

REVIEW

on the competition for the occupation of the academic position "Professor"
at the Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski"
in the field of chemical sciences, code 4.2.
(Organic chemistry – Organic synthesis)
declared in the State Gazette, issue 52/02.07.2019

Candidate (sole): Assoc. Prof. Dr. Rositca Dimitrova Nikolova

Review: Prof. Dr. Vanya Bogdanova Kurteva, IOCCP-BAS; Member of the Scientific Jury,
appointed by Order RD-09-188 from 26.07.2019

Assoc. Prof. Dr. Rositsa Nikolova presented all required documents in hard copy and electronic form, which are in accordance with the Act for the Development of the Academic Staff in the Republic of Bulgaria (ADASRB), the Regulations for the application of the ADASRB, the Regulations for the terms and conditions for acquiring academic degrees and occupying academic positions of the Sofia University "St. Kliment Ohridski" and the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field "Chemical Sciences", related to the procedure for occupying the academic position "Professor". The documentation submitted has been prepared correctly, transparently and in accordance with all requirements and recommendations.

I. Personal and professional data of the applicant

Assoc. Prof. Nikolova has almost 20 years of experience in the specialty at the Faculty of Chemistry and Pharmacy at Sofia University "St. Kl. Ohridski". In 2001, the High Attestation Committee awarded her the educational and scientific degree of "Doctor" in the specialty 01.05.03. "Organic chemistry". Since 2000 she has held the positions of assistant, senior assistant and chief assistant, and in 2009 she acquired the academic position of "assistant professor". During the period 2008-2018 she completed 5 short-term specializations at the Technical University in Munich, Germany, and 3 at the University of Cannes, France.

Since 2009, Assoc. Prof. Nikolova is Head of the Laboratory of Organic Synthesis and NMR Spectroscopy, and since 2012 she is the Chair of the Department Organic Chemistry and Pharmacognosy. In the period 2011-2015 she is the Vice-Chairman of the General Assembly of the Faculty of Chemistry and Pharmacy at Sofia University. Since 2011 she is a member of the Faculty Board of the Faculty of Chemistry and Pharmacy at Sofia University.

Assoc. Prof. Nikolova performs intensive expert activity. She is a reviewer of numerous diploma theses and scientific publications in international scientific journals. She is a member of the Scientific Jury for the award of the educational and scientific degree of "Doctor" (3) and for the occupation of the academic positions of Professor (2) and Associate Professor (11). Assoc. Prof. Nikolova participates in expert groups for program accreditation of the Standing Committee on Technical Sciences and Military Affairs and of the Standing Committee on Natural Sciences, Mathematics and Informatics. Since 2017, she is the chairman of the Standing Scientific Committee of Chemical Sciences Fund at the Research Fund. She is a member of the Expert Council at the Doctoral School of Sofia University "St. Kliment Ohridski".

Assoc. Prof. Nikolova is the chairman and co-chair of three international symposia on Organic Chemistry, two international conferences and 8 workshops in the field of Contemporary Functional Materials. She is a member of the Union of Scientists, the Union of Chemists, the European Association for Chemical and Molecular Science, the American Chemical Society.

II. General characteristics of scientific, applied and pedagogical activity and their reflection in the scientific literature

Assoc. Prof. Nikolova has presented for the current competition a list of scientific publications for her entire creative period, a list and copies of scientific publications with which she participates in the current competition and habilitation work for. A check up of compliance with the national requirements is presented. The breakdown of indicators is as follows: indicator A - 50 points; indicator C - 100 points; indicator D - 232 points; indicator E - 158 points; and indicator E - 282.6 p. As can be clearly seen, the contributions of Assoc. Prof. Nikolova exceed the national requirements. Her scientific output includes 44 scientific publications, 33 of which are in international and 2 in Bulgarian journals, 4 of scientific conference proceedings in full text and 5 textbooks. In this competition, Assoc. Prof. Nikolova participates with 22 scientific communications; 16 in refereed and indexed journals, 2 in scientific conference proceedings in full text and 4 textbooks. The distribution of scientific publications according to the rank of the journal in which they were published is as follows: 6 in journals with rank Q1 (37.5%), 7 with rank Q2 (43.8%), 2 with rank Q3 (12.5%) and 1 with rank Q4 (6.2%). An excellent impression is the fact that the predominant part of the scientific papers (81.3%) is published in the two highest categories journals, Q1 and Q2. The textbooks co-authored by Assoc. Nikolova with which she participates in the competition include "A Guide for Laboratory Exercises with a Collection of Tasks in Organic Chemistry for Pharmacy Students", University Publishing House "St. Kliment Ohridski, 2019; "Chemistry and Environmental Protection for Grade 9 in Intensive Foreign Language Learning," Anubis Ltd., 2018; "Chemistry and Environmental Protection for Grade 9

for Profiled and Vocational Education with Advanced Foreign Language Learning," Anubis Ltd., 2018; and "Organic Chemistry Problems", University Publishing House "St. Kliment Ohridski", 2011. These data clearly show that the scientific reports of Assoc. Prof. Nikolova fully cover also the additional recommended criteria set out in the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field "Chemical Sciences", related to the procedure for occupying the academic position "Professor": 42 (recommended 40) monographs and articles for the entire creative period, of which 33 (recommended 30) in journals referred to in ISI Web of Science and/or Scopus, respectively 22 (recommended 15) and 16 (recommended 10) number of monographs and articles included in the competition.

The articles of Assoc. Prof. Nikolova have found a wide response in literature. Lists of citations in refereed and indexed in the ISI Web of Knowledge and/or SCOPUS journals are presented for the entire creative period and after her selection for associate professor in 2009, including 119 citations (recommended 80 citations), of which 85 after habilitation. The latter shows a slight discrepancy between the documents presented; 79 citations after habilitation are included, omitting 6 citations from 2019, included in the list of citations for the whole creative period. A search in Scopus data base shows that Assoc. Prof. Nikolova possesses Hirsh index of 5.

The reference for the scientific contributions is written concisely and clearly outlines the personal contributions of Assoc. Prof. Nikolova. The results achieved are divided into two groups; synthetic and quantum-chemical and structural studies, with references to relevant scientific publications. The latter are placed in a table at the beginning of the document, which seriously facilitates reading.

According to indicator "C" Assoc. Prof. Nikolova participates with 4 articles in journals with rank Q1, described above. A habilitation paper entitled "3-Substituted coumarins and 1,2-benzoxaphosphorines as precursors of bioactive compounds" is also presented, written as a review article summarizing the results on the topic published in 93 literature sources and supported by over 40 schemes and figures. The preparation of this material is an indisputable benefit for the applicant who has shown recently interest in the synthesis and study of the properties of phosphorus containing coumarin derivatives. Literature sources include 3 scientific papers co-authored by Assoc. Prof. Nikolova (articles 31, 18 and 28), one of which (18) is cited twice (citations 7 and 67).

Scientific results are reported 53 times in scientific forums in Bulgaria and abroad as 32 (60%) of the presentations are in the period 2009-2016. The data are provided as an excerpt from the "The authors" system that does not allow for a breakdown by type of presentation and the person presenting the results. A detailed analysis shows that the results are reported at 25 (47.2%)

conferences abroad, at 12 (22.6%) international forums in Bulgaria and at 16 (30.2%) national events including 7 Humboldt conferences. After her habilitation, Assoc. Prof. Nikolova presented scientific results at 22 (68.8%) conferences abroad, at 5 (15.6%) international forums in Bulgaria and at 5 (15.6%) national events, including 3 Humboldt conferences. This analysis shows that the main part of the presentations is at international forums in Bulgaria and abroad (37 out of 53; 70%) and that this trend is intensified in the period after the candidate's habilitation (27 out of 32; 84%).

Assoc. Prof. Nikolova has successfully led 2 research projects funded by The Bulgarian National Science Fund of the Ministry of Education and Science, "Training and schooling of specialists" (2003-2006) and "Synthesis and structural studies of coumarin derivatives" (2009-2012), of total value of above 220000 lv. She has participated in the implementation of tasks under additional 3 international, 2 FP7 and 1 H2020, and 9 national projects.

The pedagogical activity of Assoc. Prof. Nikolova is impressive. She has given 9 lecture courses at the Faculty of Chemistry and Pharmacy and the Faculty of Biology at the Sofia University, 7 of which she leads today. Prior to habilitation, she has taken 3 lecture courses: "Organic Chemistry" Part I for distance learning undergraduate bachelor students in the specialty "Chemistry" (2003-2012), "Organic Chemistry" Part II for regular training bachelor students in the specialty "Biology and Chemistry" (2006-2015) and "Organic Chemistry" Part I for regular training undergraduate master students in the specialty "Ecochemistry" (from 2008), which is still leading today. Besides the latter, currently she is also giving the following lecture courses: "Organic Chemistry" Part I for regular training undergraduate bachelor students in the specialty "Computational chemistry" (since 2011), "Organic Chemistry" Part II for regular training undergraduate bachelor students in the specialty "Chemistry" (since 2012), "Organic Chemistry" Part II for regular training undergraduate master students in the specialty "Pharmacy" (since 2014), elective course in "Cosmetic products and care" for regular training undergraduate master students in the specialty "Pharmacy" (since 2016), compulsory course in "Organic materials in cosmetic products" for regular training and distance learning undergraduate master students in the specialty "Cosmetics and household chemicals" (since 2017), and elective course in "Active components in perfumery and cosmetics" for regular training undergraduate bachelor students in all chemical specialties (since 2018). In recent years, she has a total employment of about 550 hours and a classroom employment of about 400 hours per school year. She participates in the preparation of seminars and exercises in organic chemistry for undergraduate bachelor students in all specialties of the Faculty of Chemistry and Pharmacy and Faculty of Biology at the Sofia University. She is the chairman of the examination committee for the State Bachelor's Degree Examination and of the Master's Degree Examination of the Faculty of Chemistry and Pharmacy.

She is scientific supervisor of 1 successfully defended a PhD student (Eleonora Ilieva) and 1 graduated with the right of defence (Ana Koleva), as well as 12 graduates. She is trained 8 students in the frame of research practices.

III. Basic scientific contributions

Assoc. Prof. Rositsa Nikolova is a distinct experimenter with scientific developments that fall into two main directions:

- ✓ Synthesis of heterocyclic compounds;
- ✓ Structural investigations and quantum-chemical calculations.

The main research achievements of Assoc. Prof. Nikolova are in the area of the synthesis of heterocyclic compounds and their transformations. Among them, the research of *coumarin derivatives* occupies the most significant part (articles 1, 3, 7, and 8 of the list). The interactions of esters of coumarin-3-phosphonic acid and esters and amides of coumarin-3-carboxylic acid with nitromethane are studied and a comparison of the results obtained is performed. It is found that the reaction out-put depends on both the type of coumarin derivative and the reaction conditions. Pyrrolidinone derivatives are obtained and a putative mechanism for their formation is proposed and supported by quantum-chemical calculations.

The reaction of esters of 3-coumarin phosphonic acid with various organozinc and organomagnesium reagents (articles 2 and 4 of the list) to the corresponding 1,4-addition products is studied and is shown that the reaction proceeds smoother and with more reproducible results under ultrasound irradiation than in thermal conditions. When reacted with chloroacetic anhydride in the presence of zinc and ultrasound irradiation, a homodimerization product is isolated, while no heterodimerization product is detected. A possible mechanism of the observed homodimerization is proposed.

By decarboxylation reaction of esters of 3-acyl-3-coumarin phosphonic acid, β -ketophosphonates and propionic acids are obtained (article 17 of the list). It is found that the formation of β -ketophosphonates is favored only by thermal decarboxylation in water and that yields increase with the extension of the alkyl chain in the acyl substituent.

Salts and complexes of 3-substituted coumarins and 1,10-phenanthroline (articles 13-16 of the list) are obtained, which structures are elucidated by spectroscopic methods and X-ray diffraction analysis.

The interactions of *merocyanine dyes* with cyclodextrins (article 10 of the list) are studied and are found that nanosized supramolecular polymers are formed, some possessing solid-state fluorescence properties.

Modern *spectral methods* such as NMR, IR, fluorescent, X-ray photoelectron spectroscopy etc. are applied to assign the products' structures. The structures of a number of compounds are confirmed by *single crystal X-ray diffraction*. The proposed possible mechanisms for the formation of part of the products are supported by *quantum-chemical calculations*. The properties of compounds and systems are studied with a combination of spectral and quantum-chemical approaches. The reactivity of coumarin derivatives is investigated by X-ray photoelectron spectroscopy and theoretical calculations (article 6 of the list), and it is found that the structures are characterized by a high negative charge at C-3 atoms and that the electrophilicity of the reaction centers in the coumarin system increased in the presence of a phosphonic group. It is shown that substituted coumarins will react with soft nucleophiles preferably in position 2 and with soft nucleophiles in position 4. The processes of dissolution and dynamics of hydrogen bonds around derivatives of esters of 3-coumarin phosphonic acid are investigated (article 5 of the list). The attenuation of the H-bonds substrate-solvent upon optical excitation is found to be at odds with published data on coumarin derivatives without phosphonic groups.

IV. Critical remarks and suggestions

I have some small critical notes. In two of the articles with which Assoc. Prof. Nikolova participated in the competition (articles 11 and 14), the order of the authors does not correspond to that in the original documents. In some places, there is a discrepancy in the data indicated in the various documents. For example, in the CV it is stated that Assoc. Prof. Nikolova has 42 scientific papers, in the attached list are listed 44, and the excerpt from the "The authors" system contains 46. The CV indicates that the candidate's articles are cited 121 times in refereed and indexed journals, while 119 citations appear in the corresponding document. In the appendix describing the citations in the referenced and indexed journals after habilitation, 6 citations, mentioned in the corresponding document concerning the whole creative activity, as mentioned above, are omitted. In the CV it is stated that Assoc. Prof. Nikolova has "participated in 57 scientific conferences in the country and abroad with 28 oral presentations and 62 posters", which is in complete disagreement with the excerpt from the "The authors" system, which lists 53 participation in scientific forums. However, these small critical remarks in no way undermine the high quality of the scientific output of Assoc. Prof. Nikolova.

I also have one recommendation that does not concern the candidate personally. The habilitation work of Assoc. Prof. Nikolova does not meet the requirements laid down in the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field "Chemical Sciences". The candidate

participates in indicator "C" in the current competition with scientific publications and does not count points for the habilitation work, therefore the indicated non-compliance should not be taken into account. In this connection, I find it appropriate to be discussed that such a review material, which is very useful and important, but does not concern the applicant's personal achievement, to bear a different name from 'habilitation work', for which specific rules are laid down in those rules.

V. CONCLUSION

It is undisputed for me that Assoc. Prof. Dr. Rositca Nikolova is a productive researcher with established qualities and a promising career. Analysing the candidate's scientific achievements, the relevance and perspective of the topics, active participation in research projects, active teaching, administrative and peer review activities and her personal qualities and skills, I think that they significantly exceed the requirements of the Act for the Development of the Academic Staff in the Republic of Bulgaria, the Regulations for the application of the ADASRB, the Regulations for the terms and conditions for acquiring academic degrees and occupying academic positions of the Sofia University "St. Kliment Ohridski" and the Recommendations on the criteria for acquiring scientific degrees and occupying academic positions at the Sofia University for the professional field“ Chemical Sciences”, related to the procedure for occupying the academic position“ Professor ”, and I strongly recommend that the Faculty Council of the Faculty of Chemistry and Pharmacy at Sofia University award to

Associate Professor Dr. Rositca Dimitrova Nikolova

the academic position of "Professor" in the field of higher education 4. Natural sciences, mathematics and informatics, professional field 4.2. Chemical Sciences (Organic chemistry – Organic synthesis).

Sofia, October 28, 2019

Prepared the appraisal

(Prof. Dr Vanya Kurteva)