OPINION

of the member of Jury Professor Ivan Panaiotov on the procedure for occupation of academic position of Associate Professor announced in the State gazette issue 52 (2019)

professional field 4.2 Chemical Sciences (Theoretical Chemistry)

The candidate Miroslava Nedyalkova submits to the competition all the documents required by the Low and the Regulations on the conditions and procedures for obtaining academic degrees and occupying academic positions in the University of Sofia.

The research activity of Nedyalkova is presented at the competition with a list of 16 articles, 14 of which were published in international reputable scientific journals as Adv. Coll. Int. Sci., J. of Chem. Information and Modeling, Molecules, Ecotoxicology and Environmental Safety, J. of material science technology, J. of Chem. Physics, Open Chemistry etc..., one in bulgarian review "Comptes rendus de l'Académie bulgare des Sciences" and a Habilitation thesis. A list of all Nedyalkova's 31 publications is also included in her documentation.

The important part (12 from 16) publications presented for the procedure are based on the chemometrical combined with molecular dynamics methods. The developed approaches are directed to the environmetrics data interpretation. The obtained results are in relation with some important actual problems as the increased healthcare requirements in food industry, the risk from the environmental presence of residues of various pharmaceutics, the new opportunities that nanoparticles provide in pharmacy etc... Some examples: The presented Habilitation thesis is entirely devoted to the application of chemometrical methods in the fast growing field of nanogalenics. In publication \mathbb{N}_2 1 (following the list of 16 ones) a methodology for predicting the O/W and O/A partition coefficients is developed. In \mathbb{N}_2 2 a selection of 1400 proteins is analyzed by the discriminant and cluster analyses in order to separate allergic from non-allergic proteins. In \mathbb{N}_2 13 a multivariable statistical classification is used successfully in plant taxonomy. In \mathbb{N}_2 15 the influence of mixtures of 9 pharmaceuticals against 2 organisms is studied etc...

In general, the obtained results and corresponding conclusions are convincing and sound well. The chosen by Nedyalkova direction of research in so important and rapidly developing domains is promising for her future scientific activity. She promoted the obtained results in a large

number of international meetings and workshops in Spain, UK, Portugal, Italy, Switzerland and Bulgaria. Nevertheless, some remarks and suggestions could be made. For example, the first approach using in the modeling of mixtures toxicity (paper № 15) based on the additivity of effects needs some additional experimental and theoretical development. Some remarks concerning the part of the book devoted to the classical DLVO theory and electrical double layer can be also formulated etc...

It is important to note that the investigations are performed in the framework of a successful cooperation with leading laboratories from Spain and Poland. Nedyalkova's role in this collaboration is undeniable and present her in excellent light. Proof of such skills is the fact that she is also a leader and participant in an impressive number of scientific and teaching projects. Note that the publications No 27, 28 and 29 (from the list of all publications) are results of the specific responsibilities of the candidate in projects devoted to the electronic education, adaptation of teaching to the day after, carrier development of young scientist etc.. In these three papers some problems from the theory of higher education are discussed. That kind of ability in addition to its research and teaching activities support also her aspiration to be promoted to a higher academic rank.

The results obtained by Nedyalkova have been noted by the scientific community and cited 30 times in the issues referenced and indexed in Web of Science and Scopus.

The submitted reports №№ 12 and 15 show that the candidate has fulfilled (even exceeded) the criteria in the five groups for scientific activity as well as for teaching, required for occupation of the academic position of Associate Professor.

In conclusion, my opinion is that Nedyalkova's scientific as well as teaching and administrative activities fully comply with the requirements of the low and regulations. I suggest the Honorable Jury to propose to the Faculty Council to elect Miroslava Nedyalkova as Associate Professor.

Sofia, 25.10.2019

Prof. DSc. Ivan Panaiotov