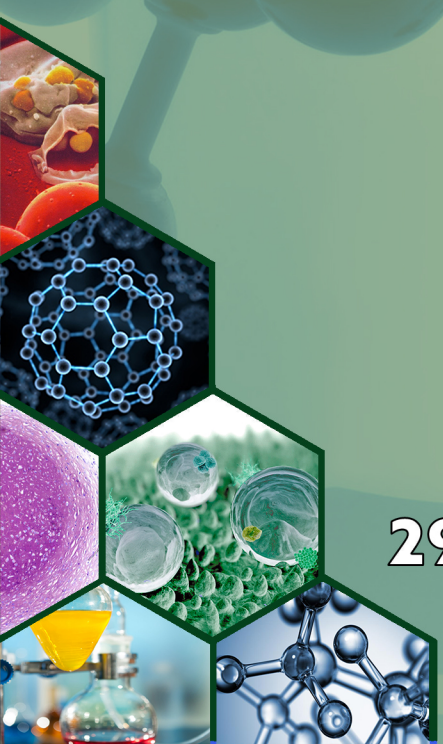
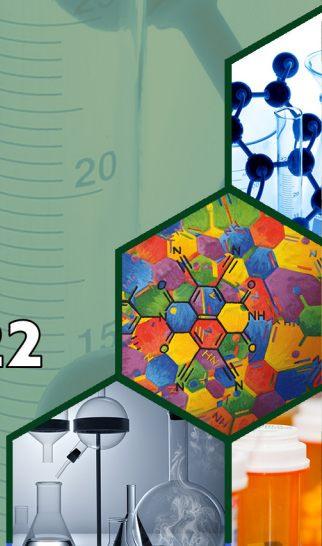
Serbian Chemical Society
Serbian Young Chemists' Club

Eight Conference
of the Young Chemists of Serbia

Book of Abstracts





Belgrade
29th OCTOBER 2022

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Scientific Program

Time	Program
9:00	*Registration of the participants* Mounting posters for the Poster Session 1 (**ODD POSTER NUMBERS**)
10:00	*Conference opening* Serbian Chemical Society – Dušan Sladić Scientific Committee – Vuk Filipović Serbian Young Chemists' Club presentation – Mihajlo Jakanovski
10:15	*Plenary Lecture* (**PP OP 01**) Ilija Cvijetić *University of Belgrade, Faculty of Chemistry*
11:00	*Oral presentations, Session 1*
	Zorica Novaković (**CMN OP 01**) *University of Novi Sad, Faculty of Sciences*
	Marija Kaluđerović (**OC OP 01**) *University of Montenegro, Faculty of Metallurgy and Technology*
	Marija Milošević (**MS OC 01**) *University Of Belgrade, Faculty of Technology and Metallurgy*
11:35	*Coffee break*
11:50	*European Young Chemists' Network (EYCN) ZOOM presentation* Maximillian Menche – Chair of the EYCN "The European Young Chemists' Network and the Power of Networking"
12:05	*Invited Lecture* (**PPP OP 01**) Ivana Kuzminac *University of Novi Sad, Faculty of Sciences*
12:40	*Oral presentations, Session 2*
	Dušica Jovanović (**TC OP 01**) *University of Belgrade, Institute of Nuclear Science Vinča* *University of Niš, Faculty of Science and Mathematics*
	Milica Đukić (**IAC OP 01**) *University Of Belgrade, Faculty of Technology and Metallurgy*
	Jovana Jovanović (**OC OP 02**) *University of Montenegro, Faculty of Medicine*
	Slađana Đorđević (**TC OP 02**) *University of Kragujevac, Faculty of Science*
13:25	***GROUP PHOTO***
13:30	*Poster session 1* (**ODD POSTER NUMBERS**)
14:15	*Lunch* Removing posters from Poster Session 1 Mounting posters for Poster Session 2 (**EVEN POSTER NUMBERS**)

15:00	*Invited Lecture* (**PPP OP 02**) Branko Kordić *University of Novi Sad, Faculty of Sciences*
15:35	*Oral presentations, Session 3*
	Dušan Ružić (**MC OP 01**) *University of Belgrade, Faculty of Pharmacy*
	Ana-Andrea Holik (**CE OP 01**) *University of Belgrade, Faculty of Chemistry*
	Aleksa Savić (**BB OP 01**) *University of Belgrade, Faculty of Chemistry*
16:10	*Poster session 2* (**EVEN POSTER NUMBERS**)
17:00	*Break*
17:15	*Closing ceremony* • ***Best Oral Presentation Award*** Board: Vuk Filipović, Ivana Kuzminac, Ilija Cvijetić • ***Best Poster Presentation Award*** Board: Jelena Milovanović, Branko Kordić
17:45	*End of the Conference*

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

VENUE:

- Lectures and oral presentations will be taken place at the **large chemistry amphitheater (VHA)** on the ground floor.
- The Poster sessions will take place in the **hallway in front of the library** on the 1st floor.

TC PP 07

Molecular docking of porphyrin-like complexes to SARS-CoV-2 main protease

Ignjat P. Filipović[1], Marko D. Radovanović[1], Maja B. Đukić[1], Marija S. Ristić[1].
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Molecular docking method, which was recently modified to allow traditional and covalent docking of organometallic compounds [1], was used to theoretically investigate the potential binding of 15 copper(II) complexes with porphyrin-like ligands to main protease of SARS-CoV-2 virion (CLpro). Method was implemented by importing published parameters into the program GOLD from the CCDC package. Target of the docking experiments was active site of the CLpro. Method was validated by redocking of N3 inhibitor, and by comparing obtained results with published crystal structure [2]. Structures of investigated complexes were obtained by filtering Cambridge Structural Database for porphyrin-like compounds with copper(II) ion. Each structure was refined using semi-empirical PM6 method implemented in MOPAC 2016 and subsequently modified for docking experiments with dummy hydrogen atoms that simulate metallic d-orbitals. Docking experiments were performed with 50 genetic algorithm runs for each investigated complex, GoldScore function was used to score fitness, no early termination was set, and rest of the settings were left at the default values. Obtained scores were then compared to the scores derived from experiment with known inhibitor to rank inhibitory potential of investigated compounds.

References

1. G. Sciortino, E. Garribba, J. D. Maréchal, *Inorg. Chem*. **2019**, 58, 294.
2. Z. Jin, X. Du, Y. Xu, Y. Deng, M. Liu, Y. Zhao, B. Zhang, X. Li, L. Zhang, C. Peng, Y. Duan, J. Yu, L. Wang, K. Yang, F. Liu, R. Jiang, X. Yang, T. You, X. Liu, X. Yang, F. Bai, H. Liu, X. Liu, L.W. Guddat, W. Xu, G. Xiao, C. Qin, Z. Shi, H. Jiang, Z. Rao, H. Yang, *Nature*. **2020**, 582, 289.

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