The Power of AI in Drug Discovery

A literature review on the research publication:

[Artificial Intelligence in Drug Discovery and Development (Debleena P. et. al, 2020)](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7577280/)

A diagram of a machine learning process

Description automatically generated

Authors:   
Rukayat Y. Omotosho-Sanni (Rxruqayyah)

Bezaleel Akinbami (B3z)

Oleh Precious ( KelHills)

Cynthia C. Eriobu(Cynthia1000)

Video Presentation: [LinkedIn Video](https://www.linkedin.com/posts/rukayat-omotosho-sanni-40459a147_hackbio-aiinpharma-drugdiscovery-activity-7238288280071340032-nadp?utm_source=share&utm_medium=member_desktop)

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HackBio Internship- Drug Discovery Track

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# INTRODUCTION

Technology is the new celebrity cutting across nearly all industries, can AI reform the process of drug discovery and development? The pharmaceutical industry has encountered challenges with the advent of data digitalization which include access, analyzing and application of knowledge in addressing clinical problems. This review focuses on the beneficial perks of AI in various pharmaceutical sectors, reducing time and work, and also addressing advancements in the field.

# HARNESSING AI FOR DRUG DISCOVERY

Drug discovery has developed through AI in the following facets: rational drug design and predictive studies. De novo designing of novel drug molecules with desired properties has indeed accelerated the drug discovery process. Bioactivity, toxicity, physicochemical properties, drug target interactions, binding affinity have all been predicted employing AI tools. ChemBank, DrugBank and ChemDB enable in silico virtual screening of compounds. Additionally, ChemMapper and SEA (Similarity Ensemble Approaches) help in assessing drug target and binding interactions.

# AI IN PHARMACEUTICAL MANUFACTURING AND QUALITY CONTROL

Pharmaceutical manufacturing processes have been able to address shortcoming in terms of stability, dissolution and product quality by employing AI. Computational Fluid Dynamics (CFD) and other AI-based simulations have helped to improve manufacturing processes while focusing on efficiency and consistency. Furthermore, the Chemputer platform has revolutionized molecule manufacture by providing digital automation. Quality Control now has more accurate and trustworthy regulation of parameters.

# AI IN CLINICAL TRIAL AND PHARMACEUTICAL PRODUCT MANAGEMENT

AI enables the analysis of enormous datasets and prediction of clinical trial outcomes. This has impacted on reducing the failure rates in the drug development process and has helped to ascertain the safety and efficacy of new drugs. Predictive Machine Learning is also employed in early prediction of lead molecules. AI also plays a pertinent role in pharmaceutical product management, from market positioning and prediction to pricing strategies by employing statistical analysis and algorithms to meet demands.

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# AI BASED ADVANCED APPLICATIONS

Advanced applications of AI include nanorobots, nanomedicines and combination drug delivery. Nanorobots will help to navigate target-based physiological conditions. At the same time, nanomedicine will integrate nanotechnology and AI to address the diagnosis, treatment and monitoring of diseases.

# CONCLUSION

The pharmaceutical industry has transformed from integration of AI into drug discovery and development. The highlight being that major challenges have been addressed, however, data access and reliability, job shift might remain a concern. Overall, AI allows for creativity and innovation in the field.

# REFERENCES

1. Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug discovery today*, *26*(1), 80–93. https://doi.org/10.1016/j.drudis.2020.10.010