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SYNTHESIS AND STUDY OF THE PROPERTIES OF SALTS OF 2-((5-PHENYL-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-phenyl-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-phenyl-1,2,4-triazole-3-thiol. The interaction of these substances contributes to the formation of 4-methylphenylisothiocyanate. At the same time, an esterification reaction was carried out with the participation of benzoic acid and ethanol under conditions of acid catalysis. Then the hydrazide of the resulting ester was synthesized. The synthesized benzoic acid hydrazide was used in the reaction with 4-methylbenzene isothiocyanate. Thus was obtained 2-phenyl-*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 included obtaining 2-((5-phenyl-4-(4-methylphenyl)-1,2,4-triazole-3-yl)thio)ethanoic acid. For this stage, the optimal conditions for the interaction of the obtained thiol and chloroacetic acid were established. The reaction was carried out in the presence of the required amount of alkali. Salts with inorganic cations were obtained with sodium and potassium hydroxides, calcium, magnesium and zinc oxides in an aqueous condition. Ammonium 2-((5-phenyl-4-(4-methylphenyl)-1,2,4-triazole-3-yl)thio)acetate was obtained using 25% ammonia solution. Salts of 2-(5-phenyl-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-phenyl-4-(4-methylphenyl)-1,2,4-triazole-3-ylthio)ethanoic acid were synthesized and their structure was proved.

Conclusions. The results of the conducted studies *in silico* confirm the prospects of the chosen direction of work.