REVIEW

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<u>Re:</u> Competition for a Full Professor position at the Faculty of Chemistry and Pharmacy, Sofia University in professional field 4.2 Chemical Sciences (Organic Chemistry - Organic Synthesis)

There is only one candidate applying for the Full Professor position, announced in the State Gazette 52/02.07.2019: Associate Professor Dr. Rositca Dimitrova Nikolova. For the competition the candidate has provided a full set of documents in accordance with the Regulations for the implementation of the Law for development of the academic community in Republic of Bulgaria. Documents are very well organised and provide ample information about the scientific and pedagogical activities of the applicant.

Rositca Nikolova obtained her M.Sc. degree in 1990 from the Faculty of Chemistry, Sofia University in the field of Organic chemistry. In 2001, under the supervision of assoc. prof. A. Bojilova, she successfully defended a Ph.D. thesis entitled "Synthesis and chemical transformations of phosphorus-containing coumarin derivatives". In 2000 she was appointed assistant professor in the department of Organic chemistry, where, in the following years she was promoted to a senior assistant professor, head assistant professor and associate professor positions. From 2009 she acts as a head of the Laboratory of organic synthesis and NMR spectroscopy at the Faculty of chemistry and pharmacy. She has been a head of the Department of organic chemistry and pharmacognosy since 2012. Dr. Nikolova has completed several specialisations abroad (Technical University of Munich and Université de Caen). She is a member of the Union of scientists and chemists in Bulgaria, European Association for Chemical and Molecular Science, and American Chemical Society.

For the competition, the candidate has presented 23 scientific works: a Habilitation thesis ("3-Substituted coumarins and 1,2-benzoxaphosphorins as precursors of bioactive compounds"), 4 textbooks and study guides and 18 scientific papers. Nine of the papers fall into Q1 and Q2 quartiles, while the rest of them are in quartiles Q3 and Q4. These papers

have been cited 79 times in the scientific literature. Generally, Dr. Nikolova is a co-author of 44 scientific papers, cited 119 times in the literature. The application materials reveal that the candidate covers the minimum national requirements for occupation of the position of professor.

The main scientific contributions of Dr. Nikolova are in the field of organic synthesis focusing on developing new methods for synthesising heterocyclic compounds (mostly coumarin derivatives), as well as characterising the synthesised products by spectroscopic and computational methods. More specifically, her investigations and achievements could be grouped into the following domains:

(1) Synthetic investigations

1.1. A new light has been shed on the process of interaction between diethyl ester of 2-oxo-2H-1-benzopyrane-3-phosphonic acid and nitromethane under different reaction conditions. Reaction parameters has been optimised in order to accelerate the reaction and increase the reaction yield.

1.2. A new, more efficient method has been developed for synthesising of 3,4disubstituted pyrrolidine-2,5-diones from 3-substituted coumarins. Both experimental and theoretical investigations have been conducted which clarify the mechanism of the reaction studied.

1.3. Studies have been conducted on the reaction of 3-phosphonocoumarin with organometallic compounds under heating and treating with ultrasound. The conditions under which the dimerisation of the 3-substituted coumarins takes place have been established. A reaction mechanism has been proposed.

1.4. Studies have been performed on reactions of decarboxylation of diethyl 3-acyl-2oxochroma-3-ilphosphonates yielding two types of new products: beta-ketophosphonates and propionic acids.

1.5. Investigations have been conducted on the interaction of seven new substituted merocyanine dyes with alpha-CD, gamma-CD and gamma-CD phosphate sodium salt. The products obtained has been characterised by powder X-ray diffraction, spectroscopic and thermal methods.

1.6. Trihydrate of the monoethyl ester of 2-oxo-2H-chromen-3-il-phosphonic acid has been synthesised, isolated and spectroscopically characterised.

1.7. Obtained are salts and complexes of 3-substituted coumarins and 1,10phenanthrolines, whose structures have been proven by spectroscopic methods and X-ray diffraction.

(2) Quantum-chemical and structural studies

2.1. Characterised in details are the electronic properties of coumarin derivatives and dependencies have been derived regarding the reaction characteristics of various atomic centres of the molecule.

2.2. Studied are the processes of dissolution and hydrogen bond dynamics in coumarins in electron exited state using time-resolved fluorescence spectroscopy and quantum-chemical calculations.

2.3. Employing X-ray diffraction, structurally characterised are 3-isonicotinoilcoumarin and co-crystal of N-(pyridine-3-il) benzamide benzoic acid.

2.4. Studied is the self-association of 2- and 3-(acetylamino)pyridines in condensed phase with the aid of conventional and linearly polarised IR spectroscopy. Molecules have been modelled by quantum-chemical methods and information has been obtained about the electronic structure and vibrational characteristics of the two compounds.

Dr. Nikolova is a successful lecturer in the Faculty of chemistry and pharmacy. She delivers lectures in Organic chemistry (I and II) to B.Sc. and M.Sc. students from chemical, biological and pharmaceutical specialties. She developed and teaches new lecture courses on "Active ingredients in perfumery and cosmetics" and "Organic materials in cosmetic products". She has supervised 12 successfully defended diploma students as well as 2 doctoral students.

Conclusion

Scientific publications presented by Dr. Nikolova fall into the scope of the announced competition and represent original scientific investigations with substantial contribution to the field of organic synthesis. The candidate is a proven scientist/lecturer with deep understanding and practical skills in the field of organic synthesis. She demonstrates creative thinking and ability to choose important problems of interest to the science and practice. As a result of the foregoing, I believe that with her scientific and pedagogical activities and

achievements Dr. Rositca Nikolova fully complies with all the requirements of the Law for the occupation of the academic position "Full Professor".

In connection with the above, I propose Associate Professor Dr. Rostca Dimitrova Nikolova to be elected Full Professor in the professional field 4.2 Chemical Sciences (Organic Chemistry - Organic Synthesis).

27.10.2019

Reviewer:

(Prof. Todor Dudev)