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SYNTHESIS AND PROPERTIES OF 3-ALKYLTHIO DERIVATIVES OF 9-METHYLPYRAZOLO[1,5-*D*][1,2,4]TRIAZOLO [3,4-*F*][1,2,4]TRIAZINE

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Topicality. The current goal of modern medicine and pharmacy is to create new drugs that exhibit high biological activity and are low-toxic substances. Many scientists work with such a heterocyclic system as 1,2,4-triazole, which is due to the valuable properties of derivatives of this system. Derivatives of 1,2-diazole, whose drugs have successfully proven themselves in Ukraine and around the world, are also attracting a lot of attention. In this work, it was used as a key compound that contains two heterocycles simultaneously – 5-methylpyrazole and 1,2,4-triazole.

The aim of this work was the targeted synthesis of 3-alkylthio-9-methylpyrazolo[1,5-d] [1,2,4]-triazolo[3,4-f][1,2,4]-triazine, the establishment of physicochemical and biological properties of the specified class of compounds.

Materials and methods. To achieve this goal in the first stage, 4-amino-5-(5-methylpyrazol-3-yl)-1,2,4-triazole-3-thiol was synthesized. Subsequently, the obtained compound was used in S-alkylation reactions with the corresponding haloalkanes. The next stage of the work involved the study of the conditions of chemical transformation of the synthesized S-derivatives of 4-amino-5-(5-R-pyrazol-3-yl)-1,2,4-triazole-3-thiol in triethyl formate medium under heating. It was confirmed that the corresponding 3-alkylthio-9-methylpyrazolo[1,5-d][1,5,4]triazolo[3,4-f][1,2,4]triazine was formed as the reaction product.

The prospects of biological research were established using the method of molecular docking. The study revealed promising objects for further study of anti-inflammatory and antifungal activity

Results. According to the results of the study, ten new compounds were obtained, the structure of which was confirmed using modern physicochemical methods of analysis. The estimation of indicators of anti-inflammatory and antifungal activity which were determined by the method of molecular docking is given. Based on the estimated estimates, a number of compounds were selected for a more in-depth study of anti-inflammatory and antifungal activity.

Conclusions. The possibility of forming 3-alkylthio-9-methylpyrazolo[1,5-d][1,2,4] triazolo[3,4-f][1,2,4]triazine based on the reaction of S-derivatives of 4-amino-5-(5-R-pyrazol-3-yl)-1,2,4-triazole-3-thiol with triethyl formate. It is shown that the obtained compounds have significant potential for anti-inflammatory and antifungal action.