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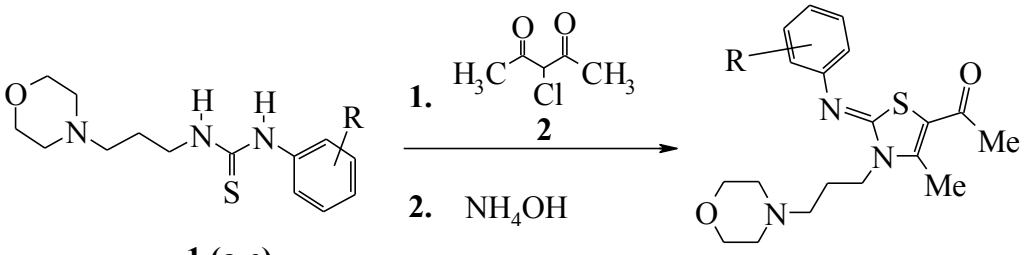
Introduction. Analysis of patent and scientific literature shows that thiazole-containing heterocycles are prospective biologically active substances with anti-inflammatory, antihistaminic, antimicrobial, immunostimulant, antioxydant activity etc.

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.