

glycerol as a moisture-retaining, emollient and moisturizing component, an emulsifier (Ercamuls NF V) and a gelling agent (Carbopol Ultrez 21). The amount of each component has been substantiated and experimentally confirmed, and the technology for creating a highlighter in the form of a cream has been selected. The structural and mechanical properties of the obtained cream have been studied.

Conclusions. The components have been selected and the composition of the cream for the care of the skin of the face and for the application of make-up has been proposed.

References

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Synthesis and properties of esters and amides of 2-(5-methyl-4-(2-methoxyphenyl)-1,2,4-triazol-3-ylthio) ethanoic acid

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Introduction. The experience accumulated over many years of research into the methods of synthesis and properties of heterocyclic compounds creates favorable conditions for the further development of this area of research. Among the great variety of compounds of this class, special attention is paid to 1,2,4-triazole derivatives. The choice of derivatives of this structure as an object of study is quite successful and well-argued. This is due to the great potential for chemical modification of derivatives of this heterocyclic system and significant biological potential. All this determines the relevance of the selected study, which, in addition to a significant contribution to the field of pharmaceutical sciences also has significant social significance.

The aim of the study. Synthesis of esters and amides of 2-(5-methyl-4-(2-methoxyphenyl)-1,2,4-triazol-3-ylthio) ethanoic acid, proof of the structure of synthesized substances and preliminary establishment of biological potential in a number of obtained compounds.

Materials and methods. Methods of organic synthesis, chemical, physical and physicochemical methods of analysis of organic compounds (melting point, elemental analysis, chromatography in a thin layer of sorbent, UV, IR, NMR ¹H spectroscopy, chromatographic spectrometry, X-ray diffraction analysis), virtual screening of compounds using methods *in silico* (molecular docking), methods for studying the biological activity of compounds (method of double serial dilutions on Mueller-Hinton medium), statistical methods of data processing.

The stepwise synthesis involved the use in the first stage of chemical conversion of carbon (IV) sulfide, ammonia and 2-methoxyaniline for the synthesis of 2-methoxyphenylisothiocyanate. Simultaneously, the reaction of ethyl acetate and hydrazine hydrate synthesized the corresponding hydrazide, which in the reaction with 2-methoxyphenylisothiocyanate followed by alkaline heterocyclization leads to the formation of the target thiol. The next step is to carry out the pharmacophore moiety by an alkylation reaction with esters (methyl, ethyl, n-propyl, iso-propyl) and 2-chloroethanoic acid alkylamides in an aqueous-alcoholic medium in the presence of an equimolar amount of potassium carbonate. Physicochemical properties of the synthesized compounds were studied in accordance with the requirements of the State Pharmacopoeia of Ukraine.

Molecular docking was performed to obtain structural information on the interaction of the synthesized compounds and the corresponding biological structure. For this purpose, the X-ray crystal structures of the corresponding biological targets from the protein database (PDB-ID) in complex with the standard ligand were previously downloaded: cyclooxygenase-1 with diclofenac (3N8Y), lanosterol 14- α -demethylase with ketoconazole (3LD6), kinases of anaplastic lymphoma in the complex of crizotinib (2XP2). The ligands (diclofenac, ketoconazole, crizotinib) were previously removed from the primary structures. It was carried out the joining of different ligands to the protein using AUTODOCK. The conformations of the ligand were analyzed in terms of energy, hydrogen bonding and hydrophobic interaction between the ligand and the receptor protein. A detailed analysis of the ligand-receptor interactions was performed, and the final coordinates of the ligand and receptor were saved as pdb files.

The study of antimicrobial and antifungal activity was conducted at the Department of Microbiology, Virology and Immunology of Zaporizhzhia State Medical University in accordance with the guidelines "Determination of sensitivity of microorganisms to antibacterial drugs" and guidelines "Study of specific activity of antimicrobial drugs". The study was performed using standard test strains: *Staphylococcus aureus* ATCC 25923, *Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 27853, *Candida albicans* ATCC 885-653. All test strains were obtained from the bacteriological laboratory of the State Institution "Zaporizhzhia Regional Laboratory Center of the State Sanitary and Epidemiological Service of Ukraine". The study determined the *minimum inhibitory concentration* and the *minimum bactericidal / fungicidal concentration*.

Obtained results. The conditions for the synthesis of esters and amides of 2-(5-methyl-4-(2-methoxyphenyl)-1,2,4-triazol-3-ylthio) ethanoic acid have been optimized and their structure has been proved. The molecular docking demonstrated the possibility of interaction with the active sites of cyclooxygenase-1, kinases of anaplastic lymphoma, lanosterol 14- α -demethylase synthesized compounds.

Compounds with pre-expected antimicrobial activity include molecules with an amide moiety. Thus, in this class of synthesized compounds were found substances to which all the studied strains were sensitive.

Conclusions. The results of the study demonstrate the prospects of the chosen direction of research.

The scientific research and development of problems, innovations education and science of the junior pharmacist in Georgia

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