STATEMENT

By Assoc. Prof. Silvia Nikolaeva Gaftandzhieva, PhD

University of Plovdiv "Paisii Hilendarski"

of a dissertation for awarding the educational and scientific degree "Doctor"

in field of higher education 4. Natural sciences, mathematics and informatics

professional field 4.6. Informatics and Computer Science

doctoral program "Informatics"

Author: Zhelyazko Petrov Terziyski

Topic: "Using techniques from artificial intelligence to analyse and predict the properties of peptides"

Scientific supervisor: Assoc. Prof. Stanka Ivanova Hadzhikoleva, PhD – University of Plovdiv "Paisii Hilendarski"

1. General presentation of the procedure and the PhD student

By order No. P21-237/29.01.2024 of the Rector of the University of Plovdiv "Paisii Hilendarski" (PU) I have been appointed as a member of the scientific jury to ensure a procedure for the defence of dissertation work on the topic "Using techniques from artificial intelligence to analysis and predict the properties of peptides" for the acquisition of the educational and scientific degree "Doctor" in the field of higher education 4. Natural sciences, mathematics and informatics, professional field 4.6. Informatics and Computer Science, Doctoral Program "Informatics". The author of the dissertation is Zhelyazko Petrov Terziyski - a full-time PhD student at the Department of Computer Informatics, supervised by Prof. Dr. Stanka Hadjikoleva from PU.

The set of materials presented by Zhelyazko Terziyski is under Article 36 (1) of the Regulations for the Development of the Academic Staff of the PU and includes the following documents:

– a request to the Rector of the PU to disclose the procedure for the defence of a dissertation work;

– curriculum vitae in European format;

– protocol from the departmental council for the opening of the procedure and with a preliminary discussion of the dissertation work;

– abstract;

– declaration of originality and authenticity of the attached documents;

– certificate of compliance with the minimum national requirements;

– list of publications;

– dissertation work;

– copies of the publications on the topic of the dissertation work;
– a document for the fee paid, according to the Tariff.

The PhD student has attached five publications.

In 1998, doctoral student Zhelyazko Terziyski obtained a Master's degree at Technical University - Sofia, Plovdiv branch. In 2019, he was enrolled as a full-time doctoral student at the "Computer Informatics" department at the FMI of the "Paisii Hilendarski" PU.

After obtaining the master's degree, he worked as the head of the "Development" department at "VITTEL Engineering" JSC (1998-2000) and "Bulsis" OOD (2000-2002). During 2002-2012, Zhelyazko Terziyski was the manager of the company "BG Factor" Ltd., engaged in web application design, development and maintenance. Zhelyazko Terziyski also has work experience as head of a department at "Engineering" EAD (2012-2021) and technical manager at "Electrolux Tabakov & Sons" OOD (2021-2022). From 2022, he works as an assistant at Thrace University.

During his training as a PhD student, Zhelyazko Terziyski conducted exercises at the Faculty of Mathematics and Informatics of PU.

2. Relevance of the topic

The topic of the dissertation work is interdisciplinary (Informatics and Biotechnology). It is related to the design, development and testing of a software application for predicting biological properties of peptides using artificial intelligence methods. Peptides are the basis of many foods and beverages, nutritional supplements, peptide medicines and cosmetic products. The study of their properties (depending on their structure), with a positive impact on human health, is of interest to medicine and people's aspiration for a natural and healthy lifestyle. The freely available data sets on the biological activity of peptides have some disadvantages, including conflicting information, duplicated information, insufficient information on the physicochemical properties of peptides, and lack of possibilities for information extraction and presentation of the result in a graphical form. These shortcomings also make it difficult to predict the biological activity of peptides. Developing software tools with an intuitive and user-friendly interface to work with a reliable database and tools for peptide prediction and analysis is of interest to biotechnologists. The current dissertation work is an attempt in this direction.

I find the topic of the dissertation completely up-to-date. I believe that the formulated tasks allow the primary goal of the research to be achieved.

3. Knowledge of the research problem

For his research, Zhelyazko Terziyski studied 150 references, of which 20 were internet sources. The bibliographic reference led me to conclude that the PhD student has thoroughly familiarized herself with the state of research on the problem considered in the dissertation work.

4. Research methodology

The chosen research methodology is standard for a dissertation in Informatics. Based on the results of a study on the essence of peptides and the possibilities of using artificial intelligence to predict the properties of peptides, the PhD student proposed a model and developed a prototype of a software application for the analysis and prediction of the properties of peptides using artificial intelligence techniques. Then, he tested the implemented SVM, RF and FFNN models on four datasets.

The research methodology allows him to achieve the set goal and fulfil the tasks solved in the dissertation work.

5. Characterization and evaluation of the dissertation work and contributions

The main text of the dissertation (189 pages in total) includes an Introduction, 4 Chapters, a Conclusion and 3 Appendices (13 pages), which complement the main statement with a description of the database of the application, statistical information on the characteristics of the peptides in the database, source data from calculation of physicochemical characteristics of a peptide. The provided lists of the abbreviations, tables and figures, and references contribute to the clarity of the exposition.

In the Introduction, the PhD student introduces the topic of the researched area and sets the main goals and objectives of the dissertation research.

In Chapter 1, he describes the nature and characteristics of peptides and presents the results of a survey of modern approaches and research for predicting their properties using artificial intelligence methods. He describes the four stages of classical algorithm for predicting the biological activity of peptides in detail. The study of available databases and datasets for the biological activity of peptides allows the PhD student to identify their shortcomings.

Chapter 2 presents the conceptual model of a software application for physicochemical properties analysis and predicting the biological activity of peptides based on the QSAR model.

Based on the conceptual model described in Chapter 2, the PhD student presents the developed Pep Lab software prototype, freely available at www.pep-lab.info. In Chapter 3, he describes the designed peptide database with information about 2775 peptides with known biological activities.

In Chapter 4, the PhD student presents results from Pep Lab experiments and proposes a feature selection method called ComStat.

The Conclusion summarizes the results of Tasks 1 - 5 and formulates the scientific, scientific-applied and applied contributions of the dissertation work and perspectives for future work in the field. The main scientific contributions of the dissertation research are the developed models for using the SVM, RF and artificial NM methods for predicting the biological activity of peptides and the ComStat feature selection method based on peptide statistical indicators. Scientific-applied contributions of the research are the developed conceptual model of a software application for analysis and prediction of peptide properties using artificial intelligence methods, the implementation of algorithms for dynamic calculation of peptide characteristics and coding of peptides and algorithms

for prediction of biological activity of peptides, based on SVM, RF and artificial NM. As applied contributions of the dissertation work, the created peptide database with entered information on 2775 peptides with known biological activities and the developed software application for analysis and prediction of the physicochemical properties of peptides can be defined.

6. Evaluation of the publications and personal contribution of the PhD student

The results obtained in the dissertation have been presented to a sufficient extent to a specialized scientific audience, and the main ones are reflected in the publications of the PhD student.

The results are presented in 5 publications - 3 in journals and 2 in Conference proceedings. Four of the publications are in English and 1 in Bulgarian. The fact that 2 of the publications are in journals indexed in the world-famous databases SCOPUS and(or) Web of Science makes a good impression. The publication indexed in Web of Science has an impact factor (Q2, IF=2.7). The minimum national requirements for acquiring the ONS "doctor" in PN 4.6 have been exceeded - 128 points against a minimum requirement of 80 points.

There are 4 citations of 3 publications on the topic of the dissertation work by 9.02.2024, which is proof of the relevance of the topic of the dissertation research and the significance of the achieved results.

I do not doubt the personal contribution of the PhD student in the attached publications.

7. Abstract

The abstract, written in Bulgarian and English, is made according to the current requirements and adequately reflects the content, main results and contributions of the dissertation work.

8. Recommendations for future use of dissertation contributions and results

I have no significant critical comments on the layout of the dissertation. In places, the text of the dissertation needs refinement.

The results obtained have the potential to be disseminated and multiplied. In this regard, I fully share the prospects for the development of the subject, as noted by the PhD student. I recommend the PhD student to continue research in the field and participate more actively in international conferences that would allow a wider international scientific community to evaluate the achieved results.

CONCLUSION

The dissertation contains scientific, scientific-applied and applied results, which represent an original contribution to science and meet the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria (ZRASRB), the Regulations for the Implementation of ZRASRB and the relevant Regulations of PU.

The dissertation work shows that the PhD student Zhelyazko Terziyski possesses in-depth theoretical knowledge and professional skills in the scientific speciality "Informatics", demonstrating qualities and skills for independent conduct of scientific research.

Due to the above, I confidently give my positive assessment of the conducted research, presented by the above-reviewed dissertation work, abstract achieved results and contributions, and I propose to the honourable scientific jury to award the educational and scientific degree "Doctor" to Zhelyazko Petrov Terziyski in the field of higher education: 4. Natural sciences, mathematics and informatics, professional field 4.6. Informatics and Computer Science, Doctoral Program "Informatics".

9.02.2024 г.   **Reviewer**: ....

Assoc. Prof. Silvia Gaftandzhieva, PhD