OPINION

by assoc. prof. Dasha Spasova Mihaylova – University of Food Technologies, Plovdiv

on dissertation for the award of the educational and scientific degree "Doctor"

in the area of higher education 4. Natural Sciences, Mathematics and Informatics, professional field 4.6. Informatics and Computer Science, Doctoral Programme “Informatics”

Author: Zhelyazko Petrov Terziyski
Title: "Using techniques from artificial intelligence to analyze and predict the properties of peptides"
Scientific supervisors: assoc. prof. Stanka Hadzhikoleva, PhD

1. General description of the procedure and the presented materials

By order No РД-21-237 от 29.01.2024 of the Rector of Plovdiv University "Paisiy Hilendarski", I have been appointed as a member of the scientific jury to ensure a procedure for the defence of a dissertation work on the topic "Using artificial intelligence techniques for the analysis and prediction of 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 Eng. Zhelyazko Petrov Terziyski - PhD student in full-time study at the "Computer Informatics" department with scientific supervisor Assoc. Prof. Stanka Ivanova Hadjikoleva, PhD.

The set of paper materials submitted by the doctoral student is in accordance with 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;

– minutes from the department council related to reporting the readiness to open the procedure and preliminary discussion of the dissertation work;

– dissertation work;

– abstract;

– a list of scientific publications on the subject of the dissertation;

– copies of scientific publications;

- declaration of originality and authenticity of the attached documents;

The doctoral student has attached 5 publications, in 1 of which he is the sole author, and in 2 of them, he is the first author. Two of the articles presented for the acquisition of the educational and scientific degree "Doctor" are indexed in international databases (Scopus and Web of Science), and 1 was published in a journal with IF (Applied Sciences, IF_{2022} - 2.7).

2. Relevance of the topic

Peptides are substances with a wide range of biological properties affecting the human body, which is why they are used both in the treatment of diseases and as food supplements or cosmetics. This is due to their biological activity, according to which the peptides are anti-cancer, anti-microbial, blood pressure-normalizing, antioxidant, anti-diabetic, etc.

It is known that the properties of peptides depend directly on their structure. Therefore, their forecasting also determines the relevance of the topic of the dissertation both in a scientific, but also in a scientific-applied sense. The main goal of designing, developing and testing a software system for predicting the biological properties of peptides using various artificial intelligence methods relates to the successful solution of an important problem facing modern man. Namely, with the help of artificial intelligence, to ease the work of laboratory researchers and shorten the time for analysis. The application of the QSAR method, with the help of artificial intelligence (AI) methods to successfully predict biological activity in this regard, is relevant.

3. Knowing the problem

The bibliography includes 150 titles of articles and books and 20 Internet sources, from which it can be concluded that the doctoral student has studied the state of research in the field under consideration. The literature reference shows that Zh. Terziyski has thoroughly approached the topic and expressed his critical remarks and offered a possible approach to overcome them, which follows the formulated goals and tasks of the dissertation work.

4. Research methodology

The research methodology used by the doctoral student is appropriately chosen and allows the achievement of the set goal and the fulfilment of the formulated tasks. Proof of this is the results achieved during the implementation of the research.

5. Characterization and evaluation of the dissertation work and contributions

The dissertation submitted to me for review consists of 189 pages, containing - an introduction, four chapters, a conclusion and appendices. The literature used includes 150 titles of articles and books and 20 Internet sources, from which it can be concluded that the doctoral student has studied the state of research in the field under consideration. In the introductory

part, the topicality of the problem, subject, goal, tasks, hypothesis and the structure of the dissertation work are presented. According to the requirements, a Declaration of originality of the obtained results and contributions was attached to the dissertation.

The individual chapters of the dissertation are developed in detail and systematically and present the author's solutions to the set tasks. Overall, the dissertation reflects the author's in-depth research work and convincingly presents the obtained results. It makes a good impression that each of the four chapters of the dissertation ends with conclusions.

I accept and positively evaluate the results noted in the dissertation and the author's reference. They can be defined as scientific, scientific-applied and only applied contributions as follows:

- Scientific contributions:

1.) Models for predicting the biological activity of peptides have been developed - SVM, RF and artificial NM.

2). A new ComStat feature selection method based on peptide statistics was developed.

- Scientific and applied contributions:

3.) A conceptual model of a software application for the analysis and prediction of peptide properties by various AI methods was developed.

4.) Algorithms for dynamic calculation of peptide features and peptide coding are implemented.

5.) Implemented artificial intelligence algorithms for predicting the biological activity of peptides based on SVM, RF and artificial NMs.

- Applied Contributions:

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. It is freely available at: www.pep-lab.info.

It is commendable that the publications related to the dissertation work are cited in the scientific community despite the short period since their availability.

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

The doctoral student has attached 5 publications to the set of documents. In 1 of them, he is the sole author, and in 2 of them he is the first author, which suggests the main contribution of Zh. Terziyski in them. Two of the articles submitted for the acquisition of the educational and scientific degree “Doctor” are indexed in international databases (Scopus and WoS), and 1 was published in an edition with IF (Applied Sciences, IF2022 – 2.7). In this way, they are

available to the general public and this is also indicative of the scientific community's high appreciation of the conducted studies.

The publications are entirely on the subject of the dissertation and reflect the conducted experiments. With the publications submitted by the doctoral student to the dissertation work, the minimum national requirements for acquiring the educational and scientific degree "doctor" in 4.6 have been met. Informatics and Computer Science.

7. Abstract

The abstract has a volume of 32 pages and sufficiently reflects the content of the dissertation work and the obtained results of the study, which is in accordance with the requirements of the relevant regulations.

8. Recommendations for future use of dissertation contributions and results

The prepared documents are according to the requirements and meet the legal requirements.

I have no significant critical remarks and recommendations for the doctoral student. I recommend the same purposefulness in his future scientific work.

CONCLUSION

The dissertation contains scientific, scientific-applied and applied results, which represent an original contribution to science and meet all 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 "Paisiy Hilendarski".

The dissertation work shows that the doctoral student, Eng. Zhelyazko Terziyski, has in-depth theoretical knowledge and professional skills in professional field 4.6. Informatics and computer sciences, doctoral program "Informatics" by 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 Honorable Scientific Jury to grant the educational and scientific degree "Doctor" to Eng. Zhelyazko Petrov Terziyski in the field of higher education: 4. Natural sciences, mathematics and informatics, professional direction 4.6. Informatics and Computer Science, Doctoral Program "Informatics".

14.02.2024 г. **Signature**: .....

assoc. prof. Dasha Mihaylova, PhD