8th Conference of Young Chemists of Serbia

Book of Abstracts

29th October 2022
University of Belgrade, Faculty of Chemistry

CIP – Категоризација у публикацији
Народна библиотека Србије, Београд

54(048)
577.1(048)
60(048)
66.017/.018(048)

CONFERENCE of the Young Chemists of Serbia (8 ; 2022 ; Beograd) Book of abstracts / 8th Conference of the Young Chemists of Serbia, [Belgrade], 29th October 2022; [organized by Serbian Chemical Society [and] Serbian Young Chemists Club]; [editors Tamara Todorović ... [et al.]]. - Belgrade : Serbian Chemical Society : Serbian Young Chemists Club, 2022 (Belgrade : Development and Research Centre of Graphic Engineering Faculty of Technology and Metallurgy). - 150 str. : ilustr. + 24 cm Tiraž 20. - Bibliografija uz većinu apstrakata. - Registar.
ISBN 978-86-7132-080-1
1. Srpsko hemijsko društvo (Beograd) 2. Klub mladih hemičara Srbije (Beograd)
a) Хемија - Апстракти b) Биохемија - Апстракти c) Биотехнологија - Апстракти d) Наука о материјалима – Апстракти

COBISS.SR-ID 78648585

8th Conference of Young Chemists of Serbia
Belgrade, 29th October 2022
Book of Abstracts

Published and organized by
Serbian Chemical Society and Serbian Young Chemists' Club
Karnegijeva 4/III, 11000 Belgrade, Serbia
Tel./fax: +381 11 3370 467; www.shd.org.rs; office@shd.org.rs

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

Editors
Jelena **MILOVANOVIĆ**
Marko **RODIĆ**
Vuk **FILIPOVIĆ**
Života **SELAKOVIĆ**
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

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

Circulation
20 copies

ISBN **978-86-7132-080-1**

Printing
Development and Research Centre of Graphic Engineering
Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

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.

MC OP 01

Epigenetic drug discovery: fragment-based drug design of novel 1-benzhydryl-piperazine derivatives as selective histone deacetylase 6 inhibitors

Dusan B. Ruzic[1], Nemanja Djokovic[1], Tatjana Srdic-Rajic[2] and Katarina Nikolic[1]
[1] *University of Belgrade, Faculty of Pharmacy, Belgrade, Serbia*
[2] *Institute for Oncology and Radiology of Serbia, Belgrade, Serbia*

Selective histone deacetylase 6 (HDAC6) inhibition with small molecules is regarded as a rational strategy to develop safer anti-cancer drugs compared to non-selective HDAC inhibitors[1]. To date, structural motifs that are important for HDAC inhibitory activity and selectivity are defined as: surface recognition group (CAP group), aliphatic or aromatic linker and zinc-binding group (ZBG).

Herein, we describe a comprehensive protocol for the computational fragment search of novel surface-recognition (CAP) groups aimed to design selective Histone Deacetylase 6 (HDAC6) inhibitors (Figure 1)[2]. Identified heterocyclic CAP group, 1-benzhydryl piperazine was employed to synthesize novel HDAC inhibitors with small structural perturbations in the hydrocarbon linker. Enzymatic *in vitro* HDAC screening identified two selective HDAC6 inhibitors (6b, IC_{50} = 186 nM and 9b, IC_{50} = 31 nM), as well as two non-selective nanomolar HDAC inhibitors (7b and 8b). The influence of linker chemistry of synthesized inhibitors on HDAC6 potency was studied using structure-based molecular modelling.

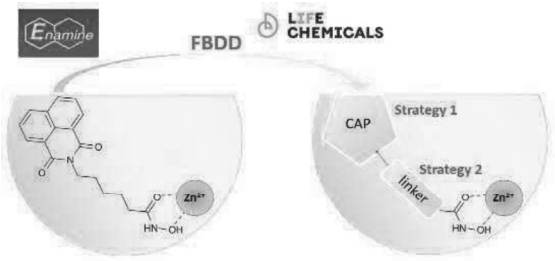

Figure 1. Design of novel selective HDAC6 inhibitors by fragment-based approach

References

1. J. Amengual, J. Lue, H. Ma, R. Lichtenstein, B. Shah, S. Cremers, S. Jones, A. Sawas, *The Oncologist*, **2021**, *26*(3), 184–e366.
2. D. Ruzic, M. Petkovic, D. Agbaba, A. Ganesan, K. Nikolic, *Mol. Inform.*, **2019**, *38*(5), 1800083.

Acknowledgments

The authors acknowledge a Ministry of Education, Science and Technological Development of the Republic of Serbia Faculty of Pharmacy project (451-03-68/2022-14/200161).