REVIEW

by Prof. Dr. Georgi Petrov Dimitrov
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dissertation for the award of the educational and scientific degree **"PhD"**

by field of higher education 4. Natural Sciences, Mathematics and Informatics,

professional field 4.6 Informatics and Computer Science,

Doctoral Program Informatics

Author.

Thread: " **Using Artificial Intelligence Techniques to Analyze and Predict Peptide Properties** "

Scientific supervisor: Assoc. Prof. Dr. Stanka Hadjikoleva , Paisii Hilendarski University - Faculty of Medical Sciences

1. General description of the submitted materials

By the order of the Rector of Plovdiv University "Paisii Hilendarski" (PU) RD-21-237 from 29.01.2024 I am appointed as a member of the scientific jury for the procedure for the defense of the dissertation on "The use of artificial intelligence techniques for the analysis and prediction of peptide properties" 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 programme Informatics. The author of the dissertation is **Zhelyazko Petrov Terziyskiy** - PhD student in full-time study at the Department of Computer Informatics with scientific supervisor Assoc. Prof. Dr. Stanka Hadjikoleva from Paisii Hilendarski University - FMI.

The set of paper materials submitted by **Zhelyazko Petrov Terziyski** is in accordance with Article 36 (1) of the Regulations for the Development of the Academic Staff of PU and includes the following documents:
  – a request to the Rector of PU for disclosure of the dissertation defense procedure;
  – CV in European format;

- Minutes of the Departmental Council relating to the reporting of readiness for the opening of the procedure and to the preliminary discussion of the thesis;
- Dissertation;
- Author's abstract;
- list of scientific publications on the topic of the dissertation;
- copies of scientific publications;
- a declaration of originality and authenticity of the attached documents;
- a reference for compliance with the National Minimum Requirements for the Acquisition of a Doctoral Degree in 4. 4.6. Informatics and Computer Science;
- et al.
- The PhD student has attached 5 publications.

2. Brief biographical data about the PhD student

The PhD student **Zhelyazko Petrov Terziyski graduated from the** Master's degree in Computer Science at the Technical University - Sofia, Branch Plovdiv in 1998.

Since his graduation he has worked in various positions, from 2022 until now he is an assistant professor at the University of Thrace.

Possesses diverse skills and competencies in the field of information technology.

3. Relevance of the subject matter and appropriateness of the set goals and objectives

The dissertation work is undoubtedly devoted to a topical issue, namely **to design, develop and approbate a software system for predicting the biological properties of peptides using various artificial intelligence methods.**

To achieve the main objective, the following tasks are set:

Task 1. Investigate the nature of peptides, current research and scientific advances for using artificial intelligence methods to predict their biological activity;

Task 2. Investigate publicly available peptide encoding databases and tools and create a database of known peptides and their biological activity;

Task 3. Create a conceptual model of a software application for analysis and prediction of peptide properties by different AI methods;

Task 4. Development of a software prototype including a database, a module for extraction of physicochemical characteristics of peptides and a module for prediction of biological activity of peptides using different artificial intelligence methods;

Task 5. Testing the software prototype and analyzing the results of the experiments.

I believe that the aims and objectives defined by the PhD student, as well as the subsequent development of the thesis, are undoubtedly relevant and of a high level of applicability.

4. Knowledge of the problem

In the presented work there are a considerable number of cited sources - 150 in total, including 19 Internet sources.

The list of author publications on the topic consists of 5 titles.

All of this to me is a testament to the thorough research done by the Ph.

5. Research methodology

The results presented in this dissertation attest to the choice of a methodologically sound approach to solving the research problems. Design, implementation, testing and technical documentation have been carried out to realize the research.

6. Characteristics and evaluation of the thesis

The submitted dissertation consists of an introduction, four chapters and a conclusion, a list of references used, appendices, a list of author's publications on the topic, appendices and a declaration of originality.

In **Chapter 1, a** survey of state-of-the-art approaches and studies to predict peptide properties using different AI methods is presented. The classical algorithm for in silico prediction of their biological activity is presented.

Chapter 2 presents a conceptual model of a software application for analysing the physicochemical properties and predicting the biological activity of peptides.

Chapter 3 describes the Pep Lab software application. It implements the functionalities and processes described in the model.

Chapter 4 presents the results of the experiments conducted with Pep Lab. These include different datasets generated and the prediction of the biological activity of peptides by several AI models.

The **conclusion** summarizes the results of the tasks. Scientific, scientific and applied contributions, the result of the dissertation research, as well as directions for future development are described.

7. Contributions and Significance of the Development for Science and Practice

I accept the following contributions as formulated:

Scientific contributions of the dissertation research:

- Developed models to predict the biological activity of peptides - SVM, RF and artificial NM.

- Developed a new ComStat feature selection method based on peptide statistics.

Scientific and applied contributions of the dissertation research:

- Developed a conceptual model of a software application to analyze and predict peptide properties using various AI methods.

- Implemented algorithms for dynamic peptide feature computation and peptide encoding.

- Implemented artificial intelligence algorithms to predict the biological activity of SVM, RF and artificial NM based peptides.

Applied contributions of the dissertation research:

- A peptide database was created and information on 2775 peptides with known biological activities was entered.

- A software application has been developed for the analysis and prediction of the physicochemical properties of peptides. It is freely available at: www.pep-lab.info.

8. Assessment of the publications on the dissertation

Results of the dissertation research are presented in 5 (five) publications Two of them are indexed in the international databases Scopus and Web of Science, and 1 is published in a journal with impact factor.

There are 2 citations on the posts.

9. Personal participation of the PhD student

After reading the materials presented by the PhD student, I have the impression that the results presented in the thesis are his personal work, of course under the supervision of the supervisor. The

achieved scientific and applied results were obtained in the fulfilment of the set tasks following the scientific supervision and are the personal work of the PhD student.

10. Abstract

The abstract contains 32 pages and presents in detail the relevance and motivation for working on the chosen topic, as well as the content of the thesis by chapter.

11. Critical comments and recommendations

From the submitted reference, I am left with the impression of the candidate's research interests and pursuits in a variety of topics.

Technically, the dissertation is well designed. The study is sufficiently voluminous and covers important aspects of the given problematic.

12. Personal impressions

I do not personally know the PhD student **Zhelyazko Petrov Terziiski**, but from the presented materials I am convinced that she is an excellently prepared and highly competent specialist, a successful participant in scientific research projects and a professional with experience in the field of information technology.

13. Recommendations for future use of the dissertation contributions and results

I recommend publishing the results of the dissertation research in other journals with impact factor, because in his further work the PhD student will certainly need more citations of the published results.

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CONCLUSION

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The dissertation *contains scientific, scientific and applied results that represent an original contribution to science* and **meet all the** requirements of the Law for the Development of Academic Staff in the Republic of Bulgaria (LADAPB), the Regulations for the Implementation of the LADAPB and the relevant Regulations of Paisii Hilendarski University. The submitted materials and dissertation results fully comply with the specific requirements of the Faculty of Mathematics and Informatics, adopted in conjunction with the Regulations of PU for the application of the Law on Mathematics and Informatics.

The dissertation shows that the PhD student **Zhelyazko Petrov Terziyski** possesses in-depth theoretical knowledge and professional skills in the scientific specialty of Informatics and Computer Science, demonstrating qualities and skills for independent scientific research.

Due to the above, I confidently give my ***positive assessment of*** the research conducted, presented by the above reviewed dissertation, abstract, results and contributions, and ***propose the Honorable Scientific Jury to award the degree of Doctor of Education and Science*** to **Zhelyazko Petrov Terziiski** in the field of higher education 4. Natural Sciences, Mathematics and Informatics, professional field 4.6 Informatics and Computer Science, doctoral programme Informatics.

19.02.2024 г.

Reviewer: ....

Prof. Dr. Georgi Dimitrov

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