

STATEMENT

regarding the quality of the doctoral thesis of the full-time doctoral student Silvia Hristova Hristova in field of higher education 4. Natural Sciences, Mathematics and Informatics, professional classification 4.2. Chemical sciences, Scientific specialty Organic chemistry

from Prof. Dr. Rositsa Dimitrova Nikolova, Sofia University "St. Kliment Ohridski ", Faculty of Chemistry and Pharmacy, member of the scientific jury

Brief biographical data

Silvia Hristova graduated with honors a bachelor's degree in chemistry in 2015 and received a gold medal for an excellent master's degree in "Modern methods for synthesis and analysis of organic compounds" in 2016 at the Faculty of Chemistry and Pharmacy of Sofia University "St. Kliment Ohridski-". During her studies she worked as a chemist at the Institute of Organic Chemistry with Center of Phytochemistry - BAS from October 2014 to December 2016. She was enrolled as a full-time doctoral student in January 2017 at the Institute of Organic Chemistry with Center of Phytochemistry - BAS with supervisor Prof. Ludmil Antonov.

Scientific contributions of the dissertation

The presented PhD thesis on the topic: "Tautomerism as an elemental mechanism for signal transfer in molecular devices" is a serious study with a strong complex nature. The research is fundamental in nature with a high potential for application.

The effect of control tautomerism on the switching action of two types of azo dyes has been studied and in my opinion the following results are the most significant:

- It has been shown that structural changes in the starting compounds allow control of the position of the tautomeric equilibrium in solution, as the processes are reversible.
- It has been found that 1- (phenyldiazhenyl) -3- (piperidinylmethyl) naphthalen-2-ol 2.3 is a suitable tautomeric switch and on the basis of experimental and theoretical studies of its behavior a concept for stimulated proton transfer has been defined by introducing into the molecule of an unconjugated functional group that transmits the action of external stimuli to the tautomeric fragment.
- It has been shown that the use of 2J constants in rotary switches in solutions makes it possible to distinguish isomers.

The work includes a large volume of experimental material and analytical interpretation of the obtained results. During its implementation the doctoral student was given the opportunity to get acquainted with and apply a number of methods of organic synthesis, UV-Vis and NMR spectroscopy and quantum chemical calculations. The results obtained by Silvia Hristova are relevant and significant in an area that enjoys serious interest from various teams in the country and abroad.

Silvia Hristova's dissertation consists of 190 standard pages and includes 15 tables, 79 figures and 37 diagrams. 193 literature sources are cited. The presented project for an abstract accurately reflects the main results and conclusions of the dissertation.

Publishing activity

Four scientific reports have been published based on the results of the research, three of which in international scientific journals with $IF > 3$ and rank Q1. Five quotations had been noted until the documents were handed over. Silvia Hristova is a co-author of a total of twelve scientific publications (eight outside the topic of the dissertation), which are cited in a total of twenty-one scientific papers. The doctoral student participated and presented her results as six oral presentations and eleven poster presentations at sixteen scientific forums, five of which were abroad.

The research performed by the doctoral student requires precision, ingenuity, developed analytical thinking and ability to independently and systematically develop specific scientific tasks. Silvia Hristova has worked successfully in various teams, both within the institute and research institutes abroad.

Conclusion

The dissertation of Silvia Hristova Hristova contains sufficient scientific results, which are original contributions and meet the requirements of the Law on the Development of Academic Staff in the Republic of Bulgaria, the Regulations for its implementation and the relevant Regulations of IOHCF-BAS.

The scientific results, their convincing presentation, as well as my personal impressions are grounds to give a positive assessment of the dissertation of PhD student Silvia Hristova Hristova for the educational and scientific degree "Doctor" and I strongly recommend the esteemed members of the Scientific Jury to award Silvia Hristova Hristova scientific degree "doctor".

August 10, 2020

Prof. Dr. Rositsa Nikolova