

STATEMENT

by prof. Vassil Borissov Delchev, DSc,
from the Department of Physical chemistry, University of Plovdiv
on the materials for the defence of a doctoral thesis
for the awarding of the academic degree *Doctor of philosophy* (PhD)
in the Department of Analytical Chemistry and Computer Chemistry,
Chemical Faculty – University of Plovdiv

Field of higher education: 4: Natural sciences, mathematics and informatics
Professional area: 4.2. Chemical sciences
Scientific field: Theoretical chemistry

PhD student: Gergana Ilieva Tancheva

Title of the doctoral thesis: „Application of chemoinformatics methods to multicomponent substances and nanomaterials”

Scientific supervisor: Assoc. Prof. Nikolay Kochev, PhD

Rector's order for the constitution of the Scientific jury: **ПД-21-1840/24.10.2024 г.**

Decision of the first meeting of the Scientific jury: **to write an academic statement.**

All materials for the defence of the doctoral thesis for the awarding of the academic degree *Doctor of philosophy* of Gergana Tancheva are presented in digital form on an internet-platform and they involve: 1) an official request to the Rector of the University of Plovdiv for start of the procedure for awarding of the academic degree *Doctor of philosophy* (PhD); 2) a standard *Curriculum Vitae*; 3) a protocol from the department council for the discussion of the thesis; 4) a statement of the scientific advisor; 5) an abstract of the PhD thesis in Bulgarian and English; 6) a list of publications; 7) a PhD thesis in Bulgarian; 8) an information for compliance with the Minimum national requirements for the PhD degree.

Biographic information

Dr. Gergana Tancheva graduated from Plovdiv University's "Medical Chemistry" bachelor's degree in 2016. In the same year, she resumed her studies in the master's program "Spectrochemical Analysis" at the University of Plovdiv, Department Analytical Chemistry and Computer Chemistry, which she completed successfully in 2017. Following that, she worked as a probationer at the Institute of Organic Chemistry with a Phytochemistry Center (BAS - Sofia), where she works on the characterization of the composition of rose oils using various analytical techniques. From 2017 to 2018 she worked as a laboratory specialist at "Sofiiska Voda", unit Drinking Water, where she analyzed drinking water for heavy metals. From 2018 to 2022 Gergana Tancheva works as an analytical chemist at "Eurofins HOS Testing Bulgaria" Ltd, Sofia. From 2022 until today, she has worked as a developer at „Ideaconsult” Ltd in Sofia, where software for automatic processing of in vitro data is developed. Gergana Tancheva has been a PhD student at Plovdiv University in the Department of Analytical and Computer Chemistry since 2019. Her research is focused on developing and evaluating methods for modeling physicochemical properties and biological activity, such as QSPR/QSAR.

Importance of the theme

The dissertation provides novel and significant conclusions for current science that are presented for the first time. A wide range of research activities have been conducted and described in the dissertation. Some modules of eNanoMapper with plugins and filters have been improved. Semantic models of Ambit/eNanoMapper have been tested for FAIR-ifying of data for multicomponent substances and nanomaterials. In this number, a software has been developed

for conversation of EXCEL data files . A software library, an in vitro data template, Orange modules, and much more have been developed either.

Dissertation

The dissertation is written on 196 pages and is structured in seven chapters. An extensive literature evaluation is offered, which spans over 60 pages. In my opinion, it could be reduced a bit, particularly with regard to the legislative information given. The literature study includes descriptions of 189 sources, the majority of which are from recent years. Chapter II clearly defines the research aim and tasks of the research. The research of the PhD student is described in Chapters III and IV, which spans 80 pages. It should be mentioned that the appendix contains templates, files, and worksheets that supplement the research in the dissertation.

Major contributions of the PhD thesis

The reported results in the dissertation have scientific and practical contributions. The scientific contributions are: 1) the developed concept of FAIR-ification of experimental data on nanomaterials to represent information on multicomponent substances, by means of a semantic data model *Ambit/eNanoMapper* and by means of *NMDataParser*; 2) a prototype is created for identifier for nanomaterials by using the linear notation *SLN*; and 3) a concept was developed to annotate HTS data with metadata and calculation of a toxicological prioritization index using *Tox5-Score*.

The practical contributions can be summarized as follows: 1) it has been applied a FAIR-ification model for 1400 EXCEL files to enrich the *eNanoMapper* database for nanomaterial safety; 2) The ontology *eNanoMapper* has been enriched with new terms in the field of ecotoxicity; 3) It has been created a *ToxFAIRy* software library for data annotation and processing, prioritization index calculation, and FAIR-ification of HTS data. 4) An *Orange3-ToxFAIRy* module has been created for the *Orange* platform. 5) An automated work process has been processed on the *Ploomber* platform, comprising the possibilities of the *ToxFAIRy* library.

All this demonstrates the PhD student's advanced scientific expertise and competence to administer databases and linked libraries.

Publications included in the doctoral thesis and participation in conferences

The results from the PhD thesis are published in three journals with a deep impact in the research area of the PhD student and its scientific supervisor. According to the SJR the first paper (DOI: 10.3390/nano10101908) has a quartile Q1, the second one (DOI: 10.1002/minf.202100027) – quartile Q2, whereas the third one does not appear in the databases *Scopus* and *WoS*. Therefore, for indicator Γ the PhD candidate should be awarded with 51 points – the required minimum is 30 points. Obviously, the candidate exceeded the required minimum. The total number of citations on the paper with quartile Q1 is 17 (*Scopus*), and not 16 as pointed out in the dissertation thesis. The publication A2 is cited 1 time for now.

The participation of the PhD candidate in scientific forums is impressive! The results of the dissertation have been presented on 12 conferences. Nine of them are poster presentations and three oral presentations, all at international conferences held in online format. There are 4 international poster participations, and 5 of them are on scientific forums in Bulgaria.

PhD thesis summary

The abstract in Bulgarian spans 32 pages. It summarizes the dissertation's major points. Point 9.3 makes a favorable impact, as it gives instructions for the future development of the problems of the dissertation. In my opinion, the bibliography in the PhD summary could be

omitted. An abstract in English is also attached, in accordance with national and local criteria for awarding of academic degree *Doctor of Philosophy*.

CONCLUSION

The provided materials for the current procedure are in agreement with the Law for development of the academic staff in Republic of Bulgaria, the Rules for its application as well as with the minimal national requirements in the professional filed. I think that Gergana Tancheva is a complete scientist in the area of research and she can guide an independent research in the field of chemoinformatics. All this and the aforementioned facts drive me to give my **positive vote** for the awarding of the academic degree *Doctor of philosophy* (PhD) to Gergana Ilieva Tancheva in the field of higher education: 4: Natural sciences, mathematics and informatics; professional area 4.2. Chemical sciences; scientific field: Theoretical chemistry.

17.12.2024 г.
Plovdiv

Author: