МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я
ЗАПОРІЗЬКИЙ ДЕРЖАВНИЙ МЕДИКО-ФАРМАЦЕВТИЧНИЙ УНІВЕРСИТЕТ

КООРДИНАЦІЙНА РАДА З НАУКОВОЇ РОБОТИ СТУДЕНТІВ, АСПІРАНТІВ, ДОКТОРАНТІВ І МОЛОДИХ ВЧЕНИХ
СТУДЕНТСЬКА РАДА

ЗБІРНИК ТЕЗ ДОПОВІДЕЙ

84 ВСЕУКРАЇНСЬКОЇ НАУКОВО-ПРАКТИЧНОЇ КОНФЕРЕНЦІЇ МОЛОДИХ ВЧЕНИХ ТА СТУДЕНТІВ З МІЖНАРОДНОЮ УЧАСТЮ

«АКТУАЛЬНІ ПИТАННЯ СУЧАСНОЇ МЕДИЦИНИ ТА ФАРМАЦІЇ - 2024»

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performed the prediction of anti-inflammatory, antifungal and anticancer activity. PDB was used as a source of three-dimensional enzyme models. The docking process was realized using the AutoDock Vina program. The preparation of ligands and enzymes was performed using AutoDock Tools, BioviaDraw, Chem 3D, HyperChem. The results were visualized using Discovery Studio Visualizer.

Results. Using *in silico* studies, the synthesized compounds are preliminarily classified as having low toxicity and minimal probability of mutagenic properties. Docking studies revealed the following regularities: the presence of a carboxyl or amide group in the structure increases the effect on cyclooxygenase, the introduction of an alkyl fragment into the structure increases the effect on lanosterol 14α-demethylase. All compounds in most cases meet the criteria for drug-like properties.

Conclusions. *S*-derivatives of 5-methyl-4-(4-methylphenyl)-1,2,4-triazole-3-thiol have great prospects as a basis for the development of biologically active compounds with potent anti-inflammatory and antifungal properties.

IN SILICO STUDY OF ANTI-INFLAMMATORY ACTIVITY AMONG NEW 2-((5-(2-BROMO-5-METHOXYPHENYL)-4-R-1,2,4-TRIAZOL-3-YL)THIO)ACETIC ACIDS AND THEIR ESTERS

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Targeted synthesis of medicinal substances involves the search for compounds with predetermined pharmacological characteristics. The creation of new drugs with predicted activity most often occurs within the same class of chemical compounds, where the directionality of the substance's action is already known. Substantial studies of 1,2,4-triazole derivatives demonstrate a great potential for inhibiting inflammatory processes. However, the analysis of scientific sources shows that this class of compounds has not been fully studied. Therefore, the development of new highly effective compounds, as well as the study of their anti-inflammatory potential, remains an urgent task for modern medicine and pharmacy.

The aim of the study. To investigate the anti-inflammatory activity of new 2-((5-(2-bromo-5-methoxyphenyl)-4-R-1,2,4-triazol-3-yl)thio)acetic acids and their esters using molecular docking.

Materials and methods. The design of research on molecular modeling included the following stages: optimization of the structure of the studied molecules according to Parr's algorithm Pariser-Pople (up to a gradient of 0.1 kcal/mol/degree), search for the COX - 2 macromolecule in the protein database, preparation of files of optimized molecules and COX -2 macromolecule (subunit A) for AutodockVina , search for the optimal placement of the ligand molecule on the COX protein -2 for each molecule, analysis and 20 visualization of docking results. The COX-2 complex with Celecoxib is obtained from the file 3LN1.pdb . File format conversion was carried out using the OpenBabel 2.4.0 program. The files for AutodockVina were prepared in AutodockTools 1.5.6 format . Docking of the studied molecules in COX -2 (subunit A) was carried out using the AutodockVina program under the condition that a flexible ligand and a rigid receptor were assumed.

The results. According to the results of molecular docking, it was established that propyl 2-((5-(2-bromo-5-methoxyphenyl)-4-methyl-4H-1,2,4-triazol-3-yl)thio was the most active among the analyzed compounds)acetate as a possible potential candidate for more in-depth investigation of anti-inflammatory activity.

Conclusions. Molecular docking was carried out for 28 new compounds, according to the results of which the most promising compounds in the biological sense were outlined for the study of anti-inflammatory activity by methods *in vivo* .