

# OPINION

**provided by Dr. Rositca Dimitrova Nikolova, Professor at Faculty of Chemistry and Pharmacy, University of Sofia "St. Kliment Ohridski",**  
on the materials submitted for participation in the competition  
to hold the academic position of 'associate professor'  
at the Institute of Organic Chemistry with the Center for Phytochemistry (IOCCP), BAS  
by field of higher education Natural sciences, mathematics and informatics professional  
direction "Chemical sciences" - 4.2, scientific specialty "Organic chemistry"

In the competition for Associate professor', announced in the State Gazette, no. 9 of 30.01.2024 and on the website of IOCCP, BAS, as a candidate participates Assistant Professor Vera Ventsislavova Deneva ,PhD, from the Center of NMR Spectroscopy at IOCCP-BAS.

The paper set of materials presented by Dr. Vera Deneva is in accordance with the Regulations for the Development of the Academic Staff of the IOCCP, and meets the criteria of the IOCCP -BAS for occupying the academic position of "Associate Professor". The candidate Dr. Vera Deneva submitted a total of 26 scientific papers. 16 scientific works, which are not in the dissertation and are counted in the final evaluation, as well as 13 scientific research projects are accepted for review. 5 scientific papers on the dissertation and 5 scientific papers outside the competition's issues are not reviewed. The distribution of scientific works by the respective Q factors is as follows: 12 (75%) publications in Q1 and 4 (25%) in Q2.

## **1. General presentation of the candidate**

Asisst. Prof. Dr. Vera Ventsislavova Deneva graduated in 2007 with a bachelor's degree and in 2009 with a master's degree at the Faculty of Chemistry of the Sofia University "St. Kliment Ohridski". Since 2009, she has been a full-time PhD student at IOCCP - BAS with scientific supervisor Prof. Dr. Ludmil Antonov. Her PhD thesis on "Experimental and theoretical studies of tautomeric systems based on aza-naphthols and their azomethine analogues" was successfully defended in 2013. In 2012, after a competitive exam, she was appointed as an assistant, in 2017 she was promoted to chief assistant at IOCCP - BAS, where she has been working until now.

In the period from 01.10.2011 to 15.06.2012 she specialized in Switzerland. Dr. Deneva was awarded the BAS "I.E. Geshov" for a young scientist in 2012.

## **1. General characteristics of the applicant's activity**

The presented documentation Dr. Vera Deneva is prepared according to all requirements and recommendations.

### **According to indicator A1.**

50

The candidate Vera Deneva defended her PhD thesis on "Experimental and theoretical studies of tautomeric systems based on aza-naphthols and their azomethine analogues" in 2013 under the supervision of Prof. Dr. Ludmil Antonov.

**According to indicator C4**

145

Six scientific publications on the subject of the competition are presented, printed in specialized international journals, referenced in SCOPUS and ISI Web of Science with an impact factor, 5 of which in Q1 and one in Q2. The average IF of the publications is 4.36. According to this indicator, the candidate exceeds the minimum requirements of 100 points.

**According to indicator D7**

235

The candidate Dr. Vera Deneva has presented as a co-author 10 scientific publications with an impact factor and they are referenced in Scopus and ISI Web of Science - 7 from Q1 (70%) and 3 from Q2 (30%). 8 of the presented publications have  $IF > 3$ , and the total IF of the publications is 34.40. Dr. Deneva is the first author in 5 of the publications and in 4 - the corresponding author.

According to this indicator, the candidate exceeds the minimum requirements of 200 points.

Research results have been presented at 13 national and international forums as 11 poster presentations and 2 oral presentations.

**According to indicator E11.**

236

During the preparation of the current opinion, 391 citations in Web of Science and Scopus were noticed. The minimum requirement for this indicator is 50 points, the candidate has submitted 118 citations for the competition, which repeatedly exceeds the requirements.

**According to indicator F.**

174

Until the submission of documents, according to the international databases - Web of Science with h-index 11 and Scopus with h-index 10, the candidate meets the minimum requirements for holding the position of Associate Professor.

Dr. Deneva develops active project activity. Participation in 10 scientific projects with FNI, 1 of which the candidate is the head of, and participation in 3 international projects are presented.

The analysis of the submitted documents shows that Dr. Deneva not only fulfills, but also exceeds the minimum requirements of the competition.

**2. Scientific results**

The submitted scientific communications of the candidate are in the scientific field for which the competition was announced. The scientific research of Dr. Vera Deneva are in the field of molecular spectroscopy and are mainly related to the study of the tautomeric equilibrium of organic compounds, their complex-forming ability and their potential applications:

- Azo dyes

The tautomeric behavior in various solvents of aryl-azo derivatives of naphthols with structural modifications to control proton transfer was investigated. Using spectroscopic methods and quantum chemical calculations, it was found that structural modifications affect the tautomerism, and the formation of complexes with alkaline earth metals leads to significant spectral shifts.

The tautomeric equilibrium of 4-(phenyldiazenyl)naphthalen-1-ol was studied and a system was developed in which complexation with metal ions completely shifts the equilibrium to the

ketotautomer. On this basis, a theoretical design of tautomeric optical sensors for the detection of metal ions has been developed.

Borderline cases of azo and hydrazo tautomers of two series of azo dyes containing a pyrazole ring were investigated using spectral and quantum-chemical methods.

Using a combination of experimental and theoretical models, the switching mechanism of ethyl 2-(2-(quinolin-8-yl)hydrozono)-2-9pyridin-2-yl)acetate was investigated. Two new 4-hydroxycoumarin-based rotary switches were also analyzed. Stator structure and solvent polarity were found to have no effect on the azohydrazone tautomerism, but did affect their emission behavior.

- Schiff bases

The tautomeric equilibrium of two 4-substituted phthalimide 2-hydroxyl Schiff bases with different 2-hydroxyaryl fragments was investigated and it was found that a solvent-dependent tautomeric equilibrium was observed for the compound containing a hydroxynaphthyl fragment, but not for the compound with a hydroxyphenyl fragment.

The results of studies of two newly synthesized Schiff bases derived from 7-hydroxyquinoline that upon irradiation exhibit rotation about a specific bond by intramolecular proton transfer in the excited state make them suitable candidates for use as bistable switches.

The tautomerism of benzothiazopicoline and isonicotinamide Schiff bases in the ground state and the proton transfer in the excited state were studied and it was found that the two compounds have the same photodynamic behavior and have potential for application as optoelectronic devices.

- Heterocyclic tautomeric systems.

The mechanism of proton transfer in 10-hydroxybenzo[h]quinoline and its derivatives was studied and it was found that the presence of an electron-withdrawing substituent at position 7 leads to the appearance of a keto tautomer in the ground state and changes in the excited state.

Using spectral methods and quantum-chemical calculations, the tautomeric behavior of favipiravir in solution was investigated. The dynamic balance between the various structural forms of the compound and their influence on its biological activity and efficiency have been studied.

The photochemical behavior of compounds containing a pyridine ring, pinene fragments and 1,3,5-triazines and the possibilities of their application were investigated.

- Other investigations.

The possibility of using near-infrared spectroscopy (NIR) to develop a rapid non-destructive method for the analysis of the pharmacologically significant components in *Arnica flos* - phenolic acids, flavonoids and sesquiterpene lactones - was investigated..

A fast non-destructive method for researching and classifying Bulgarian wines by region and variety using Raman spectroscopy is also proposed. Phenolic components in white and red wines were investigated.

The presented scientific publications are related to solving problems significant for science and practice; and the obtained results show opportunities for the potential application of the studied substances as molecular switches. A wide range of spectral and theoretical methods were used in the research. The topic is current and significant.

### **3. Evaluation of the candidate's personal contribution**

For me, the candidate's personal contribution to the current research is indisputable. In 6 of the presented publications, Dr. Deneva is the first author of the publications, and for 4 the corresponding author.

#### **CONCLUTIONS**

The documents and materials presented by the Assis.Prof. Dr. Vera Deneva meet all the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria and its Regulations for the Implementation, the Regulations for the Implementation of the BAS and the Regulations of the IOCCP-BAS. The results achieved by Dr. Vera Deneva in the research activity are fully in line with the specific requirements of the IOCCP-BAS Regulations for the application of the Low.

The candidate in the competition has submitted a sufficient number of scientific works published after the materials used in the defense of the ONS "doctor". The candidate's works contain original scientific and applied contributions that have received international recognition and response, all of which have been published in journals issued by international academic publishers. His theoretical developments have the potential for practical applicability. Dr. Vera Deneva's scientific qualifications are unquestionable.

After getting acquainted with the materials and scientific works presented in the competition, analyzing their significance and the scientific and scientific-applied results contained in them, I find it reasonable to give my positive assessment and recommend the Scientific Jury to prepare a report-proposal to the IOCCP Scientific Council -BAS to select Assist. Prof. Vera Ventsislavova Deneva, Ph.D., to the academic position of 'associate professor' at IOCCP -BAS in professional direction 4.2 Chemical sciences, scientific specialty "Organic Chemistry".

22.05.2024

**Prepared by:** .....  
(Prof. Rositca Nikolova, PhD)