AI – Driven Drug Discovery and Development

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Abstract

Artificial intelligence has transformed drug discovery and development by decreasing cost and improves successful outcome. Artificial intelligence various processes for identification of drug efficacy and includes machine learning and natural language processing. It is help to analyze large data sets and quick identification(1). Artificial intelligence also predicts bio pharmaceutics such as absorption, bioavailability and excretion, pharmacokinetics and toxicology. Artificial intelligence also improves clinical trials with minimizing risk. Artificial intelligence deals with challenges such as data quality and compliance challenges. The use of artificial intelligence increase in many sectors mainly the pharmaceutical industry. Artificial intelligence improves drug productivity, remove work load on humans. Artificial intelligence helps in overall quality of product(2)

Key words: Artificial intelligence, drug discovery, drug development, machine learning, compliance challenges

Introduction

Determining a medicine is a time taken and costly which includes high error ratio. Expanding a new medicine prices an average $1.3 billion to 2.3 billion with a long period of time(1). Artificial intelligence becomes more useful in decision making and moreover using in pharmaceutical industries. In drug discovery process artificial intelligence plays a key role. In clinical development; artificial intelligence develops a new drug, drug design and safety signal detection among drug discovery process. The success rate of new drug is very low 12-15%. There is an effect of AI in health care sector. AI mention innovation and it replaces manpower involves cause, controlling decisions

Overview of using Artificial Intelligence in drug development

Artificial intelligence is revolutionizing drug development in healthcare. Imagine machine learning algorithms sifting through millions of compounds, identifying potential drugs in a fraction of the time it used to take . Predictive modeling helps us understand how a drug will perform in the human body before it even hits the lab . Al driven drug

discovery is not just speeding up the process, it's also increasing accuracy, reducing costs, and minimizing risks. This technology is paying the way for breakthroughs and treatment , making personalized medicine a reality. The future of health care is here and it's powered by Al.(3)

Functions of AI in compound finding-

1.Target identification:

Ai boosts the objective of the compound by investigating data. Ai can find the drug, based on disease. Understanding the pathophysiology of a disease to select an appropriate molecular target. It aims for safety of selected compound.

2.Target validation:

providing information about the compound that acting on the target will have a therapeutic effect.

3.Identification:

Screening compound libraries for molecules that act on the target. (1)

4.Lead optimization:

chemically modifying to improve potency, selectivity and safety.

Ai in developing a compound

Estimation of aimed enzyme

During the discovery of a pharmaceutical active ingredient, it is necessary to aim for effective outcome. Various enzymes are included in developing the illness. Selection of target compound is very crucial.(3)

Barriers of ai in drug discovery:

Data quality

Vast data sets

Budget

Regulatory hurdles

Types

Artificial intelligence varies various , here we overview machine learning and deep learning (2)

Machine learning

Deep learning

1. **machine learning (ML)**

ML easily predict side effects and drug efficacy . ML supports preclinical and clinical trial design from this it reduces risk of failure and improves success rate and efficacy.

Ml find new therapeutic uses for approved drugs , saving time and cost compared to developing new compound from scratch

2. **Deep learning**

It involves various stages such as

Target identification, optimization, molecular generation

Target identification:

It analyze potential drug targets. And to identify proteins. It forecast the most targets and drive the disease

ADMET :

It functions safety and pharmacokinetics such as clearance, BBB.

It more likely fail in human or animal trials

Optimization:

It mainly shows patient stratification and side-effects

It contains low cost and High successful rate

Molecule generation:

It designs new molecule and another name is new drug discovery. It byself optimize absorption, distribution, metabolic, excretion and toxicology.(2)

Conclusion

The use of AI in drug discovery and pharmaceutical explores. artificial intelligence accelerates drug discovery from virtual screening to predicting drug interactions (2). Discover how machine learning algorithms analyze vast data sets to identify potential drug candidates faster and more efficiently than traditional methods gain insight into ai's role in personalized medicine and it's potential to transform health care by delivering safer and more effective treatments.(3)

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