

Attitude of Reviewer

by Assoc. Prof. Dr. Bistra Atanasova Stamboliyska, Institute of Organic Chemistry with Centre of Phytochemistry (IOHCPH), Bulgarian Academy of Sciences (BAS)

of the materials submitted for the competition for filling the academic position of an Associate Professor at IOCCPH – BAS in a field of higher education 4.0. "Natural Sciences", professional field 4.2. "Chemical Sciences", scientific specialty „Bioorganic Chemistry, Chemistry of Natural and Physiologically Active Substances”

In the competition for "Associate Professor" position, announced in the State Gazette, issue 43 of 31.05.2019 and on the website of IOCCF - BAS only Dr. Miroslav Rangelov submitted documents for participation.

General presentation of the procedure and the applicant

The presented set of documents and materials for review meets the requirements of the Rules for the conditions and procedure for acquiring scientific degrees and for occupying academic positions at IOCCPh - BAS. The candidate has attached an extended habilitation work; list and copies of articles outside the dissertation - 5 in the category "Publications in specialized scientific publications equivalent to monographs" and 11 in the category "Other original research publications"; book chapter and article citation list between 2008 and 2012. The distribution of scientific papers according to the relevant Q factors is as follows: 9 articles in category Q1, 4 articles in Q2 and 3 articles in Q4. A summary has been attached, which shows that Miroslav Rangelov exceeds in all indicators the national and additional minimum requirements of IOCCPH - BAS for occupying the position of "Assistant Professor".

Miroslav Rngelov has a Master's Degree in Organic and Analytical Chemistry from the Sofia University "St. Kliment Ohridski in 1997 and received his doctoral degree in 2008 after successfully defending a dissertation on "Participation of a vincal hydroxyl group in the biosynthesis of a peptide bond in the ribosome". From 2005 to 2011 he has been an assistant and from 2011 till now he is a senior assistant at the Laboratory of Chemistry and Biophysics of Proteins and Enzymes at IOCCPH - BAS.

General characteristic of the applicant's activity

To participate in the competition, 16 scientific publications in scientific journal, referenced and indexed in international databases were presented. Indicative of the quality and relevance of the conducted studies is the fact that 70% of the results (11 articles) were published in high impact factor journals, such as Journal of the American Chemical Society ($IF^{2018}=14.69$), ACS Chemical Biology ($IF^{2018}=5.374$), European Journal of Medicinal Chemistry ($IF^{2018}=4.83$), Journal of Organic Chemistry ($IF^{2018}=4.74$), Food Chem. Toxicol ($IF^{2018}=3.97$), Metallomics ($IF^{2018}=3.57$), The Journal of Physical Chemistry A ($IF^{2018}=2.84$), Drug Development Research ($IF^{2018}=2.64$),

International Journal of Quantum Chemistry (IF²⁰¹⁸=2.26), Journal of Molecular Graphics and Modelling (IF=1.86). The research has attracted much attention in the scientific literature. According to the latest information in the SCOPUS database, the entries in the competition paper have been cited 134 times (without self-citation) in international journals. The H factor is 8. The contribution of Dr. Miroslav Rangelov to the conducted research is indisputable. In five of the presented articles he is the first author and in five the second.

Dr. Miroslav Rangelov's scientific research is in the field of computer modeling of biological systems and processes. Much of the research has been devoted to elucidating the mechanism of aminolysis of esters as a model reaction for peptide bond formation in ribosomes. The candidate's work is impressive by the proposed new approaches and software for solving various problems related to molecular modeling of processes in biological systems. A software product (MolRan) includes automated procedures for selection of computational method based on statistical analysis as well as generation of the lowest energy transition states with pre-defined topology to define the most energetically favorable reaction route has been created. An original algorithm using catalytic maps was developed to determine the optimal position of proton-donor or proton-acceptor groups for the activation or inhibition of peptide bond formation. A new computational method was developed for neutralization of negative charge of the phosphate group in the ribosome by adding counterions.

The research with appropriate computational methods has made it possible to evaluate the various factors that influence the mechanism of peptide bond formation in living cells. These studies are essential for medical chemistry and drug design. Recent research of the candidate Dr. Miroslav Rangelov are focused on the modeling of molecular structures and complexes between biologically active molecules and their receptors, as well as prediction of their pharmacological activity towards the receptors. The studied molecules have potential application in the treatment of various pathological conditions such as cancer, hyperuricemia, epilepsy and antibodies for laboratory diagnosis and medicinal screening.

Participation in projects and scientific forums

A significant part of the research work is related to active participation in international and national projects. The candidate is the leader of two projects - one international, funded under the 7th Framework Program and one national, funded by the Nation Science Found of Bulgaria and participates in 5 international and 16 national scientific projects.

The research results were presented in 46 national and international forums with 29 poster and 17 oral communications.

Personal impressions

My personal impressions of Dr. Miroslav Rangelov are very good. He is an interdisciplinary specialist who willingly gets involved in solving various research problems. He has mastered and successfully applied advanced methods and approaches, such as molecular modeling and chromatographic (HPLC) techniques and is a good specialist in programming and processing data from scientific experiments with statistical and other computational methods.

CONCLUSION

In the announced competition, Dr. Miroslav Rangelov presents a sufficient number of high quality scientific papers, published after the materials used in the defense the PhD thesis. The large number of citations is a clear proof of the relevance of the research carried out and its use by the scientific community. The candidate is a specialist who can successfully solve various scientific problems in the field of pharmaceutical chemistry and medicinal design.

After the evaluation of the materials and scientific papers presented in the competition, analyzing their importance and their scientific contributions, I give my positive assessment and recommend to the Scientific Jury to prepare a report-proposal to the Scientific Council of IOCCPH-BAS for the selection of Dr. Miroslav Rangelov at the academic position of "Assistant Professor" in the professional field „Bioorganic Chemistry, Chemistry of Natural and Physiologically Active Substances”

16.09.2019 г.

Reviewer: