OPINION

from Assoc. Prof. Dr. Hristiyan Aleksandrov Aleksandrov
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on the application of Head Assistant Professor Dr. Miroslav Angelov Rangelov, in competition for Associate Professor in 4.2 Chemical Sciences (Bioorganic Chemistry, Chemistry of Natural and Physiologically Active Compounds) at the Institute of Organic Chemistry with Center of Phytochemistry, Bulgarian Academy of Sciences, announced in Bulgarian State Gazette No. 43 of 31/05/2019

Head Assistant Professor Miroslav Angelov Rangelov is the only candidate at the competition for associate professor. In 1997, he completed his Master's Degree in Organic and Analytical Chemistry at the Faculty of Chemistry, Sofia University "St. Kliment Ohridski". In 2008, he obtained his PhD in chemistry from the Institute of Organic Chemistry with a Phytochemistry Center, Bulgarian Academy of Sciences (IOCCP-BAS). The title of the PhD thesis is "Participation of a vicinal hydroxyl group in peptide bond biosynthesis in the ribosome - model studies". So far, the scientific career of the candidate is related to the IOCCP-BAS, occupying successively the following positions: chemist in the period 2002-2005, scientific associate III degree in the period 2005-2008, scientific associate II degree in the period 2008-2011, and since 2011 he is a Head Assistant Professor.

Dr. Rangelov participates in the competition with 17 scientific publications, 16 of which are in refereed and indexed journals with a total Impact Factor (IF) of 42.397, and one is a book chapter published by Elsevier. Most of these publications (9) are in first quartile journals (Q1), four publications are in journals from Q2 and three are in Q4. Some of these journals are among the most respected ones in the field of chemistry (*Journal of the American Chemical Society*) and in particular Bioorganic chemistry, as well as the chemistry of natural and physiologically active compounds (*The Journal of Organic Chemistry, ACS Chemical Biology, Metallomics , European Journal of Medicinal Chemistry, Food and Chemical Toxicology, Drug Development Research*). The publications of the candidate have been cited 54 times, as almost all citations are in international journals, including *Nature* and *JACS*. These scientific achievements exceed all the minimum national requirements stipulated in the Act for the Development of the Academic Staff in the Republic of Bulgaria, as well as

additional criteria of the IOCCP-BAS for occupying an academic position of "Associate Professor". Dr. Rangelov has also significant number of participations in national (16) and international (6) research projects. He is also a leader of the scientific team in one national and one international research project. He has presented his scientific results at 40 national and international forums, to which he has presented 17 oral presentations and 29 posters.

The scientific publications of the candidate are mainly in the field of computational chemistry and drug design and are focused mainly on the revealing of mechanistic aspects and characteristics of biomolecules. A major topic is to elucidate the reaction concerning the synthesis of a peptide bond in the ribosome, catalyzed by a vicinal hydroxyl group in the ribose ring, i.e. reaction of aminolysis of esters by quantum chemical calculations. Appropriate models and computational methodology have been selected for this purpose. It is noteworthy that the candidate not only relies on the available literature data and his chemical intuition in the preparation of the initial structures of reagents, transition states, intermediates and final products, but develops automation procedures for the stages of systematic investigation of similar reaction mechanisms. They have been implemented in the MolRan software package, developed by Dr. Rangelov. Personally, I have used this program and I find it very useful as it allows visualization, generation and manipulation of molecular structures as well as analysis of their properties. MolRan can work directly with input and output files from various molecular simulation packages such as: GAUSSIAN, GAMESS, MOPAC, PARAGAUSS, HYPERCHEM, etc. The program is also used in the education process of Bachelor, Master and PhD students.

I know the candidate and my personal opinion is that he has a high level of competence not only in the field of Bioorganic chemistry and chemistry of natural and physiologically active compounds, but also in the field of quantum-chemical modeling of bioorganic systems. The latter, as well as his programming skills, allow him not only to successfully use commercial software packages, but also to develop new ones when solving scientific problems.

In conclusion, taking into account the applicant's scientific results and achievements mentioned above, I consider that Head Assist. Prof. Miroslav Angelov Rangelov fully meets all the minimum national requirements as well as the criteria of the Institute of Organic Chemistry with Center of Phytochemistry at the Bulgarian Academy of Sciences for occupation of the academic position "Associate Professor" and I strongly recommend that he

should be selected as "Associate Professor" in 4.2 Chemical Sciences (Bioorganic Chemistry, Chemistry of Natural and Physiologically Active Compounds) at the Institute of Organic Chemistry with Center of Phytochemistry of BAS.

12/09/2019 Assoc. Prof. Dr. Hristiyan Aleksandrov