

STUDY OF THE BIOLOGICAL ACTIVITY OF THE COMPLEX COMPOUND $[\text{Cu}(\text{Tsk})_2](\text{Glu})_2$ USING THE PASS ONLINE PROGRAM

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<https://doi.org/10.5281/zenodo.17337714>

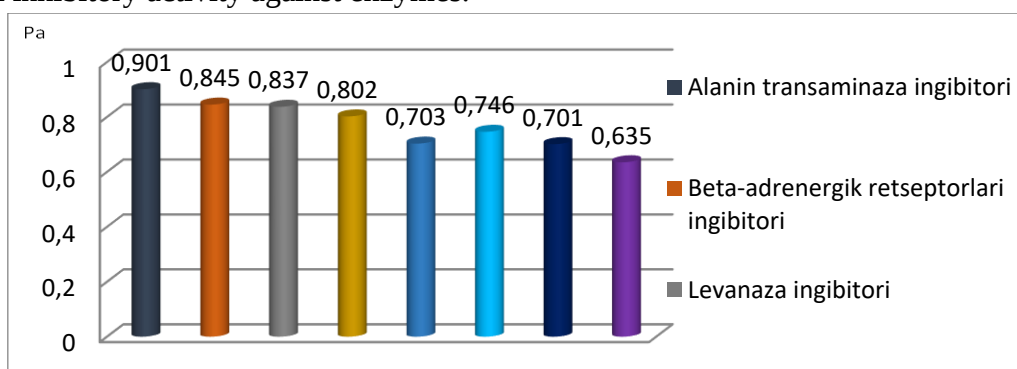
Relevance of the study. the possibility of assessing physicochemical properties directly by the structural formula of the compound is relevant. Comparison of these parameters of the synthesized compounds obtained as a result of calculations allows us to assess the contribution of a certain physicochemical characteristic to the developed activity and a better understanding of the mechanism of action of the preparation.

Purpose of the study. Study of the structure and prediction of potential biological properties of compounds: $[\text{Cu}(\text{Tsk})_2](\text{Glu})_2$.

Method and style. Pass-online application

A powerful set of methods for predicting the biological activity of chemical compounds on a computer is methods based on Bayesian probability. The Pass software package is a program capable of predicting the biological activity spectra of chemical compounds known to date. The Pass program (online) is based on the study of the biological activity of substances depending on their structure. This program contains known Pa and Pi values for the substance, these values represent the theoretical probability. That is, Pa is pharmacologically active, Pi is pharmacologically inactive. If $\text{Pa} > 0.71$, such a molecule is considered active. The online pass program works on the principle of structural biological activity. In this case, the value of Pa determines the pharmacological activity of the substance against a certain disease, and the value of Pi determines the low pharmacological activity against this disease.

Results. Computer calculations were performed using the pass-Online program to determine potential biologically active substances. It was established that the synthesized complex compounds have high inhibitory activity against enzymes.



Theoretically calculated biological activity of the $[\text{Cu}(\text{Tsk})_2](\text{Glu})_2$ molecule in the PASS-online program

Summary: According to the results of the analysis of the Pass-online program, it was established that $[\text{Cu}(\text{Tsk})_2](\text{Glu})_2$ is a high inhibitor of enzyme complexes. It was established that these complex compounds have high activity of alanine transaminase and beta-adrenergic receptor inhibitor.