

26<sup>th</sup> Young Investigators' Seminar on Analytical Chemistry  
June 24 – 27, 2019, Pardubice, Czech Republic

**YISAC 2019**  
**Book of Abstracts**



Edited by Radovan Metelka

Edition of the YISAC 2019 Book of abstracts was supported by the Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice.

Copyright © University of Pardubice, 2019

Pardubice, Czech Republic

ISBN 978-80-7560-224-4



*Dedicated to Prof. Karel Vytřas (1944–2019) and Prof. Valerija Gužvanj (1975–2019),  
great scientists, colleagues and friends.*

## **Scientific Committee**

### **University of Graz, Austria**

Kurt Kalcher (kurt.kalcher@uni-graz.at)

Kevin Francesconi (kevin.francesconi@uni-graz.at)

Walter Goessler (walter.goessler@uni-graz.at)

Doris Kühnelt (doris.kuhnelt@uni-graz.at)

Martin Mittelbach (martin.mittelbach@uni-graz.at)

Astrid Ortner (astrid.ortner@uni-graz.at)

Georg Raber (georg.raber@uni-graz.at)

### **Graz University of Technology, Austria**

Ernst Lankmayr (lankmayr@tugraz.at)

Torsten Mayr (torsten.mayr@tugraz.at)

Ingo Klimant (klimant@tugraz.at)

### **University of Ljubljana, Slovenia**

Mitja Kolar (mitja.kolar@fkkt.uni-lj.si)

Boris Pihlar (boris.pihlar@fkkt.uni-lj.si)

Helena Prosen (helena.prosen@fkkt.uni-lj.si)

Polonca Trebše (polonca.trebse@zf.uni-lj.si)

Marjan Veber (marjan.veber@fkkt.uni-lj.si)

### **National Institute of Chemistry, Ljubljana, Slovenia**

Samo Hočevar (samo.hocevar@ki.si)

Irena Grgič (irena.grgic@ki.si)

Božidar Ogorevc (bozidar.ogorevc@ki.si)

### **Slovenian Institute of Hop Research and Brewing**

Iztok Košir (iztok.kosir@ihps.si)

### **Institute Jožef Stefan, Ljubljana, Slovenia**

Vekoslava Stibilj (vekoslava.stibilj@ijs.si)

### **University of Maribor, Slovenia**

Darinka Brodnjak-Vončina (darinka.brodnjak@uni-mb.si)

Maša Islamčević Razboršek (masa.islamcevic@um.si)

Matjaž Finšgar (matjaz.finsgar@um.si)

### **University of Nova Gorica, Slovenia**

Mladen Franko (mladen.franko@ung.si)

### **University of Pardubice, Czech Republic**

Radovan Metelka (radovan.metelka@upce.cz)

Ivan Švancara (ivan.svancara@upce.cz)

### **University of Venice, Italy**

Ligia Maria Moretto (moretto@unive.it)

Paolo Ugo (ugo@unive.it)

Salvatore Daniele (sig@unive.it)

### **University of Szeged, Hungary**

Zoltán Kónya (konya@chem.u-szeged.hu)

### **AGH University of Science and Technology, Kraków, Poland**

Andrzej Bobrowski (gcbobrow@cyf-kr.edu.pl)

Agnieszka Krolicka (krolicka@agh.edu.pl)

### **University of Lodz, Poland**

Sławomira Skrzypek (skrzypek@uni.lodz.pl)

Mariola Brycht (brychtmariola@gmail.com)

### **University of Novi Sad, Serbia**

Biljana Abramović (biljana.abramovic@dh.uns.ac.rs)

Božo Dalmacija (bozo.dalmacija@dh.uns.ac.rs)

Sanja Lazić (sanjal@polj.uns.ac.rs)

Srdan Rončević (srdjan.roncevic@dh.uns.ac.rs)

**University of Belgrade, Serbia**

Dalibor Stanković (dalibors@chem.bg.ac.rs)

**University of Sarajevo, Bosnia**

Emir Turkusic (turkusic@gmail.com)

**University Zagreb, Croatia**

Sanja Martinez (sanja.martinez@fkit.hr)

**University of Split, Croatia**

Mario Buzuk (mario.buzuk@gmail.com)

Josipa Giljanovic (josipa@ktf-split.hr)

**University of Prishtina, Kosovo**

Tahir Arbnesi (tahirarbnesi@hotmail.com)

**UBT-Higher Education Institution, Kosovo**

Eda Mehmeti (eda\_mehmeti@hotmail.com)



## **Chairmen**

Kurt Kalcher

Božidar Ogorevc

## **Local Organizing Committee**

Radovan Metelka

Tomáš Mikysek

Milan Sýs

Michaela Janečková

Amir Shaaban Farag

Granit Jashari

<http://yisac2019.upce.cz>

<https://www.facebook.com/yisac2019>

## **Location and Date**

The lectures of YISAC 2019 conference will take place in the CI lecture hall, located in the first floor of building HA in Faculty of Chemical Technology, University of Pardubice, Studentská 573, Pardubice, from June 24 to June 26, 2019.

## **EXPLORING ANATOMY OF EXPERIMENT WITH DFT: QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP OF SUBSTITUTED ARYLAZO PYRIDINE DYES IN PHOTOCATALYTIC REACTION**

Vlahović F.<sup>1</sup>, Gruden M.<sup>2</sup>, Zlatar M.<sup>3</sup>, Stanković D.<sup>4</sup>

<sup>1</sup>University of Belgrade, Innovation center of the Faculty of Chemistry, Studentski Trg 12-16,  
11000 Belgrade, Serbia

<sup>2</sup>University of Belgrade, Faculty of Chemistry, Studentski Trg 12-16, 11000 Belgrade, Serbia

<sup>3</sup>University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of  
Chemistry, Njegoševa 12, 11000 Belgrade, Serbia

<sup>4</sup>University of Belgrade, The Vinca Institute of Nuclear Sciences, POB 522, 11001 Belgrade, Serbia  
filipv@chem.bg.ac.rs

A series of arylazo pyridone dyes was synthesized by changing the type of the substituent group in the diazo moiety, ranging from strong electron-donating to strong electron-withdrawing groups. The structural and electronic properties of the investigated dyes was calculated at the M062X/6-31+G(d,p) level of theory. The observed good linear correlations between atomic charges and Hammett  $\sigma_p$  constants provided a basis to discuss the transmission of electronic substituent effects through a dye framework. The reactivity of synthesized dyes was tested through their decolorization efficiency in TiO<sub>2</sub> photocatalytic system (Degussa P-25). Quantitative structure-activity relationship analysis revealed a strong correlation between reactivity of investigated dyes and Hammett substituent constants. The reaction was facilitated by electron-withdrawing groups, and retarded by electron-donating ones. Quantum mechanical calculations were used in order to describe the mechanism of the photocatalytic oxidation reactions of investigated dyes and interpret their reactivity within the framework of the Density Functional Theory (DFT). According to DFT based reactivity descriptors, i.e. Fukui functions and local softness, the active site moves from azo nitrogen atom linked to benzene ring to pyridone carbon atom linked to azo bond, going from dyes with electron-donating groups to dyes with electron-withdrawing groups [1].

1. Dostanić J., Lončarević D., Zlatar M., Vlahović F., Jovanović D. M., *Journal of Hazardous Materials* **2016**, 316, 26-33.