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SYNTHESIS, PHYSICOCHEMICAL AND BIOLOGICAL PROPERTIES 2 -((4-PHENYL-5-(((5-(PHENYLAMINO)-1,3,4-THIADIAZOL-2-YL)THIO)-METHYL)-4H-1,2,4-TRIAZOL-3-YL)THIO)ACETIC ACID AND ITS SALTS

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Introduction. The chemical ability of 1,2,4-triazole derivatives arouses an increased level of interest among many scientific teams of the world, because on the basis of this heterocyclic structure a number of substances have been obtained that are used in various spheres of human life. Analysis of the literature revealed that the combination of 1,2,4-triazolovgo and 1,3,4-thiadiazolovgo fragments leads to different types of activities (anti-inflammatory, diuretic, antioxidant, anticonvulsant). Also noteworthy is the fact that the combination within one molecule of these fragments is not fully understood.

The purpose of the study: search and optimization of synthetic ways to obtain these compounds and study their properties.

Materials and methods. The key compound used was 4-phenylthiosemi-carbazide. By reacting the starting reagent with carbon disulfide in dimethylformamide, a thione was obtained, which was subsequently alkylated with prop-2-yl ester of chloroethanoic acid.

The synthesized reaction product was further used for further transformations using hydrazinolysis reactions, nucleophilic addition of phenylisothiocyanate and intramolecular alkaline heterocyclization. The obtained thiol was further reacted with chloroethanoic acid in propan-2-ol.

Inorganic salts 2-(4-phenyl-5-(((5-phenylamino-1,3,4-thiadiazol-2-yl)thio)-methyl)-1,2,4-triazol-3-yl)thio)ethanoic acid was synthesized by the interaction of this acid with sodium hydroxide, potassium hydroxide, magnesium oxide, calcium carbonate or zinc sulfate. For analysis, the obtained salts were purified by crystallization from methanol.

Organic salts 2-(4-phenyl-5-(((5-phenylamino-1,3,4-thiadiazol-2-yl)thio)-methyl)-1,2,4-triazol-3-yl)thio)ethanoic acid is obtained by the interaction of the corresponding acid with organic bases (ammonia, diethylamine, diethylmono-ethanolamine, morpholine, piperidine) in the middle. For analysis, the synthesized substances were purified by crystallization from a mixture of water - propan-2-ol (1: 1).

The structure of the obtained compounds was confirmed by elemental analysis, ¹H NMR spectroscopy and IR spectrophotometry. The individuality of substances is established by high performance liquid chromatography. Individual calculation screening was performed for the synthesized substances with the help of the software product "PASS On-line®".

Results. During the work, the method of obtaining 2-(4-phenyl-5-(((5-phenylamino-1,3,4-thiadiazole-2-yl)thio)methyl)-1,2,4-triazole-3-yl)thio)ethanoic acids was optimized. The conditions of synthesis of organic and inorganic salts of the specified acid, their structure and physicochemical properties are established. The biological potential was preliminarily assessed using molecular docking.

Conclusions. As a result of synthetic studies, 11 new, previously undescribed compounds were obtained. The structure, composition and individuality of the synthesized substances are confirmed by a set of the latest physicochemical methods of analysis.