REPORT

by

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Member of the Academic Jury set to render a decision on the competition for filling the academic position of Professor at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski" in the Professional Field 4.2. Chemical Sciences according to the Classifier of the Areas of Higher Education and the Professional Fields (Scientific Specialty " Organic Chemistry-Organic Synthesis ")

This Report is prepared in response to Order № РД 38-444/16.07.2019 issued by the Rector of Sofia University, following the decision made by the Academic Jury that was held on 12.09.2019.

The Report is in compliance with *Development of Academic Staff in the Republic of Bulgaria Act (DASRB)*, *the Rules for the Application of the Development of Academic Staff in the Republic of Bulgaria Act,* the *Rules of* Sofia University "St. Kliment Ohridski**"**, *for applying the Act aforementioned*.

General overview of the procedure and the applicant

The competition for filling the academic position of "Professor" in the Professional Field 4.2. Chemical Sciences (Organic Chemistry - Organic Synthesis) was announced in State Gazette, issue N:52 on 02. 07. 2019, for the needs of the Department of Organic Chemistry and Pharmacognosy, Faculty of Chemistry and Pharmacy, Sofia University"St. Kliment Ohridski".

Only one candidate participates in the competition – Rositca Dimitrova Nikolova, Ph.D., currently Associate Professor at the same department.

The set of documents presented by **Associate Professor Dr. Rositca Nikolova**, is in accordance with the Rules for the Development of the Academic Staff at Sofia University "St. Kliment Ohridski" and meets the requirements for occupying the academic position of "Professor".

1. **General characteristics of the applicant's activities**

- *Assessment of the scientific and research accomplishments of the candidate*

Associate Professor Dr. Rositca Nikolova has a total of 44 scientific papers, 34 of which are in Scopus, with 219 citations, 121 of which are in Scopus. She is a co-author of 5 textbooks as well.

In this competition she participates with a total of 22 scientific papers, 16 of which are publications in foreign scientific journals, 2 papers have been published in full text in proceedings of scientific conferences and 4 textbooks. She presented habilitation work for the competition.

Most of the publications are printed in scientific journals that are referenced and indexed in world-renowned scientific information databases, having impact factor, falling in quartiles from Q1 to Q4 according to the grouping of scientific journals.

Indicator A1. Dissertation for awarding the educational and scientific degree "doctor". The candidate Assoc. Prof. Dr. Rositca Nikolova successfully defended her dissertation on the topic

"Synthesis and chemical transormations of phosphorus-containing coumarin derivatives". (50 points).

The distribution of scientific papers according to the relevant Q factors is as follows:

Indicator group C.4 - Habilitation work, scientific publications in journals that have been referenced and indexed in world-renowned scientific information databases (Web of Science and Scopus)

With respect to this indicator, Assoc. Prof. R. Nikolova has presented 4 publications which are in Q1. In 3 of these publications she has been stated as a corresponding author, which proves her significant contribution in the presented research. The points gained by this group are 100 (the required amount is 100 points). Based on the above stated, we can conclude that the criterion is unconditionally met.

Indicator Group D (Indicator D.7) – Regarding this indicator, Assoc. Prof. R. Nikolova has submitted 12 publications that have been referenced and indexed in Web of Science and Scopus. All works are in the field of the current contest and have been published in specialized international journals. They are grouped as follows: 2 in Q1 ranked journal (*Physical Chemistry Chemical Physics -IF 3,567; J. Phys. Chem.-IF 2,836*), 7 in Q2 ranked journal (*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy IF 2,93; Synlet IF 2,41; J.Phys.Org.Chem. etc.),* 2 in Q3 ranked journal, 1 in Q4 ranked journal. The total amount of points obtained in this group is 232. In this case, the requirement is not only fulfilled but significantly exceeds the needed 200 points.

Indicator Group E

All the presented scientific papers are on meaningful topics and are at a high scientific level, which is proven by the number of citations. A total of 219 citations are observed, 79 of which were submitted in this competition, bringing 158 points in indicator E.11. The points obtained in this indicator clearly show the relevance and international importance of the studies conducted and reported. The above stated proves that Assoc. Prof. R. Nikolova significantly exceeds the requirements of DASRB. Her h-index is 9.

Indicator Group F

Assoc. Prof. R. Nikolova was the co-supervisor of a successfully defended PhD student in 2012 on the topic: "Synthesis, chemical transformations and quantum-chemical studies of coumarins and their phosphorus analogues" (25 points). In addition, she participated in the development of 9 national and 3 international scientific or educational projects (150 points) and was the leader of 2 national projects - 1 educational and 1 scientific one (60 points). The funds raised from these projects bring 44 points to the applicant.

Assoc. Prof. Nikolova co-authored 2 textbooks on "Chemistry and Environmental protection" and "Tests for current self-training and matriculation exam in chemistry and environmental protection" " used in the school network, as well as of the „Handbook for Laboratory Exercises with a Collection of problems in Organic Chemistry" for students in the specialty "Pharmacy". She is also a co-author of "Problems in Organic Chemistry".

The total amount of points obtained in this group is 282,6. In this case, the requirement is not only fulfilled but significantly exceeds the needed 150 points.

Moreover, Assoc. Prof. Nikolova has participated in 57 scientific forums with posters or oral presentations.

➢ ***Assessment of educational and pedagogical activity and training of the candidate (s) (study aids, lectures, work with students, graduates, and doctoral students)***

Associate Professor Dr. Rositsa Nikolova is an established university lecturer with great experience and prestige. She is the co-author of 5 published university and school textbooks.

- ✓ She has taught lectures, seminars and exercises for students - bachelors and masters in various specialties of the Faculty of Chemistry and Pharmacy and the Faculty of Biology at Sofia University "St. Cl. Ohridski ". Assoc. Prof. Nikolova is a lecturer in the basic courses in Organic Chemistry part I and II.
- ✓ She has developed 2 new courses on „Active ingredients in perfumery and cosmetics" for bachelor's degree students and on "Cosmetic products and care" for master's degree students in the specialty "Pharmacy", as well as a new course on "Organic materials in cosmetic products".
- ✓ She participated in the preparation of tests for State and passed exams. Since 2016 she has been the chairman of the examination committee for the State Examination for the Bachelor's Degrees of the Faculty of Chemistry and the passed exams for master's degree.
- ✓ She was the head of 1 successfully defended PhD student and 12 graduates.

Auditory employment in recent years has exceeded 400 hours.

➢ ***Contributions (scientific, applied science, applied)***

All scientific papers submitted in the competition are in the field of organic chemistry and organic synthesis. The scientific interests of Assoc. Prof. Nikolova are in the field of development of new methods for the synthesis of heterocyclic compounds - mainly coumarin derivatives and their phosphorus analogues. Application of modern spectral methods for their complete identification and characterization and study of the mechanisms of organic reactions by applying quantum-chemical calculations. Dr. R. Nikolova's research might be grouped in the following main areas:

- Synthetic research / Synthetic studies
- Quantum-chemical and structural investigations.

Synthetic studies have been described in 13 publications (publications with numbers: 1, 2, 3, 4, 7, 8, 9, 10, 13, 14, 15, 16, 17) and briefly include the following developments:

Synthetic methods for the preparation of dialkyl 2-oxo-2H-1-benzopyran-3-phosphonates and alkyl-1,2-benzoxaphosphorin-3-carboxylates have been developed and studied, due to the increased synthetic and pharmacological interest to this class of compounds. Coumarins are natural heterocyclic compounds that have various biological activities. The investigations are summarized in a review article (publication 1).

The reactions of the diethyl ester of 2-oxo-2H-1-benzopyran-3-phosphonic acid with nitromethane have been studied in detail under different reaction conditions. The number of relations has been established. It was found that in the presence of nucleophilic agents, opening of the lacton ring in the product a 1,4-addition reaction is favored. A probable mechanism for the formation of a new pyrrolidine ring is proposed.

A new, effective method for the synthesis of 3,4-disubstituted pyrrolidine-2,5-dione from 3-substituted coumarins has been developed. With the help of Quantum-chemical studies of all stages of one-pot synthesis of the pirrolidinedione derivatives, the most advantageous reaction pathway

has been established, including Michael addition, migration of an oxygen atom and cyclization to a pyrrolidine ring.

The reaction of 3-phosphonocoumarin with organometallic compounds on heating and ultrasound irradiation was studied. Based on the obtained results, the mechanism of dimerization reaction was suggested.

Two new types of β-ketophosphonates and propionic acids were obtained by decarboxylation of β-ketochromanes. It was found that processes of decarboxylation of diethyl 3-acyl-2-oxochroman-3-ylphosphonates could be facilitated under reflux in water in the presence or absence of acid catalysis.

Salts and complexes of 3-substituted coumarins and 1,10-phenanthroline were also obtained. The structure of all the synthesized compounds was correctly determined using modern spectral methods. X-ray structural analysis was also used. The obtained results have been interpreted and described competently.

Quantum-chemical and structural studies have been described in publications with numbers: 5, 6, 11, 12 and 18.

Methods such as X-ray photoelectron spectroscopy and time-resolved fluorescence spectroscopy have been used. The experimentally obtained results have been compared with the theoretically calculated values as well as quantum-chemical simulations. X-ray diffraction and conventional and linearly polarized IR spectroscopy have been used for structural studies of compounds of interest to Assoc. Prof. Nikolova.

3. Critical comments and recommendations

I have no comments or recommendations for the applicant. Dr. R. Nikolova has given her best to present the materials in the finest possible way.

CONCLUSION

The documents and materials presented by Assoc. Prof. Dr. Rositca Nikolova **meet all the requirements** of the DASRB, the Rules for the Application of the Development of Academic Staff in the Republic of Bulgaria Act, and the Rules set at the Sofia University "St. Kliment Ohridski", for applying the Act aforementioned.

The candidate has submitted a **sufficient** number of scientific papers published in renowned international specialized journals. The applicant's works have original scientific and applied contributions. Their high scientific level is evidenced by the number of citations from other authors. The scientific and pedagogical qualification of Assoc. Prof. Dr. Rositca Nikolova is **undoubted.** The results achieved strongly demonstrate the applicant's competence and research experience. This gives me a reason to give my **positive assessment** and to recommend the Academic Jury to render a positive decision on **Assoc. Prof. Dr. Rositca Nikolova** filling the position of **Professor** in the professional field 4.2 "Chemical Sciences" (Organic Chemistry - Organic Synthesis) at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski".

Date: 24.10.2019

Report prepared by:

/Prof. Dr Ing. Emilia. Naydenova/