

## ABSTRACT

Master's thesis, 106 pp., 21 fig., 5 tab., 3 annexes, 78 sources.

**Topicality.** The problem of predicting the tertiary structure of protein molecules relevant in the fields of molecular biology, biochemistry, genetics, pharmacology. The ability to predict the structure of proteins is key to understanding their effects on the body, schemes of many diseases, and often find--- ways to treat them.

For many proteins the correct three-dimensional structure necessary for the operation---. Wrong structure leads to the formation of inactive proteins that often block the work of their potential partners, disrupting all cell's operation. In some cases, the wrong structure can even spread to other proteins, as happens with prions. Several neurodegenerative diseases are thought to arise from the accumulation of misfolded proteins. The accumulation of misfolded proteins in the cytosol leads to start response to heat shock. It leads to increased expression of proteins chaperones which help unfolded polypeptide fold to native conformation. If endoplasmic reticulum stress, i.e. when there is a high concentration of misfolded proteins in the organelles in the cell runs the so-called unfolded protein response. Its objective is to increase the number of endoplasmic reticulum chaperones, proteins that are involved in polypeptides retrotranslocation into the cytosol, where they are subject to degradation, and other proteins that help to increase the capacity of the endoplasmic reticulum to fold polypeptides.

**Connections with academic programs, plans, topics.** Master's thesis is written in accordance with the plan of Department of Optimization of Controllable Processes in V.M. Glushkov Institute of Cybernetics of NAS of Ukraine within the scientific research topic "Development of mathematical tools focused on the creation of intelligent information technologies for solving problems of combinatorial optimization and information security" (state registration No.0117U000323)

**Objective** Improving the accuracy of prediction of protein tertiary structure.

To achieve the goal must perform the following tasks:

- perform a review of existing models and algorithms for predicting protein tertiary structure;
- perform a comparative analysis of mathematical models used for predicting protein tertiary structure;
- perform problem formalization for prediction of protein molecules folding process
- develop a model representation of the tertiary structure of protein molecules,
- develop a method for the prediction of protein tertiary structure;
- develop algorithms and software implementation models in a form that can be used to predict protein molecules folding process;
- perform an analysis of the results.

**Object of study** - Mathematical modeling of the proteins tertiary structure formation.

**Subject of research** - approaches, mathematical models and algorithms for solving combinatorial optimization problems arising in such modeling.

**Research methods** - simulation, comparative analysis.

**The scientific novelty** of the results is to use a modified ant colony optimization algorithm and compare its performance with previously established.

**Publications.** Informatics and Computer Science" ICS-2017" - Application of various ant colony optimization algorithm implementations for the protein's tertiary structure prediction

PROTEIN FOLDING, TERTIARY STRUCTURE OF THE PROTEIN MOLECULE, DISCRETE LATTICE, COMBINATORIAL OPTIMIZATION, PROTEINS TERTIARY STRUCTURE PREDICTION, ANT COLONY OPTIMIZATION METHODS, HEURISTICS, NP-COMPLEXITY