as 'search tool for interactions of chemicals', is a database that allows users to search for information regarding interactions. It incorporates data from many sources such as metabolic pathways, crystal structures, binding tests, and drug-target relationships. Text mining and chemical structural similarity are used to forecast associations among compounds. Every suggested interaction may be tracked back to the primary data sources.
4	Super Target Hecker, et al. [12]	Super Target is a database that stores a central dataset of over 7,300 relationships between drugs and targets. Out of these, around 4,900 interactions have undergone a thorough human annotation process. Super Target offers tools for doing 2D drug screening and comparing sequences of the targets.

III DRUG TARGET VALIDATION

Bioinformatics offers methodologies and algorithms for forecasting novel drug targets and for organizing and overseeing existing drug target data. Once prospective therapeutic targets are identified, it is crucial to demonstrate a solid connection between a hypothetical target and the illness of interest [7]. The formation of such a crucial alliance offers validation for the process of developing pharmaceuticals. The process of target validation, which involves the assessment of potential therapeutic targets, is an important domain in which bioinformatics is making a substantial impact (Figure 1). Drug target validation plays a crucial role in reducing the risk of failure throughout the clinical testing and approval stages [2].

IV COST REDUCTION

Pharmaceutical businesses are very concerned about the present exorbitant expenses associated with medication research and development [13]. In addition to enhancing productivity, pharmaceutical firms also strive to mitigate the substantial failure rate in the drug development process, therefore boosting the number of pharmaceuticals that successfully reach the market [14]. The exorbitant expenses associated with different stages of clinical trials serve as constraints for the quantity of pharmaceuticals that may be created by pharmaceutical firms. Therefore, it is crucial to carefully choose the compounds with the highest likelihood of approval [15]. The expenses associated with the process of discovering and developing pharmaceuticals typically include the whole cost from the initial discovery phase to the approval phase. However, several studies have also taken into account the costs incurred by unsuccessful drug attempts and the costs involved in commercializing the treatments [13, 16]. The extended procedure, from discovery to final approval, incurs a corresponding cost [15, 17]. The progress in bioinformatics speeds up the process of discovering drugs, starting with identifying and validating drug targets (such as Docking), to developing assays, and conducting virtual-high-throughput screening (v HTS), all with the aim of finding new possible chemical compounds. Bioinformatics enhances target identification and validation methods, hence increasing the likelihood of successful drug candidates throughout the approval process and improving cost-effectiveness [3].

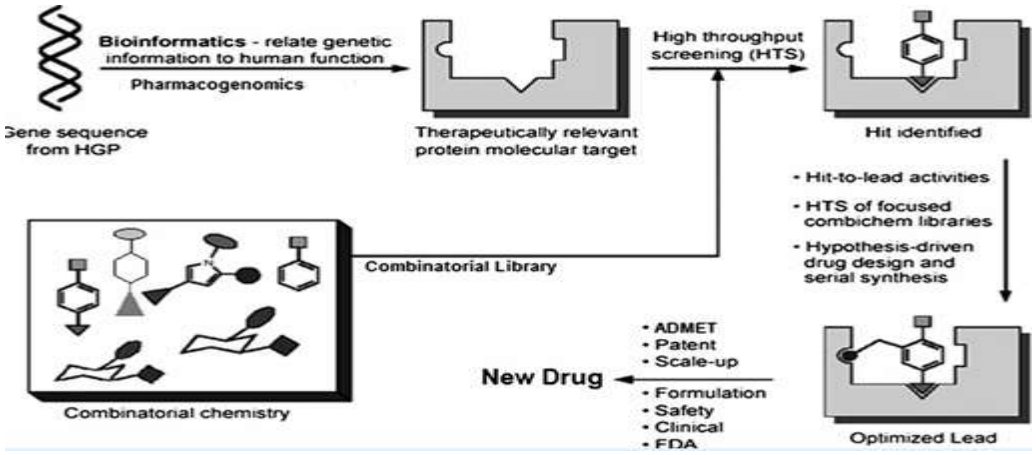

Figure 1: The role of bioinformatics in different stages of drug discovery process.

V PROMOTE NOVEL DRUG DEVELOPMENT

The pharmaceutical business is concerned about some ancillary expenses [18]. The costs mentioned include expenses related to commercialization, legal disputes, medication recalls, and overall societal expenditures [17, 19, and 20]. The high commercialization costs for new pharmaceuticals, estimated to be over $250 million per authorized drug, mostly stem from the fact that most "new" drugs that get approval are effectively functional duplicates of drugs that already exist [16, 21]. The majority of counterfeit medications are being marketed to treat illnesses for which there are already existing treatments. Therefore, there is a need for an interface that can capture the interest of both doctors and patients who already have access to comparable medication [22]. Bioinformatics serves as an effective interface, offering pharmaceutical firms new methods and possibilities to effectively identify prospective therapeutic targets and create innovative medications [2]. Commercialization costs of medications are anticipated to decrease dramatically if they are not marketed in competition with previously established alternatives [23].

VI BARRIERS TO BIOINFORMATICS PROGRESS IN DRUG DESIGN PROCESS

The use of bioinformatics did not result in any significant improvements in the process of drug discovery and development. The reason for this might be attributed to the fact that the field of bioinformatics is relatively recent and has gained significant recognition only after the partial completion of the Human Genome Project [24]. Thus far, bioinformatics has not had a significant influence, as previously anticipated, on the cost of pharmaceuticals. The pharmaceutical business is seeing an ongoing increase in expenses and the removal of pharmaceuticals from the market even after they have been licensed and made available for sale. This is due to many recorded instances of adverse drug responses [25]. Multiple pharmaceutical businesses are now encountering hurdles in medication research and development. The issues include a wide spectrum, including the exorbitant expenses associated with drug research, the protracted and hazardous nature of clinical trials and approval procedures, occasional removal of previously sanctioned products from the market, and the innovation gap arising from the relentless pursuit of blockbuster pharmaceuticals [1, 12, 13]. The field of bioinformatics was expected to significantly enhance the discovery of pharmacological targets [6]. The persistence of these unresolved issues, despite substantial expenditures in bioinformatics, suggests the existence of a more severe underlying problem [26, 27].

VII CONCLUSION

Drug design is a very intricate, costly, and complicated procedure. Bioinformatics offers significant assistance in addressing the challenges of cost and time constraints in numerous ways. Bioinformatics offers a diverse array of drug-related databases and tools that may be used for numerous objectives pertaining to the process of drug creation and development. Bioinformatics is now in its developing phase and while it is encountering certain obstacles, it has significant promise to aid in the drug development process in the not-too-distant future.

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