



INTERNATIONAL SUMMER SCHOOL

Supramolecular chemistry in Medicine and in Technology: Advances and Challenges

30.08 – 03.09.2018

Albena (near Varna), Bulgaria



SupraMedChem@Balkans.Net

SCOPES Institutional Partnership

Welcome to SupraChemWorld

Dear Friends,

On behalf of **SupraMedChem@Balkans.Net**, an initiative supported by The Swiss National Science Foundation (SCOPEs 2013-2016 Programme), we would like to welcome you in Plovdiv at the International Summer School "Supramolecular Chemistry in Medicine and in Technology: Advances and Challenges". Our idea is to strengthen your knowledge about the applicability of supramolecular chemistry in technology and life sciences.

Katharina M. Fromm (University of Fribourg)

Liudmil Antonov (Bulgarian Academy of Sciences)

Miloš Djuran (University of Kragujevac)

Local organizing committee

(Bulgarian Academy of Sciences)

Liudmil Antonov

Vera Deneva

Silvia Hristova

SupraMedChem@Balkans.Net

SupraMedChem@Balkans.Net is an Institutional Partnership funded by The SCOPES 2013-2016 Programme of The Swiss National Science Foundation, with the aim to provide training in Supramolecular Chemistry for students and young researchers in the Balkan area (and not only). Supramolecular chemistry is a truly multidisciplinary research subject with great potential for the future technology development. And logically brings need for suitable teaching.

In this Institutional Partnership we unite the efforts of the Department of Chemistry and the Adolphe Merkle Institute (AMI) (University of Fribourg), the Faculty of Science (University of Kragujevac) and the Institute of Organic Chemistry (Bulgarian Academy of Sciences) in creating of suitable educational background for teaching in supramolecular chemistry and its biomedical applications in the Balkan area. This geographic area, for long time a synonym of violence and instability, is now in a process of transition, success of which crucially depends on the availability of well-educated, motivated, beyond geographical borders minded young people. With ***SupraMedChem@Balkans.Net*** we plan to create a solid background in the modern teaching in supramolecular chemistry and to implement the best Swiss educational and research standards. This will be achieved by a three layers approach:

- ***Teaching activities (basic layer)***, which aim to develop new curricula for teaching in supramolecular chemistry and to provide conditions for training in the general concepts of supramolecular chemistry by organizing Summer/Winter schools;
- ***Training initiatives (upgrade layer)***, which are directed to increase the capacity of the staff of the partner institutions to do research and education in biomedical supramolecular chemistry through personnel exchange and organizing workshops;
- ***Strengthening the research and renewal of the infrastructure (sustainable development layer)*** in order to strengthen the training and research capacity of the participating Balkan institutions.

Number of important outcomes is expected in respect of the institutional capacity building, but the most substantial benefits are expected for the young people (high school and university students, PhD students and young researchers). This IP provides a unique opportunity to build up an educational profile and research career. We will provide basic (Summer schools) and advanced (Workshops and exchange scheme) teaching by using the complementary expertise (solid state – solution – gas phase; theory – experimental studies) of the partner groups. Through the exchange schemes the trainees will have the opportunity to work in different scientific and cultural environment, to establish new contacts and friendships and to acquire new skills in the research and management. The proposal unites 3 successful research teams, working actively in experimental supramolecular chemistry, and gives a clear perspective for strengthening their research and teaching by creating condition for expansion in the biomedical direction and for collaborative networking in future.

SYNTHESIS, MOLECULAR STRUCTURE AND ANTIOXIDANT ACTIVITY OF NEW BENZIMIDAZOLE FORMAZANS

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The chemistry of formazans have attracted the interest of many research groups due to their wide biological activity such as antioxidant, antiviral, antimicrobial, anti-inflammatory, anticancer, anti-HIV [1], [2], [3].

Herein we report the synthesis of new formazan derivatives containing benzimidazole fragments obtained by autoxidative coupling of 2-hydrazino-1*H*-benzimidazole in pyridine solutions with a variety of benzimidazole hydrazones. Tautomerization properties and geometric isomers based on conjugate π -system of formazans were theoretically studied using density functional theory (DFT) methods. It was found that according to the electronic and steric properties of the substituent at the C3 position, the azohydrazone chain adopts either closed-ring chelate configuration or half-closed ring configuration.

Selected formazans were investigated for hepatoprotective and antioxidant activity on isolated rat hepatocytes. In tert-butyl hydroperoxide induced oxidative stress, the studied compounds showed cytoprotective and antioxidant effects similar to those of Quercetin. Different possible mechanisms of antioxidant action such as hydrogen atom transfer (HAT), single-electron transfer (SET-PT), sequential proton loss electron transfer (SPLET) were estimated by DFT computations in polar and nonpolar medium.

References:

- [1] A. S. Shawali, N. A. Samy, *J. of Adv. Res.*, **6**, 241 (2015).
- [2] J. D. Bhosale, A. R. Shirolkar, *J. of Pharm. Res.*, **7**, 582 (2013).
- [3] N. P. Bednyagina, I. Ya. Postovskii, *Rus. Chem. Rev.*, **44**, , 493 (1975).