

*University of Plovdiv „Paisii Hilendarski“
Faculty of Chemistry*



11th Chemistry Conference

Plovdiv, 11 –13 October 2018

<https://11cc.uni-plovdiv.net>

Book of abstracts



LECTURES

Friday 12 October 2018

Conference Hall Paldin

SECTION 1 Theoretical chemistry and Analytical chemistry

Chairman

K. Simitchiev

LECTURES

14:00 – 14:20	S1L1	Tautomerism in azodyes and related Schiff bases: if theory meets experiment. <u>L. Antonov</u> BAS, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgaria
14:20 – 14:40	S1L2	DFT study of interactions between hydroxamic acids and histone deacetylases <u>N. Toshev, D. Cheshmedzhieva, T. Dudev</u> University of Sofia "St. Kliment Ohridski", Bulgaria
14:40 – 15:00	S1L3	One-pot synthesis of formamide-based prebiotic compounds after heating and proton irradiation <u>V. Enchev</u> BAS, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgaria
15:00 – 15:30		COFFEE BREAK
15:30 – 15:50	S1L4	Artificial intelligence applications in drug discovery <u>D. Hristozov</u> Evotec, UK
15:50 – 16:10	S1L5	Profile of volatile organic compounds (VOCs) emitted from the point of combustion of charcoals produced from three potentially toxic tree plants in Nigeria <u>J. Gushit</u> University of Jos, Nigeria
16:10 – 16:30	S1L6	Analysis of some illicit drugs and abused pharmaceuticals in municipal wastewaters (effluents) of Nottingham <u>M. Aliru Olajide</u> Kwara State University Malete, Nigeria
16:30 – 16:50	S1L7	Chemical reagents for detection of fluoroquinolones by immunoassays <u>S. Eremín</u> A.N. Bach Institute of Biochemistry, Research Centre of Biotechnology of the Russian Academy of Sciences, Moscow, Russia

**ONE-POT SYNTHESIS OF FORMAMIDE-BASED PREBIOTIC COMPOUNDS AFTER HEATING AND PROTON IRRADIATION**

V. Enchev¹, I. Angelov¹, N. Markova¹, N. Stoyanova¹, M. Kapralov²,
E. Krasavin², M. Rangelov¹, L. Avramov³

¹*Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Science, 1113 Sofia, Bulgaria, e-mail: venelin@orgchm.bas.bg*

²*Joint Institute for Nuclear Research,*

JINR's Laboratory of Radiation Biology, Dubna, Russia

³*Institute of Electronics, Bulgarian Academy of Science,
72 Tsarigradsko chaussee blvd., Sofia 1784, Bulgaria*

S1L3

Understanding the formation of biogenic molecules in abiotic conditions is a prerequisite in the origin-of-life studies. Determining the conditions allowing an efficient one-pot synthesis of the largest possible panel of biogenic compounds may shed light on the plausible scenario in which the processes that started life might have occurred. We report experiments describing the syntheses taking place from formamide. The warming of formamide at 170°C and 180°C in vacuo yielded large panels of different compounds: purine and nucleobases (adenine, cytosine and uracil), amino acids (glycine, alanine), hypoxanthine, pterine, urea and urocanic acid. After that to model the Solar Wind radiation, these probes were irradiated at 25°C with 170 MeV protons generated by the Phasotron facility of the Joint International Nuclear Institute (Dubna, Russia). The absorbed dose was 6 Gy. New panel of compounds was detected: timine, 2-methylpurine, 6-methylpurine, 4-methylcytosine and one nucleoside – 6-carboxamido-9-β-D-ribofuranosylpurine. Mechanism of reactions affording nucleic bases and amino acids were simulated by high-level (MP2 and SCS-MP2) ab initio quantum chemical methods.

Acknowledgements: Financial support from the grant DN09/7/2016 of the National Science Fund, Bulgaria, is greatly acknowledged.

**CYTOTOXIC AND ANTI-VIRAL ACTIVITIES OF THE PLANT
GRAPTOPETALUM PARAGUAYENSE E. WALTHER**

N. Markova¹, P. Genova-Kalu², I. Dincheva³,
I. Badjakov³, V. Enchev¹

¹*Institute of Organic Chemistry with Centre of Phytochemistry,
Bulgarian Academy of Sciences, Sofia 1113, Bulgaria; nadya@orgchm.bas.bg*

²*National Reference Laboratory "Rickettsia and tissue cultures", National Centre
of Infectious and Parasitic Diseases, Sofia, Bulgaria; petia.d.genova@abv.bg*

³*AgroBioInstitute, Plant Genetic Resources Group, 8 Dragan Tsankov blvd.,
1164 Sofia, Bulgaria; ivadincheva@yahoo.com*

Infectious diseases are the leading cause of global morbidity and mortality. 90% of infectious diseases in humans have viral aetiology. Frequent human infections of viral origin could be exemplified as common cold, influenza, varicella, AIDS, herpes simplex, infectious mononucleosis, avian influenza etc. Herpes simplex virus types 1 (HSV-1) and 2 (HSV-2) are common human pathogens associated with orofacial infections, genital lesions and encephalitis. Due to the increase of antibiotics resistance, there is an urgent need to develop new and innovative antimicrobial agents. Plants have long been investigated among the potential sources of new agents.

S2P50

The objective of our examination is to evaluate the *in vitro* anti-herpetic and cytotoxicity of *G. paraguayense* extracts using colorimetric assay.

Three main fractions were obtained – A (lipids), B (amino and organic acids, carbohydrates) and C (phenolic acids). The composition of each was determined by GC-MS analysis. The capacity for inhibition the lytic activity of HSV-1 Victoria strain and HSV-2 Bja strain and the reduction of viability of infected or uninfected cell cultures were defined by MTT assay. Data were used to calculate CC₅₀. The cytopathic effect (CPE) was expressed as a percentage of the optical density of the sample compared with untreated virus-infected cells. Acyclovir was used as positive control.

Fraction C has not CPE on human cell lines RD 64 and Lep and inhibits HSV replication in dose-dependent manner more efficiently against HSV-1, whereas its effect to HSV-2 was significantly lower. A and B fractions showed no antiviral effect.

The mechanism of the antiviral action of fraction C is not yet completely identified. Further studies are needed in order to verify which compounds could be responsible for this activity and how they exert their antiviral effects.

Acknowledgements: We acknowledge the financial support of the Bulgarian Fund for Scientific Research under Grant DH19/16.