

## REVIEW

of the materials submitted for the competition for the academic position "Professor" in the professional field 4.2 Chemical Sciences (Organic Chemistry – Organic Synthesis), announced in State Gazette, issue. 52 of July 02, 2019

The only candidate is **Associate Professor Dr. Rositca Dimitrova Nikolova**

Reviewer: Professor Dr. Nikolay Georgiev Vassilev, Institute of Organic Chemistry with Centre of Phytochemistry, BAS

### **1. Biographical information and eligibility**

Associate Professor Dr. Rositsa Nikolova has graduated as a Master of Science in Organic and Analytical Chemistry at the Faculty of Chemistry, Sofia University "St. Kl. Ohridski" in 1990. In 2000, she obtained her scientific and educational degree "Doctor" in the scientific specialty 01.05.03 "Organic chemistry", defending her doctoral thesis on "Synthesis and chemical transformations of phosphorus-containing coumarino derivatives" at the Faculty of Chemistr of Sofia University "St. Kliment Ohridski". In 2000 the candidate began her carrier in Faculty of Chemistry and Pharmacy at Sofia University "St. Kl. Ohridski", where his entire career goes up to an associate professor, which academic position she still holds. Associate Professor Dr. Rositsa Nikolova has been the Head of the Organic Synthesis and NMR Spectroscopy Laboratory since 2009 and since 2012 has been the Head of the Department of Organic Chemistry and Pharmacognosy.

The documents for participation in the competition of the candidate fulfill the requirements of the Regulations of the Sofia University "St. Kliment Ohridski" for the implementation of the Law on the Development of the Academic Staff in the Republic of Bulgaria, and her scientific and educational profile is in accordance with the requirements for a professor in the professional field 4.2. Chemical Sciences (Organic Chemistry – Organic Synthesis).

### **2. General characteristics of the applicant's activities**

Associate Professor Dr. Rositsa Nikolova participates in the competition with a list of 16 scientific papers, 2 publications in proceedings of scientific conferences and 4 textbooks. All

publications are related to the competition, all of which are published in specialized international journals, referenced in the ISI Web of Knowledge and/or in SCOPUS and with Impact Factor (IF). In reputable international journals such as *Molecules* (with IF = 3.060 for 2018), the candidate has published 3 articles, in *Physical Chemistry Chemical Physics* (with IF = 3.567 for 2018), *RSC Advances* (with IF = 3.049 for 2018), in *J. Phys. Chem. A* (with IF = 2.641 for 2018), *Synlett* (with IF = 2.418 for 2018) and *J. Phys. Org. Chem.* (with IF = 1.53 for 2018) has one article published, *Spectrochimica Acta Part A* (with IF = 2.931 for 2018) has 2 articles published, etc. What is noteworthy is the fact that the publications are printed in various reputable journals, depending on the thematic focus of the research. The distribution of the 4 scientific publications equated to habilitation thesis according to the rank of scientific journals is as follows: all are in scientific publications with Q1. The distribution of the other scientific publications with which the applicant participates in the competition for the academic position of Professor according to the rank of scientific journals is as follows: two are in scientific publications with Q1, seven are in scientific publications with Q2, two are in scientific publications with Q3 and one is in scientific publications with Q4.

The competition materials contain a list of 79 quotations of the scientific works of Associate Professor Dr. Rositsa Nikolova with whom she participated in the competition. Four articles are most cited: one in *Molecules* from 2012 and three earlier in *Tetrahedron*. It is not surprising that mostly articles from the beginning of the candidate's scientific career have elicited more resonance in the literature, and more recent ones, though in more renowned journals, are yet to be cited.

Associate Professor Dr. Rositsa Nikolova has included in her documents habilitation work on the topic "3-Substituted coumarins and 1,2-benzoxaphosphorins as precursors of bioactive compounds". The habilitation work contains 39 pages, 37 schemes and 93 literature sources are cited. It summarizes her own research on the coupling reactions of nucleophilic reagents to 3-substituted coumarins and 1,2-benzoxaphosphorines. The habilitation work is divided into three chapters on: Tandem Hydration Reactions, CH-Acid Reactions, and Organometallic Reagents. They describe in detail the developed preparative methods for the targeted synthesis of different coumarin derivatives, focusing on the comparative consideration of the reactivity of the newly prepared substances with nucleophilic reagents in order to identify differences in their behavior and the factors responsible for this difference.

The attached report shows that Associate Professor Dr. Rositsa Nikolova fulfills the minimum national requirements for occupying the academic position of "Professor" (Indicator A

and C fulfill national requirements, Indicator D is 232 with a minimum value of 200, indicator E is 158 with a minimum value of 100 and indicator E is 282.6 with a minimum value of 150).

### **3. Publications submitted for participation in this competition**

Associate Professor Dr. Rositsa Nikolova summarized in the "Reference for Scientific Contributions" her own scientific achievements in the scientific papers presented for the competition, all her works are in the field of organic chemistry and organic synthesis.

The scientific contributions of Associate Professor Dr. Rositsa Nikolova, according to the attached reference, are divided in two directions: A. Synthetic studies and B. Quantum-chemical and structural studies.

A. Synthetic studies include a detailed study of the interaction of diethyl 2-oxo-2H-1-benzopyran-3-phosphonic acid with nitromethane under various reaction conditions (Publications 1 and 8) and a mechanism for the formation of pyrrolidinedione is supposed, including successive Michael reaction, Nef reaction and molecular rearrangement leading to the opening of the lactone and the formation of a new pyrrolidine ring. In addition, a new, effective method for the synthesis of 3,4-disubstituted pyrrolidine-2,5-dione from 3-substituted coumarins has been developed. The reaction of 3-phosphonocoumarin with organometallic compounds on heating and ultrasound irradiation was also investigated (Publications 2 and 4). Decarboxylation reactions of diethyl 3-acyl-2-oxochroman-3-ylphosphonates were also investigated, yielding two new product types  $\beta$ -ketophosphonates and propionic acids (Publication 17). The interaction of seven new substituted merocyanine dyes with  $\alpha$ -CD,  $\gamma$ -CD, as well as the functionalized  $\gamma$ -cyclodextrin phosphate sodium salt was studied (Publication 10). The 2-oxo-2H-chromen-3-yl phosphonic acid trihydrate of the monoethyl ester is characterized, isolated, spectral and structural. Using quantum-chemical DFT calculations, the electronic structure and its vibration properties were determined to be focused on the relationship between structure and spectral characteristics (publication 9). Salts and complexes of 3-substituted coumarins and 1,10-phenanthroline were obtained (publications 13, 14, 15 and 16). Their structure was proved by spectral methods and X-ray diffraction analysis.

B. Various local reactivity descriptors have been tested to explain the reactivity of 3-substituted coumarins (1,2- versus 1,4-addition). The atomic charges, the atomic electrostatic potential and the Fukui atomic index were theoretically calculated and the binding energies were determined experimentally by X-ray photoelectron spectroscopy (XPS) (publication 6). The solvation processes and the dynamics of H bonds around 3-phosphono-7-aminocoumarin and 7-aminobenzoxaphosphorin in an electronically excited state were investigated using time-

resolved fluorescence spectroscopy as well as quantum chemical simulations (publication 5). The crystal structures of 3-iso-nicotinoylcoumarin and the co-crystal of N- (pyridin-3-yl) benzamide and benzoic acid have been determined (Publications 11 and 18). The self-association of 2- and 3- (acetylamino) pyridines in the condensed phase was investigated using conventional and linearly polarized IR spectroscopy. Theoretical quantum-chemical calculations of the electronic structure and vibration characteristics of the two compounds promote the analysis of the results (Publication 12).

Scientific works of Associate Professor Dr. Rositsa Nikolova are at a very high scientific level, are relevant to the subject of the competition and are in the field of organic chemistry. Various spectral and theoretical characterizations of the studied systems have been used in scientific publications. The carried out studies can be categorized as novelty for science as well as enrichment of scientific knowledge by clarifying mechanisms of chemical reactions and predicting qualitatively, and sometimes quantitatively, the reactivity of the systems under study.

#### **4. Teaching and project activity**

As a lecturer in Faculty of Chemistry and Pharmacy at Sofia University "St. Kl. Ohridski" Associate Professor Dr. Rositsa Nikolova has developed five courses for both undergraduate and master students, has been a lecturer for 9 courses, has conducted classes and seminars in "Organic Chemistry" for undergraduate students in all specialties of the Faculty of Chemistry and Pharmacy and the Faculty of Biology, she was the chairman of the examination committee for the State Examination for the Bachelor's Degrees of the Faculty of Chemistry and the Admissions Exam for Masters (from 2016 until now). Associate Professor Dr. Rositsa Nikolova has one successfully defended PhD student and one defended PhD student and has managed 12 graduate defense students. The academic workload in the last 4 years is well above the minimum required.

Associate Professor Dr. Rositsa Nikolova was: Head of 13 successfully reported and one current contract funded by the Scientific Research Fund of Sofia University "St. Kliment Ohridski"; member of the working group of 9 contracts and manager of two contracts financed by the Ministry of Education and Science - Research Fund; Member of the Board of Directors of two contracts funded under FP7, Everest and Beyond Everest and one under H2020 Materials Networking. She has chaired and co-chaired three international symposia on Organic Chemistry, two international conferences, and 8 workshops on Contemporary Functional Materials. Associate Professor Dr. Rositsa Nikolova has several short-term specializations at both the Technical University of Munich and the Université de Caen.

**CONCLUSION:** Associate Professor Dr. Rositsa Nikolova fulfills all the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria and the Rules for the Conditions and Procedures for Acquiring the Academic Position "Professor" at the Sofia University "St. Kliment Ohridski". The valuable scientific production presented for participation in the competition is sufficient in volume, has been published in renowned scientific journals with high IF and has found wide echo in the literature.

Based on the above, I am convinced of my positive assessment and suggest Associate Professor Dr. Rositsa Nikolova to be elected to the academic position of "Professor" in the professional field 4.2. Chemical Sciences (Organic Chemistry - Organic Synthesis) in the Faculty of Chemistry and Pharmacy at Sofia University "St. Kl. Ohridski".

25.10.2019

Reviewer: .....

Prof. Dr. Nikolay Vassilev