Polish Italian Conference on Heteroatom Chemistry

Book of Abstracts

Katowice, 23.05.2025 r.

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Contents

Schedule

godz.	Name - Surname /Affiliation
9^{30} – 10^{00}	Rejestracja/Registration, spinPLACE, ul. Bankowa 5 KATOWICE
10^{00} – 10^{10}	Komitet organizacyjny/Organizing committee
Section 1	
10^{10} – 10^{50}	***Claudio Santi***, Università degli Studi di Perugia, Italy
10^{50} – 11^{20}	***Cecilia Scimmi***, Università degli Studi di Perugia, Italy
11^{25} – 12^{00}	***Agnieszka Kudełko***, The Silesian University of Technology, Poland
12^{00} – 12^{40}	***Anna Maroń,*** University of Silesia in Katowice, Poland
12^{40} – 13^{10}	***Paweł Ręka***, Jagiellonian University, Poland
13^{10} – 13^{30}	Coffee break
13^{30} – 14^{00}	***Beata Morak-Młodawska***, Medical University of Silesia in Katowice, Poland
14^{00} – 14^{30}	***Jacek Nycz,*** University of Silesia in Katowice, Poland
14^{30} – 15^{00}	
15^{00} – 15^{50}	Lunch break
15^{50}	***Award ceremony***

Unveiling the Biological Role of Organoselenium Compounds: The Se–S Bond as a Key Player in Anti-SARS-CoV-2 Activity and Beyond

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The chemistry of selenium-sulfur (Se–S) bonds plays a fundamental role in redox regulation and enzymatic activity, yet its full biological significance remains underexplored. Organoselenium compounds, particularly those containing Se–S motifs, exhibit remarkable reactivity with thiols, influencing protein function and oxidative stress responses. In this study, we leverage these properties to investigate the antiviral potential of Se-containing molecules against SARS-CoV-2. Given the virus's capacity to generate immune-evading mutants, there is a pressing need for alternative therapeutic strategies targeting conserved viral proteins such as the main protease (Mpro). A series of benzisoselenazolones and diselenides were screened for Mpro inhibition, followed by in vitro antiviral assays to assess their efficacy. Mechanistic insights were gained through density functional theory (DFT) calculations, molecular docking, and molecular dynamics simulations, revealing key protein-drug interactions. Furthermore, a bio-organic model was developed to elucidate the reactivity of these selenorganic compounds with biologically relevant thiols, providing critical insights into their metabolic pathways. New results based on a series of biophysical analyses will be presented, offering deeper insight into the interaction between organoselenium compounds and Mpro, further clarifying their mechanism of action and potential as antiviral agents. Beyond their immediate pharmacological relevance, our findings shed light on the evolutionary role of Se–S bonding in biochemical systems, highlighting its impact on redox homeostasis and host-pathogen interactions. By bridging fundamental chemistry with applied virology, this study paves the way for the rational design of novel selenium-based therapeutics.

Unprecedented Use of Selenium Catalysts for Lignin Oxidative Discoloration

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Lignin (LI), cellulose and hemicellulose are the main component of plants cell wall. LI is a non-regular biopolymer able to confer to the plant mechanical resistance, and resistance against pests and pathogens[1]. On the other hand, LI is also considered one of the most abundant biomass produced as a waste by the paper industries in a huge estimated amount of 50-70 millions of tons. The aromatic structure of LI makes it one of the most interesting natural polymers, as it confers unique properties. Indeed, the phenyl propanoid units are the responsible of the UV-blocker property of LI and for this reason it can be considered as a natural alternative to the synthetic and not-ecofriendly ones. However, the major drawback is the dark brown colour because of the formation of quinonic structures during the extraction process. Treatments able to lightening lignin without losing the UV-blocker properties are highly requested[2]. In this context, we decided to use the approach of the chemical modification of LI to discolorate it without losing its UV-blocker ability. In this work, we propose a catalytic oxidative protocol based on the use of organoselenium compounds as catalyst and H2O2 as oxidant. First, the protocol was tested on lignin model compounds, and later applied to the Kraft-Lignin biomass.

References

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1,3,4-Thiadiazole – a Versatile Scaffold for Diverse Applications: Synthesis and Transformations into Azo Derivatives and Luminescent Compounds

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1,3,4-Thiadiazole belongs to the group of five-membered heterocyclic compounds containing two nitrogen atoms and one sulfur atom in the ring. Many compounds featuring this scaffold exhibit a broad spectrum of biological activities, including antifungal, antimicrobial, anti-inflammatory, and anticancer effects. In addition to biological applications, it is worth mentioning their use as viscosity stabilizers in rubber processing, additives in the production of lithium battery electrodes, and lubricants. Conjugated thiadiazoles are also highly attractive moieties in materials science due to their electron-deficient nature, electron-accepting properties, and the presence of π-conjugated rings, especially relevant in optical, electrochemical, and photochemical applications. There are also reports on the use of 1,3,4-thiadiazole-based azo dyes in the production of inkjet printer cartridges, owing to their wide range of colors.

Our initial work on the use of acid hydrazides in the synthesis of 1,3,4-oxadiazoles inspired us to explore their potential in the construction of corresponding 1,3,4-thiadiazoles. The encouraging results prompted us to expand the range of reagents and adopt additional synthetic procedures to obtain a broad array of 1,3,4-thiadiazole derivatives. The presentation will show the results of a study on the synthesis and properties of new derivatives of 2-aryl-1,3,4-thiadiazole and 2,5-diaryl-1,3,4-thiadiazole, prepared from acyclic reagents such as acid hydrazides, *N,N'*-diacylhydrazines, *N*-acylhydrazones, or *N'*-aroylhydrazinecarbothioamides. We further employed the heterocyclic thiadiazole precursors in Suzuki cross-coupling reactions [1-3] and in cyclization reactions [4-5] to obtain more extended conjugated systems incorporating other aromatic and heterocyclic scaffolds (e.g., quinazoline, *s*-tetrazine). Transformations of 2-amino-5-aryl-1,3,4-thiadiazoles and *N'*-(arylhydrazinecarbonyl)-benzhydrazides leading to azo compounds containing a 1,3,4-thiadiazole unit [5-6] will also be presented.

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Can one molecule be either an early bird or a nigth owl? The photodynamics of the 2,2':6',2"-terpyridine with triphenylamine motive

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2,2':6',2"-Terpyridine (*terpy*) and its derivatives play a crucial role as building blocks in coordination and supramolecular chemistry[1]. Since Morgan and Burstall described the synthesis of *terpy*[2], the enormous number of *terpy*-based complexes with a wide range of transition metal ions was obtained. Compared to bidentate 2,2'-bipyridines and 1,10-phenanthrolines, the tridentate coordination mode of *terpy* leads to unprecedented stability of transition metal complexes and is crucial for the design of isomerically pure multicomponent systems[3,4]. *Terpys* can also be readily synthesized using the environmentally friendly and cost-effective Kröhnke condensation method, which provides access to virtually unlimited possibilities for modifying their structures and the photophysical properties of both the ligands and their coordination compounds. Especially, by introducing suitable substituents at the 4′-position, photophysics of *terpy*-like systems can be tuned. Substitution of strong electron-donating substituents makes *terpys* interesting push-pull dyes[5], which display intramolecular charge transfer (ICT), a fundamental phenomenon occurring in an ultrafast time domain. Particularly interesting can be sensitiveness of *terpy*-based ICT molecules to polarity and viscosity of the environment. This makes them good candidates for enviromental sensors. Here, the photophysical properties of 4′-(4-(di(4-tert-butylphenyl)amino)phenyl)-2,2′,6′,2″-terpyridine (*tBuTPAterpy*) as a model push-pull building block for transition metal coordination compounds will be discussed. Combining the femtosecond transient absorption (fsTA) and femtosecond fluorescence up-conversion (fsFU) we will show the dependence of the deactivation pathway on the polarity and viscosity of the medium used. The time scale and yield of light-induced conformational changes can be tuned up two orders of magnitude by changing the solvent. Thus, *tBuTPAterpy* either can act as "an early bird" or as "a night owl" depending on the local environment.

Acknowledgments

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Regioselective Synthesis and Investigation of Spectroscopic Properties, and Biological Activity of *N*-substituted Phenazine

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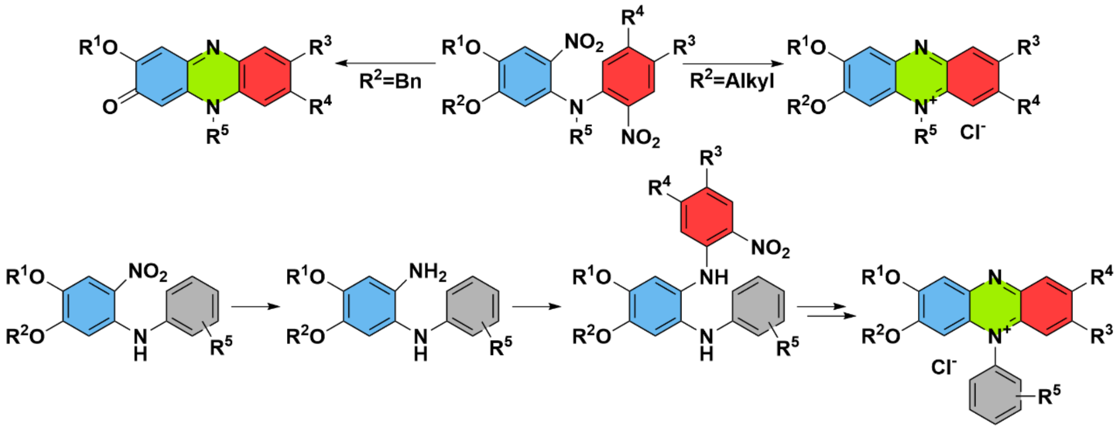
From the *N*-substituted phenazines, there are *N*-alkyl and *N*-aryl derivatives of phenazinium salts and phenazin-2-ones, which were under our investigation. Compounds were obtained with the modification of the previously described synthetic protocol,[1] providing both efficiency and regioselectivity. In the synthesis, nonsymmetrically substituted 4,5-dialkoxy-2-nitroanilines[2] are coupled with 1-bromo-2-nitrobenzene derivatives by Buchwald-Hartwig amination, yielding bis(2-nitrophenyl)amines. The obtained compounds are then alkylated with alkyl halides, and after reduction and oxidative cyclisation, yield *N*-alkylphenazinium salts. In this reaction, substrates substituted with a benzyloxy group (**Scheme 1: R2**) yield phenazin-2-ones instead of phenazinium salts. *N*-aryl substituted phenazinium salts were obtained in a new synthesis route presented in **Scheme 1**. The compounds obtained in this research have been investigated for their spectroscopic properties and biological activity. The *N*-alkyl phenazinium salts bearing four electron-donating alkoxy substituents exhibit intense fluorescence with maxima at approximately 490 nm, with fluorescence quantum yields of 0.53 in solution. Investigated phenazin-2-ones exhibit fluorescence maxima at approximately 560 nm in solution, which shift to 490 nm under acidic conditions, with a change in fluorescence quantum yield from 0.10 to 0.46, respectively. Cell culture experiments indicate that *N*-alkyl and *N*-aryl phenazinium salts exhibit cytotoxic effects against the 4T1 cell line (murine mammary carcinoma) at concentrations below 1 µM, whereas the phenazin-2-ones at concentrations below 10 µM.



Scheme 1. Regioselective synthesis of *N*-alkyl phenazinium salts and phenazine-2-ones.

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New Tool in Heavy Metal Detection: Synthesis, Spectroscopic and Quantum Chemical Characterization of Unique Water-Soluble Phosphorus Derivative of AzoQuinoline

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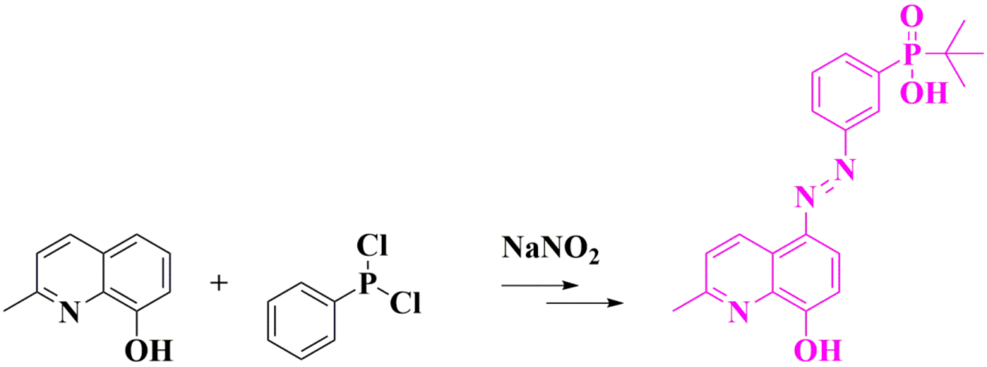
Phosphorus(V) species containing an azo (RN=NR) moiety prepared by standard azo coupling reactions are poorly studied compounds, and quinoline derivatives are unknown. Developing efficient and convenient syntheses of them would result in new interesting applications because of the importance of quinolines. We will show a novel and practical way to introduce an azo group as a bridge between quinoline and phosphine oxide units under mild reaction conditions. This strategy enables highly efficient and practical synthesis of suitable organophosphorus compounds with high added value, high chemoselectivity, and a broad substrate range. Due to the chirality center located on the phosphorous atom, the new compounds expressed anisotropy of diastereotopic methylene protons within the ethoxy moiety. The diastereotopic methylene protons of precursor of final molecule, presented below in Scheme 1, appear as an ABMX3 system.



Scheme 1. Synthesis of (*E*)-tert-butyl(3-((8-hydroxy-2-methylquinolin-5-yl)diazenyl)phenyl)phosphinic acid.

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Notatki

Notes