

МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я УКРАЇНИ  
ІВАНО-ФРАНКІВСЬКИЙ НАЦІОНАЛЬНИЙ МЕДИЧНИЙ УНІВЕРСИТЕТ  
ТОВАРИСТВО МОЛОДИХ ВЧЕНИХ  
СТУДЕНТСЬКЕ НАУКОВЕ ТОВАРИСТВО

## **ТЕЗИ ДОПОВІДЕЙ**

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## **ABSTRACTS**

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## HIBISCUS SABDARIFFA AS A PERSPECTIVE MEDICINAL PLANT

Ezeh Franklin Chinecherem

Scientific adviser – Candidate of Biological Science Svitlana Danyliv

Ivano-Frankivsk National Medical University

Department of Pharmaceutical Management, Drug Technology and Pharmacognosy

Ivano-Frankivsk, Ukraine, e-mail: ezefranklinn@gmail.com

**Actuality.** A wide range of expectorant drugs does not exclude the possibility of studying new types of medicinal plant raw materials in order to expand the range of drugs with similar effects. *Hibiscus sabdariffa* is a species of flowering plant, native to West Africa, and also found in India. In the 16th and early 17th centuries, it was distributed in the West Indies and Asia, respectively, where it has since become naturalized in many places. In everyday life, the plant is often called rosella, Sudan rose. The stems are used to make bast fiber, and the dried cranberry-flavored calyxes are commonly used to make a popular tea known as karkade. It is an annual or perennial herbaceous plant or woody subshrub, reaching 2–2.5 m in height. The leaves are deeply three- to five-lobed, 8–15 cm long, located alternately on the stems. Flowers 8–10 cm in diameter, white to pale yellow with a dark red spot at the base of each petal; have a powerful, massive calyx at the base, 1–2 cm wide, which grows during the season to 3–3.5 cm and becomes fleshy and deep bright red when the fruit ripens, which takes about six months.

**The aim** of work was a studying the anatomical structure of *Hibiscus sabdariffa* flowers.

**Materials and methods.** The preparation of micropreparations was carried out according to the method of SPhU 1.4, 2.8.23 “Microscopic examination of medicinal plant raw materials.” The reagent for microscopic examination was a 5 % chloral hydrate solution. The study was carried out using a Delta optical microscope.

**Results and Conclusions.** When examining the upper epidermis of the calyx and subcup, polygonal cells with slightly convoluted lateral walls with a pronounced clear-like thickening are visible. Well-formed pointed drusen of calcium oxalate are visible through the epidermis in the mesophyll. Drusen are also contained in smaller isodiametric thin-walled cells of the epidermis. The cells of the lower epidermis of the calyx and subcup have more convoluted lateral walls. Stomata of the anisocytic type are located only on the lower side of the epidermis. Hairs are of 3 types: simple (up to 700  $\mu\text{m}$  long), unicellular, pointed, with thickened walls, oblique transverse pores and a slightly expanded base, which is surrounded by a rosette of epidermal cells; simple (up to 500  $\mu\text{m}$  long) unicellular, narrow, tortuous, often fused at 2–4 bases; capitate on a one-two-cell stalk with an oval multicellular head, the cells of which are arranged in 3–5 tiers in 2 rows. Mesophyll cells are round or oval with calcium oxalate drusen occurring mainly along the vascular bundles. Vascular-fibrous bundles contain scalariform, reticular, spiral vessels and are accompanied by spindle-shaped mechanical fibers with thickened walls. Among the mesophyll cells, round or oval idioblast cells of a yellowish-brown color with mucus are sometimes found.

## SYNTHESIS AND PROPERTIES OF 5-METHYL-4- (4-METHYLPHENYL)-1,2,4-TRIAZOLE-3-THIOL DERIVATIVES

Oumaima Khaloua

Supervisor - Doctor of Pharmacy, Associate Professor Andrii Gotsulya

Zaporizhzhia city, Ukraine, e-mail: andrey.goculya@gmail.com

**Objective.** The chemistry of 1,2,4-triazole derivatives has significant potential for the development of truly effective drugs. This opinion is confirmed by the successful history of the use of drugs that have a heterocyclic 1,2,4-triazole nucleus in their structure. Among the representatives of this class are fluconazole, voriconazole, alprazolam, triazolam, anastrozole, letrozole and other well-known medicines.

**Material and methods.** Modern methods of organic chemistry allowed the synthesis of 5-methyl-4- (4-methylphenyl)-1,2,4-triazole-3-thiol in high yield. Acetohydrazide was used as a starting compound, which was converted to 2-acetyl-*N*- (4-methylphenyl) hydrazinocarbothioamide in a reaction with 4-methylphenyl-isothiocyanate. The resulting compound was converted to 5-methyl-4- (4-methylphenyl)-1,2,4-triazole-3-thiol in alkaline medium. Further transformation involved alkylation reactions on the Sulfur atom. For this purpose, halogenalkanes, halogenalkane carboxylic acids, halogen ketones and chloroacetamides were used. The structure of all the compounds was proved by elemental analysis,  $^1\text{H}$  NMR spectroscopy and their individuality by chromatography-mass spectrometry. The pharmacological potential was determined using *in silico* methods. The acute toxicity and mutagenicity parameters were determined using the T.E.S.T. program. The current level of drug-like properties was determined by using the SwissADME online resource.

The prediction of anti-inflammatory, antifungal and anticancer activity was performed by molecular docking to the active sites of cyclooxygenase-2, lanosterol 14 $\alpha$ -demethylase, and anaplastic lymphoma kinase, respectively. PDB was used as a source of three-dimensional enzyme models. The docking process was realized using the AutoDock Vina program. The preparation of ligands and enzymes was performed using AutoDock Tools, BioviaDraw, Chem 3D, HyperChem. The results were visualized using Discovery Studio Visualizer.

**Results.** The *in silico* studies allow us to preliminarily identify the obtained compounds as low-toxic substances with a low risk of mutagenic properties. Docking studies revealed the following regularities: the presence of a carboxyl or amide group in the structure increases the effect on cyclooxygenase, the introduction of an alkyl fragment into the structure increases the effect on lanosterol 14 $\alpha$ -demethylase. All compounds in most cases meet the criteria for drug-like properties.

**Conclusions.** *S*-derivatives of 5-methyl-4- (4-methylphenyl)-1,2,4-triazole-3-thiol are a promising source for the development of biologically active substances with anti-inflammatory and antifungal activities.