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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).

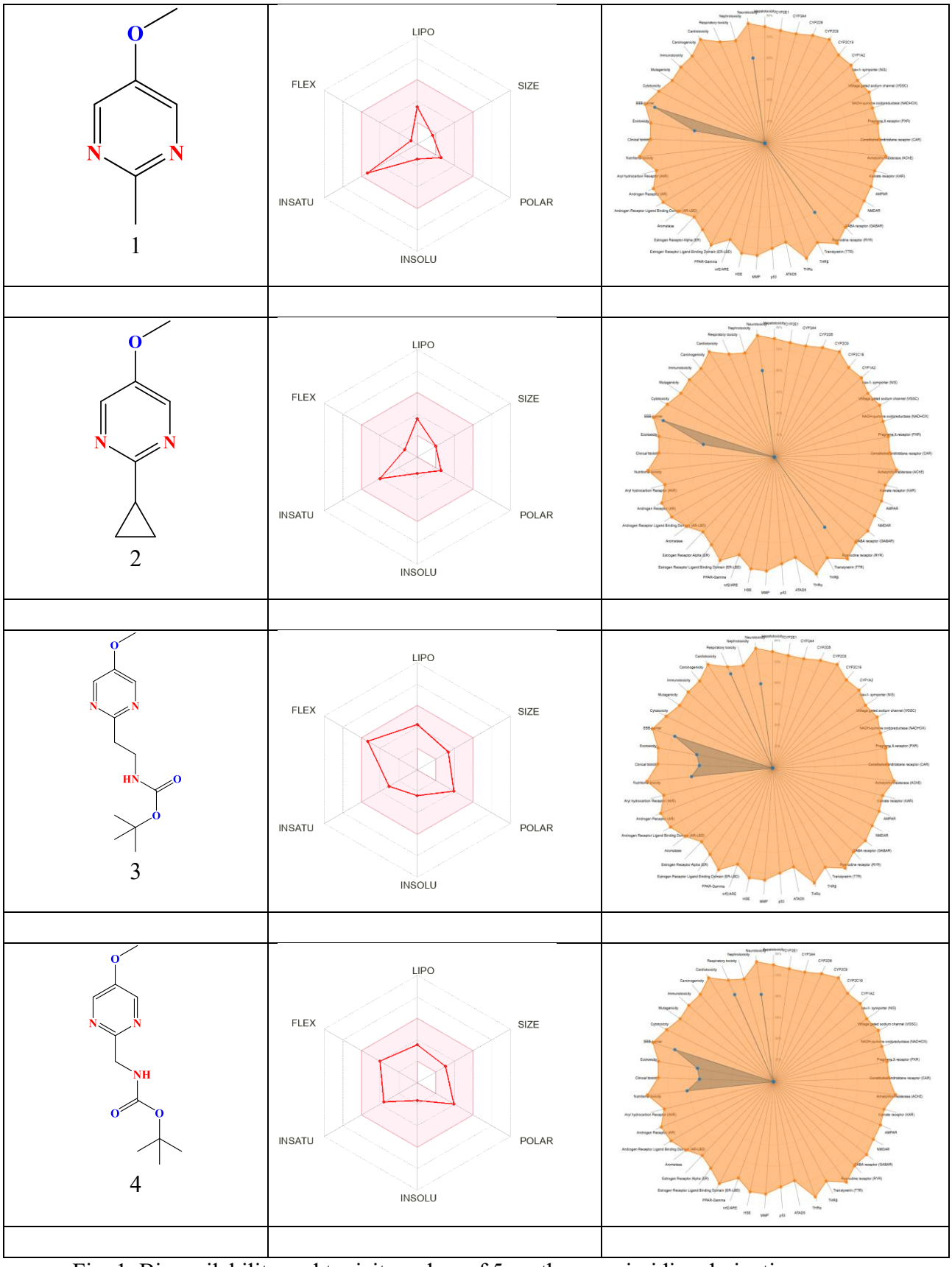

Fig. 1. Bioavailability and toxicity radars of 5-methoxypyrimidine derivatives

To establish the appropriate druglikeness compounds (1-4), compliance with the rules given in the table was assessed using the online program SwissADME:

Table 1. Prediction of the druglikeness of 5-methoxy pyridine derivatives

Compound	Lipinski	Ghose	Veber	Egan	Muegge
1	Yes	No	Yes	Yes	No
2	Yes	No	Yes	Yes	No
3	Yes	Yes	Yes	Yes	Yes
4	Yes	Yes	Yes	Yes	Yes

According to this study, compounds (3) and (4) fully comply with the above 5 filters. All pyrimidine derivatives (1-4) comply with the Lipinski, Veber and Egan rules. They do not comply with the Ghose rule (1-2), since the molecular weight is less than 160, the number of atoms is less than 20 and the molecular weight according to the Muegge rule must be more than 200.

Conclusions. The analysis of 4 pyrimidine derivatives was carried out using *in silico* methods. According to the results of online prediction of pharmacokinetic parameters, the compounds are orally bioavailable, meet the parameters of druglikeness and are low-toxic. This study proves the feasibility of synthesizing 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) as biologically active compounds and have prospects for further research.

RATIONAL DESIGN OF HYBRID THIENOPYRIMIDINE DERIVATIVES AS POTENTIAL MODULATORS OF NEURODEGENERATION

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Introduction. Neurodegenerative disorders such as Alzheimer's disease, Parkinson's disease, and other forms of cognitive decline represent one of the most significant medical and social challenges of modern healthcare. Their pathogenesis is multifactorial, involving disturbances in cholinergic and glutamatergic neurotransmission, oxidative stress, neuroinflammation, imbalance of neurotransmitter systems, and the accumulation of pathological protein aggregates. This complexity of biological mechanisms makes it impossible to effectively modify the course of neurodegeneration using drugs with narrowly targeted mechanisms of action.

Current therapeutic approaches provide only symptomatic relief and do not influence the key pathways driving disease progression. This underscores the need to develop new chemical platforms and molecular architectures capable of simultaneously modulating several pathogenetically relevant targets. In this context, multitarget hybrid molecules that combine pharmacophoric elements of different origins are considered a promising direction in medicinal chemistry.

The integration of biogenic fragments and synthetic structural modules within a single chemical scaffold enables the reproduction of biologically relevant interaction patterns while providing optimal pharmacokinetic and pharmacodynamic characteristics. Particular attention has been directed toward heterocyclic systems, including thienopyrimidines, which have demonstrated