



# ***Serbian Biochemical Society Thirteenth Conference***

***“Amplifying Biochemistry Concepts”***

**Proceedings**

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# Serbian Biochemical Society

## Thirteenth Conference

International Scientific Meeting

September 19-20, 2024, Kragujevac, Serbia

**“Amplifying Biochemistry Concepts”**

## FOREWORD

Dear Colleagues,

Welcome to the 13<sup>th</sup> Conference of the Serbian Biochemical Society, entitled “Amplifying Biochemistry Concepts”.

I would like to express my gratitude to all the participants who chose to present their valuable work at the conference and share their results with auditorium.

On behalf of the Organizing Committee, I would like to dedicate this year conference to our colleague and friend, and above all a great biochemist and scientist, professor Mihajlo Spasić.

*On behalf of the Organizing Committee  
Editor of the Proceedings  
Dragana Robajac*

# Serbian Biochemical Society

## Thirteenth Conference

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**“Amplifying Biochemistry Concepts”**

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# Identification of novel ligands of human cytochromes P450 among steroidal 1,2,4,5-tetraoxanes

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Cytochrome P450 enzymes (P450s) are involved in a wide variety of biotransformations including endogenous substrates (e.g. steroids, fatty acids, prostaglandins and leukotrienes) as well as exogenous compounds (xenobiotics, as drugs or environmental toxins). P450s are responsible for most of the important reactions (drug metabolism, hormone synthesis etc.) in tissues such as liver, gastrointestinal tract, brain, lung, kidney and heart. 1,2,4,5-tetraoxanes are specific class of peroxide compounds exhibiting antimalarial and antitumor activity, and very low cytotoxicity against normal cell lines. In the present work we examined binding potency of a group of steroidal mixed 1,2,4,5-tetraoxanes in the active site of four isoforms of human cytochrome P450 (CYP7A1, CYP7B1, CYP2E1 and CYP21A2). UV-VIS spectroscopy, reconstruction of enzymatic activity and SAR analysis were used in this study. A group of compounds with high affinity to the active site of all the enzymes was found, among which 2 new CYP7A1 ligands, 1 new CYP7B1 ligand, 3 ligands for CYP2E1 and 4 for CYP21A2. For a group of molecules  $K_d$  values were in the micromolar range: 3.91 $\mu$ M and 4.51 $\mu$ M (CYP7A1), 7.1 $\mu$ M (CYP7B1), 2.1 $\mu$ M and 3.8 $\mu$ M (CYP2E1) and 2.6 $\mu$ M (CYP21A2). This is comparable with the  $K_d$  values for natural ligands – cholesterol, DHEA, arachidonic acid and testosterone. SAR analysis of novel ligands allowed to identify pharmacophore features of the molecules that are crucial for compound binding. The data obtained are of great importance for the in-depth understanding of the mechanism of the molecular recognition/interaction of human P450s and their ligands in facilitating the discovery, design and development of novel bioregulators of the enzymes.

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