We believe that the uncontrolled use of the aforementioned drugs, in particular by the respondents involved in our study, confirms the fact of irresponsible self-medication and needs increased attention from a pharmacist (clinical pharmacist) in the form of professional pharmaceutical care in order to establish positive compliance, maximize the effectiveness of self-treatment and change the lifestyle of the patient (complete rest, normalization of sleep (≥ 8-9 hours); optimization of a food mode; provision of adequate psychological microclimate).

IN SILICO STUDY OF 4-R-3-SUBSTITUTED-4*H*-1,2,4-TRIAZOLE-5-THIOLES DERIVATIVES

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The study of the biological activity of the new synthesized compounds is one of the tasks for the creation of the original drug. The new synthesized 1,2,4-triazole derivatives are not exception. Strategic study of biological activity of new synthesized substances should begin with computer analysis and molecular docking research.

The aim of our work was to conduct virtual screening and molecular docking of 4-R-3-substituted-4*H*-1,2,4-triazole-5-thioles derivatives.

Virtual screening was held using PASS software. Molecular docking research was done using Autodock 4.2.6 software. The screening was held on the crystallographic structure of the “EC 1.15.1.1 Superoxide dismutase” (1SHN) enzyme

Visualized with Discovery Studio Visualizer. The grid for binding was as follows, 60 Å × 60 Å × 60 Å, which was spacious enough to cover the entire enzyme region. All the programs we used were shared.

The increase in the level of free radical processes at maximal and submaximal physical loads is explained by the activation of the sympathoadrenal system in response to muscular work. The essence of this mechanism is as follows: reactive oxygen species capable of initiating free radical reactions can be generated both in the biosynthesis of catecholamines and in their decay, when adrenaline is oxidized to adrenochrome.

Actoprotective activity is known in many cases due to the induction of protein synthesis, including antioxidant enzymes.

The most promising compounds for molecular docking were the compounds with the highest affinity for the enzyme "EC 1.15.1.1 Superoxide dismutase", which were -8.12, -7.21kcal / mol and -6.95 kcal/mol.

All docked molecules have zero RMSD values.

Nitrogen atoms of 1,2,4-triazole ring have been found to form 2 hydrogen bonds with water molecules that are part of the enzyme.

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