Editorial

Journal of Applied Pharmaceutical Science
Vol. 13 (Suppl 1), pp. i-ii, September, 2023
DOI: 10.7324/JAPS.2023.9.1ed
Available online at https://japsonline.com

Applications of Artificial Intelligence in Drug Design, Discovery and Development

Kalirajan Rajagopal *

Recently, Artificial Intelligence (AI) has been a model tool and technique which occupied most of the areas such as information technology as well as pharmaceutical industries including drug discovery and development, repurposing of drugs, pharmaceutical productivity clinical trials etc. The advantages of utilizing AI, mainly reducing the involvement of human in many sectors in short period and also cost effective to create novel medicines. AI also can be handling huge no. of data with the enhanced automation technique (Paul *et al*., 2021; Miles *et al*., 2006). With the advancement of deep learning techniques, there is an increase in drug-related data, and a variety of methodologies are emerging at all phases of the drug discovery processes (Zhang *et al*., 2017).

Nowadays, AI is also used for drug design and discovery process in the pharmaceutical industry with the advent of established physics-based modelling, make-on-demand commercial libraries as well as generative AI/ML models, the millions of purchasable or synthesizable compounds available for virtual screening and lead-optimization has grown explosively and the methods ranging from ultra-fast, approximate approaches through AI-enhanced physics-based *in-silico* simulation methods to advanced ligand docking approaches. AI technologies such as machine learning support which integrates biological, psychological, and social factors approaching diagnosis and treatment of disease. In parallel, our ability to computationally predict key design properties has grown tremendously.

Computer-aided formulation design is an area of interest that attracts many researchers around the globe and especially, pharma industry is especially keen to understand the molecular mechanisms which predict the physio-chemical properties of pharmaceutical formulations and capable of handling various formulation-related issues such as physical and chemical degradation of components, chemical and physical stability, excipient compatibility, impurity profiling, solubility and stability issues etc (Lamberti 2019).

The applications of AI in the drug discovery such as target prediction, drug-target interaction, toxicity prediction and determination of physicochemical properties (Pu *et al*., 2019). AI is also used in pharmaceutical product management like market prediction and analysis and costing. In the pharmaceutical product development, AI is used for ensuring in-process specification compliance and deciding suitable excipients etc. AI also helps in automated manufacturing process by adjusting various parameters to ensure quality control and quality assurance regulations and in the clinical trial design and monitoring (Yang *et al*., 2019, Harrer 2019).

In the year 2020, the first drug molecule known as DSP-1181which will be used for the treatment of obsessive-compulsive disorder (OCD) was invented by artificial intelligence (AI), using algorithms through potential molecules by checking against huge database of parameters. The above drug will be in human trials and it was the world first for machine learning in medicine. The drug was created by British start-up company Exscientia and Japanese pharmaceutical company Sumitomo Dainippon Pharma. Generally, drug discovery and development process take about five years to get into clinical trial, but the AI drug took only just one year (https://www.bbc.com/news/technology-51315462, Jan, 2020).

In-silico Medicine INS018_055, a small molecule inhibitor for the treatment idiopathic pulmonary fibrosis (IPF) has been granted by FDA which is the first orphan drug discovered and designed by using artificial intelligence which

Department of Pharmaceutical Chemistry, JSS College of Pharmacy, JSS Academy of Higher Education & Research, Ooty – 643001, The Nilgiris, Tamilnadu, India.

***Corerspondence Authors**

enters phase-II clinical trial in early 2023 (https://www.genengnews.com/news/insilico-gains-fdas-first-orphan-drug-designation-for-ai-candidate/).

In future, AI plays a major role in the drug design and discovery of novel drugs against various disease targets.

FUNDING

There is no funding to report**.**

DISCLOSURE

The author declares to report no conflicts of interest for this work. This includes expert testimony, honoraria, stocks or options ownership, employment, royalties, grants, or patents received or pending.

REFERENCES

Harrer S. Artificial intelligence for clinical trial design. Trends in Pharmacological Sciences, 2019; 40:577–591. http://doi.org/10.1016/j.tips.2019.05.005

Jane Wakefield, Artificial intelligence-created medicine to be used on humans for first time. https://www.bbc.com/news/technology-51315462, 30, Jan, 2020.

Lamberti M.J. A study on the application and use of artificial intelligence to support drug development. Clinical Therapeutics.2019;41:14141426. http://doi.org/10.1016/j.clinthera.2019.05.018

Miles J., Walker A. The potential application of artificial intelligence in transport. IEE Proceedings-Intelligent Transport Systems, 2006;153:183–198

Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug Discovery Today. 2021; 26(1): 80-93. http://doi.org/10.1016/j.drudis.2020.10.010.

Pu L. eToxPred: a machine learning-based approach to estimate the toxicity of drug candidates. BMC Pharmacology and Toxicology, 2019;20:2. http://doi.org/10.1186/s40360-018-0282-6

Yang X. Concepts of artificial intelligence for computer-assisted drug discovery. Chemical Reviews. 2019; 119:1052010594. http://doi.org/10.1021/acs.chemrev.8b00728

Zhang L. From machine learning to deep learning: progress in machine intelligence for rational drug discovery. Drug Discovery Today, 2017; 22: 1680–1685. http://doi.org/10.1016/j.drudis.2017.08.010

https://www.genengnews.com/news/insilico-gains-fdas-first-orphan-drug-designation-for-ai-candidate/, 10, Feb, 2023.

How to cite this article

Rajagopal K. Applications of Artificial Intelligence in Drug Design, Discovery and Development. J App Pharm Sci, 2023; 13 (Suppl 1): i-ii.