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ЗБІРНИК ТЕЗ ДОПОВІДЕЙ

ВСЕУКРАЇНСЬКОЇ НАУКОВО-ПРАКТИЧНОЇ КОНФЕРЕНЦІЇ З МІЖНАРОДНОЮ УЧАСТЮ

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30 °C and an injection volume of 4 μL [3]. Detection was carried out using a diode-array detector, recording signals at 280 and 365 nm and acquiring UV-absorption spectra within the range of 210–700 nm.

Identification and quantitative analysis were performed using standard solutions of flavonoids.

Results. Using the HPLC method, the following compounds were identified in the herb of *Gazania rigens* 'Tiger Stripes': rutin, isoquercitrin, naringin, fisetin, neohesperidin, quercetin, rhamnetin, and casticin. Among the detected flavonoids, rhamnetin predominated, with a quantitative content of 1530.50 μg/g.

Conclusion. The obtained results provide a basis for future pharmacognostic researchon *Gazania rigens* 'Tiger Stripes' and will contribute to the development of quality control procedures for the plant's raw material.

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DERIVATIVES OF N-((5-PHENYL-6,11-DIHYDRO-5H-[1,2,4]TRIAZOLO[1′,5′:1,6]PYRIDO[3,4-B]INDOL-2-YL)METHYL)-R-CARBOXYLIC ACID: SYNTHESIS AND THEIR PROPERTIES

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Introduction. 1,2,4-Triazole and indole derivatives belong to the "privileged" chemical scaffolds that are widely used in the creation of pharmacologically active molecules. The 1,2,4-Triazole fragment is a component of many drugs with antifungal (fluconazole, itraconazole, voriconazole, posaconazole), anxiolytic (alprazolam, triazolam), antitumor (anastrozole, letrozole) and cardio- and hepatoprotective (thiotriazoline) activity. The indole pharmacophore, due to its polyfunctionality, exhibits a wide spectrum of action - antifungal, antiprotozoal, antioxidant, neuroprotective and antitumor - through various molecular targets and mechanisms of action.

The aim of the work was to determine the optimal synthesis conditions and study the properties of N-((5-phenyl-6,11-dihydro-5H-[1,2,4]triazolo[1′,5′:1,6]pyrido[3,4-b]indol-2-yl)methyl)-R-carboxylic acid, their esters and amides as candidates for new biologically active substances**.**

Materials and methods. (Indol-3-yl)ethanoic acid was used as the starting compound, which was sequentially subjected to esterification, hydrazinolysis, and addition of 2-oxoacetate. As a result, 2-methyl-6,11-dihydro-5H-[1,2,4]triazolo[1',5':1,6]pyrido[3,4-b]indole-5-carboxylic acid was obtained - a key intermediate for the synthesis of ester and amide derivatives.

Molecular docking was used to evaluate potential antimicrobial, antifungal, anti-inflammatory and anticancer activities. Ligand and target preparation was performed in MarvinSketch, HyperChem, Discovery Studio and AutoDockTools, and calculations were performed in AutoDock Vina with analysis of affinities, binding modes and spatial orientations in the active sites of enzymes.

Discussion. Molecular docking of a series of compounds (1 acid, 5 esters, 10 amides) showed that amides of N-((5-phenyl-6,11-dihydro-5H-[1,2,4]triazolo[1′,5′:1,6]pyrido[3,4-b]indol-2-yl)methyl)-R-carboxylic acid exhibit the highest affinity for their respective protein targets. They form stable complexes through hydrogen bonding and π-π stacking interactions, indicating their potential as antifungal, anti-inflammatory, antioxidant, and antitumor agents. N-((5-phenyl-6,11-

dihydro-5H-[1,2,4]triazolo[1′,5′:1,6]pyrido[3,4-b]indol-2-yl)methyl)-R-ethanoates were characterized by slightly higher values of the minimum energy of interaction with the active sites of model enzymes, however, while maintaining the optimal orientation of the pharmacophore fragment, which allows us to consider them as promising compounds for further optimization. The starting acid demonstrated weaker stabilization in the hydrophobic regions of the active centers of enzymes, which indicates lower affinity. Summarizing the results, amides can be considered the most promising structures for further experimental studies in vitro.

Conclusions. N-((5-phenyl-6,11-dihydro-5H-[1,2,4]triazolo[1′,5′:1,6-]pyrido[3,4-b]indol-2-yl)methyl)-R-carboxylic acid amides represent a promising class of compounds for further in vitro studies aimed at evaluating their antifungal, anti-inflammatory, antioxidant and antitumor activity, which is consistent with the results of docking analysis and confirms their potential as lead structures for further pharmacological optimization..

QUALITATIVE AND QUANTITATIVE STUDY OF FLAVONOIDS IN *IRIS GERMANICA* L. FROM UKRAINE

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Medicinal plants serve as valuable sources of biologically active compounds with therapeutic properties, used in both the prevention and treatment of numerous human diseases. In this context, particular attention is drawn to German iris (*Iris germanica* L.), a member of the Iridaceae family that is widely grown in Ukraine as an ornamental species.

Different parts of *Iris germanica* are valued for various traditional and practical applications. The rhizomes possess strong pesticidal and anticancer properties, contain blood-cleansing constituents, and are used in the treatment of venereal diseases. The leaves serve as a notable source of vitamins, particularly vitamin C (ascorbic acid). The underground organs, especially the rhizomes, are regarded as the primary medicinal raw materials of the plant. In addition, numerous secondary metabolites have been reported in *I. germanica*, contributing to its therapeutic potential [1, 2].

Therefore, the aim of the work was to determine the qualitative composition and quantitative content of flavonoids by HPLC in German iris herb.

Identification and quantitative content of flavonoids were investigated by high-performance liquid chromatography (HPLC) on an Agilent 1200 liquid chromatograph (Agilent Technologies, USA) [3]. Separation was performed using a Zorbax SB-C18 column (5 μm, 150 mm × 4.6 mm, i.d., Agilent, USA). The temperature of the column was set at 30˚C and the flow rate was 1.0 ml/min, 20 μl of injection. Mobile phase A – 0.1% trichloroacetic acid, mobile phase B – acetonitrile was used. Peak purity and absorbance were automatically detected by a DAD (UV–Vis) detector at 200-400 nm. Purified fractions of hydroxycinnamic acids and flavonoids were identified by matching retention time and spectra of standards with unknown peaks. External standards were used for the identification and quantification of compounds [4].

The analysis revealed the presence of nine flavonoids in the herb of *Iris germanica*: rutin, isoquercitrin, naringin, neohesperidin, quercetin, naringenin, apigenin, rhamnetin, and castesin. Among these compounds, rhamnetin (1794.35 μg/g), naringenin (708.11 μg/g), and rutin (356.39 μg/g) were the predominant constituents. Given the significant role flavonoids play in the therapeutic activity of plants, these findings provide valuable preliminary data and highlight the potential of *I. germanica* for further phytochemical and pharmacological investigations.

Thus, the herb *Iris germanica* L. exhibits a special flavonoid composition that may be of great interest to the pharmaceutical industry.

References:

1. Ibrahim S.R. (2012). New constituents from the rhizomes of Egyptian *Iris germanica* L. *Molecules*.17(3): 2587-2598.