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ЗАПОРІЗЬКИЙ ДЕРЖАВНИЙ МЕДИКО-ФАРМАЦЕВТИЧНИЙ УНІВЕРСИТЕТ

МАТЕРІАЛИ

ВСЕУКРАЇНСЬКОЇ НАУКОВО- ПРАКТИЧНОЇ КОНФЕРЕНЦІЇ З МІЖНАРОДНОЮ УЧАСТЮ

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A compensation solution was prepared as follows: 2.0 mL of 0.5 M hydrochloric acid solution and 2.0 mL of 8.3% sodium hydroxide solution were mixed, and the volume was adjusted with distilled water to the mark. The content of the total hydroxycinnamic acids, expressed as chlorogenic acid, was calculated using the formula:

$$X(\%) = \frac{A \times K_{dil} \times 1000}{188 \times V}$$

where, A – absorbance of analyzed solution; 188 – specific adsorption coefficient of chlorogenic acid; V – volume of tincture, mL; K_{dil} – coefficient of dilution, mL.

Results and discussions. The total content of hydroxycinnamic acids was 0.45 ± 0.02 mg/mL in the in the tincture of green tea leaves.

Conclusions: The green tea leaf tincture has the perspectives in the developing new medicines, dietary supplements and cosmetologically products.

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DESIGN AND BIOLOGICAL POTENTIAL OF 5-PHENYL-4-(*PARA*-TOLYL)-1,2,4-TRIAZOLE-3-THIOL DERIVATIVES

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Introduction. The introduction of new medicines into practice is an urgent problem for the pharmaceutical, chemical and medical industries today. The scientific work associated with the creation of modern medicines is a thorny path with various obstacles that pharmacists and doctors have to overcome for years to achieve the desired goal. Medicines based on heterocyclic systems occupy a significant segment among the rich variety of pharmaceuticals. This fact convincingly demonstrates the relevance and expediency of research aimed at developing new methodologies for the preparation of azaheterocyclic systems with powerful pharmacological potential.

The aim of the work has been to create a virtual library of compounds with subsequent prescreening assessment of the biological potential of S-derivatives of 5-phenyl-4-(*para*-methylphenyl)-1,2,4-triazole-3-thiol. To achieve this goal, it had been necessary to solve the following tasks: 1) to propose a rational method for the synthesis of 2-(5-phenyl-4-(*para*-methylphenyl)-1,2,4-triazole-3-ylthio)ethanoic acid, ester and amide based on it; 2) to determine the predictive level of pharmacokinetic and pharmacodynamic parameters and discriminators using available online computer programs.

Carbon (IV) sulfide, ammonia and *para*-methylaniline are proposed as starting reagents for the construction of the structure of the intermediate in the form of 4-(*para*-tolyl)-5-phenyl-1,2,4-triazole-3-thiol. The interaction of these substances will lead to the formation of *para*-

methylphenylisothiocyanate. In parallel, the chemical reaction of the interaction of benzoic acid ethyl ester with hydrazine hydrate will contribute to the synthesis of benzoic acid hydrazide. The synthesized benzoic acid hydrazide will be used in the process of chemical interaction with para-methylphenylisothiocyanate to form 2-benzoyl-*N*-(*para*-methylphenyl)hydrazinecarbothioamide. Subsequently, the heterocyclicization process will be implemented to form the corresponding thiol. Further conversion will involve alkylation of the starting thiol with halogenated carboxylic acids, as well as their amides and esters.

The predictive level of the biological potential of the studied compounds has been established using in silico modeling. For this purpose, the following molecular docking tools have been used: AutoDock 4.2.6, Open Babel 3.1.1, MGL Tools-1.5.6, BIOVIA, which allowed us to determine the binding energy, conformational arrangement of the ligand in the active site of the model enzyme, as well as the nature of amino acid residues and the type of interaction. Further studies were based on the use of the SwissADME resource and the Toxicity Estimation Software Tool (TEST) application, which allowed us to assess compliance with the drug-like criteria. It was noted that the appearance of carboxylic, ester and amide groups in the structure of the studied substances has a general positive effect on the formation of pharmacological properties. The high affinity of the constructed ligands for the active sites of cyclooxygenase-2 and lanosterol-14α-demethylase has been demonstrated. It has been determined that most types of chemical interactions are hydrophobic in nature. Among the amino acid residues, aliphatic ones prevail. The studies made it possible to identify the most promising compounds. The SwissADME prediction data showed that almost all compounds have the required molecular weight and fall within the required standard. As for the criterion of topological surface area and molecular flexibility: most compounds meet the required criteria. The molecular refraction of all compounds is almost at the same level and has the required values. All compounds also meet the lipophilicity criteria. The study also revealed a diverse effect on a number of cytochrome P450 (CYP) enzymes (CYP1A2, CYP2C19, CYP2C9, etc.), which, for example, may affect elimination from the human body. The optimal vector for the creation of promising 1,2,4-triazole-3-thiol derivatives with significant potential for anti-inflammatory and antifungal activity has been developed and determined.

THIN LAYER CHROMATOGRAPHY ANALYSIS OF ORGANIC ACIDS FROM *HYDRANGEA ARBORESCENS* L. LEAVES

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Introduction. Organic acids (OA) are a prospective group of biologically active compounds (*BACs*) of natural origin. They are show anti-inflammatory, antioxidant, hepatoprotective, antimicrobial activity, as well as take part in metabolic processes. It is common knowledge that, all plants, regardless of the species and family, contain OA to a small or large extent [2]. Smooth Hydrangea (*Hydrangea arborescens* L.) contains a complex of *BACs* [1]. The scientific literature does not contain any data about research of OA in the leaves of Smooth Hydrangea. Therefore the research upon this group of *BACs* in *Hydrangea arborescens* L. plant material is of great current interest. The aim of the research is determination of OA in the leaves of *Hydrangea arborescens* L. by Thin Layer Chromatography (TLC) and calculation the value of retention factor (Rf).

Materials and methods. *Sample preparation*. OA are the water-soluble compounds and for the their identification we used a previously obtained water extract from leaves of *Hydrangea*