МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я УКРАЇНИ
БУКОВИНСЬКИЙ ДЕРЖАВНИЙ МЕДИЧНИЙ УНІВЕРСИТЕТ

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професорсько-викладацького колективу
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У збірнику представлені матеріали 106-ї науково-практичної конференції з міжнародною участю професорсько-викладацького колективу Буковинського державного медичного університету (м. Чернівці, 03, 05, 10 лютого 2025 р.) зі стилістикою та орфографією у авторській редакції. Публікації присвячені актуальним проблемам фундаментальної, теоретичної та клінічної медицини.

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EVALUATION OF THE INFLUENCE OF AI AND MACHINE LEARNING APPROACHES ON DRUG DISCOVERY

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Introduction. Drug discovery has historically been an expensive and time-consuming process, often taking more than a decade and billions of dollars to bring a new drug to market. However, the emergence of artificial intelligence (AI) and machine learning (ML) offers an opportunity to enhance the efficiency and accuracy of the important drug discovery stages such as target identification, drug design and lead optimization, and clinical trial predictions. AI and ML approaches also have the potential to reduce both the time and cost of drug development.

The aim of the study is to investigate the influence and transformative potential of artificial intelligence (AI) and machine learning (ML) technologies on the drug discovery process.

Material and methods. Literature search, data extraction, analysis, and systematization.

Results. Several modern AI and ML techniques were found to be improving the drug discovery process:

1. Target Identification. AI algorithms, particularly natural language processing (NLP) models, are employed to mine biomedical literature and genomic data to identify potential drug targets. For example, BenevolentAI utilized AI-based knowledge graphs to identify baricitinib, an existing arthritis drug, as a potential treatment for COVID-19 by analyzing the relationship between the drug's known properties and viral infection pathways. Baricitinib was predicted to reduce the ability of the virus to infect lung cells and then these results were proved clinically.

2. Drug Design Using Generative Models. For drug design, generative adversarial networks (GANs) and variational autoencoders (VAEs) can be applied to generate new chemical structures. These generative models use molecular fingerprint data to propose molecules with high binding affinity to specific targets. A notable example of AI-driven drug design is Insilico Medicine's use of generative models to discover a DDR1 kinase inhibitor for fibrosis treatment. Within 46 days, AI predicted promising molecules, one of which later advanced to clinical trials.

3. Simulation and Lead Optimization. ML models such as graph neural networks (GNNs) are used to predict the binding affinity of potential drug molecules to target proteins. Additionally, reinforcement learning (RL) techniques are employed to optimize the chemical properties of lead compounds, balancing efficacy with safety and pharmacokinetics. AtomNet is an example of convolutional neural networks used to predict bioactivity, identifying novel inhibitors for proteins involved in diseases like Ebola and multiple sclerosis.

When compared with traditional high-throughput screening (HTS), AI-driven methods achieved up to 50% reduction in early-stage discovery time (Pfizer). AI-driven predictions of ADMET (absorption, distribution, metabolism, excretion, and toxicity) profiles reduce the number of failed drug candidates in later stages, thus the success rate of compounds moving from early-stage discovery to clinical trials increased by 20%.

Conclusions. The integration of artificial intelligence (AI) and machine learning (ML) into drug discovery processes has revolutionized the pharmaceutical industry by significantly reducing the time and costs associated with new drug development. AI and ML methodologies significantly improve efficiency in drug discovery, particularly in target identification and early-stage compound screening. However, there are also challenges such as the quality and availability of training data, model interpretability, and regulatory hurdles. The pharmaceutical industry will need to adapt to these challenges to fully realize the potential of AI-driven discovery. Future research should focus on refining AI models, expanding the use of real-world data, and fostering collaborations between computational scientists and pharmacologists.