

SCI-121 – Medical Science For AI Engineering AI in Drug Discovery

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Drug discovery has always been a slow, expensive, and risky process. The process of developing a new medicine can exceed \$2.5 billion and can potentially take more than a decade, while only a small percentage of (drug) candidates actually succeed in clinical trials. These challenges come from labor-intensive screening, complex biological validation, and high trial failure rates leading to delays in the delivery of treatments to the patients.

Artificial intelligence or A.I. is reducing these challenges by improving every stage of the pharmaceutical process. For target identification, AI integrates genomic, proteomic, clinical trial, and electronic health record data to find disease-relevant genes and examine druggability faster than traditional methods. Machine learning, deep learning, and natural language processing algorithms may detect patterns in these large datasets and find promising biological targets that may be missed through usual / manual processes.

In a new discovery, AI-powered virtual screening speeds up the evaluation of millions of chemical structures. Techniques such as quantitative structure activity relationship (QSAR) modeling help predict biological activity, toxicity, and pharmacokinetics early in development reducing the need for expensive screenings. DL models and generative AI, such as, GANs, are also able to design novel molecules with therapeutic properties, expanding the chemical space explored by researchers.

AI also improves preclinical and clinical development as predictive algorithms estimate absorption, metabolism, and drug-to-drug interactions identify safer compounds before human trials. In clinical research, AI accelerates patient recruitment, optimizes trial protocols, and enables real-time monitoring to detect safety concerns sooner making clinical trials more efficient and adaptable.

Many AI methods contribute to these advancements like Machine Learning approaches such as support vector machines and random forests support classification tasks, while convolutional and recurrent neural networks drive drug design and protein interaction modeling. Natural Language Processing discovers more scientific literature for new insights, and reinforcement learning helps optimize treatment decisions or molecular structures. Graph neural networks model complex molecule-protein relationships, and large language models support knowledge findings and generative workflows.

Despite rapid progress, there are still several challenges and concerns regarding the use of A.I. Model accuracy depends on high-quality, unbiased data, however, real-world biomedical data can be biased, fragmented and incomplete. Many DL models function as “black boxes”, this means that decisions made by these models are difficult to understand or interpret. Integration into existing pharmaceutical processes requires a lot of changes to the existing infrastructure and this creates concerns about workforce disruption and intellectual property. Ethical risks, such as data privacy, cybersecurity, and informed consent in clinical scenarios must also be looked into.

In summary, AI will continue reshaping drug development by enabling personalized medicine, supporting quick responses to emerging diseases, and reducing costs that limit access to healthcare worldwide. By improving transparency, strengthening regulation, and advancing collaboration between data scientists and biomedical experts, AI can accelerate the development of safer, more effective medicines ultimately transforming global health outcomes.

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