International Journal of Scientific Research in Engineering and Management (IJSREM)
Volume: 07 Issue: 03 | March - 2023 Impact Factor: 7.185 ISSN: 2582-3930

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT-A REVIEW

Mr CHETAN S.H[1], Mrs DEEKSHA[2]

[1] Department of Pharmaceutical Chemistry, Srinivas College of pharmacy
[2]Department of Electronics and Communication Engineering, Srinivas institute of Technology

---

Abstract – Artificial Intelligence (AI) has recently been developed into a sizzling topic in the area of medical care industry. The biopharmaceutical industries are making efforts to approach AI to enhance drug discovery process, reduce research and development expenses, diminish failure rates in clinical trials and ultimately generate superior medicines. This article describes the use of artificial intelligence and machine learning to augment drug discovery and development to make them more efficient and accurate. This body of work supported the roles of machine learning and artificial intelligence in facilitating drug development and discovery processes, making them more cost-effective or altogether eliminating the need for clinical trials, owing to the ability to conduct simulations using these technologies

Key Words: Artificial intelligence, Machine learning, Drug discovery

1. INTRODUCTION

Every aspect of life is constantly subject to change, and one of the main aims of humans is to control these changes for our benefit; this is especially true in the field of medicine and pharmaceuticals. These disciplines focus on the creation or discovery of chemical compounds and mixtures and their use to ease physical and psychological suffering. For many decades, the manufacturing of drug products has been controlled by a regulatory framework that safeguards the quality of final products by testing of raw materials, in-process materials, end-product characteristics, batch-based operations and fixed process condition. The drug and biopharmaceutical industries have been limited source of inventive and novel technologies or machinery, and have led the development of novel principles or interpretations in general chemical and mechanical engineering. The pharmaceutical industry is in critical need of mechanical innovation, easing the creation of medications for human use

The use of artificial intelligence (AI) is increasing, and is likely to change how clinical examination and training is carried out. Doctors can participate in the development of this technology for use in the medical and pharmaceutical industries; this will ensure that the potential of AI to significantly improve medical care is fulfilled [2]. AI is currently used in the pharmaceutical industry in four main ways. The first is in the assessment of the severity of disease and the prediction of whether treatment will be successful for an individual patient, even prior to its administration. Secondly, it is used to prevent or solve complications during treatment. Its third main use is as an assistive technology to during treatment procedures or operations on patients. Lastly, it is used was created which was the first system that had overwhelming commercial success leading to a million-dollar industry

2. BACKGROUND

The use of machine learning is increasing in various avenues of the pharmaceutical industry, including drug discovery, enabling improvements in the industry as a whole. The achievements of machine learning are demonstrated by the expanding number of companies in which ML is key to their business structure. They stated that machine learning techniques has also been investigated by large pharmaceutical companies for use in drug research and development [10]. The extent of the capability of machine learning and its usefulness in the field of drug discovery; it is thus imperative that it must be incorporated in future advances in the field of drug discovery. The goal is to use high-throughput screening technologies to reduce the asset and work seriousness of medicine necessity for live animal testing [10]. These studies demonstrate that machine learning is an extremely useful tool in drug discovery. Some factors relating to chemical and biological information are needed to enhance and develop machine learning technologies for drug discovery and development. These data would help to design more advanced and accurate systems by the insights drawn from data [11]. In order to gather these data, medicinal features such as cellular toxicity, cell structure heterogeneity, animal model efficacy, on-target activity, pharmacokinetic endpoints, microsomal stability, and cytochrome P450 (CYP) inhibition values will need to be measured using assay

Fig 1 shows a simplified cycle of the events that take place during the implementation of machine learning in the pharmaceutical industry, specifically in the development and manufacturing sectors of this industry, and also shows how machine learning functions in general [12]. The data consist of different components, such as orthogonal data and applicability domain and termination data. These data are put into a previously-designed algorithm that takes into account model choices, selection functions, and orthogonal computations. The algorithm generates results as well as iterative improvements to the current methodology and procedures in order to make it more efficient and reliable. The technique is then modified, and the cycle is repeated until a final product is designed and manufactured.

One study that demonstrates the application of machine learning in the area of drug discovery was done by Margulis and colleagues [13], which looks at how intensely bitter molecules can be identified with the help of machine learning in the early stages of drug development. The aim was to determine a certain machine learning algorithm could be used

as a substitute for animal testing to predict the bitterness of different molecules used in drugs. Overall, 80% of the identified bitter molecules matched those obtained from a brief access taste aversion (BATA) experiment, indicating that this study was successful. After the BATA experiment the results demonstrated that toxicity and bitterness are not always linked, as was previously assumed. This demonstrates that machine learning was able to provide sufficiently accurate results as well as new information

Enhanced computational power and the development of innovative techniques in the field of AI could be used to reform drug discovery and development processes. At the time of this literature review, the pharmaceutical industry is facing drops in efficiency of their drug improvement programs and simultaneous rises in research and development costs [23]. In recent years, there has been a radical expansion in the digitalization of information in the pharmaceutical industry; efficiently obtaining, examining, and applying this information to tackle complex clinical issues is a current challenge. AI can deal with enormous volumes of information with upgraded computerization [24]. It can also integrate and use machine learning algorithms to increase efficiency and productivity. In this section, the main uses of AI to improve the effectiveness of the drug discovery cycle are discussed

above shows how and where AI can be integrated into drug discovery and development processes and the novel applications of AI in the pharmaceutical industry [25]. Drug discovery can be usefully split into four parts: drug design, polypharmacology, drug repurposing, and drug screening. The primary use of AI is in predicting drug properties, which may reduce the need for clinical trials and live study participants, which would be beneficial from both financial and ethical standpoints. The studies identified in this review that support the integration of AI into the drug discovery procedure to improve efficiency, accuracy and productivity are discussed in this section

3. CONCLUSIONS

The main potential of AI in the pharmaceutical industry is to reduce costs and increase efficiency [39]. Extensive research has demonstrated that dynamic learning can distinguish profoundly exact AI models while using half or less information than traditional AI and information subsampling approaches. Although the reason for this increased productivity is not fully understood, it appears that reduced repetition and predisposition, as well as gaining more significant information to traverse choice limits, are key components in this improved execution. As a result, without taking into account the expected mechanical overhead for actually carrying out dynamic learning efforts, screening expenses appear to be reduced by up to 90% [12]

Machine learning techniques can manage complex analyzes with huge, heterogeneous, and high-dimensional information collections with no manual input, which has proved helpful in the writing business applications. Combining machine learning, particularly deep learning, with human skill and experience might be the best way to coordinate numerous enormous data stores. The amazing information-mining capacity of AI innovation has given new essentiality to computer supported medication plans that incorporate multiple clinical considerations are better than piecemeal information, which can speed up prescription process.

In summary, many factors impact the successful integration of AI and machine learning into drug discovery and development and the pharmaceutical industry for ploypharmacology, drug design, drug screening and drug repurposing. Advances in technology, including those based on AI, will always be required to reduce the time and money spent on research, development and production, and to increase efficiency.

REFERENCES

1. Baldonado, M., Chang, C.-C.K., Gravano, L., Paepcke, A.: The Stanford Digital Library Metadata Architecture. Int. J. Digit. Libr. 1 (1997) 108–121
2. Bruce, K.B., Cardelli, L., Pierce, B.C.: Comparing Object Encodings. In: Abadi, M., Ito, T. (eds.): Theoretical Aspects of Computer Software. Lecture Notes in Computer Science, Vol. 1281. Springer-Verlag, Berlin Heidelberg New York (1997) 415–438
3. van Leeuwen, J. (ed.): Computer Science Today. Recent Trends and Developments. Lecture Notes in Computer Science, Vol. 1000. Springer-Verlag, Berlin Heidelberg New York (1995)
4. Michalewicz, Z.: Genetic Algorithms + Data Structures = Evolution Programs. 3rd edn. Springer-Verlag, Berlin Heidelberg New York (1996)