

Opinion

by **Prof. Milena Petkova Popova, PhD,**

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on the materials submitted in a competition for the academic position of **Professor** at the Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences (IOCCP-BAS), in professional field 4.2. Chemical Sciences, scientific specialty "Organic chemistry"

Assoc. Prof. Dr. Svilen Plamenov Simeonov from IOCCP-BAS, Laboratory "Organic synthesis and stereochemistry" is the only candidate in the competition for the academic position of Professor, announced in the State Gazette, issue 89 dated 8 November 2022, and on the website of IOCCP-BAS.

1. General presentation of the procedure and the candidate

The set of materials submitted by Assoc. Prof. Dr. Svilen P. Simeonov is in accordance with the Regulations of the Development of the Academic staff of the IOCCP-BAS, and meets the criteria of the Institute for the academic position of Professor.

The candidate participates in the competition with 17 scientific papers (5 included in indicator "B" and 12 in indicator "Г"), of which 15 are research articles, and 2 are review articles. Sixteen of the papers are published in Q1 journals and 1 is in Q4 journal. Citations noticed in WoS and Scopus are 901; the candidate's h-index is 17 (Scopus). Dr. Simeonov has been a leader of 4 international and 2 national research projects, two of them on-going, with 1 248 060 BGN of funding. He is a participant in other three national projects. Materials and data for participation in scientific forums and awards received are also provided.

Assoc. Prof. Dr. Svilen P. Simeonov began his scientific career in 2006 as an assistant at IOCCP-BAS (2006-2010). In 2010-2014, he was a PhD student at the Faculty of Pharmacy of the University of Lisbon, where in 2014 he obtained his PhD degree. In the same year, he returned to IOCCP and successively held the positions of assistant (until 2017) and associate professor (at present). In the period 2014-2016, Dr. Simeonov realized two specializations in the field of (bio)organic synthesis at Universities of Vienna, Austria. He is currently Head of the Laboratory "Organic synthesis and stereochemistry" at IOCCP-BAS, a leader of the Bulgarian team on a project financed under H2020-WIDESPREAD, and leader of project under the national science program "Vihren". The candidate is a supervisor of one PhD student. Assoc. Prof. Dr. Simeonov has published 38 scientific papers, which have received over 2 000 citations. He is a member of the editorial board of *Catslyst* and *Frontiers in chemistry*. Dr. Simeonov was awarded the "Green Chemistry for Life" from UNESCO, FOSAGRO and YUPAK for young researchers (2015) and the "Acad. Bogdan Kurtev" for achievements in the field of organic chemistry (2019).

2. General characteristics of the candidate's activities. Evaluation of the contributions and their significance

Dr. Simeonov's research is in the scientific field of Organic synthesis and Green chemistry. The studies are focused mainly on biorefinery, undoubtedly modern and perspective area, with an emphasis on production of various products based on furan derivatives. In his research, a drive to overcome difficulties and challenges faced by science and industry stands out, the results of which have led to innovative solutions and results expanding the possibilities for a more rational use of biorenewable resources.

The contributions presented in the habilitation work (set of publications) are summarized in the direction New methods for the intensification of the furanic platform, Synthetic modifications of natural products, and Other topics. They are formulated clearly and precisely, and can be classified as original fundamental and scientifically applied contributions.

The contributions in the direction **new methods for the intensification of the furanic platform** are related to the *development of new approaches and methods for obtaining industrially valuable chemical products, and for biologically active substances, including newly obtained catalysts, optimization of the methods in terms of yield and guided by the principles of green chemistry*. The contributions can be summarized as follow:

✓ An new concept to achieve pentane-1,2,5-triol from furfuryl alcohol *based on Achmatowich rearrangement* and subsequent hydrogenation of the resulting intermediate was proposed. Initially, the transformation was achieved in a liquid phase. Further, a highly effective green method was developed by gas-phase hydrogenation. *For these contributions, the candidate was awarded the "Acad. Bogdan Kurtev" for achievement in the field of organic chemistry*. The obtained product was used for preparation of a new nanogel with an application as an antitumor drug delivery system of doxorubicin.

✓ The first, *and so far only*, effective stabilizer ($\text{Na}_2\text{S}_2\text{O}_4$) of 5-hydroxymethylfurfural was proposed in conditions of preparation, processing and vacuum distillation as well as a new concept for synthesis of substituted furans (potential biologically active substances) based on furan-2,5-dicarboxylic acid in a sequence of biocatalyzed desymmetrization and functionalization of unreactive furan core. *The results are published in ChemSusChem, and distinguished as very important papers (VIPs)*.

✓ A new synthetic route towards biorenewables and biologically active lactones by using Ru-catalyzed isomerization of Achmatowich derivatives was developed. In the process, *transformations utilize the reduction of the C=C bond*.

✓ A method for the synthesis of 5-hydroxymethyl furfural from glucose was developed. Using 5-hydroxymethyl furfural as a starting material, in a suitable reaction media, using suitable catalysts and flow reactors, and *by developed new green methods*, other industrially important furan derivatives were also obtained.

Contributions in the direction of **synthetic modifications of natural products** are related to the obtained *new biologically active substances and valuable for the asymmetric synthesis*: a set of C2 modified analogues of the alkaloid sparteine, using lupanine, and showed as a potential new class of therapeutic agents with a long-lasting analgesic effect; biologically active compounds based on the monoterpene unit of oleuropein; (+)-(1R,5S,11 α S)-tetrahydrodeoxycytisine as free base, mono- and dihydrochloride, which were characterized by NMR for the first time. *The studies are based on readily available natural compounds/waste products as a starting material*.

Last but not least are the contributions in the direction **other topics**. Nanoporous materials with a high CO_2 adsorption capacity were obtained based on modified with organic amines mesoporous silicates, and the process's mechanism was studied by ^{13}C NMR. A new comprehensive green method for the synthesis of amides from amines and esters was developed. Significant contributions to the candidate's work are also the review articles devoted to shikimic acid and its epimers in terms of their production (*paper in Chem. Rev. with IF2018 54.301*) and methods for noncovalent control in the functionalization of arenes.

The results achieved are undoubtedly a reflection of critical and creative thinking as well as of precise implementation of the studies. This is supported by the fact that the papers are published in high impact journals such as *ChemSusChem* (IF2018 7.804; IF2019 7.962), *Green Chem.* (IF2019 9.480), *ACS catal.* (IF2021 IF 13.700), *ChemCatChem* (IF2018 4.495) and *Nanomaterials* (IF2021 IF 5.719). The results were presented at international conferences and symposia.

The candidate's results, presented in 30 publications, have received a high number of citations - 901 for a 5 year period (after holding the position of Associate Professor).

The scientific qualification, the leading and personal contribution of Assoc. Prof. Dr. Svilen Simeonov in the submitted papers is indisputable. He is the author of correspondence of a significant part of them, and is a leader of research projects within the field. These indicators, along with his established scientific collaborations, are a prerequisite for successful implementation of his

research plans, aimed at deepening and expanding research in the field of organic synthesis and green chemistry.

3. Critical comments

I have no substantial critical remarks. Materials are precisely organized and presented as required. I have only one note regarding the numbering of the publications presented in the habilitation thesis. There is an inconsistency in their numbering and that in the lists and evidentiary material of the publications according to indicators “B” and “I”, which makes it difficult to track them.

4. Personal impressions

I know Assoc. Prof. Dr. Svilen Simeonov as a colleague at IOCCP, including in his position as a head of the lab "Organic synthesis and stereochemistry" and vice-chairman of the Scientific Council of the Institute. My personal impression, supported by his overall activity and future research plans, is that he is a cooperative and correct person; he is a researcher with personal scientific style and innovative thinking. I wish him to keep his scientific curiosity, thoroughness and precision, and to reach new achievements.

CONCLUSION

The research work and research metric indicators of Assoc. Prof. Dr. Svilen Plamenov Simeonov, reflected in the documents and materials submitted for the competition cover and exceed the requirements for the academic position of Professor. The documents and materials enclosed are in accordance with the Act for the Development of the Academic Staff in the Republic of Bulgaria, the Regulations of BAS, and the Regulations of IOCCP-BAS.

The candidate has presented enough number of scientific papers, not presented in other competitions, with original fundamental and scientifically applied contributions, which are published in high impact international journals and have received high recognition.

Based on analysis of the research output of Assoc. Prof. Dr. Svilen Simeonov, its importance and the scientific contributions reflected therein, I give convincingly my **positive assessment** and recommend to the Scientific Jury to prepare a report-proposal to the Scientific Council of IOCCP-BAS for **election of Assoc. Prof. Dr. Svilen Plamenov Simeonov to the academic position of Professor at IOCCP-BAS** in the Area of higher education 4. Natural Sciences, Mathematics and informatics, professional field 4.2. Chemical Sciences, scientific specialty "Organic chemistry".

Sofia, 16 March 2023

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/Prof. Dr. Milena Popova/