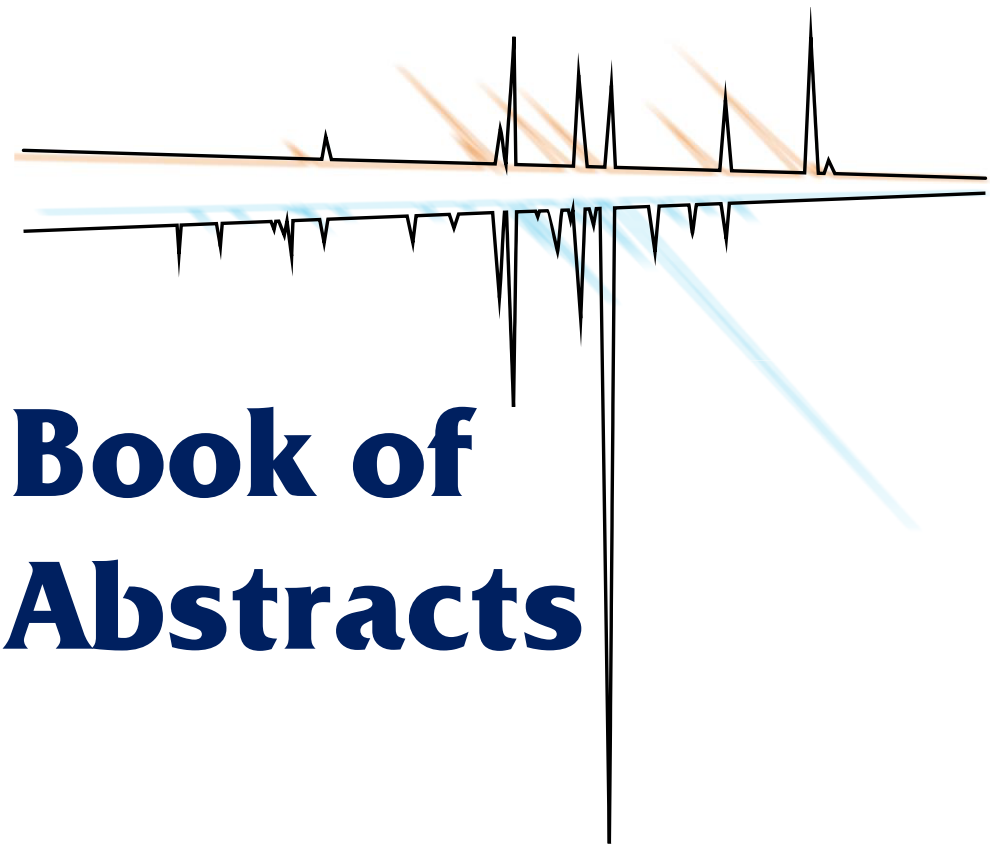
10th IAPC Meeting

Tenth World Conference on Physico-Chemical Methods in Drug Discovery & Sixth World Conference on ADMET and DMPK



Book of Abstracts

10th IAPC Meeting

Tenth World Conference on Physico-Chemical Methods in Drug Discovery
&
Sixth World Conference on ADMET and DMPK
Belgrade, Serbia, September 4-6, 2023

Book of Abstracts

Organized by
International Association of Physical Chemists
&
Faculty of Chemistry, University of Belgrade, Serbia

Published by
International Association of Physical Chemists
E-mail: office@iapchem.org, URL: http://www.iapchem.org

For Publisher
Zoran Mandić

Editor
Tatjana Verbić & **Zoran Mandić**

Design, page making and computer layout
Aleksandar Dekanski

On Line version only

The Scientific and Organizing Committee:

Tatjana Verbić, Conference Chair
University of Belgrade, Serbia,

Alex Avdeef
ADME Research, New York, USA

Kiyohiko Sugano
Ritsumeikan University, Osaka, Japan

Kin Tam
University of Macau, Macau

Zoran Mandić
University of Zagreb, Croatia

Klara Valko
Biomimetic chromatography Ltd. UK

Godefridus J. Peters
Amsterdam University Medical Centers, The Netherlands

Hong Wan
WHDeX Consultng AB, Sweden

Local Organizing Committee

Tatjana Verbić, Conference Chair
University of Belgrade, Faculty of Chemistry, Serbia

Goran Roglić
University of Belgrade, Faculty of Chemistry, Serbia

Ilija Cvijetić
University of Belgrade, Faculty of Chemistry, Serbia

Miloš Pešić
University of Belgrade, Faculty of Chemistry, Serbia

Olivera Marković
University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Serbia

Aleksandar Dekanski
University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Serbia

Marija Popović Nikolić
University of Belgrade, Faculty of Pharmacy, Serbia

P 07

Biomimetic characteristics of dual TLC retention mechanism

Darija Obradović[1], Lukasz Komsta[2], Marija Popović-Nikolić[3], Jovana Milutinović[4], Saša Lazović[1]

[1]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade, Serbia*
[2]*Department of Medicinal Chemistry, Faculty of Pharmacy, Medical University of Lublin, Jaczewskiego 4 20-090 Lublin, Poland*
[3]*Department of Pharmaceutical Chemistry, University of Belgrade-Faculty of Pharmacy, Vojvode Stepe 450, Belgrade, Serbia*
[4]*Promontis, Koste Stamenkovica 6, Niš, Serbia*

Most biomimetic chromatography measurements provide information on the ability of drugs to pass through cell membranes, their interaction with protein-based structures and distribution properties. The biomimetic properties of thin-layer chromatography (TLC) conditions have not been investigated so far. In our previous research, the presence of dual retention mechanisms for selected imidazoline and serotonin receptor ligands was confirmed under TLC conditions on C-18, diol, and a silica-based phases. The mobile phase was a mixture of ACN and water with 20 mM ammonium acetate and 0.1 volume % of acetic acid [1]. In this research, the average retention parameters were determined by using the integration procedure [2]. The parameter R_M^H is the average retention in the hydrophilic-dominated (HILIC), while R_M^R is the average retention in the region of reversed-phase interactions (RP). The parameter R_M^A corresponds to the average retention within the overall HILIC/RP region. The lipophilicity successfully correlates with the C-18 and silica based behaviour. For plasma protein binding affinity, the best correlations were found within C-18 and silica-based systems ($r > 0.70$). There is also a correlation of average silica gel and C-18 mechanism of interaction with the volume of distribution ($r > 0.73$), and the intestinal absorption ($r > 0.70$). The retention behaviour on the diol phase showed a good correlation with the P-gp inhibitor activity ($r = 0.80$). TLC systems that provide dual retention mechanisms can be successfully used in the rapid biomimetic profiling of serotonin and imidazoline receptor ligands in the first steps of drug discovery.

[1] D. Obradović, T. Kowalska, D. Agbaba, J. Chromatogr. Sci. 60 (2022) 372-386.
[2] D. Obradović, L. Komsta, D. Agbaba, J. Chromatogr. A 1619 (2020) 460951.

Acknowledgments: Institute of Physics Belgrade, grant from the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia, and University of Belgrade-Faculty of Pharmacy, grant No: 451-03-47/2023-01/200161.