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SYNTHESIS AND PROPERTIES OF SOME 3-(5-(4-METHOXYPHENYL)PYRAZOL-3-YL)-6-R-[1,2,4]TRIAZOLO[3,4-B][1,3,4]THIADIAZOLE

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Heterocyclic compounds, as well as their physical and chemical properties, began to be studied by scientists more than a century and a half ago. And nowadays, not only scientific, but also practical interest in 1,2,4-triazole and pyrazole derivatives is steadily increasing. This is primarily due to their high reactivity and the possibility of obtaining a biologically active substance with acceptable toxicity indicators.

The aim of the work was to study the conditions for obtaining 3-(5-(4-methoxyphenyl)-pyrazol-3-yl)-6-R-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazoles and studying the properties of these compounds.

Methods and results. Diethyloxalate and 1-(4-methoxyphenyl)ethan-1-one with the participation of sodium hydride in toluene were used for the synthesis of the original thiol. The obtained ethyl 4-hydroxy-4-(4-methoxyphenyl)-2-oxobut-3-ethanoate at the next stage was used in the process of transformation into ethyl 5-(4-methoxyphenyl)pyrazole-3-carboxylate with the participation of hydrazine hydrate. Further modification of the molecule consisted in the stepwise formation of the structure of 4-amino-5-(5-(4-methoxyphenyl)pyrazol-3-yl)-1,2,4-triazol-3-thiol. The next stage of the work involved interaction with carboxylic acids in the environment of phosphorus oxychloride. To establish the composition and identify the structure of the isolated substances, 1H NMR and infrared spectra were recorded, as well as qualitative and quantitative indicators of the elemental composition of the synthesized structures were obtained. The individual nature of the presence of substances and the degree of their purity were determined using high-performance liquid chromatography. For docking analysis, 3D models of ligands and receptor were prepared in the AutoDock Tools software package. Docking was performed using the AutoDock Vina package. Information regarding the structure of the model enzyme was taken from the Protein Data Bank (PDB) database.

The results. The synthesis of 3-(5-(4-methoxyphenyl)pyrazol-3-yl)-6-R-[1,2,4]triazolo [3,4-b][1,3,4]thiadiazoles was carried out and the optimal conditions were determined the process of obtaining these substances. The structure of the chemical transformation products has been confirmed and the results of the physical properties study have been recorded.

Conclusions. As a result of the conducted molecular docking, data were obtained that form an idea of a certain level of probability of the effect of the synthesized compounds on the activity of lanosterol-14α-demethylase, which substantiates the possibility of further research of antifungal activity.

ANTIMICROBIAL ACTIVITY OF DERIVATIVES OF N-ACYL THIOSULFANYL ACIDS

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Introduction. Our previous research found thiosulfonates with moderate and low toxicity, high antimicrobial and antiviral activity in low concentrations among the class of sulfur-containing compounds that became a good basis for further search for new effective active substances and design of composite drugs with biosurfactants. Therefore, the aim of the work was the synthesis of compounds, derivatives of N-acyl thiosulfanyl acids, and evaluation of their antimicrobial and antiviral activity.