hydroxy-3-methylglutaryl-CoA synthase 2. Indicators of the effects that, at least indirectly, may affect the CNS functions are significantly lower.

Conclusions. The obtained results emphasize that, in spite of real usefulness of *in silico* approaches for prediction and study of properties of new classes of compounds, the probability of incorrect conclusions based on them always exists.

SYNTHESIS AND PROGNOSIS PHARMACOLOGICAL ACTIVITY OF DERIVATIVES OF N1-(4-(4-R- PHENYL)-1,3-THIAZOLYL-2)- N1-(4'-R'- PHENYL)ACETAMIDE

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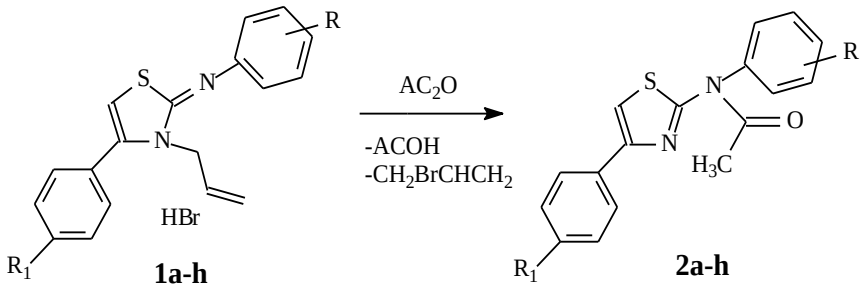
Introduction. Analysis of the scientific literature indicates that the derivatives of thiazole have a sufficiently wide spectrum of pharmacological activity and a large number of drugs is created on their basis. Therefore, the search for new biologically active substances based on thiazoles is a promising area of modern pharmaceutical science.

Aim. Synthesis of new biologically active compounds in a series of derivatives of N1-(4-(4-R-phenyl)-1,3-thiazolyl-2)-N1-(4'-R'-phenyl)acetamide, confirmation of their structure with ^{1}H-NMR spectroscopy and thin layer chromatography, prognosis pharmacological activity of synthesized compounds.

Materials and methods. The starting materials, auxiliary substances and solvents used in the work were obtained and purified using standard techniques. ^{1}H-NMR-spectra were recorded on a Varian Gemini 400 MHz instrument in DMSO-d_6. The forming of the final products of reaction was monitored by thin layer chromatography through the use of Fluka silica gel (60 F254) plates (0.25 mm). The visualization was carried out by UV-radiation.

Results and discussions. A new series of derivatives of N1-(4-(4-R- phenyl)-1,3-thiazolyl-2)-N1-(4'-R'-phenyl)acetamide (2a-h) was obtained by acetylation of hydrobromide derivatives of 3-allyl-4-(R-phenyl)-N-(R^1-phenyl)thiazole-2-imine (схема 1).

Scheme 1



2a R = CH_3, R_1 = OCH_3; 2b R = CH_3, R_1 = Cl; 2c R = CH_3, R_1 = 2',4'-$(Cl)_2$;
2d R = Br, R_1 = Cl

The structure of the compounds obtained is confirmed by modern physicochemical methods of analysis: ^{1}H-NMR spectroscopy and thin layer chromatography.

The signals of protons of the allyl fragment and proton NH^+ are absent on ^{1}H-NMR-spectra of the synthesized compounds, that indicates the formation of derivatives of N1-(4-(4-R-phenyl)-1,3-thiazolyl-2)-N1-(4'-R'-phenyl)acetamide.

Prediction of pharmacological activity for new derivatives of N1-(4-(4-R-phenyl)-1,3-thiazolyl-2)-N1-(4'-R'-phenyl)acetamide (2a-h) is made using the PASS program. According to the results obtained, the synthesized compounds have a wide range of pharmacological activity and act as mucomembranous protector, insulin promoter, ubiquinol-cytochrome-c reductase inhibitor, transcription factor STAT3 inhibitor, calcium channel N-type blocker, antianorexic, anti-Helicobacter pylori etc.

Conclusions. The synthesis of derivatives of N1-(4-(4-R-phenyl)-1,3-thiazolyl-2)-N1-(4'-R'-phenyl)acetamide is made. The structure of the synthesized compounds is confirmed by the integrated use of modern physicochemical methods of analysis: ^{1}H-NMR spectroscopy and thin layer chromatography. The results of PASS prediction allow us to state that the synthesized substances have a fairly wide range of pharmacological activity.

SYNTHESIS OF 2-AMINO-4-ARYL-3-CYANOBENZOPYRANS BASED ON METHYL ESTER OF 2-HYDROXY-4-OXO-6-PHENYLCYCLOHEXENE-2-CARBOXYLIC ACID

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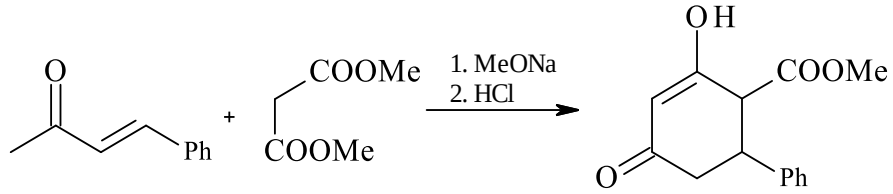
Introduction. Progress in the pharmaceutical industry always accompanied by synthesis of new biologically active substances. A message about synthesis of fused 4-substituted 2-amino-4*H*-pyrans based on interaction of nitriles with cyclohexane-1,3-diones and aldehydes has recently shown up in literature. Compounds above are promising biologically active substances.

Aim. Current research was aimed to synthesize new derivatives of methyl ester of 2-hydroxy-4-oxo-6-phenylcyclohexene-2-carboxylic acid by interaction of benzylideneacetone with dimethyl malonate with further three-component interaction with aromatic aldehydes and malononitrile to obtaining new derivatives of 4-aryl-2-amino-3-cyanobenzopyrans.

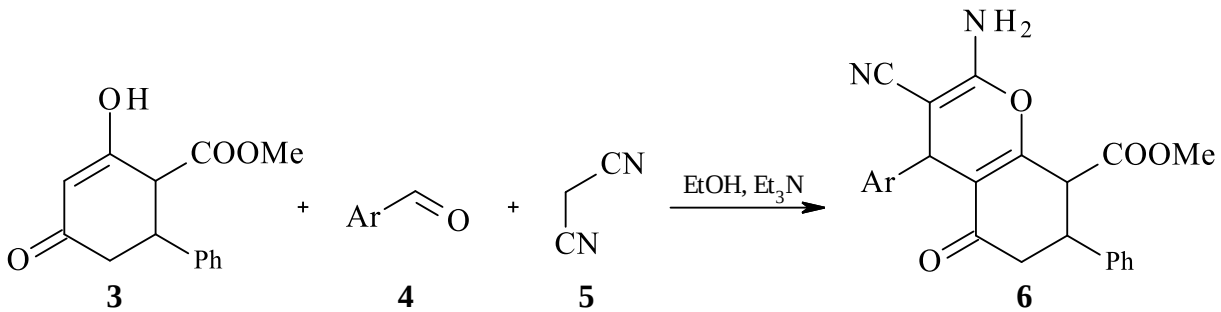
Materials and methods. Starting compounds and reagents: benzylideneacetone, dimethyl malonate, aromatic aldehydes, malononitrile, triethylamine, ethanol. The methods of organic synthesis and IR-, ^{1}H NMR spectroscopy methods were applied in the course of the research.

Results and discussion. Interaction between benzylideneacetone (1) and dimethyl malonate (2) proceeds in the presence of sodium methylate with refluxing in ethanol for 3 hours as domino transformation by the «Michael addition / Claisen condensation» type. As a result, methyl ester of 2-hydroxy-4-oxo-6-phenylcyclohexene-2-carboxylic acid (3) was obtained:



1 **2** **3**

By further three-component interaction of ester (3) with aromatic aldehydes (4) and malononitrile (5) in the presence of catalytic quantity of triethylamine in ethanol medium 2-amino-4-aryl-8-methoxycarbonyl-5-oxo-3-cyano-5,6,7,8-tetrahydro-7-phenyl-4*H*-chromenes (6) were synthesized with high yields:



3 **4** **5** **6**

Ar = Ph, p-MeOPh, p-NO_2Ph