

ARTIFICIAL INTELLIGENCE IN PHARMACY DRUG DESIGN**NISHAV KALAYIL*, SHONA S D'SOUZA, SHOWKHIYA Y KHAN, PALLAVI PAUL**

Department of Pharmaceutics, St. John's College of Pharmacy and Research, Palghar, Maharashtra, India. Email: nishavk@stjohns.edu.in

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ABSTRACT

Drug discovery is said to be a multi-dimensional issue in which different properties of drug candidates including efficacy, pharmacokinetics, and safety need to be improved with respect to giving the final drug product. Current advances in fields such as artificial intelligence (AI) systems that refine the design through support investigations, microfluidics-assisted chemical synthesis, and biological testing are now giving a cornerstone for the establishment of greater automation into detail of this process. AI has stimulated computer-aided drug discovery. This could likely speed up time duration for design and discovery and enhancement and authorize more productive paths of related chemicals. However, such a paradigm is also increases substantial theories, technical, and organizational quarters, as well as suspicion about the ongoing boom around them. Machine learning, in particular deep learning, in multiple scientific disciplines, and the development in computing hardware and software, among other factors, continue to power this development worldwide.

Keywords: Drug discovery, Artificial intelligence systems, Computer-aided drug discovery, Quantitative structure-activity relationship approach.

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INTRODUCTION**Drug discovery**

The process of Drug Discovery affects the whole Pharmaceutical sector including all the phases such as a preliminary phase of research from target Discovery and validation to the discerning of molecules. A variety of streams can be used to initiate the identification of small therapeutic molecules [1]. New research can lead to awareness of different diseases with different routes of drug administration and can be developed to take part in pharmaceutical companies to run large-scale trials and other waste programs, in order to identify the targeted molecular compounds. This process is mostly performed at the beginning of lead Discovery, with the prospect of taking identified compounds in the right way through pre-clinical and clinical trials [2,3].

The steps involved in the process of drug discovery**Step 1 – Target identification and validation**

The first step involves target identification and validation as it starts the whole drug discovery process. The basic targets for therapeutic use are cellular or molecular structures which materialize naturally and take part in prime roles in pathogenesis [3]. The target molecule should be conveniently safe and efficacious and should meet the clinical demands of the patient to get the desired drug molecule after identification of the drug target system approach should be performed in the modification of the API to be qualified for efficacy (Fig. 1).

Step 2 – Hit identification and validation

The next step is to recognize whether the small molecule leads have the desired effect against the identified targets. Hits can be identified using several techniques, such as high-throughput screening, knowledge-based approaches, and virtual screening. Validation of hits is important during the initial stage of screening.

Step 3 – moving from a hit to a lead validation

The aim now is to clarify each hit series to develop more selective compounds based on the various series of hits introduced to facilitate particularly important to work on multiple series in parallel since some successful series will fail due to unique characteristics. Focusing on multiple series structurally, different sets of hit series will help to offset this possibility.

Step 4 – lead optimization

To develop a pre-clinical drug candidate, it is necessary to improve on the deficiencies of lead compounds and maintain their desired properties. Using this step, you can determine whether your drug metabolizes in the right area of your body, or whether you have any current side effects of concern. An integrated approach is recommended for the same. Bringing together experts in computational chemistry, medical chemistry, drug metabolism, and other fields will allow them to provide unique insight into the late stages of the process [4-7].

Step 5 – late lead optimization

Before progression to pre-clinical and clinical trials, late-stage optimization, in which further pharmacological safety of a lead compound is assessed, is a vital step. A drug's efficacy, pharmacokinetics, and safety will be more likely to be compromised later in development if this phase is ignored. As part of safety optimization, the aim is to identify and progress leads with the best overall safety profile, remove the most toxic leads, and establish a well-defined hazard and translational risk profile necessary for further in vitro testing. By thoroughly calculating the risks at this point, more opportunities can be taken when investments are made into leads. Further, if the drug is approved for development it is passed to perform pre-clinical and clinical trials [8].

Artificial Intelligence (AI)

AI and the area of machine learning (ML) are the study of the processes and viability of functioning machines to cleverly execute intelligent tasks, without obviously being pre-programmed for those tasks [9,10]. At present, AI systems have approached or exceeded human performance in multiple tasks, such as game playing and image recognition, but these have generally been quite limited and focused domains. However, AI in its varied forms is being effectively used across several domains and for complex tasks, such as robotics, speech synthesis, image analysis, and logistics, as well as its application in the design of molecules (Fig. 2).

Since 1960, medicinal chemistry has been applied to AI in different forms and with an assorted degree of progress in designing compounds. It involves supervised learning, in which labeled training datasets are used to train models broadly. One example is the quantitative structure-activity relationship (QSAR) approach, which is frequently

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