

МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я УКРАЇНИ  
НАЦІОНАЛЬНИЙ ФАРМАЦЕВТИЧНИЙ УНІВЕРСИТЕТ

Серія «Наука»

## **ЛІКИ – ЛЮДИНІ.**

### **СУЧАСНІ ПРОБЛЕМИ ФАРМАКОТЕРАПІЇ І ПРИЗНАЧЕННЯ ЛІКАРСЬКИХ ЗАСОБІВ**

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Збірник містить статті і тези доповідей IV Міжнародної науково-практичної конференції «Ліки – людині. Сучасні проблеми фармакотерапії і призначення лікарських засобів», де розглядаються проблеми фармакотерапії захворювань людини, наводяться результати експериментальних та клінічних досліджень, аспекти вивчення й упровадження нових лікарських засобів, доклінічні фармакологічні дослідження біологічно активних речовин природного і синтетичного походження. Наведено також праці, присвячені особливостям викладання медико-біологічних і клінічних дисциплін у закладах вищої освіти.

Видання розраховано на широке коло наукових і практичних працівників медицини і фармації.

Відповідальність за зміст наведених матеріалів несуть автори.

**УДК 615:616-08**

336 nm (MeOH). IR spectrum is (KBr,  $\nu_{\max}$ ,  $\text{cm}^{-1}$ ): 3103-3612  $\text{cm}^{-1}$  (OH), 1647  $\text{cm}^{-1}$  (C=O), 1110  $\text{cm}^{-1}$  (C-O).  $^1\text{H}$  NMR spectrum is (600 MHz: MeOH, 300K):  $\delta$ 12.97 (1H, s, 5-OH), 7.85 (2H, d,  $J=8.9$  Hz, H-2', H-6'), 6.93 (2H, d,  $J=8.9$  Hz, H-3', H-5'), 6.60 (1H, s, H-3), 6.46 (1H, d,  $J=2.1$  Hz, H-8), 6.21 (1H, d,  $J=2.1$  Hz, H-6).  $^{13}\text{C}$  NMR spectrum is (150 MHz: MeOH, 300K):  $\delta$ 183.9 (C-4), 166.3 (C-2), 166.1 (C-7), 163.2 (C-5), 162.7 (C-4'), 159.5 (C-9), 129.6 (C-2', C-6'), 123.3 (C-1'), 117.1 (C-3', C-5'), 105.3 (C-10), 102.9 (C-3), 100.2 (C-6), 95.0 (C-8).

**Conclusions.** Compound 1 and 2 was obtained as yellow powder. Further studies can be carried out by using different extraction methods such as isolation and identification of active compounds.

### SYNTHESIS, STRUCTURE AND PROPERTIES OF 3-HYDROXYMETHYLPYRIDINIUM HEXAFLUOROSILICATE MONOHYDRATE AS A NEW POTENTIAL ANTICARIES AGENT

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The present communication describes of the synthesis, crystal structure, spectral data and properties of 3-hydroxymethylpyridinium hexafluorosilicate monohydrate – a new ammonium hexafluorosilicate, which may find an application as anti-caries agent. Dental caries remains one of the most common chronic diseases with considerable economic and quality-of-life burdens. The search for new effective anticaries agents is therefore an urgent task of modern pharmacy.

The crystalline salt with composition  $(3\text{-HOCH}_2\text{C}_5\text{H}_4\text{NH})_2\text{SiF}_6\cdot\text{H}_2\text{O}$  (**I**) was obtained by reaction of hexafluorosilicic acid (45 %) with methanol solution of 3-hydroxymethylpyridine. The ionic complex **I** was characterized by elemental analysis, IR, mass-spectrometry, solubility data and X-ray crystallography. Compound **I** crystallizes in the monoclinic crystal system (space group  $C2/c$ ). The anions and cations in **I** are held together *via*  $\text{OH}\cdots\text{O}$ ,  $\text{NH}\cdots\text{F}$ ,  $\text{OH}\cdots\text{F}$  hydrogen bonds and  $\text{CH}\cdots\text{F}$  contacts. The  $\text{SiF}_6^{2-}$  anion occupies the position of inversion center in **I** and has the geometry of a distorted octahedron, with Si–F distances running from 1.645(4) till 1.6938(11) Å. In IR spectrum for **I**, bands in the range 3275 – 3000  $\text{cm}^{-1}$  can be assigned to the  $\nu(\text{OH})$ ,  $\nu(\text{N}^+\text{H})$ ,  $\nu(\text{CH})$  vibrations of cations and water molecule. The superposition of vibration bands  $\nu(\text{SiF})$  for  $\text{SiF}_6^{2-}$  anion and deformation vibrations for cations and water molecule were registered in the range 800 – 650  $\text{cm}^{-1}$ . Deformation vibrations  $\delta(\text{SiF}_2)$  for the anion in the form of triplet were registered in the range 485 – 425  $\text{cm}^{-1}$ , free of natural oscillation of cations. The multiple character of the  $\delta(\text{SiF}_2)$  vibrations were in agreement with the X-ray data indicating the distortion of the octahedral geometry of the  $\text{SiF}_6^{2-}$  anion in **I** due to interionic H-bonds.

The solubility of **I** was determined according to the recommendations of the State Pharmacopeia of Ukraine. Compound **I** was very easily soluble in water, easily

soluble in DMSO, soluble in methanol and slightly soluble in ethanol (96 %) at 25 °C. The relationship between the solubility in water of complex **I** and related ammonium hexafluorosilicates and the salts structure is noted. The study of biological activity of hexafluorosilicate **I** is subject to further investigations.

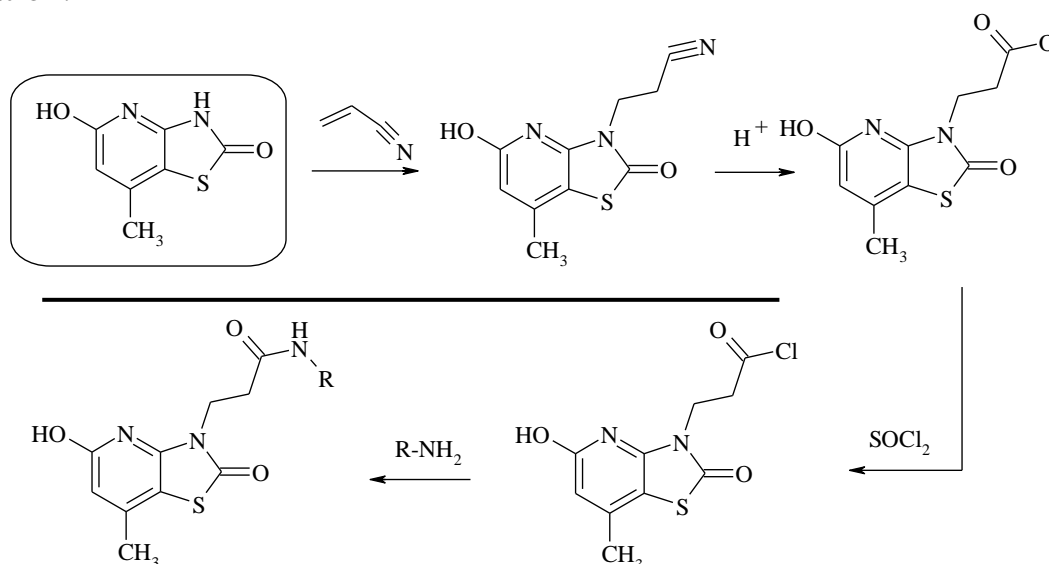
## SYNTHESIS AND ANTI-INFLAMMATORY PROPERTIES OF NOVEL THIAZOLOPYRIDINES

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According to World Health Organization data, about 20% of the world's population regularly apply NSAIDs, based on the most important features of this group of drugs - their antipyretic, analgesic and anti-inflammatory effects. Despite NSAIDs centuries-old clinical practical application history, issue of eliminating side effects still remains unresolved. Now heterocyclic nature organic compounds account for about 70% of all clinically applied drugs. Thiazolopyridines, as purine bioisosters, are an important type of heterocyclic systems, intensive study of which is prompted by considerable range of their pharmacological activity and synthetic derivatives functionalization possibilities at different positions.

The objective of the present work was to synthesize a series of novel thiazolo[4,5-*b*]pyridin-2-ones by the structural modification of the core heterocycle in its N<sup>3</sup> position for further pharmacological screening *in vivo* as anti-inflammatory activity. The target 5-hydroxy-7-methyl-3*H*-thiazolo[4,5-*b*]pyridin-2-ones were synthesized via reactions [3+3]-cyclocondensations, cyanoethylation, hydrolysis as well as acylation.



Researched substances impact effect on the inflammation exudative phase course was studied on the basis of white rats paws inflammatory edema carrageenan model. A series of novel compounds testing over the carageenin induced rat paw

Demchenko S.A., Palamarchuk Yu.O., Yadlovskiy O.E., Fedchenkova Yu.A. ANXIOLYTIC AND ANTICONVULSANT ACTIVITY OF 3-ARYL-1-(4 <sup>1</sup> -METHOXYPHENYL)-1-(6,7,8,9-TETRAHYDRO-5H-[1,2,4]TRIAZOLO [4,3-a]AZEPINE-3-YL-METHYL)-UREA DERIVATIVES .....	25
Dielievska V. Yu., Dobrovolska I. M. TO THE DISCREPANCIES IN ABO TYPING.....	26
Dotsenko R., Orobchenko O., Roman'ko M., Dubinina N., Morozenko D. TOXICITY DETERMINATION OF PREPARATIVE MIXTURE OF AMOXICILLIN TRIGHIDRATE BY ORAL ADMINISTRATION .....	27
Fursenco C., Calalb T., Uncu L. ANTIBACTERIAL AND ANTIFUNGAL ACTIVITIES OF SOME <i>SOLIDAGO</i> SPECIES .....	28
Garibli A.S., Suleymanov T.A. ISOLATION AND IDENTIFICATION OF KAEMPFEROL AND APIGENIN FROM <i>MEDICAGO FALCATA L.</i> ....	30
Gelmboldt V.O., Shyshkin I.O., Anisimov V.Yu., Fonari M.S., Kravtsov V.Ch. SYNTHESIS, STRUCTURE AND PROPERTIES OF 3-HYDROXYMETHYLPYRIDINIUM HEXAFLUOROSILICATE MONOHYDRATE AS A NEW POTENTIAL ANTICANCER AGENT .....	31
Goncharenko O.V., Chaban T.I., Matiychuk V.S., Chaban I.G., Ogurtsov V.V., Nektegayev I.O. SYNTHESIS AND ANTI-INFLAMMATORY PROPERTIES OF NOVEL THIAZOLOPYRIDINES.....	32
Hayrullayeva G.B., Rakhimova O.R., Botirmukhamedova S.T., Khudoykulova Yu.A., Rakhimova G.R. STUDY OF IMMUNOSTIMULATING EFFECT OF STYBIO TABLETS .....	33
Iskandarova Sh. F., Abdukhalilova N.S., Kholboyeva M. U. MICROBIOLOGICAL RESEARCH OF THE OINTMENT BASED ON RAW MATERIALS.....	35
Karatsuba T.A., Bondarenko L.B., Shayakhmetova G.M., Khavich O.V., Sharykina N.I. , Kovalenko V.M. , Kalachinska M.M. THE EFFECT OF 2 (3-ALLYL-4-OXO-3,4-DIHYDRO-QUINAZOLIN-2-YL-SULFONYL) -N- (2,6-DICHLOROPHENYL) -CERAMIDE ON CHROMATIN COMPONENTS AND ANTIOXIDANT SYSTEM IN GUERIN'S CARCINOMA AND UNCHANGED UTERINE TISSUES.....	36
Kholboeva M.U., Khamdamov U.I., Fatkhullaeva M. SYNTHESIS OF MIXED LIGAND COORDINATION COMPOUNDS OF Cu(II), Zn (II) WITH ASPARAGINE AND GLUTARIC ACIDS.....	37
Kholboyeva M. U, Sharipov A. T, Aminov S. N. THE CONTENT OF LOCAL PLANTS, PRODUCING OF PHYTO DRINK FOR DIABETES AND LEARNING ITS PROPERTIES .....	38
Kvizhinadze N., Tchumburidze T., Tophuria D., Matoshvili M. GENERICS USING PERSPECTIVES IN GEORGIA .....	40