## **STANDPOINT**

by Prof. Dr. Ivelina Mircheva Georgieva

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of the materials for participation in a competition for the academic position "Associate Professor" at the Institute of Organic Chemistry with Centre for Phytochemistry (IOCCP), BAS in the field of higher education 4. Natural sciences, mathematics and informatics professional field 4.2. Chemical Sciences, scientific specialty "Organic Chemistry" for the needs of the Laboratory "Organic Synthesis and Stereochemistry" (OSS)

In the competition for 'Associate Professor', announced in the State Gazette, № 9/30.01.2024 and on the website of IOCCP-BAS, only one candidate participated: Chief Assistant Professor Vera Ventsislavova Deneva, PhD from IOCCP-BAS; Vera Deneva; ORCid: 0000-0002-1285-9037; Scopus ID: Deneva, 35078441400

*General description of the submitted materials and the applicant.* The submitted set of materials (in paper and electronic format) for participation in the competition is in accordance with the requirements of the Law on the Development of the Academic Staff in the Republic of Bulgaria, the Regulations for its implementation at the BAS and the recommended criteria of the IOCCP-BAS on PF 4.2. Chemical Sciences. The verification of the above requirements for the AP "Associate Professor" showed that Vera Deneva fulfills the required minimum in all groups of indicators (A, C, D, E, (F), G) and collects **860 pts** out of a total required minimum of 445 pts.

Vera Deneva completed her higher education at the FCPh at Sofia University with a master's degree in Organic Chemistry in 2009, and in 2013 at IOCCP-BAS, she obtained the educational and scientific degree "doctor" in PF 4.2 Chemical Sciences, specialty "Organic Chemistry". With a PhD degree, the candidate fulfills indicator "A" (50 pts). As a young scientist, in 2012, Deneva was awarded the "Ivan Evstratiev Geshov" prize of the BAS for scientific achievement on the topic "New molecular switches and sensor systems based on tautomeric proton transfer". In her consistent career development in the field of Organic Chemistry, as Senior Assistant Professor (2012-2017) and Chief Assistant Professor since 2017 in the Laboratory "Organic Synthesis and Stereochemistry" at IOCCP-BAS, Dr. Deneva has accumulated over 10 years of work experience in the specialty. During her scientific career, the candidate conducted an 8-month specialization in Switzerland.

*Research activity.* In her current research activity, Dr. Deneva is a co-author in **26 scientific publications** (according to the attached list) and 28 - according to the SCOPUS database, all of which have been published in indexed journals in the SCOPUS and Web of Science. At the time of drafting the document, the total number of citations of the publications is **391**, **H-index 10** (SCOPUS) (without self-citations of all co-authors), which exceeds the required H-index 5.

In the current competition, Dr. Deneva participates with **16 original scientific publications**, excluding those from her PhD thesis. The papers correspond thematically to the competition's specialty "Organic Chemistry" and have been published in prestigious journals such as *Dyes and* 

*Pigments* (IF = 4.9), *Journal of Molecular Liquids* (IF = 6.6), *Physical Chemistry Chemical Physics* (IF = 3.7), *Spectrochimica Acta Part A* (IF = 3.2), *Molecules* (IF = 4.6), etc., which is a recognition of the importance of scientific research with the participation of Dr. Deneva. The scientometric indicators of the candidate are impressive: all articles for participation in the competition were published in highly indexed scientific journals and distributed by quartiles (for the year of publication), they are as follows: 14 in Q1 and 2 in Q2. With her publication activity, Dr. Deneva fulfills the minimum criteria: 1) under GI "C" for habilitation work on 6 scientific papers with Q1 (required 100 pts/completed 150 pts); under GI "D" for scientific works and patents (required 220 pts/completed 240 pts); 3) under GI "E" for 118 citations in SCOPUS of the publications included in the competition (without self-citations of co-authors) (required 70 pts/completed 236 pts). In 6 of the scientific papers on the competition, Dr. Deneva is the first author.

In fulfillment of the requirements for the competition for AP "Associate Professor", Dr. Deneva presented a habilitation thesis on the topic "*Tautomeric studies of organic compounds: Spectral properties, structural modifications and potential applications*". The 16 publications on the competition are included in this reference at the candidate's discretion. Her research interest and competence are in the development of materials based on tautomeric systems with optical applications such as molecular switches and sensors. A major contribution of Dr. Deneva is the skillful application of molecular spectroscopy (absorption and fluorescence in the UV-Vis region) to study the tautomeric properties of organic compounds, the factors that activate their switching and the mechanisms of tautomeric conversion. The more important results of the research work can be summarized as follows:

1) The tautomeric behavior of a series of azonaphthol dyes in the ground state is studied.

The role of solvent and substituents in controlling the keto-enol equilibrium in aryl azo naphthol derivatives is evaluated. Suitable ligands are identified that selectively bind alkali and alkaline earth ions, induce a bathochromic shift of the absorption band, and are potential optical sensors for the detection of metal ions.

Two series of azo dyes are studied in solution and solid state, which are stabilized in azo enol and hydrazo tautomeric forms, respectively. Both groups have the potential to be used as reference compounds to establish azo or hydrazo tautomerism with NMR spectroscopy.

The Z/E isomerization process of ethyl-2-(2-(quinolin-8-yl)hydrazono)-2-(pyridin-2-yl)acetate is studied and the most likely switching mechanism is predicted to be by proton transfer via chain-forming water molecules.

The tautomeric equilibria of two new 4-hydroxycoumarin azo (naphthyl or quinoline) dyes in the ground and excited states in different solvents are investigated. They are found to exist as keto (hydrazone) tautomers that were unaffected by solvent polarity. Protonation is shown to be a suitable stimulus for E/Z switching and a possible mechanism of the process is proposed.

2) The tautomeric behavior of three groups of Schiff bases are investigated: 4-substituted phthalimide 2-hydroxy, 7-hydroxy quinolone and benzothiazo picoline/isonicotinamide bases. The influence of the solvent type, possible rotations, protonation, etc. on the tautomeric equilibrium of Schiff bases is estimated by combining experimental methods of UV-Vis

spectroscopy, crystallography and fluorescence spectroscopy. By elucidating the photophysics and dynamics of proton transfer in molecular switches, their potential applications as optoelectronic devices have been revealed.

3) The tautomeric behavior of 10-hydroxybenzo[h]quinoline (HBQ) and 1,3,5-triazine and their derivatives in ground and excited states are studied. Molecular spectroscopy is used to evaluate the influence of the solvent and the type of substituents in the skeleton on the tautomeric equilibrium and the mechanism of proton transfer (one- and two-step).

4) An unusual anti-Kasha behavior for a rotary switch featuring a pyridyl ring and a carboxyl group as mobile substituents is predicted based on experimental spectroscopic data from UV-Vis, excitation and fluorescence spectra, fluorescence quantum yield, fluorescence lifetime.

5) Of interest is the investigation for the first time of the keto-enol tautomerism of the bioactive compound, favipiravir in solution. Molecular spectroscopy has shown that the keto tautomer is stabilized in water, while the enol tautomer is preferred in organic solvents. The possibility of the deprotonated ligand forming complexes with alkaline earth ions ( $Mg^{2+}$ ,  $Ca^{2+}$ ) is predicted.

6) Methodological studies: i) Development of calibration models using near-infrared spectroscopy to quantify the content of active components in samples of *Arnicae flos* substance obtained from the plants *Arnica montana L*. and *Arnica chamissonis Less*; ii) Development of calibration models for the measurement of phenolic compounds in wine using Raman spectroscopy, which is a rapid, non-destructive analytical technique. With the assessment of the chemical composition, the aim is to classify the Bulgarian wines.

The scientific activity of Dr. Deneva is closely related to the implementation of 13 projects: two international (scientific networks in supramolecular chemistry suprschem@balkans.eu suprsmedchem@balkans.net, funded by the Swiss Science Foundation), 11 at Bulgarian National Science Fund – Ministry of education and science, for one project for young scientists, she is a supervisor. For the dissemination of scientific results, Dr. Deneva participated in 13 scientific forums, 10 international and 3 national, giving 2 oral and 11 poster presentations.

*Comment:* In the publications for the competition, Dr. Deneva is a co-author in a 6-7 member team and the research is multidisciplinary. It would be clearer, if the candidate explicitly stated her personal contribution and competence in the joint research.

In conclusion, the high evaluation of the research with the participation of Dr. Deneva, published in prestigious journals, her scientific contributions and her active participation in projects prove that she is a highly qualified and established scientist in the field of tautomeric organic systems and molecular spectroscopy for their research, in full accordance with the scientific specialty "Organic Chemistry" of the competition. The presented analysis of the competition materials gives me reason **to vote positively with a convinced "yes"** and I recommend to the Scientific Jury to propose to the Scientific Council of the IOCCP-BAS that the Chief Assistant Professor **Dr. Vera Ventsislavova Deneva be elected to the academic position "Associate Professor" in IOCCP-BAS** in the PF 4.2. Chemical Sciences, scientific specialty "Organic Chemistry".

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Prepared the standpoint: Prof. Dr. Ivelina Georgieva