

## **REPORT**

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Member of the Academic Jury set to render a decision on the competition for the academic position of "Professor" at the Institute of Organic Chemistry with a Centre of Phytochemistry - Bulgarian Academy of Sciences

in the Professional Field 4.2. Chemical Sciences, Scientific Specialty "Organic Chemistry"

This Report is prepared in response to Order No ПД-09-200/15.12.2022 issued by the Director of the Institute of Organic Chemistry with a Centre of Phytochemistry - Bulgarian Academy of Sciences

In the competition for the academic position of "Professor", announced in State Gazette, issue 89 of 08.11.2022, as well as on the website of the Institute of Organic Chemistry with Centre of Phytochemistry - Bulgarian Academy of Sciences (IOCCP-BAS), application documents were submitted by Assoc. Prof. Dr. Svilen Plamenov Simeonov. Assoc. Prof. Simeonov has been working at the IOCCP-BAS since 2006 (with a short break), and since 2017 he has held the academic position of an associate professor.

### **1. General Information**

Assoc. Prof. Dr. Svilen Simeonov has submitted all required documents for participation in the competition, both on paper and in an electronic format, in compliance with the Development of Academic Staff in the Republic of Bulgaria Act (DASRBA), the Rules for the implementation of the DASRBA at the BAS and the Rules on the terms and conditions for acquiring scientific degrees and for occupying academic positions at IOCCP-BAS. The candidate has attached a total list of 38 publications. In the current competition he participates with 17 publications. They were published after 2017 and are assigned as follows: 5 publications under indicator B, and 12 - under indicator D (forth indicator). In addition, Assoc. Prof. Simeonov has included a list of 5 participations at scientific forums and 2 participations as an invited lecturer. Information on participation and coordination of eight research projects has been also included.

### **2. Brief Biographical Data of the Applicant**

Assoc. Prof. Svilen Simeonov graduated in 2002 with a bachelor degree in "chemistry", and in 2004 he obtained a master degree in "organic chemistry" at SU "St. Kl. Ohridski", Faculty of Chemistry and Pharmacy. The candidate was a doctoral student at the Faculty of Pharmacy,

University of Lisbon, where in 2014 he acquired the scientific degree "Doctor" in "Organic Chemistry". He worked as an analytical chemist at Unipharm AD. Since 2018, Assoc. Prof. Simeonov has been elected as the head of the laboratory Organic Synthesis and Stereochemistry (OSS).

### **3. General Characteristics of the Applicant's Activity**

Assoc. Prof. Simeonov has applied with 17 publications in the competition, as well as with a habilitation reference for scientific contributions in Bulgarian and English, in accordance with the requirements. Sixteen of the presented articles are in journals ranked in the Q1 quartile and one article in a journal within the Q4 quartile of the corresponding scientific fields. Proof of the high level and relevance of Prof. Simeonov's research is the large number of citations - 2082 citations (without self-citations according to a Scopus reference) in refereed and indexed journals and in monographs abroad. The candidate's Hirsch index is 17. The citations of the works presented in the competition are 901.

It should be noted that Assoc. Prof. Simeonov has been the principle investigator of 3 international projects (financed by UNESCO and H2020) and 2 projects financed by the National Science Fund. He has been participating in 3 more projects financed by Bulgarian funds with a total contribution of about 1 250 000 BGN. Assoc. Prof. Simeonov is the head of the ReCat4VALUE project under the VIHREN National Scientific Programme. The applicant has been actively involved in educational activities - supervisor of a postdoctoral researcher (Dr. Adolfo Fernández-Figueiras) and two doctoral graduates, as well as co-supervisor of a master student at the Faculty of Pharmacy, University of Lisbon. He is currently the supervisor of a PhD student. For his excellent scientific results, Assoc. Prof. Dr. Simeonov was awarded in 2015 with the UNESCO, FOSAGRO, IUPAK "Green Chemistry for Life" award for young researchers and the "Acad. Bogdan Kurtev" award 2017-2019 for achievements in the field of organic chemistry.

### **4. Analysis of the main scientific contributions**

The main research conducted by Assoc. Prof. Svilen Simeonov has been focused on organic synthesis and green chemistry, results of which have been successfully included in the development of new biorefinery technologies. The contributions are of a fundamental and applied research nature and can be assigned to the following areas:

- Biorefinery of furan derivatives with emphasis on new green methods
- Synthetic modifications of natural products
- Other research lines

Within these studies, the potential of the Achmatowicz rearrangement as a key synthetic transformation for the biorefinery of furfural and 5-hydroxymethyl furfural was demonstrated for

the first time. An entirely new synthetic strategy has been developed to obtain the industrially important pentane-1,2,5-triol. A number of drawbacks of liquid-phase reactions have been overcome by the application of mesoporous silicas containing Ni and/or Pt nanoparticles, which catalyzed the conversion of the intermediate into the gas phase. A high selectivity of the reaction was achieved, which took place under mild conditions and in the absence of a solvent, i.e. the advantages of green chemistry have been demonstrated.

Research has been extended to the development of Ru-catalyzed isomerization of Achmatowicz products leading to biorenewable monomers and biologically active lactones. The reaction has also been used as a key step in the total asymmetric synthesis of biologically active products. The reaction mechanism was studied using the isotopic labeling technique and confirmed by DFT calculations.

As part of the research aimed at the biorefinery of 5-hydroxymethyl furfural (HMF), Assoc. Prof. Simeonov and co-authors have shown for the first time that  $\text{Na}_2\text{S}_2\text{O}_4$  is an effective stabilizer in the HMF production, purification and synthetic applications. In this way, a major industrial problem, namely the chemical instability of HMF, could be overcome. In addition to increasing the yield, the use of  $\text{Na}_2\text{S}_2\text{O}_4$  resulted in a product with a high purity of >99.9%.

A new strategy for biorefinery of furan-2,5-dicarboxylic acid based on enzymatic desymmetrization of carboxyl groups and subsequent catalytic activation of C-H in the furan ring has been developed. In the framework of this research, the preparation of new structurally complex furan derivatives with potential application in medicinal chemistry was achieved. The results of these studies are of particular importance considering also the growing industrial application of furan-2,5-dicarboxylic acid as a substitute for terephthalic acid in the production of polyesters.

Research aimed at the utilization of widespread and accessible raw materials, from which valuable products can be obtained, expands the perspectives of green chemistry. An example of such research is the developed method for the synthesis of HMF from glucose using  $\text{Cr}^{3+}$ -modified commercial acid resins as catalysts, in which yield of 70% and high purity of the target product was achieved.

Other thematic lines developed by Assoc. Prof. Simeonov include synthetic modifications of natural products such as lupanin and oleuropein, aimed at applications in medicinal chemistry; the development of new  $\text{CO}_2$  absorption materials; new synthetic approaches for direct amidation of esters, etc.

The candidate has presented the directions for his future research, which are in the field of organic synthesis with the application of green chemistry approaches - a topic which importance will increasingly grow and will impact the industry.

Assoc. Prof. Simeonov is the corresponding author of 11 publications and the first author of 3 publications out of the 17 research articles presented in the competition, which clearly demonstrates his leading role in the presented works. The publications are in journals with a high IF and leading in the scientific field in which Assoc. Prof. Simeonov works, such as: ChemSusChem, Green Chemistry, ACS Catalysis, ChemCatChem, Chemical Reviews, etc. According to the presented list of a total of 12 publications under the the forth indicator, Assoc. Prof. Simeonov has been the corresponding author of 6, and in 1 of them he has been also the first author.

## **5. Critical remarks and recommendations**

I have no critical remarks on the materials presented in the competition.

## **CONCLUSIONS**

Based on the documents and scientific works presented in the competition, I believe that Assoc. Prof. Dr. Svilen Simeonov fully meets the requirements for occupying the academic position of "professor" according to the DASRBA and the specific requirements laid down in the Rules on the terms and conditions for acquiring scientific degrees and for occupying academic positions at IOCCP-BAS. His scientific production and competence with a clear thematic focus on industry-priority methods and technologies, as well as his strong project activity and participation in the training of young specialists, is a strong ground to express a positive opinion and recommend to the members of the Scientific Council of IOCCP-BAS to vote positively for the election of Svilen Simeonov to the academic position of "professor" in the Professional Field 4.2. Chemical Sciences, Scientific Specialty "Organic Chemistry".

15.03.2023

Prof. Dr. Neli Koseva