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VIRTUAL SCREENING OF PYRROLO[1,2-A] QUINOLINE DERIVATIVES

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Relevance. Every year, chemists around the world synthesize from 200 to 250 thousand new chemical compounds. Complex experimental testing of biological activity *in vitro* and *in vivo* is not always possible, therefore it is rational to carry out the preliminary computer screening of compounds before starting synthesis. The biological activity of the compounds is determined by the chemical structure of the molecules. Using PASS allows predict biological activity to fast. The theses present information obtained through PASS online developed under the guidance of V. Porojkoff, D. A. Filimonov. At the present stage development of organic and bioorganic chemistry, considerable attention is paid to the synthesis of pyrrolo[1,2-a]quinolines, which are interest primarily as bioregulators with a wide spectrum of biological activity. Experimental testing of the interaction of many millions chemical compounds with thousands molecular targets is impossible both from an economic and a practical point of view. Thus, it is necessary to pre-select the molecules with the highest probability of interaction with the target molecular targets. One of the main directions of the development chemical science is the search substances with high biological performance, which can become the basis of new biologically active substances. Nitrogen-containing heterocyclic compounds are known as natural and synthetic molecules and exhibit a wide range of biological effects. Among the various N-heterocycles, pyrrolo[1,2-a] quinoline derivatives pay considerable attention to the unique biological activity.

Purpose of research: The purpose of our work was to conduct a screening of biological properties for some pyrrolo[1,2-a] quinolines derivatives for further biological research.

Experimental Set-up and Procedure. Internet resource PASS Online (http://www.way2drug.com/passonline) was used. The algorithm of the program's work is based on the analysis structural descriptors of multilevel atomic orbits. This set of descriptors is generated on the basis of a structural formula, which is a list of atoms that form a molecule, and a list of bonds between them. Description the structure of chemical compounds in the PASS system is based on 2D structural formulas. Derivatives of pyrrolo[1,2-a] quinoline containing the substituents in the 2nd and/or 5th positions were selected for analysis. The result of the prediction is issued in the form of a list of activity names with estimated values of probabilities presence (Pa) or absence (Pi) for each type activity. They can be considered as measures of affiliation the predicted compound to the classes "active" and "inactive" substances. The prognosis of some types biological activity, which gives the probability $Pa>0.7$, indicates that this compound will detect this type of activity in the experiment, and the chance that this substance is an analogue of the known medicinal product is also quite significant. There is a high probability that the compound will detect this type of biological activity in the experiment if $0.5 <Pa <0.7$. If $Pa<0.5$, the probability that the test substance detects this type of biological activity in the experiment is less, but if its presence is experimentally confirmed, then such the substance may be a fundamentally new base structure. These probabilities are calculated independently of the sub-assemblies of active and inactive compounds and their sum is not equal to one. The greater value of Pa for a particular activity and the smaller value of Pi, the greater chance to detect this activity in the experiment.

Results and discussions. The results obtained for compounds similar in structure demonstrate that biological activity depends on substituents in positions 2 and 5. As a result of calculations and analysis of the data obtained. As a result of the calculations and analysis of the data obtained, it is possible to reduce a wide range of biological activities and select the most likely ones for further practical research.

Conclusions. Using PASS allows predict biological activity to fast. Thus, we can conclude that the introduction substituents in positions 2nd and 5th leads to change in the values of Pa and Pi and biological activity in general. Possible cases when one biological action manifests itself to varying degrees or when the types of activity disappear/appear.