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THE WAY TO OPTIMISE PHARMACEUTICAL CARE FOR GASTROENTEROLOGICAL PATIENTS

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The socially important strategy of public health care is to increase the average life expectancy of the population and to maintain at an appropriate level such an important indicator of the well-being of the Ukrainian population as 'health'. Diseases of the digestive organs occupy one of the first places in the structure of morbidity in Ukraine.

High prevalence of gastroenterological pathology, tendency to chronic recurrent course and, as a consequence, deterioration of the quality of life of patients, determines its social importance in the structure of the health care system. An individual approach to drug treatment and improvement of the quality of life of patients with specific pathology are included in the concept of modern pharmaceutical care, which includes two aspects: drug assistance to the population and information support for specialists and consumers of medicines.

Significant expansion of the range of drugs for the prevention and treatment of digestive diseases by updating the segment of reference and reproduced drugs significantly complicates the timeliness of updating the information resource. The rapid growth of information flow about gastroenterological medicines inhibits the process of purposeful transfer of information from specialists to consumers, which may lead to a decrease in the quality of pharmaceutical care for patients and information satisfaction of specialists and consumers of gastroenterological medicines.

The search for effective directions of optimisation of pharmaceutical care for gastroenterological patients contributes to the solution of these issues.

At the same time, urgent issues of identification of priority directions of improvement of pharmaceutical care for gastroenterological patients and development of methodological solutions for their implementation have not been the subject of scientific research so far. The above-mentioned determined the choice of the research topic.

At the initial stage, the state of medical and pharmaceutical care of gastroenterological patients was assessed, acting as the first direction of the process of optimisation of pharmaceutical care. The processing of medical statistics data revealed a high prevalence of digestive organ pathology and growth trends in gastroenterological morbidity. In the course of marketing analysis of the market of gastroenterological medicines it was established that there is sufficient assortment coverage of drug therapy for gastroenterological patients: the group of gastroenterological medicines under study in the pharmaceutical market is represented by 551 trade names and 152 International non-proprietary names. Domestically produced gastroenterological medicinal products (57 %) prevail.

As a result, two components of the scientific justification of the priority of this direction were identified for the first direction of optimisation of pharmaceutical care: determination of the level and structure of morbidity of gastroenterological pathology, as well as assessment of the assortment coverage of pharmacotherapy and satisfaction of consumers' requests for gastroenterological medicines.

5-(PYRROL-2-YL)-4-PHENYL-1,2,4-TRIAZOLE-3-THIOL DERIVATIVES IN MOLECULAR MODELLING OF ANTIFUNGAL AGENTS

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The development of a biologically active substance with antifungal activity based on 1,2,4-triazole derivatives is highly relevant. The combination of this heterocycle with other pharmacophores can lead to the enhancement of a number of useful pharmacological properties.

The aim of the study was to substantiate the search for biologically promising agents with antifungal activity among the derivatives of 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol.

Materials and methods. The design of the library of compounds under study was based on the general theoretical principles of organic chemistry and, if necessary, the synthetic availability of all stages of chemical transformation. Theoretical *in silico* studies have been carried out in three stages and included the determination of the toxicological properties of 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol derivatives, their general pharmacodynamics and pharmacokinetic profile. The first stage involved the active use of the online application TEST (Toxicity Estimation Software Tool), which made it possible to determine the predictive level of acute toxicity and the likelihood of mutagenic properties. The second stage, based on docking studies using the lanosterol 14α-demethylase model, allowed us to form a preliminary idea of the possible identification of substances with antifungal activity. This stage has been implemented with the help of AutoDock 4.2.6, Open Babel 3.1.1, MGL Tools-1.5.6, BIOVIA and AUTOGRID. The third stage broadly covered the compliance of the designed 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol derivatives with the basic pharmacokinetic criteria. This stage has been carried out using a multifunctional set of tools of the SwissADME platform. Thus, the necessary physical and chemical properties (related to the structure, hydrophilic-lipophilic properties, formation of intermolecular chemical bonds, etc.) have been determined step by step, the ability to overcome barriers (placental, blood-brain and skin) and influence some cytochromes (CYP1A2, CYP2C19, CYP2C9, CYP2D6, CYP3A4) and P-glycoprotein, and the likelihood of being involved in adsorption processes in the gastrointestinal tract.

Results. The 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol derivatives predictably demonstrate an acceptable level of harmlessness at the level of moderately or slightly toxic compounds. Additionally, it should be noted that there is a low probability of mutagenicity formation. Subsequently, it was determined that the formation of bonds of the test substances with the active site of lanosterol 14α-demethylase occurs in sufficient quantities. This phenomenon has been further supported by the values of the minimum energy of complexation. Among the 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol derivatives, S-alkyl derivatives demonstrate the greatest potential for antifungal activity. The heptyl and octyl substituents demonstrated the most favourable conformation for the studied activity. At the same time, the hydrophobic nature of the bonds significantly prevailed.

Conclusions. The obtained results of *in silico* studies of 5-(pyrrol-2-yl)-4-phenyl-1,2,4-triazole-3-thiol derivatives allow us to reasonably recommend them for further research to create a biologically active substance with antifungal activity.

ANTHELMINTIC DRUGS. ANALYSIS OF THE PHARMACEUTICAL MARKET

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- Over the past 5 years, there has been a clear upward trend in the incidence of invasive aetiology, in particular, helminthiasis.
- Among the main 250 species of helminths in Ukraine, more than 25 pathogens have been identified, mainly of the digestive system. The reasons for this phenomenon are active population migration, including tourism, as well as the ability of helminth eggs, cysts and larvae to persist in the environment for a long time and pose a threat of new infections.
- According to the WHO, about 4.5 million people worldwide are affected by parasitic diseases. According to official statistics, 25-30 of the 342 known species of helminths are widespread in Ukraine. Among them, 73.7% are enterobiasis, 22.4% are hookworm, 3.3% are trichocephalosis, and up to 0.6% are other helminths.
- The purpose of our study is to analyse the range of albendazole-based medicines as the most common anthelmintic.