МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я УКРАЇНИ
НАЦІОНАЛЬНИЙ ФАРМАЦЕВТИЧНИЙ УНІВЕРСИТЕТ

YOUTH PHARMACY SCIENCE

МАТЕРІАЛИ
VI ВСЕУКРАЇНСЬКОЇ НАУКОВО-ПРАКТИЧНОЇ
КОНФЕРЕНЦІЇ З МІЖНАРОДНОЮ УЧАСТЮ

10-11 грудня 2025 року
м. Харків

Харків
НФаУ
2025

бо для щоденного догляду бажано використовувати засоби без силіконів, а для інтенсивного відновлення – з силіконами.

Висновки. Силікони в шампунях є доцільним та ефективним інструментом догляду, коли вони використовуються диференційовано. Вони є необхідними для інтенсивного відновлення пошкодженого волосся і також можуть бути виключені із споживання для здорового волосся. Вибір шампуню має ґрунтуватися на хімічному типі силікону (леткий/нелеткий; водорозчинний/не водорозчинний), стані і типі волосся.

THE ROLE OF ARTIFICIAL INTELLIGENCE IN THE DEVELOPMENT OF DRUGS FOR THE TREATMENT OF ONCOLOGICAL DISEASES

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Introduction. Humanity has always sought ways to obtain medicines, and these efforts continue to this day. Especially labor-intensive and resource-intensive research involves the discovery of effective agents for oncological diseases. Cancer remains one of the leading causes of death worldwide. For example, in 2020 alone, nearly 10 million deaths were registered, along with an even greater number of cases of the disease, although many patients achieve remission through treatment. Despite decades of research and billions of dollars in investment, bringing a single effective drug to market remains challenging. Traditional drug development often involves a high attrition rate of candidates, which is especially noticeable in oncology, where tumor heterogeneity, the emergence of resistance, and the complex conditions of the tumor microenvironment significantly complicate the translation of activity from *in vitro* (in a test tube) to *in vivo* (in the human body). In recent years, computational technologies have been introduced into the field of new drug development to accelerate research time and minimize costs; this is precisely the main reason for implementing Artificial Intelligence (AI) in new drug development processes.

Aim. To study how AI optimizes the process of searching for and developing anticancer drugs, particularly through the use of Computer-Aided Drug Design (CADD) and Generative Artificial Intelligence (GAI).

Materials and methods. Generalization, logical and analytical methods were used when reviewing information, applying literary sources from electronic databases of scientific publications such as PubMed and searching tools such as Google and Google Scholar.

Research results. Traditional sources of pharmacological solutions, particularly plant-based agents, continue to play an important role — as evidenced by the discovery of compounds such as Paclitaxel (Taxol), Vinblastine, Vincristine, Camptothecin derivatives, Etoposide, Irinotecan, and Topotecan. However, their transition from the laboratory to clinical practice is often hindered by objective pharmacological barriers: unfavorable pharmacokinetic profiles, insufficient efficacy, or unacceptable levels of toxicity, particularly nephrotoxicity. The potential of AI in oncology is realized through numerous successful applications, among which the accelerated development of new drugs holds a special place. Modern research demonstrates how machine learning algorithms, by analyzing complex relationships between tumor biology and molecular structure of compounds, enable the identification and prioritization of the most promising candidates, including agents for targeted

therapy and immuno-oncology. By leveraging powerful modern datasets, AI not only accelerates the drug discovery cycle but also directs it towards the development of safer and significantly more effective therapeutic solutions.

Since AI should be considered as a collection of computational approaches, the most relevant ones in oncology drug development are: Machine Learning (ML), which allows algorithms to detect patterns in data and make predictions; Deep Learning (DL), where neural networks can process large and complex datasets such as histopathological images or omics data; Natural Language Processing (NLP), which extracts knowledge from unstructured biomedical literature and clinical notes; and Reinforcement Learning (RL), which optimizes the decision-making process and finds application, for example, in de novo molecular design. Using these methods together helps reduce research time and cost by combining computational precision with researcher expertise.

As mentioned above, three main AI algorithms are used: Computer-Aided Drug Design (CADD), which minimizes the risk of lead molecule rejection and increases the efficiency of identifying and prioritizing active compounds; Generative Artificial Intelligence (GAI), which allows for the de novo creation of new molecules and prediction of their target interaction, capable of generating original molecules absent from the training set, using neural networks to predict physicochemical and biological properties. Examples include the development of EXS-21546 for solid tumors characterized by high adenosine content, and the identification of Ouabain as a potential drug for lung cancer treatment. Application examples include EXS-21546, INS018_055 (an AI-discovered drug that progressed from initial discovery to preclinical trials in 18 months, faster than traditional methods, and is currently in Phase IIa studies for idiopathic pulmonary fibrosis), and Petosemtamab, TNT005, and HRS-1893, which have undergone clinical trials thanks to organoid/ organ-on-a-chip modeling, demonstrating the efficacy and safety of new drugs.

Reviews published in 2025 show that nearly 72.8% of studies on AI application in drug discovery relate to oncology. Research on solid tumors indicates that through the integration of multi-omics data, specifically transcriptomics, and powerful computational models via AI, the traditional drug discovery cycle is shortened to 2–3 years. The use of Graph Neural Networks (GNN) for analyzing molecular structures, virtual screening, compound generation, and synthesis planning is growing, as are partnerships between biotech companies and pharmaceutical giants implementing AI platforms for oncology research.

The advantages of using AI for drug development are also significant: reducing the time from target discovery to candidate drug; increasing the probability of success in early stages (improved identification of “hits” and optimization of “leads”); better therapy personalization: AI can guide drug selection for a specific tumor subtype or patient; optimization of clinical trial design, reducing the number of failed attempts, and improving participant selection. However, there are also certain challenges and limitations in using AI for the development of these drugs. These include: a lack of high-quality, standardized, and well-annotated data. The transition from the *in silico* (in computer) models to *in vivo* remains a major barrier: many AI-generated candidates have not yet gained approval in oncology. Problems with model interpretability: it is important for doctors and regulators to understand why a model recommends a particular solution. Ethical, legal, and regulatory issues: data usage, algorithm transparency, liability in case of errors. The biological complexity of oncological diseases: multiple mutations, tumor heterogeneity, unexpected resistance mechanisms. AI is not a “magic wand”; it assists but does not replace experimentation and clinical validation.

Conclusions. The future of oncology is hard to imagine without the use of artificial intelligence, which makes traditional drug development faster and more precise. AI is transforming traditional technology through its ability to analyze complex and unstructured data, rapidly replicate

virtual experiments, and optimize clinical trials. Despite problems such as data quality, model interpretability, and regulatory aspects, AI is already significantly changing the approach to fighting cancer. This makes it a key driving force being used to create major progress in the field of oncology, especially by providing patients worldwide with access to safe, effective, and personalized treatment methods.

Therefore, the use of AI in developing drugs for oncological diseases has great potential. But to fully realize it, issues concerning data, verification, interpretation, and regulation need to be addressed. This direction could become a key in the transition from “one-drug-fits-all” to truly “precision” oncology.

CALCULATION OF PHARMACOKINETIC PARAMETERS AND TOXICITY OF 5-METHOXYPYRIMIDINE DERIVATIVES

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Introduction. Heterocyclic compounds with a pyrimidine core are characterised by a wide range of biological activity and significant potential for medical applications as therapeutic agents, in particular, they exhibit pharmacological activity within the central nervous system, and antitumor, antiviral, antibacterial, and antimalarial activity have been reported. Despite the wide range of synthetic drugs on the pharmaceutical market, the search for new biologically active compounds remains relevant, while *in silico* prediction methods allow the selection of potentially effective molecules at an early stage.

Aim. Virtual prediction and assessment of pharmacokinetic, physicochemical properties and toxicity of 5-methoxypyrimidine derivatives for further synthesis of the most potential biologically active substances.

Materials and methods. For *in silico* prediction of pharmacological parameters of a number of 5-methoxypyrimidine derivatives, an online service was used. 4 pyrimidine derivatives were selected as objects of study: 5-methoxy-2-methylpyrimidine (1), 2-cyclopropyl-5-methoxypyrimidine (2), *tert*-butyl (2-(5-methoxypyrimidin-2-yl)ethyl)carbamate (3) and *tert*-butyl ((5-methoxypyrimidin-2-yl)methyl)carbamate (4). The software SwissADME, Pro-tox III were used to determine druglikeness parameters, predict ADME properties and determine toxicity, respectively.

Research results. Thanks to the radar of the online program SwissADME, the compliance of the molecules of 5-methoxypyrimidine derivatives with the bioavailability criteria was assessed. The range on each parameter axis does not go beyond the limited area. Considering the physicochemical properties such as lipophilicity, size, polarity, solubility, elasticity and saturation, it can be concluded that compounds (1-4) meet all the requirements of bioavailability (Fig. 1).

According to the ProTox-3.0 prediction, the results indicate a favorable toxicological profile of the studied compounds. Compound (4) belongs to toxicity class III, compounds (1) and (3) to class IV, and the safest is the pyrimidine derivative (2), which is predicted to have toxicity class V. Importantly, all substances in this series demonstrate predictable activity in overcoming the blood-brain barrier and only a slight level of potential neurotoxicity, which is an encouraging indicator for further studies as potential CNS agents (Fig. 1).