THE CONCEPT OF COMPUTERIZATION IN BIOCHEMISTRY

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Modern methods of scientific research in the biological field are less and less consistent with applied problems for many reasons. As science advances, the main reason is the increasing complexity of the required experiments. In other words, if a century and a half ago it was enough to examine the internal structure of a cell in a microscope or to decompose the light of the flame of certain chemical compounds into a spectrum, today we set ourselves the task of understanding complex and ambiguous processes, such as changing the genome or predicting the chemical properties of non-existent compounds. Today, we cannot rely solely on observation due to the limited capabilities of the observer. Naturally, modern research methods and their development should be based on the available empirical data, but their further development is impossible without the active introduction of information technologies. Data hybridization, in turn, requires multidisciplinary knowledge from a specialist. The next-generation researcher should be comfortable both in the laboratory and at the computer.

According to the analysis of literature data, an accelerating growth of interest in bioinformatics is observed. To confirm the promise of computational methods in biology, an analysis of scient metric data such as Web of Science, Elsevier, and Google Scholar was carried out based on software solutions for simulating the software requirements of the cholinergic system without laboratory testing. The usable options of proposed software were determined.

Currently, there are many functional highly specialized implemented solutions in the fields of bioinformatics. At the same time, the term “solutions” refers to products of various profiles: from the unified bioinformatics bases mentioned above to software implementations of individual methods or models. Nevertheless, the field of problems in this young area is still vast, and further pace of development depends on our ability to solve these problems.

It is proposed to create a software product in the form of a complex of modules that comprise a single working environment capable of simulating the cholinergic system, considering dynamic processes considering all direct and indirect factors, predicting possible interactions, assessing the effectiveness of the process and the quality of the result, and modelling processes at the micro-level and macrosystems.

The interface should be intuitive and user-friendly, be comfortable in working with specific information in the, have some universal base of implemented techniques and a wide range of settings for typical procedures, as well as the ability to create custom processes and algorithms for solving highly specialized tasks.

An important aspect of the work of the proposed product is a powerful mechanism for preprocessing the incoming data, which will be able to increase the quality of raw data to the required quality and level of trust; if necessary, to generate additional data samples based on a small sample or increase/ decrease the amount of noise. Also, an urgent task is to solve the problem of a full-fledged, unified, and complete coding format for specific information in the fields of bio- and chemoinformatics, which would be supported by all methods and algorithms included in the solution, exclude the loss or the possibility of ignoring important special information, and at the same time would imply the possibility of convenient visualization for the researcher [1].

References

1. V. Vasylenko, M. Martynova, S. Mickevičius, Development and application of the complex model of the cholinergic system, BIOLOGIJA. 2021. Vol. 67. No. 1. P. 1–10, Lietuvos mokslų akademija, 2021, DOI: 10.6001/biologija.v67i1.4399