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ЗБІРНИК ТЕЗ ДОПОВІДЕЙ

ВСЕУКРАЇНСЬКОЇ НАУКОВО-ПРАКТИЧНОЇ КОНФЕРЕНЦІЇ СТУДЕНТІВ ТА МОЛОДИХ ВЧЕНИХ

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Materials and methods. A substantial portion of modern anticancer drug discovery yet concentrated on the lead finding and optimization of ligands by evaluating, among other properties, their affinity to the primary target, because such targets are proteins that are related to diseases. If a drug interacts with a target, that drug can possibly be used to treat the corresponding disease. An anticancer-drug target should be essential, have a unique function in the pathogen and show an activity that can be rearranged over by tiny molecules.

Results and discussion. To faster the process, a possible direction is to predict new interactions for novel drugs based on known drug-target interactions using in silico approaches before conducting laboratory experiments. Existing computational approaches, that are widespread, are docking simulation and machine learning.

Conclusion. At this time, the search for new drugs is aimed at reprocessing known structures and refining and adjusting them to design new substances. Research on 3-methylxanthine derivatives fits well with this trend, nevertheless, 3-methylxanthines are not currently the drug of choice for cancer treatment, they are promising and valuable group of substances in medical chemistry.

SYNTHESIS AND STUDY OF THE PROPERTIES OF SALTS OF 2-((5-METHYL-4-(4-METHYLPHENYL)-1,2,4-TRIAZOLE-3-YL)THIO)ACETIC ACID

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The aim of this study synthesis of salts of 2-((5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-yl)thio)ethanoic acid, study of their structure, physico-chemical properties and determination of the level of biological potential of synthesized groups of substances.

Materials and methods. Methods of organic synthesis, physico-chemical methods of analysis, virtual screening of biological activity (molecular docking). Carbon (IV) sulfide, ammonia and 4-methylaniline were used as the starting structure for the formation of the molecule 4-(4-methylphenyl)-5-methyl-1,2,4-triazole-3-thiol. The interaction of these substances led to the formation of 4-methylphenylisothiocyanate. Simultaneously, the interaction of the ethyl ester of ethanoic acid with hydrazine hydrate in ethanol allowed to synthesize the hydrazide of ethanoic acid. Synthetic acetohydrazide is involved in the reaction with 4-methylphenylisothiocyanate to form 2-acetyl-*N*-(4-methylphenyl)hydrazinocarbothioamide. The obtained compound in an alkaline medium was subjected to alkaline intramolecular heterocyclization with the formation of thiol. The next stage of work involved obtaining 2-((5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-yl)thio)ethanoic acid. For this purpose, the obtained thiol and chloroacetate acid were used. The reaction was carried out in an alkaline condition. Salts with inorganic cations were obtained with sodium and potassium hydroxides, calcium, magnesium and zinc oxides in an aqueous condition. Ammonium 2-((5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-yl)thio)acetate was obtained using 25% ammonia solution. Salts of 2-(5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-ylthio)ethanoic acid with organic bases (monoethanolammonium, diethylammonium, diethanolammonium, morpholine, piperidine) synthesized by heating the starting materials in ethanol and subsequent evaporation of the solvent. Physicochemical properties of synthesized compounds have been studied in accordance with the requirements of the State Pharmacopoeia of Ukraine.

Results. Salts of 2-(5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-ylthio)ethanoic acid were synthesized and their structure was proved.

Conclusions. The results of the molecular docking demonstrate the prospects of the chosen direction of research.

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