

REVIEW

from **prof. Todorka Atanasova Glushkova, PhD,**

Plovdiv University „Paisii Hilendarski“

on the **Thesis** for awarding educational and scientific degree **PhD,**

under the Scientific Field: 4. Natural Sciences, Mathematics and Informatics, the

Professional Area: 4.6. Informatics and Computer Sciences,

the Scientific Specialty: **Informatics**

Author of the PhD Thesis: **Zhelyazko Petrov Terziyski**

Thesis Title: “**Using techniques from Artificial Intelligence to analyze and predict the properties of peptides**“

This review is prepared on the basis of Art. 30, para. 3 of the Regulations for the Implementation of the Law on the Development of the Academic Staff in the Republic of Bulgaria (ZRASRB), as well as in compliance with order No. RD-21-237/29.01.2024, of the Rector of Plovdiv University "Paisiy Hilendarski", prof. Dr. Rumen Dimitrov Mladenov, regarding the decision of the Faculty Council at the Faculty of Mathematics and Informatics, with protocol No. 3 of 24.01.2024, to disclose the procedure for the defense of the dissertation work of the full-time PhD student **Zhelyazko Petrov Terziyski**, to obtain the educational and scientific degree "doctor" in the scientific field 4. Natural sciences, mathematics and informatics, by professional direction 4.6. Informatics and computer science, doctoral program **Informatics**, on the topic "**Using artificial intelligence techniques for analysis and prediction of the properties of peptides**". The scientific advisor is Assoc. Prof. Stanka Ivanova Hadjikoleva, PhD.

As a member of the Scientific Jury I have received:

1. Order No. RD-21-2231/27.11.2023 of the Rector of the Plovdiv University “Paisii Hilendarski”;
2. Application for opening a procedure for acquiring the educational and scientific degree PhD;
3. European Curriculum Vitae;

4. Protocol No. 2-23/24 from 27.10.2023 of the preliminary discussion of the PhD Thesis in the Department “Computer systems” at the Plovdiv University “Paisii Hilendarski”;
5. Opinion of the scientific advisor.
6. Reference to the implementation of the minimum requirements of the of the Faculty of Mathematics and Informatics at the Plovdiv University “Paisii Hilendarski” for obtaining the educational and scientific degree PhD;
7. Abstracts of the PhD Thesis – in Bulgarian and in English;
8. PhD Thesis;
9. Declaration for the original scientific and applied scientific contributions;
10. List of the publications included in the PhD thesis;
11. Copies of the publications included in the PhD thesis;

In order to form the final evaluation of the dissertation, the requirements of the Development of Academic Staff Act in the Republic of Bulgaria are implemented the specific requirements in the Act’s Institutional Regulation shall be taken into consideration, where the respective norms are:

- Pursuant to Art. 6 (3) of the Development of Academic Staff Act in the Republic of Bulgaria, PhD thesis should contain scientific or scientific-applied results, which represent an original contribution in science. The PhD thesis must indicate that the candidate **has in-depth theoretical knowledge of the relevant specialty and ability for independent research.**
- According to Art. 27 (2) of the specific requirements in the Act’s Institutional Regulation, PhD thesis should be presented in a form and volume corresponding to the specific requirements of the primary unit. **The PhD thesis should contain: a cover page; content; introduction; exhibition; conclusion - a summary of the results obtained with a declaration of originality; bibliography.**

Zhelyazko Petrov Terziyski completed his master's degree at the Sofia Technical University - Plovdiv branch in 1998 as an electronics engineer. He works successively in several companies as a specialist in the design, implementation and maintenance of hardware and software components. The desire of the PhD student to share his knowledge with the students is confirmed by the fact that from 2022 he is realized as an assistant professor and participant in the research activity of the Thracian University in

Stara Zagora. The experience of the PhD student gained over the years is a prerequisite for the high level of research related to the subject of the dissertation.

I. Actuality and significance of the PhD thesis

The relevance of the dissertation work is based on the relevance of the considered scientific field related to artificial intelligence and its application in solving various practical tasks. The PhD student has focused his research on using techniques from artificial intelligence to analyze and predict the properties of peptides. On the other hand, the development of software products to facilitate the use of the selected methods, as well as the analysis of the obtained results, is timely, necessary and useful. Based on this, I define the topic of the dissertation research as current and significant.

The main goal of the PhD Thesis is "**To design, develop and validate a software system for predicting the biological properties of peptides using various artificial intelligence methods.**"

To achieve this goal, the following scientific tasks have been formulated:

1. Study of the essence of peptides and current research and scientific achievements for the use of artificial intelligence methods for predicting their biological activity;
2. Study of publicly available databases and tools for coding peptides and creation of a database of known peptides and their biological activity;
3. Creation of a conceptual model of a software application for the analysis and prediction of peptide properties by various AI methods;
4. Development of a software prototype, including a database, a module for extracting physicochemical characteristics of peptides and a module for predicting biological activity of peptides, using different methods of artificial intelligence;
5. Testing of the software prototype and analysis of the results of the conducted experiments

II. Summary of the PhD thesis

The dissertation consists of 175 pages. Its structure includes an introduction, four chapters, a conclusion, a declaration of originality of the results, publications on the subject of the dissertation, a list of noted citations, a bibliography and appendices.

In the introduction of the PhD thesis, the need for research on peptides that have a positive effect on human health is presented. The QSAR - Quantitative Structure Property Relationships method, which in the dissertation is based on the study of a sequence of amino acids, is one of the most used methods for studying quantitative structure-activity relationships. In view of this, this dissertation is aimed at predicting the biological activity of peptides by the QSAR method, using artificial intelligence (AI) methods. The goal of the dissertation work is formulated and the main tasks that will be followed in order to realize the goal are described. The strategy for the work of the conducted research is also presented.

In the **First chapter**, the nature and characteristics of peptides are described and a survey of current approaches and research is made to predict their properties using various AI methods. The classic algorithm for in silico prediction of biological activity of peptides is presented.

In the **Second chapter**, a conceptual model of a software application for analyzing the physicochemical properties and predicting the biological activity of peptides is presented.

The **Third chapter** presents a Pep Lab software application that implements the functionalities and processes described in the model.

In the last **Fourth chapter**, the results of the Pep Lab experiments are presented. These include generating various datasets and predicting the biological activity of peptides through several AI models.

In the conclusion, the results of the fulfillment of the tasks of the dissertation research are summarized. Future directions for continuing work on the topic are also discussed.

The list of used literature includes 150 titles, of which 20 are Internet sources.

Each chapter is a separate part of the PhD thesis that deals with the results obtained. The connection between the chapters is provided by the logic of the exposition and allows to gain an overall idea of the scientific research.

The cited sources are sufficiently diverse and present the scientific research on the subject in sufficient detail.

The language rules and the scientific style of writing research papers are observed. The text of the dissertation is clear and analytical.

III. Evaluation of the PhD thesis's contributions

The results of the dissertation work, requested by the PhD student, are seven and are divided into three directions: scientific, scientific-applied and applied. The first group includes:

1. Developed models for predicting the biological activity of peptides - SVM, RF and artificial NN.
2. Developed a new ComStat feature selection method based on peptide statistics.

The second group includes three contributions as follows:

3. Developed a conceptual model of a software application for the analysis and prediction of peptide properties by various AI methods.
4. Implemented algorithms for dynamic calculation of peptide characteristics and peptide coding.
5. Implemented artificial intelligence algorithms for predicting the biological activity of peptides based on SVM, RF and artificial NNs.

The contributions from third group are defined as:

6. A peptide database was created and information was entered on 2775 peptides with known biological activities.
7. A software application was developed for the analysis and prediction of the physicochemical properties of peptides, which is freely available on the Internet at www.pep-lab.info.

I accept the obtained results and contributions, as well as their division by the author.

IV. Assessment of the submitted publications

In the presented list of publications on the dissertation work of Zhelazko Terziyski included five publications, of which:

- one with IF=2.7, Q2, referenced in Scopus and WoS;
- one referenced in Scopus;
- two journal publications and
- one in a collection of scholarly works.

Four of the publications are in English and one in Bulgarian. The main results of the research were reported at two international and one national conferences, as well as at three research seminars.

A good impression is made by the author's desire to pass on his knowledge to university students. A textbook "Introduction to Databases" was published in coauthorship with other colleagues.

All publications are original and I am not aware of plagiarism. The qualities of the presented papers have been proven by being published in papers at national and international conferences and in scientific journals. The data thus presented give me reason to conclude that the research presented in the dissertation has been provided with the necessary publicity among the scientific community. Proof of this is also the independent citations in scientific works in the field under consideration, indicated in the PhD thesis.

V. Evaluation of the PhD abstract

The abstract has a volume of 32 pages. It faithfully reflects the essence and content of the dissertation work, including the purpose, subject, object and tasks of the dissertation research and the ways of their realization.

VI. Remarks and recommendations

I have not critical notes. To improve the quality of the dissertation and considering future research on the topic, I have the following notes and recommendations, which do not reduce the quality of the conducted research:

- There are some stylistic inaccuracies in the text, as well as some technical errors.
- Given the quality of the scientific research and the results obtained, I recommend that the doctoral student direct his efforts to self-publishing in refereed scientific publications.

VII. Conclusion

I accept that the requirements of the Development of Academic Staff Act in the Republic of Bulgaria and the specific requirements in the Act's Institutional Regulations for its implementation, the Rules for the conditions and the order for acquiring academic degrees and the Rules for the specific conditions for acquisition of academic degrees and occupation of academic positions at the Plovdiv University "Paisii Hilendarski" are accomplished. After my introduction to the PhD thesis and its publications, an analysis

of their significance and the contributions they make, I give my positive assessment and I recommend to the Honorable Jury to award the educational and scientific degree “Doctor of Philosophy” (PhD) to **Zhelyazko Petrov Terziyski** in the Scientific Field **4. Natural Sciences, Mathematics and Informatics**, the Professional Area **4.6. Informatics and Computer Sciences**, the Scientific Specialty. **Informatics**.

15.02.2024

Signature:

Plovdiv

/prof. Todorka Glushkova, PhD/