STATEMENT

from Prof. DSc Sonia Varbanova Ilieva,
Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski"
on the materials submitted for the competition for the academic position of **'Associate Professor'**
at the Laboratory of Structural Organic Analysis (SOA),
Institute of Organic Chemistry with Centre of Phytochemistry (IOCCP), BAS
in higher education professional field **4.2. Chemical Sciences (Theoretical chemistry)**

In the competition for the academic position 'Associate Professor' announced in the State Gazette, issue 79/08.10.2019, **Assist. Prof. Dr Nadezhda Vasileva Markova**, Laboratory of Structural Organic Analysis (SOA), IOCCP, BAS is the only candidate.

The electronic and hard copy materials submitted by Dr Nadezhda Markova **meet all the requirements** of the Law for the Development of the Academic Staff in the Republic of Bulgaria and the relevant regulations for its implementation (including those of BAS and IOCCP). The applicant meets the criteria (minimum requirements) for the academic position 'Associate Professor', as well as the additional requirements of IOCCP-BAS.

N. Markova graduated with a Master Degree in Organic Chemistry from the University of Shumen "Konstantin Preslavski" in 2000, after that she completed her doctorate at IOCCF, BAS. In 2005 she defended her doctoral dissertation on *"Theoretical studies of tautomeric equilibria in organic molecules taking into account the specific influence of the solvent"* under the guidance of Prof. Venelin Enchev, with whom she continues collaborative research to this day. Since 2006 she has been Assistant Professor at IOFCF.

Dr Markova has published a **total of 32 scientific publications** (with 314 citations according to the information provided, h index 7 (Scopus), 9 (Google Scholar), with 27 publications being in Impact Factor (IF) journals, in 4 of these she is the corresponding author. To participate in the present competition, she has submitted **18 scientific papers,** for 6 of these being the first but not the corresponding author. The publications correspond to the subject of the competition and do not repeat the papers included in her doctoral thesis. The scientific articles are published in reputed international journals with impact factor and are distributed in the respective quartiles as follows: 5 - in Q1, 5 - in Q2, 4 – Q3, 3 – Q4, thus demonstrating the **quality of the research studies.** The average impact factor (IF) of these publications is 2.06, varying from 0.238 (*Bulg. Chem. Commun. – 3 papers*) to 7.346 (*Acta Biomaterialia – 1 paper*). The science metrics demonstrate the level of Dr Markova scientific work and therefore the Associate Professor position is a natural result in her scientific career.

The overall scientific activity of Dr Markova is in the field of theoretical chemistry, with tautomeric equilibrium research taking a major role. The presented **habilitation thesis** is dedicated to the study of the role of water as a medium and catalyst in tautomeric transformations of nucleic bases and nucleosides, covering five scientific publications. The mechanism of proton transfer reactions in the compounds studied is clarified. The approach in which the influence of the solvent is considered both as a continuous reaction medium and explicitly incorporated water molecule(s) has been proven to be the most correct in theoretical

studies of tautomeric transformations. In the introductory part of the habilitation work, the main scientific contributions of the research are defined: elucidation of the structure of organic compounds and the mechanism of proton transfer processes by theoretical quantum-chemical approaches. In the thesis the candidate's view on further research developments is presented: widening of the research in a new scientific field is envisaged - application of quantum-chemical and docking methods in phytochemistry for elucidating the active components and the mechanism of their action.

N. Markova has managed three **scientific projects**, two of which are ongoing. She has participated in eight national scientific projects, three of which comprising international collaboration. She has participated in a number of national and international scientific congresses / conferences.

The **educational and pedagogical activity** of the applicant is expressed in: (i) guidance of the practices of 9 students under the Student Practices project; (2) guidance of 1 graduate in the preparation of their diploma works for obtaining Bachelor and Master Degrees.

CONCLUSION

According to the submitted materials and scientific publications, the above analysis of their importance and scientific contributions, I am convinced in my **positive assessment** and firmly recommend to the Scientific Jury to prepare a report-proposal to the Scientific Board of IOCCP-BAS for the selection of **Dr Nadezhda Vasileva Markova** for the academic position of **'Associate Professor'** at IOCCP-BAS in the professional field 4.2. Chemical Sciences (Theoretical Chemistry).

12/02/2019 Reviewer: *Prof. Sonia Ilieva*