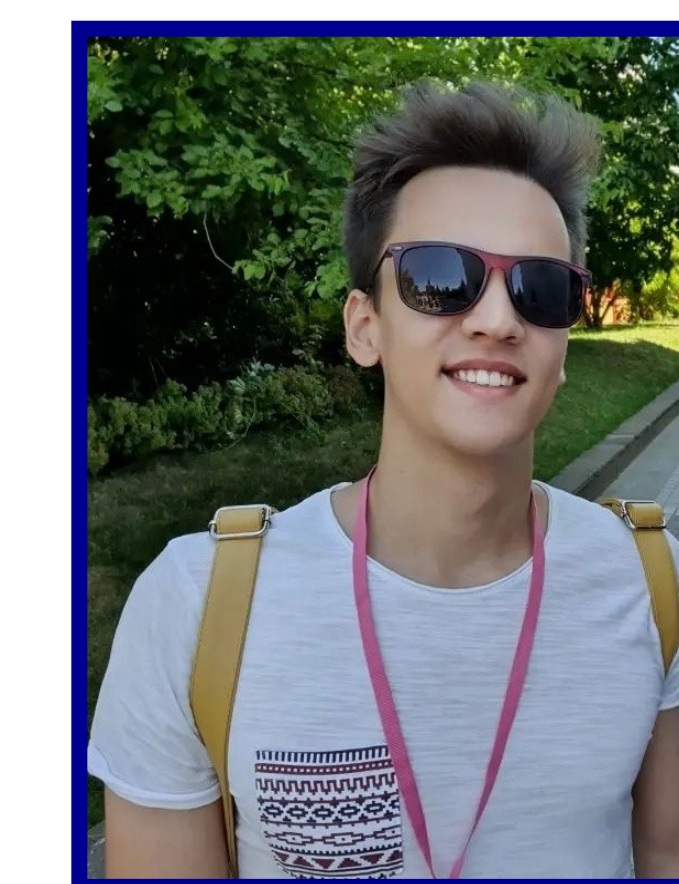


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# Topological analysis of protein surfaces and its role in the development of new medicines. *Oleg V. Bystrov*<sup>\*1</sup>, *Sergey D. Kulik*<sup>2</sup>.

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## SUMMARY

The paper addresses the challenges of managing and organizing data in the research of protein structures and it is organized into sections that introduce the topic, discuss mathematical research and topology, present the prototype of the information system.

## INTRODUCTION

Information technologies and cognitive technologies have gained significant importance in various fields, including medicine, telemedicine, education, and biochemistry.

The study focuses on the use of information technology and mathematical methods, particularly topology, in understanding protein structures and interactions. Proteins are complex objects that have not yet been fully studied, but thanks to the use of topology and mathematical analysis, the study of protein interactions is crucial for understanding their functions and properties, as well as for the development of new drugs and the creation of proteins with desired characteristics.

The article aims to present a biological information system that can store and utilize research data, samples, and analysis results for future researches.

## APPROACH

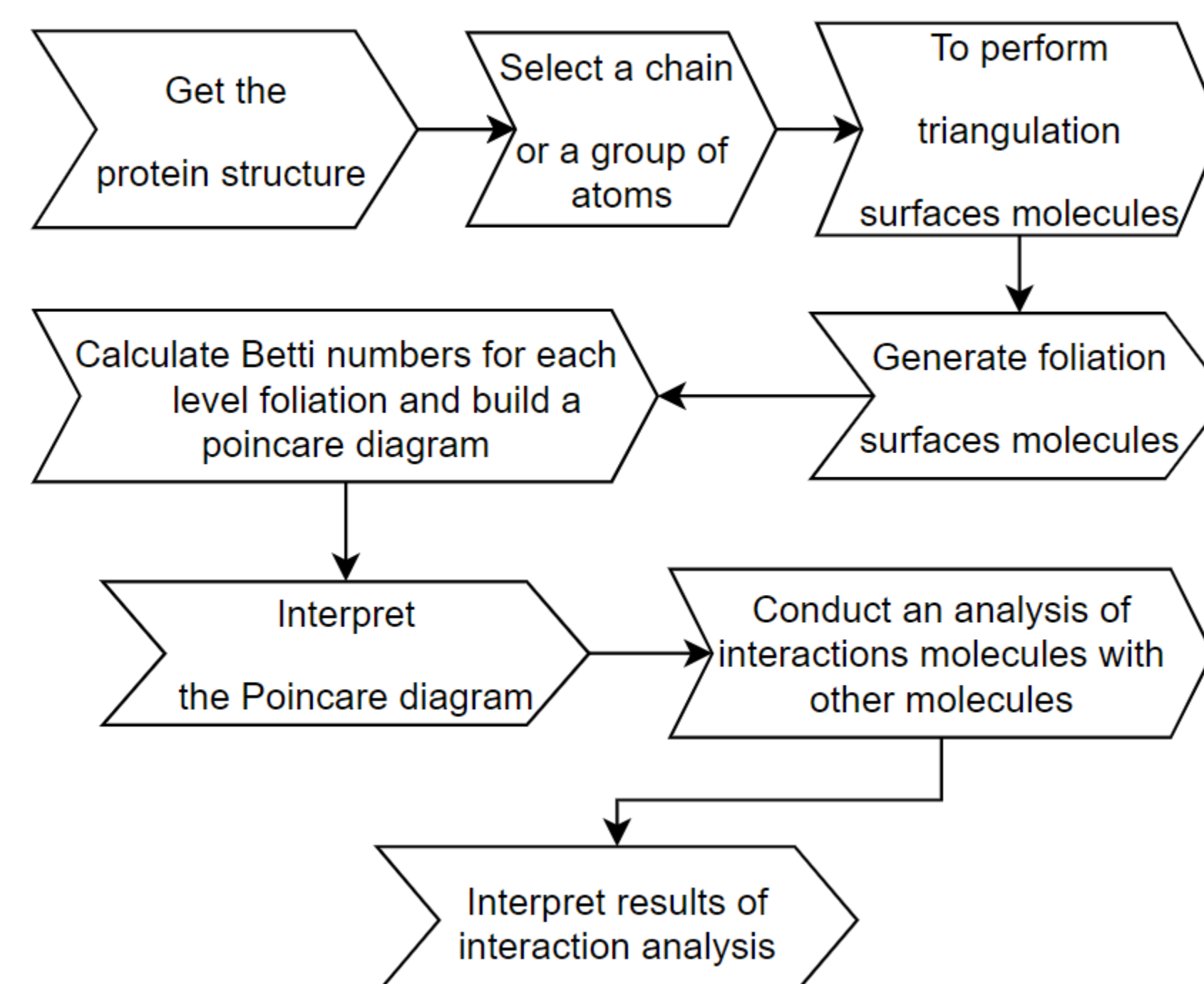


Fig. 1. The algorithm of the biological information system

## METHODS

Assume that the biological information system for scientific research consists of a variety of different blocks. These blocks have a rather complex structure. It includes a database, a special format for storing protein structures PDB, a query repository and a block for processing it, a query repository and a block for receiving it, a block for preparing for research, a block for conducting research (including conducting a topological analysis of the protein surface) and a block for preparing responses to requests. Each of the listed blocks implies a specific software with a user interface for a laboratory employee.

## RESULTS

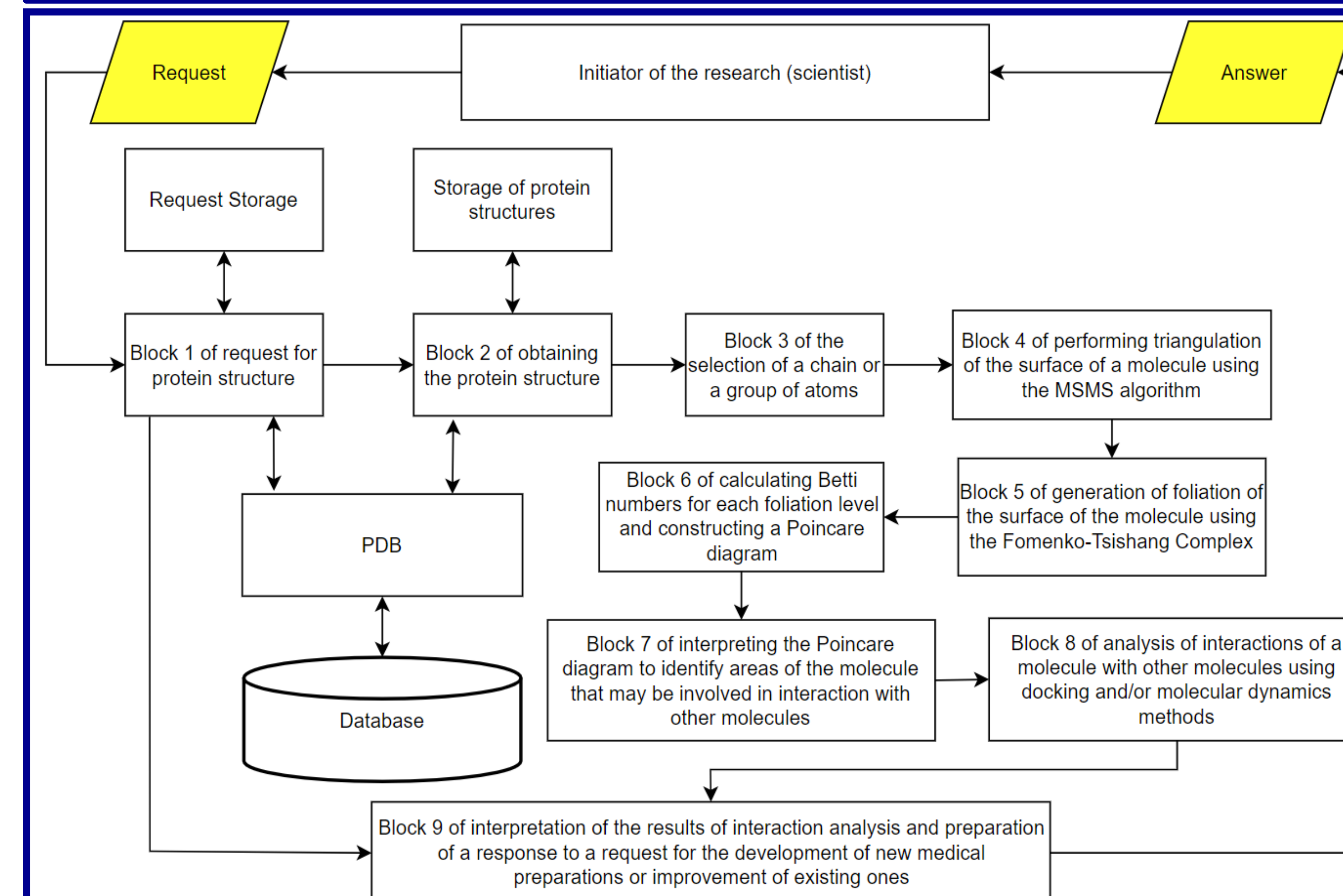


Fig. 2. Structural diagram of the biological information system for scientific research

## ANALYSIS

The research focuses on studying the three-dimensional structure of proteins using various computational techniques. It involves obtaining protein structure data from public databases, selecting specific atoms or protein chains for investigation, performing surface triangulation and foliation, calculating Betti numbers and constructing a Poincare diagram to analyze the structural features of the molecule. The interactions between the molecule and other molecules are then analyzed using docking and molecular dynamics methods. The data obtained are interpreted in the context of the function of the protein and its role in the body and a response is prepared to a request for the development of new drugs or the improvement of existing ones.

## DISCUSSION

Proteins are particularly complex objects. Despite this, there has been some progress in scientific research of the structures of molecules and their interactions with each other through the joint use of information technology and mathematical methods, including topology, that can increase the effectiveness of medical research and improve the tools of employees involved in protein analysis. Understanding the three-dimensional structure of proteins allows the development of targeted drugs aimed at specific protein targets in the brain. This may be an important in the development of medicaments for the treatment of cognitive disorders.

## CONCLUSIONS

1. A structure of the biological information system for scientific research was designed.
2. The scheme and algorithm of the information and biological system were developed.
3. The development of special software for the study of the three-dimensional structure of proteins in order to determine the areas of the molecule that can be involved in interaction with other molecules is the subject of our future research.

## ACKNOWLEDGMENTS

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