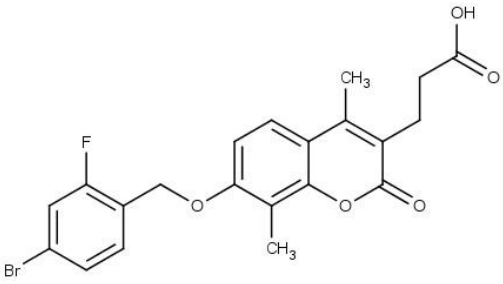
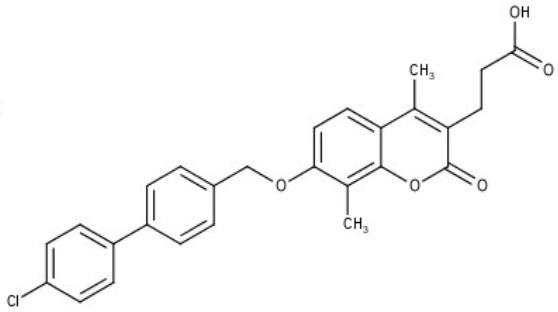


II



III

Results and discussion. As a result of the research, a large-scale variation of various electron density substituents in the benzene ring of the quinolone heterocycle was carried out. Substitution groups were also ranked by the number of rotating bonds, and parameters such as lipophilicity, topological polar surface areas, molecular volume, etc. The variation of the substituents was carried out at the C-7 position of the quinolone heterocycle. Molecular docking studies have shown the ability to interact with minimal binding energy between helicase enzyme and derivatives of 3-(4-oxo-2-methylquinoline-3-yl) propanoic acids.

Conclusions. Carried out studies using CADD methods did not disprove our assumption about the possibility of antimicrobial activity of the derivatives of 3-(4-oxo-2-methylquinoline-3-yl) propanoic acids as inhibitors of replicative DNA helicases, in particular, DnaB type.

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1. O'Neill, J. Review on Antimicrobial Resistance: tackling a crisis for the health and wealth of nations (HM Government, 2014).

2. Rossolini, G. M., Arena, F., Pecile, P. & Pollini, S. Update on the antibiotic resistance crisis. Curr. Opin. Pharmacol.18, 56–60 (2014).

3. Tanwar, J., Das, S., Fatima, Z. & Hameed, S. Multidrug resistance: an emerging crisis. Interdiscip. Perspect. Infect. Dis.2014, 541340 (2014).

THE USE OF THE IN SILICO STUDIES WITH PURPOSE OF SEARCHING POTENTIAL ANTIMICROBIAL DRUGS

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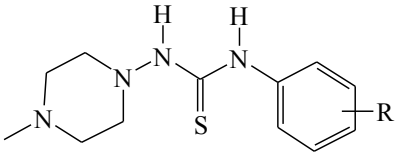
Introduction. The problem of finding new biologically active compounds with a specific biological activity and low toxicity is one of the most important tasks of pharmaceutical chemistry. Pre-experimental studies *in silico* successfully used at various stages of the search and optimization of the structures of biologically active compounds.

Purpose of our work is *in silico* studies of biological activity, adverse effects and acute toxicity of thiourea derivatives**.** It allows us to eliminate the potentially toxic substances as unpromising objects for experimental pharmacological screening.

Materials and methods. The objects of our study – 1-(N-methylpiperazin-1-yl)-3-(R-phenyl)thioureas *I (a-i)* of general formula:



I (a-i)

where, a) R=H, b) R=2-CH_3, c) R=3-CH_3, d) R=2,3-diCH_3, e) R=4-C_2H_5, f) R=4-OCH_3, g) R=3,6-diOCH_3, h) R=4-OC_2H_5, i) R=4-Br.

To optimize the pharmacological screening of thiourea derivatives computer prognosis of biological activity, adverse effects by PASS-online programme and computer prognosis of acute rat toxicity using GUSAR-online programme were carried out by the structural formula of compounds.

Results and discussion. Possible biological activity profile was predicted by the PASS-online (All Activities) programme and according to the results obtained, test compounds probably have antimycobacterial (with Pa=0.70-0.74), antituberculosic (with Pa=0.67-0.75) and antiviral (with Pa=0.40-0.57) activity. According to the results of PASS-online (Adverse Effects & Toxicity) prognosis, test compounds **Ia-g**,**i** probably have such adverse effects as twitching (with Pa=0.70-0.82) and inflammation (with Pa=0.48-0.55). Results of GUSAR-prognosis showed that the compounds probably belong to class 4 of toxicity (low-toxic substances).

Conclusions. All synthesized 1-(N-methylpiperazin-1-yl)-3-(R-phenyl)thioureas ***I (a-i)*** can be recommended for further pharmacological screening as antimicrobial agents in *in vitro* and *in vivo* systems.

PREDICTIVE TECHNOLOGIES IN THE STUDY OF 1,3-THIAZOLINE DERIVATIVES

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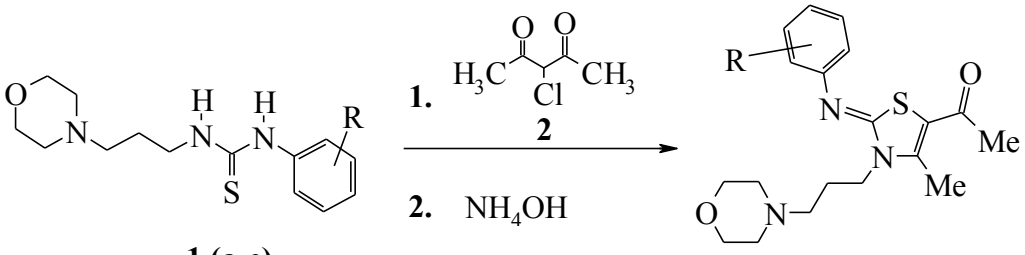
Introduction. Analysis of patent and scientific literature shows that thiazole-containing heterocycles are prospective biologically active substances with anti-inflammatory, antihistaminic, antimicrobial, immunostimulant, antioxydant activity etc.

Aim. To continue the search of new biologically active substances among 1,3-thiazole derivatives and to optimize the pharmacological screening of 1,3-thiazoline derivatives, namely 4-aryl-3-[3-(morpholin-4-yl)propyl]-N-phenyl-1,3-thiazol-2(3*H*)-imine derivatives using predictive technologies**.**

Materials and methods. 4-aryl-3-[3-(morpholin-4-yl)propyl]-N-phenyl-1,3-thiazol-2(3*H*)-imine derivatives were synthesized by Hantzsch reaction in the ethanol medium in accordance to the Scheme:

Scheme



1 (a-e) **3 (a-e)**

a) R=3-OCH_3, b) R=3,4-diOCH_3, c) R= 4-OCH_3, d) R=4-Cl, e) R=4-Br.

To optimize the pharmacological screening of 4-aryl-3-[3-(morpholin-4-yl)propyl]-N-phenyl-1,3-thiazol-2(3*H*)-imine derivatives «drug-like» parameters using Molinspiration and ACD/Labs programmes were calculated and computer prognosis of acute rat toxicity using GUSAR-online programme was carried out.

Results and discussion. According to the test results, determined «drug-like» properties are in the range of permissible values for all test compounds and comply with requirements Lipinski. Results of GUSAR-prognosis indicates that the compounds probably belong to class 4 and 5 of toxicity (low-toxic and practically non-toxic substances).

Conclusions. All compounds synthesized comply with requirements Lipinski and probably belong to low-toxic and practically non-toxic substances, so can be recommended for experimental biological tests.