STATEMENT

by Prof. Vesselin Petrov Baev,
from the Department of Molecular Biology,
Faculty of Biology, University of Plovdiv
regarding materials submitted for the defense of a dissertation
for awarding the academic degree Doctor of philosophy “PhD”

Field of Higher Education: 4. Natural Sciences, Mathematics and Informatics
Professional Field: 4.2. Chemical Sciences
PhD Program: Theoretical Chemistry
PhD Student: GERGANA ILIEVA TANCHEVA
Title: "Application of Chemical Informatics Methods to Multicomponent Substances and Nanomaterials"
PhD Supervisor: Assoc. Prof. Dr. Nikolay Kochev
Rector's Order for determining the Scientific Jury composition: RD-21-1840/23.10.2024

The materials related to the defense of the aspirant Gergana Tancheva for awarding the academic degree PhD were presented to me in electronic format.

The set of materials presented by Gergana Tancheva in electronic format complies with Article 36 (1) of the Regulations for the Development of the Academic Staff at Plovdiv University "Paisii Hilendarski". The documents include:

1) Application to the Rector of Plovdiv University for initiating a defense procedure and awarding the educational and scientific degree PhD;
2) Curriculum vitae in the required format;
3) Protocol from the Department Council for preliminary discussion of the dissertation and opinion of the PhD supervisor about the doctoral student;
4) Abstract of the dissertation in Bulgarian and English;
5) Declaration of originality;
6) Reference for minimum requirements;
7) List of publications;
8) Dissertation thesis in Bulgarian;
9) Full-text publications.

Biographical Data

In 2016, Gergana Tancheva completed her bachelor's degree in "Medical Chemistry" at the Faculty of Chemistry of Plovdiv University. A year later, she obtained a master's degree in "Spectrochemical Analysis" at the same institution. Since 2019, she has been a PhD student in the Department of "Analytical Chemistry and Computer Chemistry" at the same university. It should be noted that simultaneously, Gergana Tancheva has worked as a laboratory specialist at Sofia Water Supply and Sewerage (2017-2018), as a specialist in food and environmental analysis and control at "Eurofins HOS Testing Bulgaria" EOOD (2018-2022), and as a chemist-informatician at "Ideaconsult" Ltd. (2022-present).

Relevance and Significance of the Topic

The dissertation topic is extremely relevant as it involves work in the interdisciplinary field of "Chemical Informatics" or "Chemoinformatics" and its applications in the developing production of multicomponent substances. The dissertation's main objective is to explore the possibilities of chemoinformatics for processing and storing data on multicomponent substances, nanomaterials, and new materials, and discovering prospects for effective information processing through semantic FAIR analysis. I believe that the research objective is well-defined, significant, and relevant.

Dissertation Thesis

The presented dissertation thesis is 196 pages long and is divided into four sections: 1) Literature Review; 2) Aim and Objectives of the Dissertation; 3) Results Achieved on the Dissertation Tasks; and 4) Summary of the Dissertation.*It is notable that the dissertation thesis does not have a clearly defined "Materials and Methods" section, and the main sources of materials and methods used are scattered throughout the literature review and results.*

Research Methodology

The semantic data model of Ambit/eNanoMapper was selected and used to represent information about multicomponent substances and nanomaterials, through which the FAIR principles for the presented chemical objects were implemented. A platform for FAIR-ification of chemical object data was used, as well as external tools such as Jupyter notebooks, machine learning and data analysis platforms like KNIME and Orange, workflows in the Ploomber platform, etc. I believe that the methods and materials are well-chosen for the purpose and tasks of the dissertation.

Results and Contributions of the Dissertation

The dissertation presents a development/concept for FAIR-ification of experimental nanomaterial data based on the Ambit/eNanoMapper data model. A prototype for nanomaterial identifier has been created, demonstrating the capabilities of SLN linear notation. The eNanoMapper database and ontology have been enriched with high-quality FAIR data, including safety information on nanomaterials from several major European projects. A software library and module for the Orange platform - ToxFAIRy, has been developed for annotation and processing of HTS data.

Publications, Participation in Scientific Forums and Training Courses

The results of the dissertation have been published in 2 scientific articles in the following high-quartile journals: Nanomaterials (Q1), Mol. Informatics (Q2), and in one book chapter "Data Integrity and Data Governance". The Scopus database shows that both articles have been cited, one of which has accumulated a large number of citations - 17 (Nanomaterials), demonstrating high recognition of the topic and achieved results.

In addition to scientific publications, doctoral student Gergana Tancheva has actively participated in various national and international forums with 9 posters and 3 presentations. Additionally, the

doctoral student's participation in 5 projects, as well as numerous training courses enhancing the candidate's skills in Python programming language and QSAR.

Abstract

An abstract has been presented in Bulgarian (32 pages) and English (30 pages), prepared according to requirements and reflecting the main results of the dissertation.

Conclusion

The materials presented in this procedure **meet the requirements** of the Law on the Development of Academic Staff in the Republic of Bulgaria and the minimum national requirements. The dissertation shows that the doctoral student Gergana Tancheva possesses in-depth knowledge, professional skills, and significant results in the field of Chemical Informatics. In this regard, I give my **positive vote** for awarding the academic degree PhD to Gergana Ilieva Tancheva in the field of higher education: 4. Natural Sciences, Mathematics and Informatics; professional field: 4.2. Chemical Sciences; scientific area: Theoretical Chemistry.

December 17, 2024
Plovdiv

Statement prepared by:

Prof. Dr. Vesselin Baev