Conclusions. By the interaction of 4-R-5-(5-brom-thiophen-2-yl)-4*H*-1,2,4-triazole-3-thiols in an alcoholic medium in the presence of an equimolecular amount of alkali with the corresponding 1-bromo-alkanes (1-bromobutane, 1-bromohexane, 1-bromoheptane, 1-bromoctane, 1-bromononane, 1-bromodecane), 10 new compounds were synthesized. The structure of synthesized compounds is confirmed by the complex use of elemental analysis, chromatographic mass spectrometry, IR spectrophotometry and ^{1}H NMR spectrometry. Some theoretical calculations coincide with experimental data.

SYNTHESIS AND STUDY OF MOLECULAR STRUCTURE OF A NEW 2-AMINO-4-ARYL-3-CYANO-5,6,7,8-TETRAHYDRO-4*H*-CHROMENES

Voronovich A.S., Levashov D.V.
Scientific supervisor: Shemchuk L. A.
National University of Pharmacy, Kharkiv, Ukraine
voronovichandrey@gmail.com

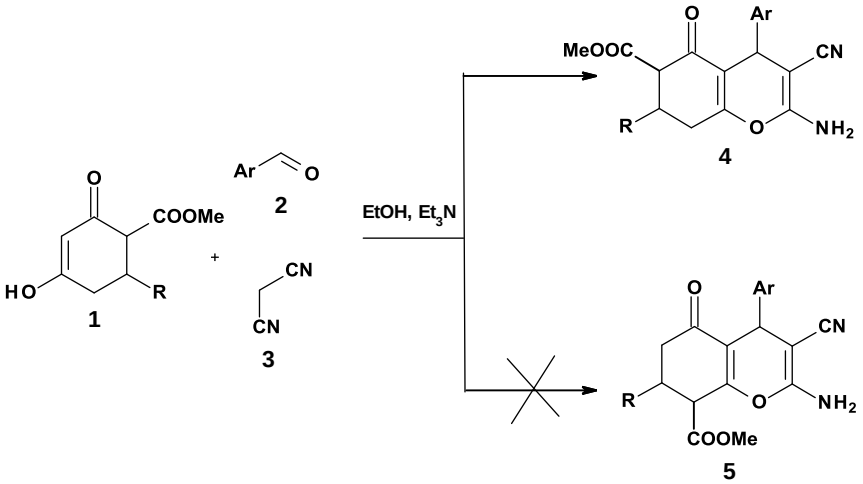
Introduction. The work is devoted to the synthesis of new carbanelated derivatives of 2-amino-4*H*-pyran, in particular 2-amino-3-cyano-5,6,7,8-tetrahydro-4*H*-chromenes. Among the synthetic derivatives of such heterocyclic system, many substances with a high level of certain types of pharmacological activity are known (anti-inflammatory, antibacterial, antitumor, etc.).

Aim. In the present work we described the synthesis of new derivatives of 2-amino-4-aryl-3-cyanochromenes via three-component one-pot interaction of esters of 2-hydroxy-4-oxo-6-arylcyclohexene-2-carboxylic acid with aromatic aldehydes and malononitrile.

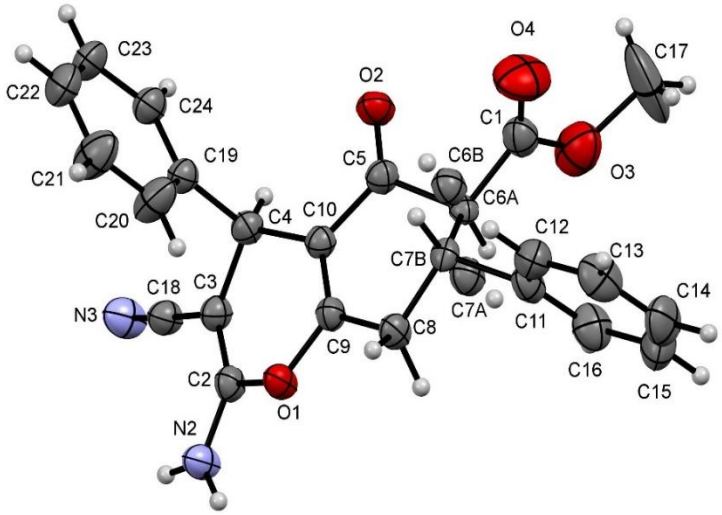
Materials and methods. Starting compounds and reagents: aromatic aldehydes, malononitrile, triethylamine, ethanol. The methods of organic synthesis and IR-, ^{1}H, ^{13}C NMR spectroscopy, chromatography-mass spectrometry, single crystal X-ray diffraction methods were applied in the course of the research.

Results and discussion. One of the effective methods that can be used to construct the 2-amino-4*H*-pyranes and its carbanelated derivatives are multicomponent reactions. Enolnucleophils, carbonyl compounds and methylene active nitriles are used in such reactions.

A series of new 2-amino-4-aryl-3-cyano-6-methoxycarbonyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromenes (4) were synthesized in high yields via three-component interaction of methyl esters of 2-hydroxy-4-oxo-6-arylcyclohexene-2-carboxylic acid (1) with aromatic aldehydes (2) and malononitrile (3) in the presence of catalytic quantity of triethylamine in ethanol medium.



Theoretically, the interaction can proceed in two directions: with the formation of 6-methoxycarbonyl chromene (4) or 8-methoxycarbonyl chromene (5). IR-, ^{1}H, ^{13}C NMR spectroscopy, chromatography-mass spectrometry data may correspond both structures. The Single Crystal X-ray diffraction analysis showed that the reaction results in the formation of structure (4).



Conclusions. New 2-amino-4-aryl-3-cyano-6-methoxycarbonyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromenes were obtained. Their molecular structure was studied according to X-ray diffraction data.

COMPUTER FORECASTING AND QUANTUM-CHEMICAL CALCULATIONS OF DERIVATIVES OF THE CYTISINE ALKALOID

Zhasymbekova A.R., Nurmaganbetov Zh.S., Nurkenov O.A., Mazhitov A.S.
Scientific supervisor: Mukusheva G.K.
Karagandy University of the name of academician E.A. Buketov, Kazakhstan;
mukusheva-1977@list.ru

Introduction. Work on the transformation of available alkaloids, the use of which in medicine is not possible due to significant side effects, is being successfully developed.

The availability of the source of cytisine and the analysis of its structure leads to the conclusion that it is promising to carry out its synthetic transformations with the production of compounds structurally similar to a number of natural metabolites and other practically significant substances.

Aim. Study of the reactivity of molecules of cinnamoylcytisine (1), lipoylcytisine (2), cytisine isoalantholactone (3) and computer bioprediction.

Materials and methods. The calculations were carried out by semiempirical methods of quantum chemistry in the parametrization of AM1 and PM6. In terms of a detailed study and the probable establishment of the biological activity of synthesized cytisine derivatives, we carried out a bioprediction using one of the most effective and well-known to date, computer programs - PASS (Prediction of Activity Spectra for Substances), developed by Russian scientists, which has in its arsenal and uses in its calculations a unified description of the chemical structure and a universal mathematical algorithm for establishing structure-activity relationships.