9th Conference of Young Chemists of Serbia

Book of Abstracts

4th November 2023

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Dušan **SLADIĆ**, president of Serbian Chemical Society

Editors
Jelena **MILOVANOVIĆ**
Vuk **FILIPOVIĆ**
Života **SELAKOVIĆ**
Snežana **PAPOVIĆ**
Branko **KORDIĆ**
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

Page Layout and Design
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

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Scientific Committee

Dr. Jelena Milovanović - University of Belgrade - Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia

Dr. Vuk Filipović - University of Belgrade - Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia

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ИНОВАЦИЈА

Acknowledgement

Acknowledgement to the University of Novi Sad - Faculty of Sciences for the use of the space of the faculty during the 9th Conference of Young Chemists' of Serbia.

Thanks to the Board of the Serbian Chemical Society for the supporting during organization of the Conference.

Deeply acknowledgments to the European Young Chemists' Network for the financial support of the best oral and poster presentations.

Thanks to the Analysis doo for confidence and the promoting material.

Contents

Scientific Program

Time schedule	Program
8:30	*Registration of the participants* Mounting posters for the Poster Session 1 (**ODD POSTER NUMBERS**)
9:30	*Conference opening* Serbian Chemical Society Scientific Committee Serbian Young Chemists' Club presentation
9:45	*Plenary Lecture* **PP OP 01 – Gordana Krstić** University of Belgrade, Faculty of Chemistry, Belgrade, Serbia *"Determining the structure of natural products using NMR spectroscopy - is it enough or not?"*
10:20	*Popular Scientific Lecture* **Luka Mihajlović** (Analysis doo)
10:50	*Invited Lecture* **PPP OP 01 – Jelena Lazić** University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia *"From waste streams to biotherapeutics: making a connection using bacteria"*
11:15	*Coffee break*
11:30	*Invited Lecture* **PPP OP 02 – Alen Albreht** National Institute of Chemistry, Ljubljna, Slovenia *"Towards future food supplement ingredients: chemical modification of natural antioxidants"*
11:55	*European Young Chemists' Network (EYCN)* **Gaia De Angelis** – Global Connection Team Leader Soft-skill presentation

12:25	*Oral presentations, Session 1*
	DSC OP 01 – Nikola Radnović University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"Syntheses and structures of Ag(I) complexes with pyrazole-type ligand"*
	PFC OP 02 – Nikola Horvacki Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia *"Comparative assessment of preeminent sugars and organic acids in fruits of several apple cultivars"*
	PCC OP 02 – Katarina Ćeranić Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia *"Benzene coordination strengthens cation-π interactions: A DFT study"*
	SCCE OP 01 – Andrija Vukov University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"Hydration properties of the antidiabetic drug metformin in the presence of selected artificial sweeteners"*
	SCFM OP 01 – Daliborka Odoboša University of Belgrade, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, Belgrade, Serbia *"A novel gamma rays dosimeter based on organic dye and PVA: microwave synthesis and spectroscopic studies"*
	PFC OP 03 – Nikolina Sibinčić Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia *"Arthrospira platensis and Porphyra sp. – prospective serum-substitute in HEK293T cell culture"*
13:25	***GROUP PHOTO***
13:30	*Poster session 1* (**ODD POSTER NUMBERS**)
14:20	*Lunch* Removing posters from Poster Session 1 Mounting posters for Poster Session 2 (**EVEN POSTER NUMBERS**)

15:10	*Workshop* University of Novi Sad, Faculty of Sciences – Parliament University of Belgrade, Faculty of Chemistry – Parliament Young Division of Croatian Chemical Society
15:55	*Invited Lecture* **PPP OP 02 – Tatjana Majkić** University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"Polyphenols as modulators of prostaglandin E_2 and thromboxane A_2 production"*
16:20	*Oral presentations, Session 2*
	PCC OP 01 – Milica Bogdanović University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"The crystal structure of 3-(1-pyrazolyl)-L-alanine and its Ag(I) polymeric complex"* **PFC OP 01 – Mihajlo Jakanovski** Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia *"Validation and optimization of ion chromatography based method for citric acid determination in Robinia pseudoacacia honey"* **CS OP 01 – Branislav Kokić** Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia *"Teaching chirality on dynamic systems"* **CB OP 01 – Ana Matošević** Institute for Medical Research and Occupational Health, Zagreb, Croatia) *"Design, synthesis and biological evaluation of carbamates as cholinesterases inhibitors in the treatment of Alzheimer`s disease"* **EA OP 01 – Marija Kuč** University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"Photodegradation of organic UV filters in water using UV/chlorine and UV/H_2O_2"* **EA OP 01 – Sara Pepić** University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia *"Physico-chemical and structural characterization of the pharmacologically active ionic liquid tetracainium-ibuprofenate"*

17:10	*Poster session 2* (**EVEN POSTER NUMBERS**) *and Coffee break*
	Closing ceremony
18:00	• **Best Oral Presentation Award** • **Best Poster Presentation Award**
18:15	*End of the Conference*

POSTER NUMBER is the last part of the contrubition code, e.g. XY PP 15.

VENUE:

- Lectures and oral presentations will be taken place at the "Mihajlo Pupin" amphitheater on the ground floor at the Department of Matematics and Informatics and the Department of Physics, Faculty of Science, University of Novi Sad (address: Trg Dositeja Obradovića 4, Novi Sad).
- The Poster sessions will take place in the hallway in front of the "Mihajlo Pupin" amphitheater.

CB PP 19

Identification of the new candidate NLRP3 inhibitor using combined computational approach

Kristina Stevanović[1], Milan Senćanski[2], Vladimir Perović[1], Sanja Glišić[1]
[1] *University of Belgrade - Vinča Institute of Nuclear Sciences, Belgrade, Serbia*
[2] *University of Belgrade - Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia*

The NOD-like receptor pyrin domain-containing protein 3 (NLRP3), an important intracellular sensor in the innate immune system, detects a plethora of exogenous and endogenous stimuli, leading to inflammasome formation and caspase-1 activation. More recently, it emerged as an attractive drug target due to abnormal NLRP3 inflammasome activation implicated in many acute and chronic diseases (including diabetes, atherosclerosis, metabolic syndrome, cardiovascular, and neurodegenerative diseases) [1]. Several direct NLRP3 inhibitors that block its ATPase activity by keeping it in closed conformation have been reported [1,2]. Some of them have entered clinical trials, but still, none of them is FDA approved.

A powerful strategy in identifying potential NLRP3 inhibitors can be *in silico* drug repurposing of compounds with already known safety profiles. In this study, we performed a virtual screening protocol that considers both long- and short-range interactions between molecules. First, the Informational spectrum method developed for small molecules was applied for searching the Drugbank database. Selected candidates were filtered by successive cross-correlation spectra analysis. Finally, after molecular docking, we identified the most promising candidate and proposed it for further experimental testing.

References

1. R. Coll, K. Schroder, P. Pelegrín, *Trends Pharmacol. Sci.* **2022**, *43* (8), 653-668.
2. I. Hochheiser, M. Pilsl, G. Hagelueken, J. Moecking, M. Marleaux, R. Brinkschulte, E. Latz, C. Engel, M. Geyer, *Nature*. **2022**, *604* (7904):184-189.

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