XXVI International Symposium

“Advances in the Chemistry of Heteroorganic Compounds”

SYMPOSIUM MATERIALS

Łódź, November 21, 2025

XXVI International Symposium

“Advances in the Chemistry of Heteroorganic Compounds”

Organized by:

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in cooperation with

Jan Dlugosz University in Czestochowa

Czestochowa Branch
Polish Chemical Society

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University of Lodz

Łódź, November 21, 2025

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XXVI International Symposium

“Advances in the Chemistry of Heteroorganic Compounds”

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Programme

XXVI International Symposium

"Advances in the Chemistry of Heteroorganic Compounds"

November 21, 2025		
9:00 – 9:15	**OPENING**	
SESSION I – chairman: Włodzimierz Stańczyk		
9:15 – 9:30	ML	**Witold Fortuniak** Centre of Molecular and Macromolecular Studies of PAS, Łódź *Professor Chojnowski in our memory*
9:30-10:15	PL-1	**Sławomir Rubinsztajn** Silicone Experts LLC, Ballston Spa, USA Centre of Molecular and Macromolecular Studies of PAS, Łódź *Bonded by Siloxanes: A 46-Year Scientific Journey and New Insights – In Memory of Professor Julian Chojnowski and His Enduring Legacy*
10:15 – 11:00	PL-2	**György Keglevich** University of Technology and Economics, Hungary *Four decades in organophosphorus chemistry: from P-heterocycles via new reactions to green chemistry*
11:00-11:10		**Wolfgang Weigand** The Editor-in-Chief of Phosphorus, Sulfur, and Silicon and The Related Elements *Information*
11:10-11:30	**COFFEE BREAK**	
11:30-12.30	**POSTER SESSION I (P001-P064)**	
SESSION II – chairman: Marcin Jasiński		
12:30-13:15	PL-3	**Yosuke Uchiyama** Kitasato University, Japan *Recent Aspects of Intermediates in the Wittig Reaction: 1,2-Oxaphosphetanes and Betaines Containing a Phosphaheteratriptycene*
13:15-14:00	PL-4	**Zbigniew J. Witczak** Wilkes University ,USA *Synthesis of new S-and N- functionalized heterocycles from exo-cyclic enone with 1,4-dithiane-2,5-diol and 2-mercaptotriazole*
14:00-15:00	**LUNCH**	
15:00-16:00	**POSTER SESSION II (P065-P128)**	
SESSION III – chairman: K. Michał Pietrusiewicz		
16:00-16:45	PL-5	**Daniel B. Werz** Albert Ludwigs University of Freiburg, Germany *Gain by Strain: Donor-Acceptor Cyclopropanes to Access Carbo- and Heterocyclic Compounds*
16:45-17:15	PL-6	**Grzegorz Mlostoń** University of Lodz, Poland *The Novel hetero-Diels-Alder Reactions with Thiochalcones Used as Active 1-Thia-1,3-dienes*
17:15-17:30	**CLOSING**	

PLENARY LECTURES

PL-1

Bonded by Siloxanes: A 46-Year Scientific Journey and New Insights – In Memory of Professor Julian Chojnowski and His Enduring Legacy

Sławomir Rubinsztajn[1,2]

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[2]*Centre of Molecular and Macromolecular Studies of PAS, Łódź, Poland*
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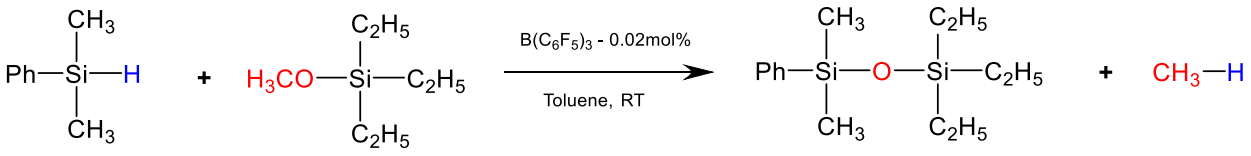
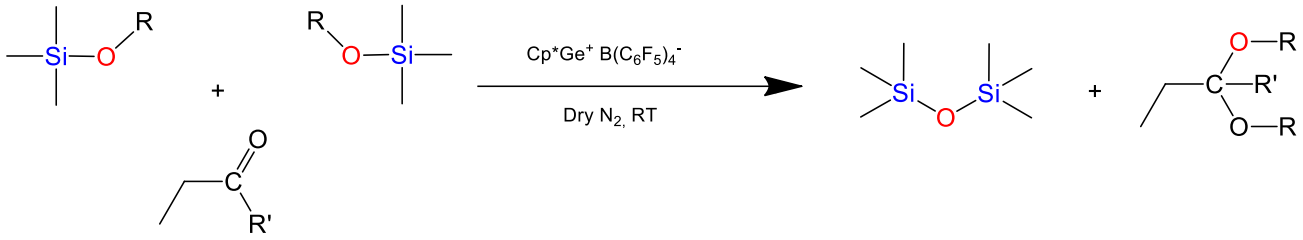
My scientific journey in siloxane chemistry began in 1979, when I joined the research group of the late Professor Julian Chojnowski at the Centre for Molecular and Macromolecular Studies of the Polish Academy of Sciences. Under his mentorship, I completed my Ph.D. in Chemistry in 1986, focusing on the mechanism of polycondensation of siloxane oligomers. In 1988, I relocated to the United States to continue my research at the GE Corporate Research Center, yet our collaboration in siloxane chemistry endured across decades and continents, sustained by shared curiosity, trust, and friendship.

This lecture, presented in memory of Professor Chojnowski and in celebration of his scientific legacy, will highlight key milestones from our joint investigations into the dehydrocarbonative condensation of alkoxysilanes with hydridosilanes - commonly referred to as the Piers-Rubinsztajn reaction.[1]



I will also present recent findings from my ongoing work at the Centre for Molecular and Macromolecular Studies, including a novel siloxane bond formation pathway via dealkoxylation of alkoxysilanes in the presence of stoichiometric amounts of aldehydes or ketones.[2,3]



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PL-2

Four decades in organophosphorus chemistry: from P-heterocycles via new reactions to green chemistry

György Keglevich

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This lecture is a summary of the results of the Keglevich group obtained in the previous decades. The lecture is a repetition of the talk presented on the occasion of the decoration with the International Arbuzov Price (Kazan, Sept. 4, 2025). The following topics will be included:

- The synthesis of 6- and 7-membered P-heterocycles by ring enlargement
- Optical resolution of racemic P-heterocycles
- The problem of aromaticity of phospholes
- Transition metal complexes of P-heterocycles
- The synthesis of bridged P-heterocycles and their utilization in fragmentation-related phosphorylations
- Deoxygenation of bridged phosphine oxides
- The inverse-Wittig type reaction of P-trialkylphenyl heterocycles and dialkyl acetylene dicarboxylates
- The MW-assisted direct esterification of phosphinic-, phosphonic- and phosphoric acid derivatives
- Scope and limitation of the MW assistance in organic reactions
- Transesterifications, amidations and hydrolyses
- P-ligand-free Hirao P–C couplings
- Application of the Kabachnik–Fields reaction and the Pudovik addition
- The synthesis of dronic acid derivatives.

PL-3

Recent Aspects of Intermediates in the Wittig Reaction: 1,2-Oxaphosphetanes and Betaines Containing a Phosphaheteratriptycene

Yosuke Uchiyama

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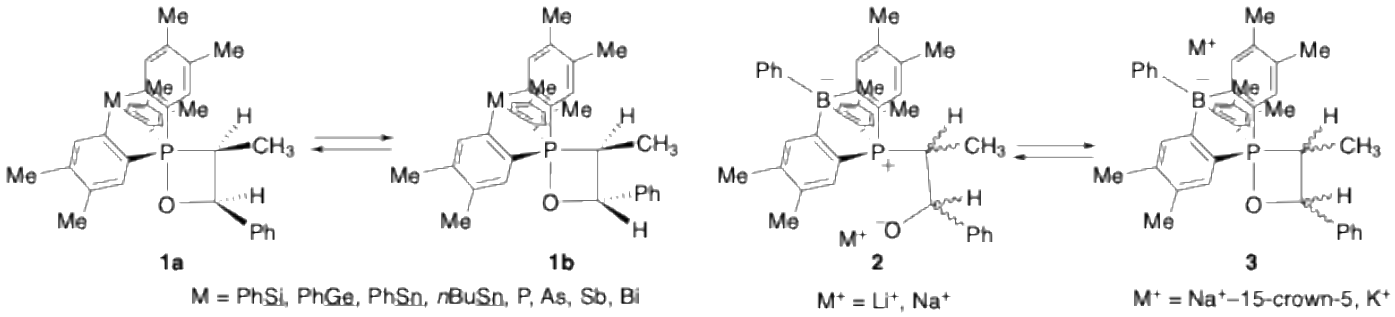
To investigate the relationship between 1,2-oxaphosphetanes and betaines in the Wittig reaction, intermediates containing phosphaheteratriptycenes with Group 13, 14, and 15 elements (PhB$^-$, PhSi, PhGe, PhSn, *n*-BuSn, P, As, Sb, Bi) were observed using VT-^{31}P{^{1}H} NMR spectroscopy over a temperature range from –90 °C to 25 °C. The Wittig reactions of non-stabilized phosphonium ylides containing phosphaheteratriptycenes with Group 14 and 15 elements with PhCHO afforded both (*E*)- and (*Z*)-olefins *via* 1,2-oxaphosphetane intermediates **1** (**Scheme 1**). VT-^{31}P{^{1}H} NMR spectroscopy revealed the isomerization of intermediates **1a** to **1b** was observed in systems involving Group 14 and 15 elements, showing the origin of stereochemical drift. In the system containing a phosphaboratatriptycene (Group 13), the reaction with PhCHO did not yield olefins. Instead, betaine intermediates **2** were detected by VT-^{31}P{^{1}H} NMR spectroscopy. Deprotonations of the corresponding □-hydroxyethylphosphonium salts containing a phosphaboratatriptycene with MHMDS (M = Li, Na) provided betaines **2-Li**, which were thermodynamically stable at 0 °C, whereas betaines **2-Na** were unstable at the same temperature. On the other hand, 1,2-oxaphosphetanes **3-Na** and **3-K** were observed when NaHMDS (with 15-crown-5) and KHMDS were used, respectively, giving PhCHO instead of the corresponding olefins.

DFT calculations were performed to evaluate the energies and P–O bond strengths of 1,2-oxaphosphetanes. The results indicated that *trans*-isomers were approximately 2 kcal/mol more stable than *cis*-isomers. Additionally, the P–O bond strength decreased with increasing atomic number due to elongation of the P–O bond. In phosphaboratatriptycene system, the relative stabilities of betaines and 1,2-oxaphosphetanes were estimated both in the presence and absence of alkali metal ions. The interaction between the alkali metal ion and the oxide ion of the betaine significantly influenced stabilities of betaines in the order of Li > Na > K. However, this interaction had little effect on the stabilities of betaines and 1,2-oxaphosphetanes when the metal ion was placed near the phenylborata ion.



Scheme 1. Equilibra of 1,2-oxaphosphetanes **1a–1b** and betaines **2**–1,2-oxaphosphetanes **3**.

Acknowledgement

The authors thank Prof. Takayuki Kawashima of the University of Tokyo for his valuable advice.
The computation was performed at the Research Center for Computational Science, Okazaki, Japan (Project: 23-IMS-C174, 24-IMS-C217, and 25-IMS-C249).

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PL-4

Synthesis of new *S*-and *N*- functionalized heterocycles from *exo*-cyclic enone with 1,4-dithiane-2,5-diol and 2-mercaptotriazole

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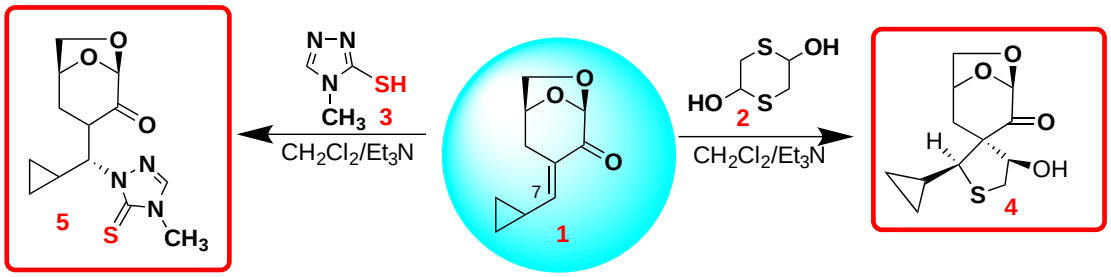
In continuation of our studies on aldol condensation of active methylene compounds, such as dihydrolevoglucosenone (Cyrene^{R}), with aromatic and heterocyclic aldehydes [1-2] containing no α-hydrogen atoms, we decided to extend the synthetic approach to functionalize conjugated system present in our representative *exo*-cyclic enone shown in the reaction scheme below.

In order to examine the potential chemical reactivity and electronic effect of bioisosteric scaffold at C-7 position we selected the enone **1** for the stereoselective reaction with 1,4-dithiane-2,5-diol **2** [3] under base catalyzed thio Michael addition. The adduct product **4** was isolated as an attack of thiol **2** on C-7 with cyclization product *via* domino cyclization reaction conditions.

The addition of thiol **3** to the conjugated system *of exo*-cyclic enone **1** was performed under base (Et_3N) catalyzed reaction condition to functionalize C-7 enone position. The adduct product **5** was identified as *N*-linked heterocycle formed *via* stereoselective addition of triazole moiety through *N*- bridge, not *S*-thiol addition and compared to other derivatives produced earlier.

In both additions, the crystalline products **4, 5** were isolated in good yield (58-65%) and characterized by ^{1}H and ^{13}C NMR spectroscopy. A plausible reaction mechanism of both stereoselective additions will be presented in details.



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PL-5

Gain by Strain: Donor-Acceptor Cyclopropanes to Access Carbo- and Heterocyclic Compounds

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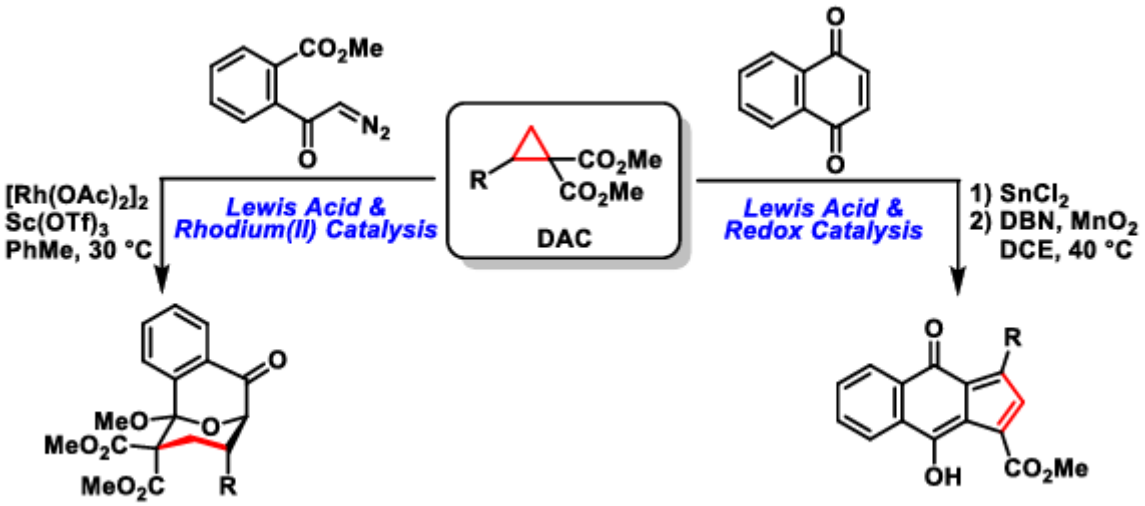
Donor-acceptor cyclopropanes (DACs) are highly strained entities which are unique building blocks for hetero- and carbocyclic systems.[1,2] For the last decade, we have been developing novel methodologies starting from these type of three-membered rings leading to oligopyrroles, chalcogen-containing heterocycles, and 1,3-bisfunctionalized products,[3] just to name a few. To get deeper insights into their intrinsic reactivity in-depth physical organic studies were performed recently.[4] Besides the common activation of DACs by Lewis acids leading to a wide variety of ring-opening and cycloaddition products even synergistic catalytic approaches can be applied to generate fleeting intermediates which react with the strained systems. Scheme 1 depicts two representative examples, one using Lewis acid and Rh catalysis (affording intermediate carbonyl ylides)[5] and another using Lewis acid and redox catalysis are presented.[6] More recently, electrochemical methods were applied to activate donor acceptor cyclopropanes.[7]



Scheme 1. Donor-acceptor cyclopropanes in dual catalyses.

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PL-6

The Novel *hetero*-Diels-Alder Reactions with Thiochalcones Used as Active 1-Thia-1,3-dienes

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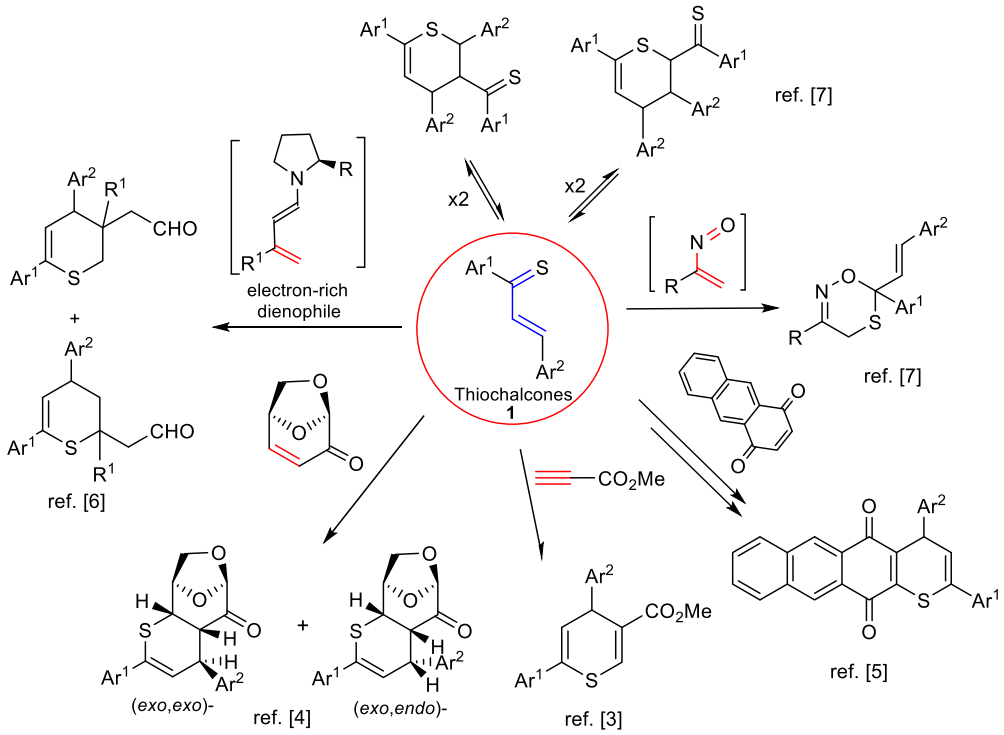
In contrast to chalcones which are widely applied as useful building blocks in organic synthesis, e.g. as easily accessible Michael acceptors [1], their thio-analogues, i.e. thiochalcones **1**, have not yet found spectacular applications. In a series of our recent publications, a remarkable usefulness of thiochalcones **1** for preparation of diverse sulfur heterocycles, via (3+2) and (4+2) cycloaddition reactions, was demonstrated and special attention was focused on diverse exploration as reactive 1-thia-1,3-dienes in *hetero*-Diels-Alder reactions leading to thiopyran derivatives [2].



In the lecture, *hetero*-Diels-Alder reactions performed with acetylene carboxylates [3], levo-glucosenone [4], benzoquinones [5], and in situ-generated, chiral dienamines [6], and will be discussed in detail. In the extension of the main topic, *hetero*-Diels-Alder reactions with thiochalcones **1** used as heterodienophiles towards electron deficient nitrosoalkenes, leading to 1,5,2-oxathiazine derivatives, will also be presented [7].

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ABSTRACT POSTERS

P-001

The use of Huisgen 1,3-dipolar cycloaddition in the synthesis of new conjugates with potential dual anticancer and antimicrobial properties

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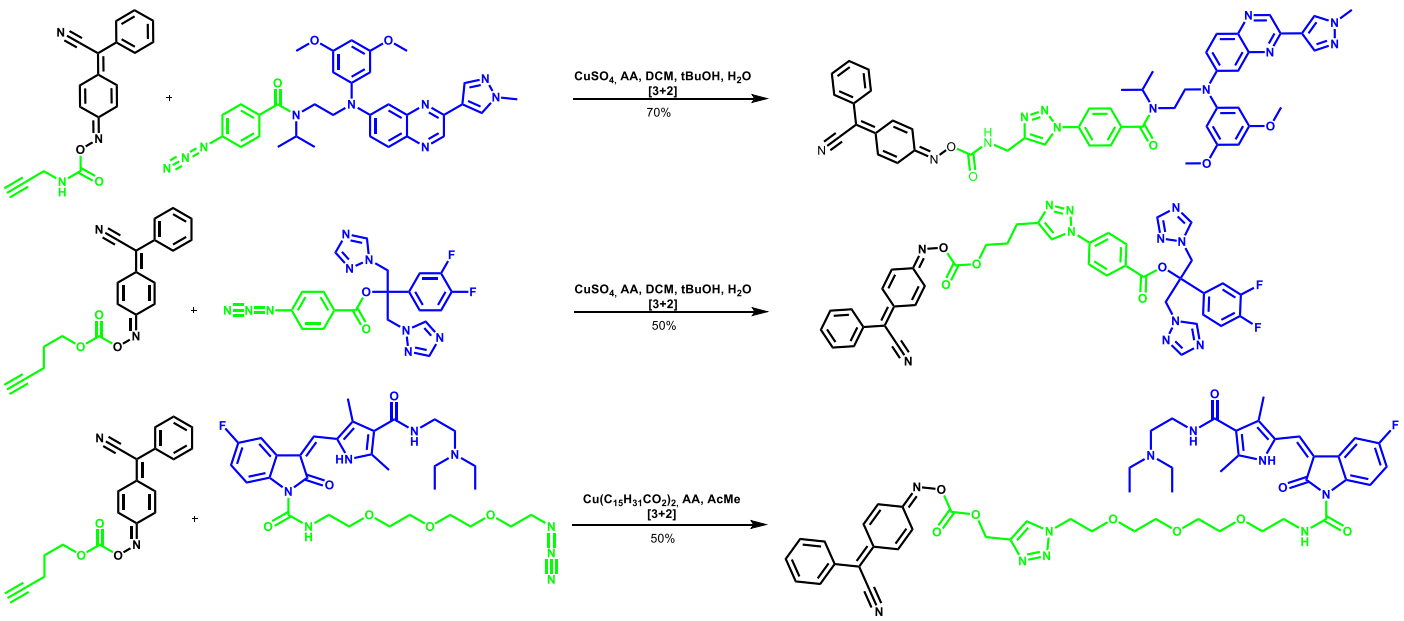
Over the past few decades, there has been an increasing trend in fungal resistance to antibiotics, with cancer patients being particularly vulnerable to such threats. Consequently, there is an urgent need to explore and develop new, effective therapeutic strategies that enable simultaneous treatment of microbial infections and oncological diseases.

We have recently presented novel properties of the 4-AN molecule as well as its derivatives and analogues, such as high activity against Candida species, leading to a reduction in the relative expression of genes involved in the virulence of these pathogens [1].

The combination of 4-AN derivatives and analogues with molecules exhibiting anticancer activity may lead to the development of new therapeutic agents with dual therapeutic potential. One possible approach to implementing this idea will be presented through the following transformations:



Scheme 1. Synthesis of selected conjugates.

Acknowledgement

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P-002

Synthesis, Spectroscopy, and Computational Studies of Unique α-Conjugated *N*-Alkylated Phenazinium Salts and Their Precursors

Filip Milewski[1], Daniel Swoboda[1], Jolanta Kolińska[2], Nataliya Karaush-Karmazin[3], Magda Adamczyk[2], Radosław Podsiadły[2] and Jacek E. Nycz[1]

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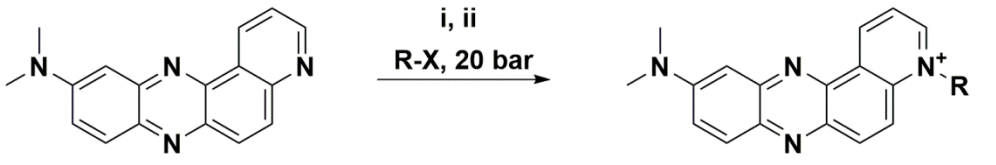
Two unique structures, 10-(dimethylamino)-4-methylpyrido[3,2-*a*]phenazin-4-ium iodide (**PZS1**) and 10-(dimethylamino)-4-(2-fluorobenzyl)pyrido[3,2-*a*]phenazin-4-ium bromide (**PZS2**), were received from the *N*-alkylation reactions of *N*,*N*-dimethylpyrido[3,2-*a*]phenazin-10-amine (**PZ1**) and appropriate electrophile **RX**, under pressure conditions of 20 bar (Scheme 1). Without the application of pressure, the reactions did not occur. A combination of IR, NMR, MS, HRMS, GC-MS, and electronic absorption spectroscopy characterized the nine selected symmetrical and unsymmetrical pyridine-embedded phenazines, and two *N*-alkylated salts.[1]

The absorption maxima were determined, and molar extinction coefficients were calculated, enabling a quantitative analysis of absorption capacities. Additionally, the fluorescence properties were determined, including the lifetimes of excited singlet states and the quantum emission yields. This allowed the efficiency of the photoemission processes to be assessed, as well as their dependence on the chemical structure of the compounds studied.

Quantum chemical calculations using density functional theory (DFT) and B3LYP/6-31G(d,p) level were performed to study the electronic structures and conformational peculiarities of the novel synthesized *N*-alkylated phenazinium salts are presented in Scheme 1. The DFT calculations provided insight into the electronic distribution across the π-conjugated phenazine core and the influence of the alkyl substituents on charge localization, molecular planarity, and frontier molecular orbitals. Particular attention was paid to the effect of the electron-donating dimethylamino group and the electron-withdrawing fluorobenzene moiety in modulating the HOMO-LUMO gap and electronic transitions of **PZS1** and **PZS2**.



PZ1

R = CH_3; X = I; PZS1 = 87%
R = Bz2F; X = Br; PZS2 = 27%

Scheme 1. Synthetic route of *N*-Alkylated phenazinium salts (**PZS**), where i = **RX** = MeI, 60 ˚C ii = ACN, **RX** = 1-(bromomethyl)-2-fluorobenzene, 100 ˚C.

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P-003

Synthesis and study of new xanthene dyes

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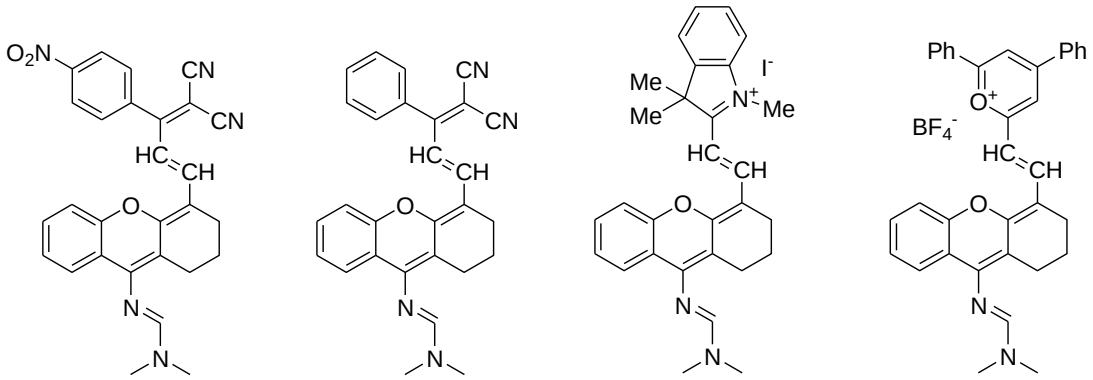
Xanthene dyes have found widespread application in numerous fields, particularly in the textile, food, pharmaceutical, cosmetic, and biomedicine industries. The broad practical application of this method has contributed to the development of methods for the synthesis of xanthene derivatives and the study of their properties.

Xanthene dyes 1-4, each with a distinct acceptor group at the 4-position, were synthesized through a reaction of N'-(4-formyl-2,3-dihydro-1H-xanthen-9-yl)-N,N-dimethylimidoformamide with CH-acids.

The present study analyzes the influence of end groups on the absorption maximum in two polar solvents. Absorption spectra were recorded at a concentration of 5*10-6 mol/L in dimethylformamide and acetonitrile. The most significant shift of the absorption maximum to the near infrared region is observed for 2-(9-{[(1E)-(dimethylamino)methylene]amino)-2,3-dihydro-1H-xanthen-4-yl}vinyl-4,6-diphenylpyrylium tetrafluoroborate 4.



	1	2	3	4
DMF:	λ_{abs} – 675 nm	λ_{abs} – 668 nm	λ_{abs} – 645 nm	λ_{abs} – 724 nm
MeCN:	λ_{abs} – 648 nm	λ_{abs} – 658 nm	λ_{abs} – 634 nm	λ_{abs} – 713 nm

Scheme 1. Xanthene dyes 1-4 with different acceptor groups in the 4th position.

The existence of two conjugated reaction centers enables the selective chemical modification of the structure, thereby forming dyes with predicted photophysical properties. It is evident that the resulting compounds have considerable potential for further exploration within the domain of photonic-active materials.

P-004

Synthesis and conformational studies of 1,10-*N,N′*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane

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Drug delivery systems (DDS) are used to transport therapeutic substances whose physicochemical properties hinder direct application. To achieve the desired therapeutic effect, an increased drug dosage is often required. This poses a particular challenge for anticancer drugs used in chemotherapy, as they are rapidly metabolized and eliminated from the body. These compounds are typically characterized by low molecular weight and high toxicity [1–2].

To improve efficacy and reduce non-selective toxicity, drugs are often modified by forming complexes with carriers. One example of such a carrier is 1,10-*N,N′*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane (Figure 1). The synthesis of this cryptand was carried out using the Staudinger–aza-Wittig method.

The poster presents results obtained from theoretical analysis. Calculations were performed using an approximate computational method with the Universal Force Field (UFF). The most stable conformers and their corresponding energy values are shown.

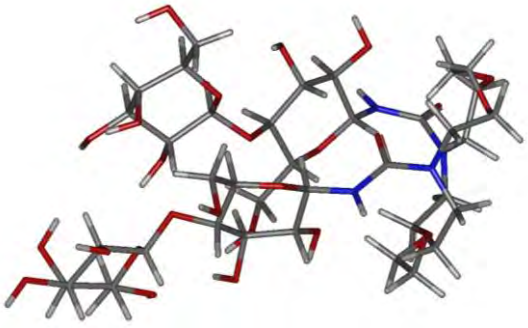

Figure 1. Molecular structure of 1,10-*N,N'*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane.

Acknowledgement

M.H. gratefully acknowledges Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018176.

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P-005

Theoretical investigation of the newly synthesized lactose cryptand

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Drug carriers are substances used to transport pharmaceuticals whose direct administration into the body is either ineffective or harmful. The most common limitation is the poor water solubility of the drug. This property prevents the drug's effective use, as the human body consists mainly of water. Other factors that exclude the possibility of direct drug administration include high cytotoxicity, low molecular weight, and rapid metabolism. These characteristics are particularly relevant to anticancer drugs used in chemotherapy [1-2].

One method of improving the pharmaceutical properties of a drug is, for example, the formation of a complex with a drug carrier. A potential carrier may be 1,10-*N,N'*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane (**TL**; Figure. 1).

The poster will present the most stable conformers of TL obtained through molecular mechanics calculations using the OPLS force field.

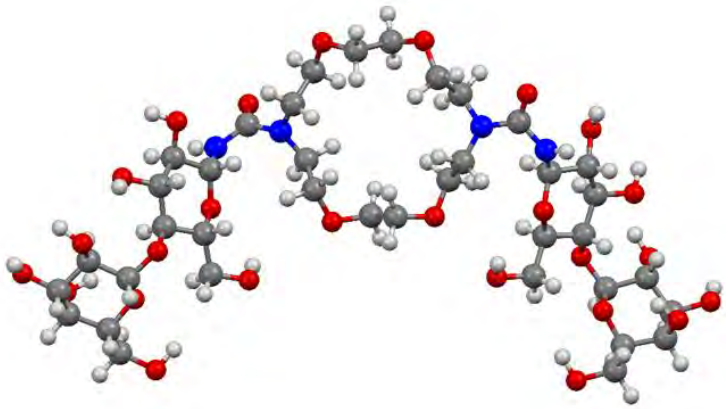

Figure 1. The structure of 1,10-*N,N'*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane.

Acknowledgement

M.H. gratefully acknowledges Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018176.

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P-006

Theoretical study on a new lactose cryptand

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Drug delivery systems (DDS) are designed to transport therapeutic agents that, due to their pharmacological properties, are unsuitable for direct administration. As the human body consists of approximately 60% water, one of the key challenges in drug formulation is the poor aqueous solubility of many active pharmaceutical ingredients. To achieve the desired therapeutic effect higher doses of such drugs are often required [1–2].

One strategy to overcome this limitation involves modifying the drug's properties by forming a complex with an appropriate carrier. A recently synthesized compound with potential as a drug carrier is 1,10-*N,N'*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane (Figure 1).

The poster will present the results of computational studies carried out in vacuum using molecular mechanics with the MMFF94 force field. The most stable molecular structures are shown along with their corresponding energetic properties.

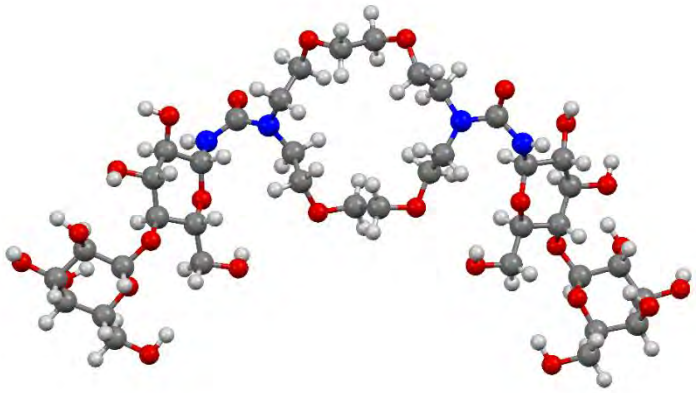

Figure 1. The molecule 1,10-*N,N'*-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane.

Acknowledgement

M.H. gratefully acknowledges Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018176

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P-007

Application of theoretical chemistry methods to the analysis of a cryptand containing glucose and its complex with a fluoromethyl derivative of busulfan

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The potential anti-cancer drug 1,4-butanediol di-2,2,2-trifluoroethane sulfonate (BFS, Fig. 1) is a compound poorly soluble in water [1,2]. Drug carriers can be used to increase solubility in water and reduce cytotoxicity to healthy tissues. Diazacrown ether 1,10-*N,N′*-bis-(β-D-ureidoglucopyranosyl)-4,7,13,16-tetraoxa-1,10-diazacyclopentadecane (STM, Fig. 1; 11a in [3]) has a sufficiently high molecular weight and its complexing abilities have been preliminarily tested with p-toluenesulfonamide [3].

In the study a conformational analysis of the STM carrier and the configurational analysis of the STM:BFS complex were carried out as part of the research. The poster will present the results obtained using computational chemistry methods. The conformation of the carrier with the lowest potential energy and the most energetically favourable configuration of STM and BFS relative to each other will be presented. For this purpose DFT methods were used, taking into account the continuous medium model PCM, where water was the solvent.

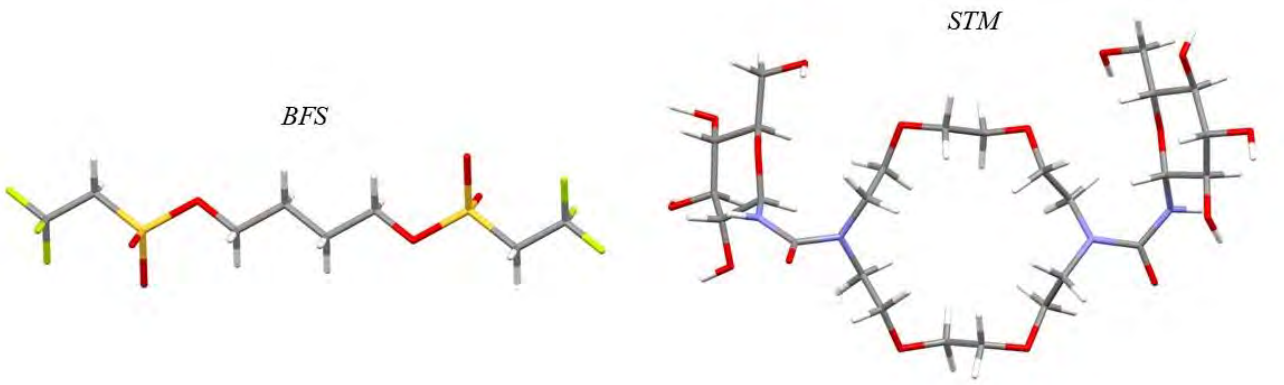

Figure 1. 1,4-butanediol di-2,2,2-trifluoroethanesulfonate and 1,10-*N,N′*-bis-(β-D-ureidoglucopyranosyl)-4,7,13,16-tetraoxa-1,10-diazacyclopentadecane.

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P-008

NHC-Catalyzed Dearomative Higher-Order Cycloaddition: Access to Dihydropyrimidin-4(1*H*)-one Frameworks

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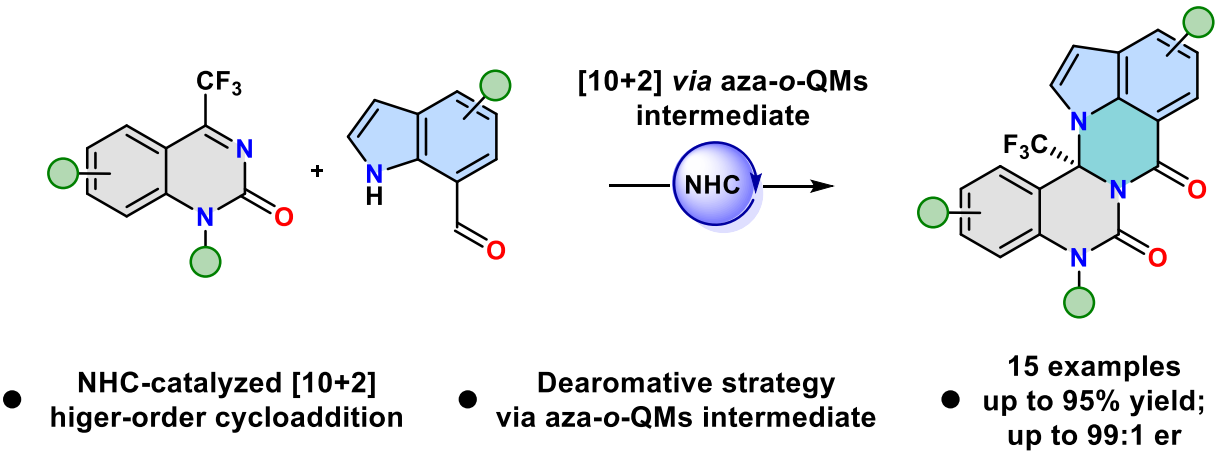
Cycloadditions and related higher-order cycloadditions (HOCs) represent a powerful and versatile tool in modern organic synthesis, providing a well-established approach to the construction of heterocyclic systems. [1] In HOCs, more than 6π electrons participate in bond-forming processes. [2] The development of asymmetric higher-order cycloadditions has been advanced through the use of organocatalysis. Among these methods, NHC catalysis offers unique reactivity profiles of aromatic compounds via dearomative functionalization. This strategy relies on the temporary dearomatization of aromatic carbonyl compounds, enabling the generation of highly reactive intermediates such as aza(benzo)fulvenes and *o*- or *p*-quinodimethanes. [3]

In our research, we present a new dearomative [10+2]-hetero-higher-order cycloaddition realized under NHC catalysis. [4] The reaction occurs between indole-7-carbaldehydes, serving as higherene precursors, and cyclic trifluoromethyl ketimines, which act as higherenophiles. Under *N*-heterocyclic carbene (NHC) catalysis, this process generates NHC-bound aza-*o*-quinodimethanes. The transformation proceeds in a fully enantioselective manner. Using this strategy, we prepared a series of structurally diverse and biologically relevant dihydropyrimidin-4(1*H*)-one scaffolds. Moreover, the synthetic utility of the obtained cycloadducts was demonstrated through selected chemoselective transformations.



Scheme 1. Dearomative higher-order cycloaddition for the synthesis of dihydropyrimidin-4(1*H*)-one scaffold.

Acknowledgement
This project was realized within the Opus programme (grant number: UMO-2021/41/B/ST4/03385) from the National Science Centre, Poland.

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P-009

Synthesis and structural analysis of new phosphonates with an *N*-substituted fluorine-containing acetanilide core

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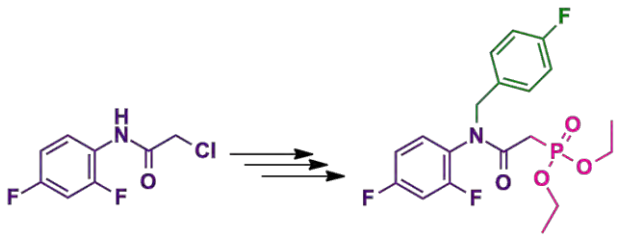
Despite ongoing medical advances, cancer still poses a major public health challenge. Cancers account for 3 out of 10 premature deaths caused by non-communicable diseases worldwide. [1] The main therapeutic approach is still based on chemotherapy, which uses small-molecule chemical compounds to inhibit the growth and invasion of cancer cells. These drugs usually cause many side effects due to their toxicity to healthy cells, and at the same time, their effect is limited by low efficacy and drug resistance. Therefore, the design and development of new, more effective chemotherapeutics with a lower side effect profile is a major challenge for medicinal chemists. [2,3]

Phosphorus- and fluorine-containing compounds play a significant role in medicinal chemistry due to their ability to form specific interactions with selected molecular targets. [4,5]

With this in mind, new compounds containing both pharmacophores: fluorine, a phosphonate group, were designed, and their synthesis based on acetanilide derivatives was initiated.



Scheme 1. Example of obtaining new phosphonates containing an *N*-substituted acetanilide core.

Acknowledgement
The work was financed partially within the framework of the project "ID-UB" No. 181/13/SNŚ/0002.

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P-010

Bioreduction of 3*n*-phenacyl derivatives of tri- and tetramethylenepyrimidines

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In recent decades, increasing attention has been directed toward environmental protection, as natural ecosystems are being disrupted by intensive and often uncontrolled anthropogenic activity. The chemical and pharmaceutical industries represent major sources of waste with a high environmental burden, which necessitates the search for innovative, alternative methods of synthesis and production. In this context, particular emphasis is placed on strategies aligned with the paradigm of green chemistry, whose fundamental objective is the minimization of harmful and non-degradable by-products.

Biocatalysis, which employs enzymes as natural catalysts of chemical processes, represents one of the most promising technologies within this framework. It is characterized by a high degree of environmental sustainability and economic efficiency, enabling reactions to be carried out under mild physicochemical conditions (e.g., moderate temperature, pressure, and aqueous environments). Compared with conventional chemical catalysts, enzymes offer several advantages: they are biodegradable, can be reused multiple times, exhibit remarkably high substrate selectivity and stereo-/regioselectivity, and are safe for both humans and ecosystems. Owing to these properties, biocatalysis constitutes a key tool for the development of sustainable industrial technologies and aligns with global efforts to reduce the negative environmental impact of industrial activities.

The aim of the present study was a detailed evaluation of the enantiomeric purity of products obtained through the bioorganic synthesis of chiral compounds in the presence of fungal bioreagents and isolated oxidoreductases. This research is in line with current trends in bioorganic and green chemistry, focusing on the application of biocatalysts for the stereoselective transformation of prochiral substrates. In the investigated enzymatic reduction of prochiral 3-*N*-phenacyl derivatives of tri- and tetramethylenopyrimidines, the key step involves the selective transfer of one of the enantiotopic hydride ions from the dihydropyridine ring of the cofactors NADH or NADPH to a specific face of the carbonyl group. This process, catalyzed by oxidoreductases, leads to the formation of secondary alcohols with high enantiomeric purity. The resulting products exhibited enantiomeric excess values of up to 99%, confirming the high precision and efficiency of the applied biocatalysts.

Such a high degree of enantioselectivity in bioreduction is of considerable importance both from the perspective of organic synthesis and pharmaceutical applications, as the enantiomeric purity of biologically active compounds critically determines their pharmacological efficacy and safety. These findings demonstrate that bioreduction mediated by fungal bioreagents and oxidoreductases constitutes an effective, environmentally friendly, and promising strategy for obtaining stereochemically homogeneous alcohols with potential applications in drug synthesis and other bioactive compounds.

P-011

Diphenyl diselenide decorated with a long carbon chain as an additive to new chitosan-based edible films

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Organoselenium compounds have been widely utilized as reagents, catalysts, bioactive agents or antioxidants across various fields of chemistry, including organic synthesis, asymmetric catalysis, medicinal chemistry and material science. Within this class of compounds, diselenides are particularly interesting due to the presence of a reactive Se-Se bond, which can be readily cleaved, transformed into diverse types of reagents, used to scavenge reactive species such as peroxides, or interact with key molecular targets.[1]

Herein, we present a different strategy of using the unique properties of diphenyl diselenides – as antioxidant and antibacterial additives to innovative chitosan edible film for extending poultry meat quality during storage. The synthesis and activity evaluation of a series of diphenyl diselenides possessing lipophilic long carbon chains, solely or with additional polar insets: phenyl linkers and ester groups will be presented.[2]

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P-012

A new route to ethynyl(2-ethynylphenyl)phosphine oxides

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Ethynylphosphine oxides have become a key motif in organophosphorus chemistry.[1] Typically, ethynylphosphine oxides are synthesized through metal-mediated coupling of a terminal alkyne with sec-phosphine oxides[2] or chlorophosphines[3]. Another important method employs an acetylene anion in reactions with an electrophilic phosphorus reagent.[4] Recently, we observed the formation of a small amount of ethynyl(2-ethynylphenyl)phosphine oxide in the reaction of benzo[*b*]phosphol-3-yl triflate with ArMgX.[5] Here, we present a new approach to these compounds.

Acknowledgement

This work was supported by standard university statutory funding.

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P-013

Nucleophilic substitution vs ring opening – dual reactivity of benzo[*b*]phosphol-3-yl triflates towards alkyl Grignard reagents

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We previously reported the application of benzo[*b*]phosphol-3-yl triflates in the ring-opening reaction [1]. Herein, we demonstrate the dual reactivity of benzo[*b*]phosphol-3-yl triflates towards alkyl Grignard reagents.[2] We clarify the conditions needed to prevent competition between the nucleophilic substitution and the ring opening.

Acknowledgement
This work was supported by standard university statutory funding.

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P-014

Development and implementation of new technology of obtaining of non-opioid analgesic active substance

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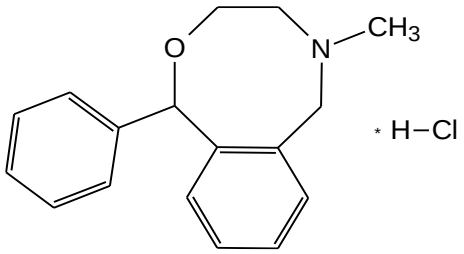
Nefopam hydrochloride is a non-opioid, non-steroidal, centrally acting analgesic active pharmaceutical ingredient with anti-inflammatory potency. It is used for the prevention of postoperative pain, severe hiccups, chronic pain and has relaxant, anticholinergic and antihistamine activity. It is only indicated in the treatment of acute painful conditions. [1] [2] [3]



Scheme 1. Nefopam hydrochloride

Pharmaceutical Works Polpharma S.A., Production Department API Warsaw, Poland are one of global manufacturers of Nefopam hydrochloride, which is produced in four countries around the world only. That is why maintenance of continuity of production and national export of Nefopam is highly anticipated. As the current route of synthesis involves the use of genotoxic solvent, which is supposed to be forbidden, the development of completely new technology of obtaining of Nefopam with use of more safety and environment-friendly organic solvents, reagents and raw materials is a matter of concern.

The aim of this project was the development and optimization of route of synthesis in laboratory scale, determination of impurity profile of active pharmaceutical ingredient and full spectral and chromatographic analysis of new intermediates and impurities which will extend the knowledge on chemistry of heterocyclic compounds. Moreover, performance and development of all analytical methods either of in-process control or quality control were done. The technology transfer to the production scale is set, followed by process validation batches and the final implementation of new technology of obtaining of Nefopam hydrochloride.

Acknowledgement
This research was financed by PIW Ipochem Sp. z o.o.

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P-015

Polyfluoroalkanethioamides: new aspects of reactivity and areas of application in the synthesis of organofluorine compounds

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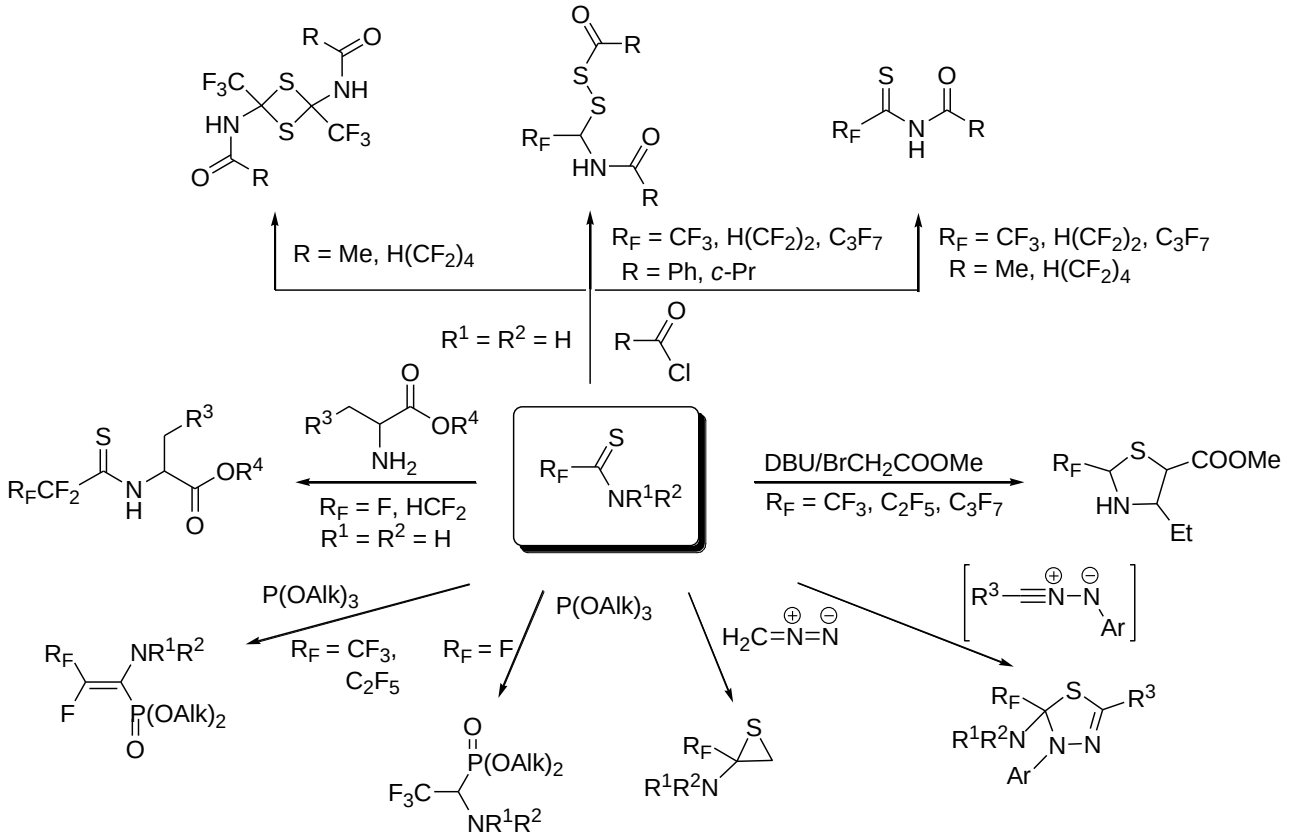
Amides of polyfluoroalkanethiocarboxylic acids (polyfluoroalkanethioamides) are among promising fluorine-containing building-blocks, which possess a significant synthetic potential. Divergent transformations of these compounds arise from the high versatility of the thioamide functionality and the presence of a polyfluoroalkyl group. Polyfluoroalkanethioamides are able to interact with different types of reagents – electrophiles, nucleophiles, as well as participate in cycloaddition reactions. A systematic study of these reactions involving polyfluoroalkanethioamides allowed to develop the methods for the synthesis of new fluorine-containing compounds of the acyclic and heterocyclic structure.



Scheme 1. Synthetic applications of polyfluoroalkanethioamides.

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P-016

Chiral benzothiophenyl *β*-amino alcohols – synthesis and properties

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Sulfur-containing heterocycles represent a versatile class of compounds with significant biological, pharmacological, and material science applications. Among them, benzothiophene is a unique aromatic scaffold found in natural sources such as petroleum derivatives and coffee beans, as well as in bioactive natural products. Benzothiophene derivatives exhibit a wide range of biological activities, including anti-inflammatory, antifungal, anticancer, antidepressant, antimalarial, and enzyme inhibitory effects. In addition, they serve as potential agents in neurodegenerative disease diagnostics and as modulators of diverse molecular targets such as estrogen receptors, kinases, and enzymes.[1] Several benzothiophene-based drugs have reached the market, including raloxifene (osteoporosis), zileuton (asthma), and sertaconazole (antifungal therapy), highlighting their therapeutic relevance. Due to its broad pharmacological profile, the benzothiophene ring system is considered a privileged structure in drug discovery and continues to attract intensive research interest across medicinal and materials chemistry.

A new series of benzothiophenyl *β*-amino alcohols was developed by asymmetric transfer hydrogenation of the corresponding *α*-amino ketones. ATH is established as an excellent reduction method due to its versatility, operational simplicity, avoiding the use of explosive hydrogen gas, catalysts resistant to moisture and air oxidation, and high stereoselectivity. The starting *α*-amino ketones were traditionally prepared[2] by condensation of variously substituted 1-(benzothiophen-2-yl)-2-bromoethanone with 1*H*-imidazole, 1*H*-1,2,4-triazole, 2-aminothiazole, 1*H*-1,3-benzimidazole, and 1*H*-benzotriazole. The asymmetric reduction was carried out with formic acid as a hydrogen donor, catalyzed by both, RhCl[(*R*,*R*)-TsDPEN](C_5Me_5) and RhCl[(*S*,*S*)-TsDPEN](C_5Me_5), in dichloromethane at reflux for 24-48h. All new chiral benzothiophenyl *β*-amino alcohols were obtained in high yields and excellent enantioselectivities (97-99%). The absolute configuration of products was confirmed by means of ECD spectroscopy supported by theoretical calculations. Selected racemic and optically active amino alcohols were tested against four bacterial and two fungal species. It was found that 1-(benzo[*b*]thiophen-2-yl)-2-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)ethan-1-ol, both racemic and chiral-*S*, exhibit excellent antifungal properties against *Malassezia furfur* (MIC = MBC = 4 μg mL^{-1}).

Acknowledgement

Heartfelt thanks Prof. Patrycja Golińska for performing biological test.

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P-017

Synthesis and Structure-Activity Relationship of Pyrazino[1',2':1,5]pyrrolo[2,3-*d*]pyrimidines as Acetylcholinesterase Inhibitors

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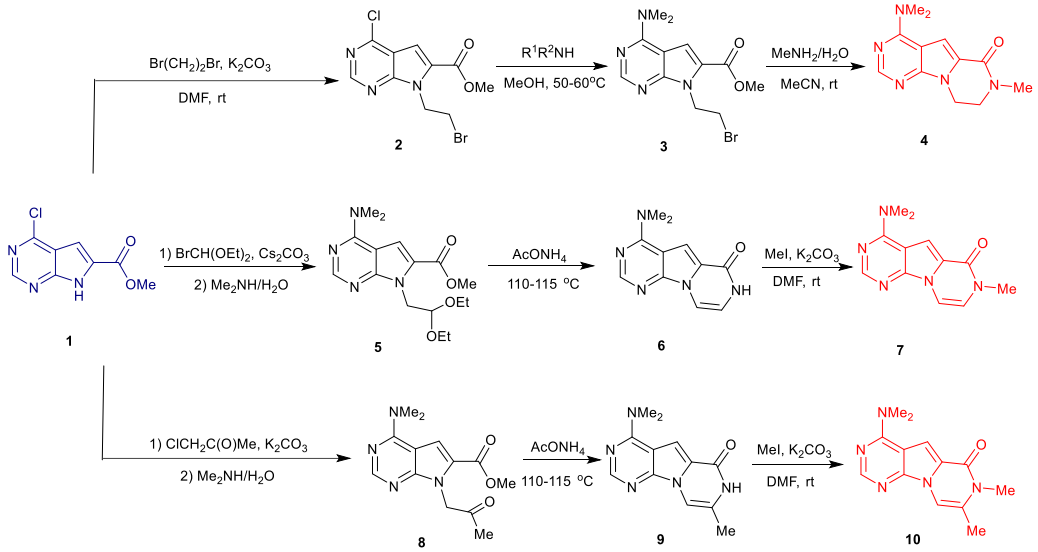
Alzheimer's disease is a neurodegenerative disease associated with decreased levels of acetylcholine. Acetylcholinesterase inhibitors such as donepezil, rivastigmine and galantamine are used to alleviate the symptoms of the disease, and many tricyclic compounds have been developed as new inhibitors of acetylcholinesterase.

Inspired by our previous results [1], we synthesized and tested a series of pyrazino[1′,2′:1,5]pyrrolo[2,3-d]pyrimidine derivatives to study how the ring system (dihydropyrazine vs. pyrazine) and the presence of methyl substituents at positions 7 and 8 affect acetylcholinesterase inhibition. Methyl 4-chloro-7*H*-pyrrolo[2,3-*d*]pyrimidine-6-carboxylate (**1**) was used as a starting material for the synthesis of potential inhibitors (Scheme 1).



Scheme 1. Synthesis of pyrazino[1',2':1,5]pyrrolo[2,3-*d*]pyrimidine derivatives **4**, **7**, **10**.

The presence of the pyrazine moiety in the inhibitor structures was found to increase their potency compared to the compounds with a dihydropyrazine. For example, compounds **4** and **7** inhibited acetylcholinesterase with IC_{50} values of 7.17±1.01 and 2.43±0.26 μM, respectively. Among the synthesized compounds, compound **10** was the most potent inhibitor with an IC_{50} value of 0.22 ± 0.02 μM. Thus, the methyl group at position 8 of the pyrazino[1',2':1,5]pyrrolo[2,3-*d*]pyrimidine core played an important role in the enzyme inhibition. The obtained data can be used for the development of more potent acetylcholinesterase inhibitors with a pyrazino[1',2':1,5]pyrrolo[2,3-*d*]pyrimidine scaffold.

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P-018

An example of the synthesis of bis-pyrazole molecular segment based on conjugated nitrodienes: DFT mechanistic study

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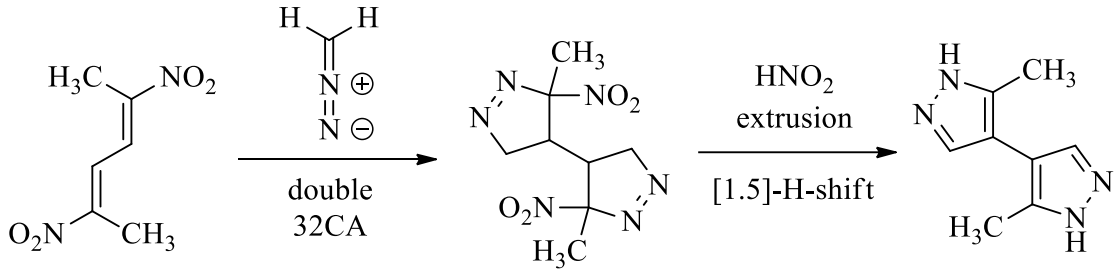
The molecular mechanism underlying the reaction between (2E,4E)-2,5-dinitrohexa-2,4-diene and diazomethane leading to the formation of 3(5),3′(5′)-dimethyl-4,4′-bis-pyrazole was investigated on the basis of the results of the DFT calculations. A topological analysis of the Electron Localization Function (ELF) confirmed the conjugated character of the nitrodiene system and revealed the allenic pseudoradical electronic structure of diazomethane. The reactivity studies demonstrated that the nitrodiene, as well as both nitrovinyl pyrazolines, behave as electrophilic species, whereas diazomethane acts as a nucleophilic agent. Furthermore, evaluation of both kinetic and thermodynamic parameters, together with the analysis of all critical structures, indicated that the formation of bis-pyrazoline through the pmr-type double cycloaddition proceeds via a one-step polar asynchronous mechanism.

Subsequent transformation of the initially formed bis-pyrazoline into the corresponding bis-pyrazole was shown to occur through a sequence of competing processes: a one-step elimination of HNO_2 and a one-step [1,5]-H shift. Importantly, both of these transformations proceed through non-polar asynchronous one-step mechanisms without the involvement of ionic intermediates. This mechanistic insight highlights the subtle interplay between polar and non-polar pathways, providing a deeper understanding of the reactivity of nitrodienes with diazomethane within the MEDT framework [1]



Scheme 1. The formation of 3(5),3′(5′)-dimethyl-4,4′-bis-pyrazole.

Acknowledgement

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017868.

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P-019

In Silico Evaluation of Isoxazolidines: Reactivity and Activity Prediction

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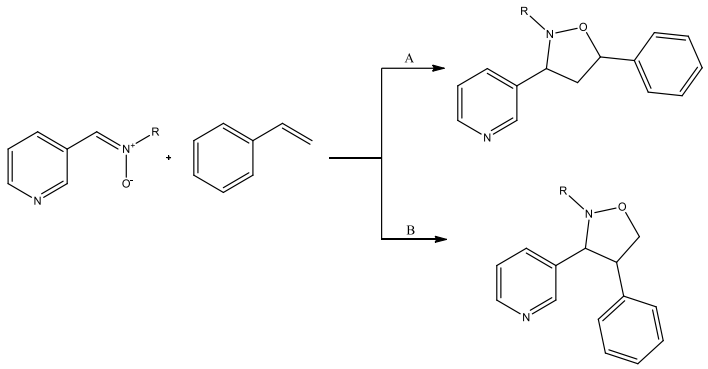
Isoxazolidine derivatives, obtained via the cycloaddition reaction of styrenes with nitrones, represent a valuable class of heterocycles with promising biological activities. To rationalize their reactivity and potential pharmacological relevance, we employed a combination of conceptual density functional theory (CDFT), PASS prediction, ADME evaluation, and molecular docking studies. CDFT descriptors indicated that styrenes act as nucleophiles in these reactions, whereas nitrones behave as strong electrophiles. Among the possible pathways, pathway A was identified as the most favorable route leading to the cycloadducts. The resulting isoxazolidines were further evaluated in silico using PASS-based activity prediction, which suggested a broad spectrum of biological potential. ADME profiling confirmed their drug-like properties, while molecular docking revealed favorable interactions with selected biological targets.



Scheme 1. Alternative cycloaddition pathways for styrene and nitrones.

In silico biological profiling highlighted the importance of structural modifications: the presence of a pyridine ring enhanced biological potential, while alkyl-substituted derivatives satisfied all six bioavailability radar criteria (LIPO, SIZE, POLAR, INSOLU, INSATU, FLEX), suggesting favorable pharmacokinetic profiles. Structural effects were reflected in lipophilicity, with alkyl-substituted analogs showing lower log P values than aryl analogs. All compounds were predicted to exhibit high gastrointestinal absorption and blood–brain barrier permeability.

PASS predictions indicated that all derivatives possess a favorable probability of activity (Pa > 0.7), suggesting strong biological relevance. The most probable pharmacological profiles included nicotinic receptor antagonism and 5-HT2C receptor antagonism, pointing to potential applications in CNS-related disorders. Additional predicted activities involved (S)-6-hydroxynicotine oxidase inhibition and CYP2A8 substrate properties, underscoring the need to evaluate metabolic stability and safety. Molecular docking further supported favorable interactions with selected targets.

Overall, these findings demonstrate that isoxazolidine derivatives promising drug-like features. Substituent effects strongly influence their pharmacokinetic behavior, while PASS and docking results point to potential CNS-related applications, warranting further pharmacological evaluation.

Acknowledgement
We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017645.

P-020

MEDT exploration of the new type of intermediate in the course of (2 + 2) cycloaddition with the participation of conjugated nitroalkenes

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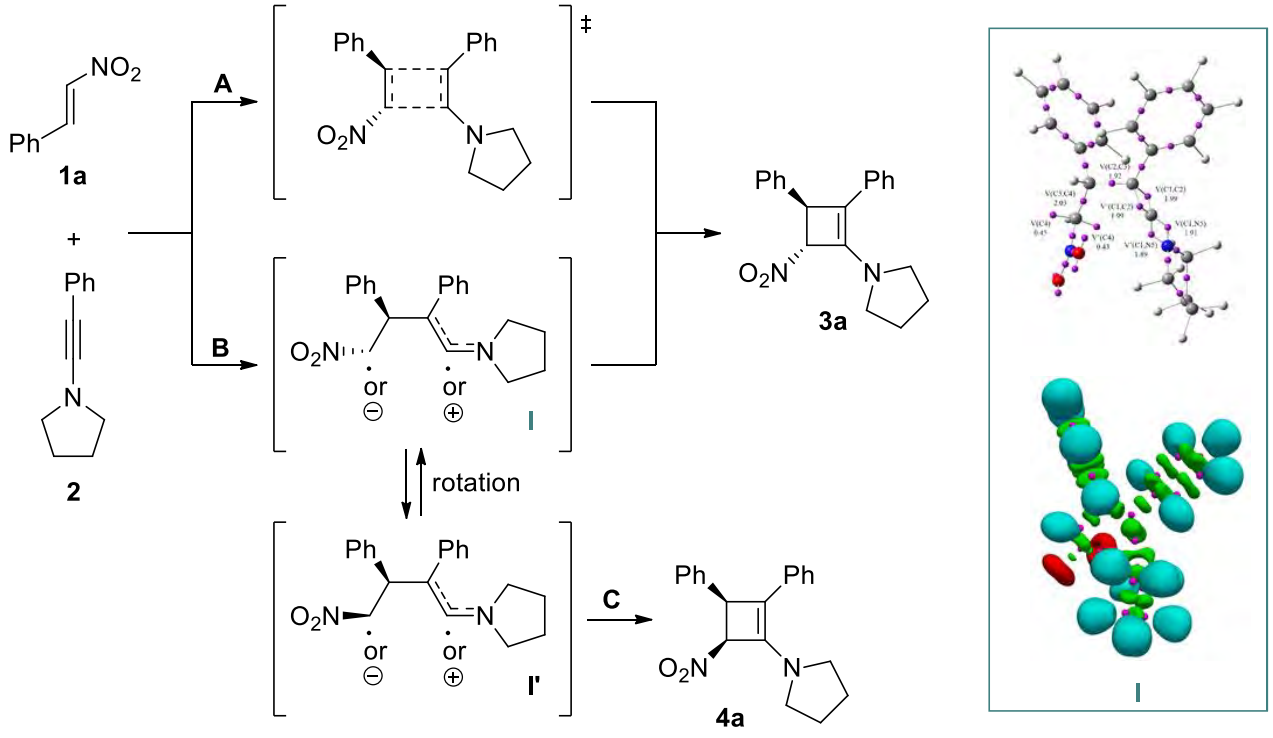
The phenomenons of the regio- and stereoselectivity and the molecular mechanism of the (2+2) cycloaddition (22CA) reaction between (E)-2-phenylonitroethene (**1a**) and ynamine (**2**) molecular system were analysed based on quantumchemical calculations.[1] The analysis of the electronic properties of localized reaction intermediate suggest its possible zwitterionic nature. In the consequence, the proposed mechanism can be treatment as a general for some group of 22CA processes. Lastly, for the model process, the full Bonding Evolution Theory (BET) analysis along the reaction coordinate was performed. It was found, that 22CA reaction between **1a** and **2** begins with formation of two *pseudoradical* centers at C2 and C3 atoms. First C2-C3 single bond is formed in phase V by combining of two *pseudoradical* centers while the formation of a second C4-C1 single bond begins at the last eleven phase of the reaction path. A BET analysis of intermediate (**I**) allows to classified it as a compound with a *pseudoradical* structure. Next to zwitterions and biradicals, it is evidently new type of intermediate on the path of the 22CA reaction.



Scheme 1. Theoretically possible course of 22CA reaction between **1a** and **2**.

Acknowledgement

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017842.

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P-021

A comprehensive insight on the course of the Diels-Alder reaction between hexachlorocyclopentadiene and dichloroethylene

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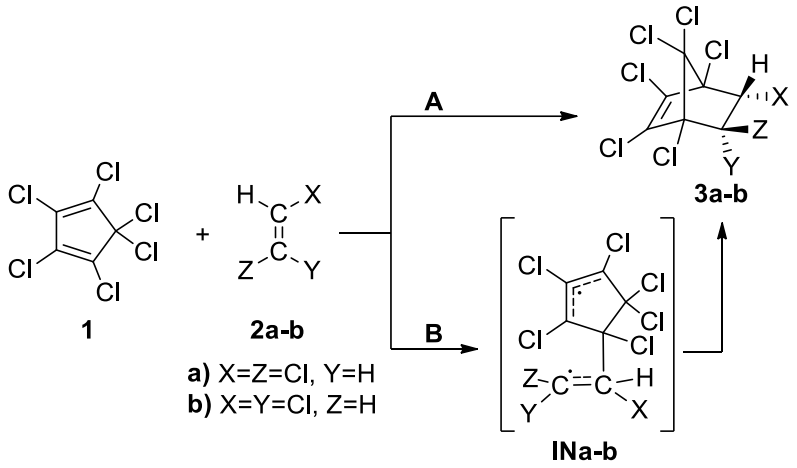
The Diels-Alder (DA) reaction between hexachlorocyclopentadiene (**1**) and 1,2-dichloroethylene (**2a-b**) has been studied using the Molecular Electron Density Theory (MEDT) through Density Functional Theory (DFT).[1] The electronics structure of the reagents has been characterized through the Electron Localization Function (ELF) and the Conceptual DFT (CDFT). The DA reaction of **1** with **2a-b** proceeds via a synchronous or low asynchronous one-step mechanism. Based on the conducted research, two-step mechanism with biradical intermediate was completely ruled out. Bonding Evolution Theory (BET) study of the DA reaction shows that this reaction is topologically characterized by nine different phases. The reaction begins by the rupture of the double bonds in substrate molecules. Formation of first C-C single bond takes place in phase VII, while the second C-C single bond take place in the phase IX. Formation of these two single bonds takes place by sharing the non-bonding electron densities of the two pairs of *pseudoradical* centers. In addition this study evaluates some ligands as potential HIV-1 inhibitors. Docking results identified as the most promising candidates, surpassing AZT in theoretical affinity.



Scheme 1. Two possible path of the DA reaction paths between **1** and **2a-b**.

Acknowledgement

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P-022

On the question of the zwitterionic intermediates on the cycloaddition reaction with the participation of the 2-methoxyfuran and ethyl (Z)-3-phenyl-2-nitroprop-2-enoate

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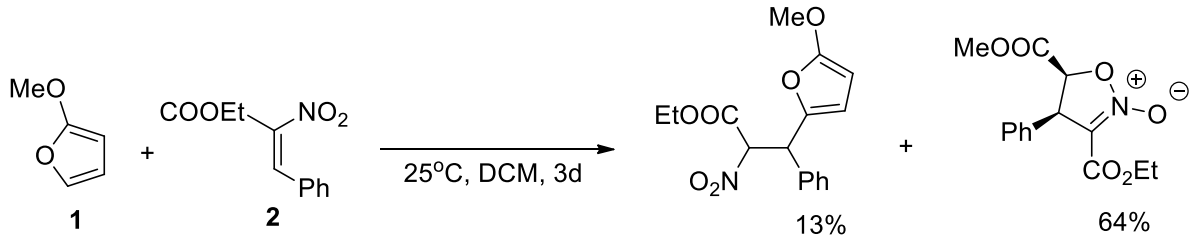
Molecular mechanism for the reaction between 2-methoxyfuran (**1**) and ethyl (Z)-3-phenyl-2-nitroprop-2-enoate (**2**), was investigated applying ωb97xd/6-311+G(d,p)(PCM) quantum chemical computations [1].

The substrates were characterized using MEDT approach [2]. Reaction pathway was thoroughly studied, with the simulated influence of dichloromethane. Intermediates on the reaction pathway were found and characterized by ELF topological analysis. The nature of the intermediates was further studied via Natural population analysis. Thermodynamic aspects of the reaction were also studied.

As a result a molecular mechanism for the reaction was proposed.



Scheme 1. Experimental results of the studied reaction (**1** + **2**) as reported by *Itoh and Kishimoto* [3].

Acknowledgement

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P-023

Hetero Diels-Alder reaction between N-(2,2,2-trichloroethylidene)Carboxamides and Dicyclohexylcarbodiimide: MEDT quantumchemical analysis

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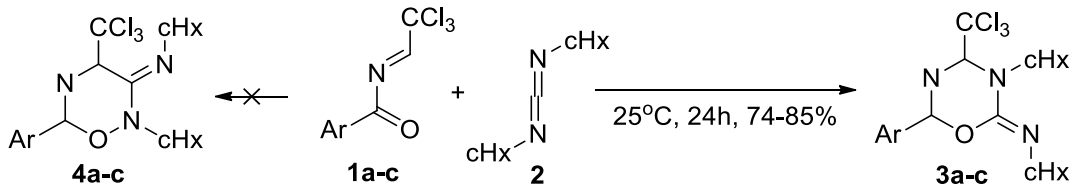
The regioselectivity and the molecular mechanism of the Diels–Alder reactions between N-(2,2,2-trichloroethylidene)carboxamides and dicyclohexylcarbodiimide were explored based on the ωB97xd/6-311G(d) (PCM) calculations [1]. It was found that the reaction course is determined by polar local interactions. It is interesting that the most favored reaction channel is realized not via classical single-step Diels–Alder mechanism, but according to the stepwise scheme with the intervention of the zwitterionic intermediate. The details of the electron density redistribution along the reaction coordinate were explained using the ELF technique.



Ar = Ph (a), 4-Me-C_6H_4 (**b**), 4-CF_3-C_6H_4 (**c**)

Scheme 1. Experimentally observed course of the hetero Diels-Alder reactions between N-(2,2,2-trichloroethylidene)carboxamides (**1a-c**) and dicyclohexylcarbodiimide (**2**).

Acknowledgement

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018201.

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P-024

Review of anticancer sulfonamide complexes with metals

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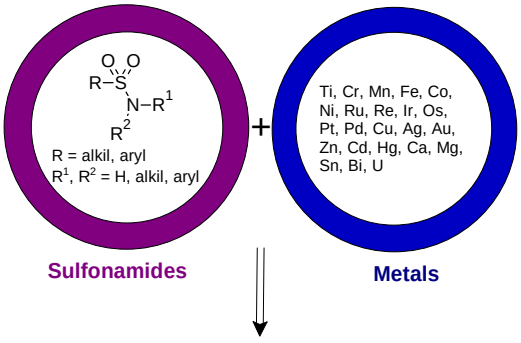
Sulfonamides are organic compounds widely used in medicine as drugs: antibacterial, anti-inflammatory, drugs for the treatment of erectile dysfunction, antidiabetic drugs, diuretics, neuroleptics, and even anticancer drugs. Anticancer sulfonamide drugs include, for example: amsacrine, pazopanib, belinostat and venetoclax [1]. Currently, there are many sulfonamides with anticancer activity described in the literature, which act according to various mechanisms, e.g., through enzyme inhibition [2]. Among the most commonly used anticancer drugs that are metal complexes as cisplatin and its analogues: carboplatin, nedaplatin, oxaliplatin, heptaplatin, etc. Currently, various platinum complexes with other organic ligands are being studied, as well as complexes of other metals, such as palladium, ruthenium, etc. Sulfonamides, which also exhibit anticancer activity, can also be organic ligands in such complexes [3]. Sulfonamide ligands form such complexes with the following metals: Ti, Cr, Mn, Fe, Co, Ni, Ru, Re, Ir, Os, Pt, Pd, Cu, Ag, Au, Zn, Cd, Hg, Ca, Mg, Sn, Bi, U. Popular sulfonamide ligands that form complexes with d-block metals include for example: saccharin [4], sulfamethoxazole [5], sulfafurazole [6], and sulfathiazole [7].



Scheme 1. Sulfonamide metal complexes exhibiting anticancer activity

Acknowledgement

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P-025

Synthesis of New Imidazolidinone Derivatives as Potential Antibacterial Drugs

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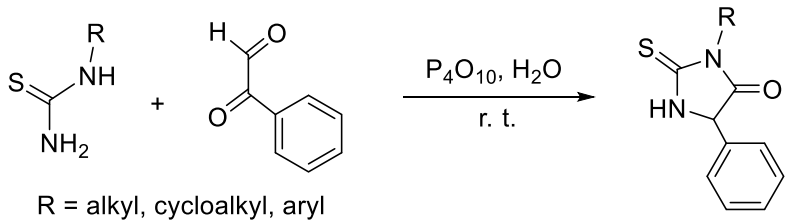
Imidazoles and their hydrogenated derivatives are a group of compounds that exhibit a range of biological activities, including antibacterial, antifungal, antiprotozoal and anticancer effects. [1] Many of them are commonly used in treatment (for example: clotrimazole, metronidazole, dacarbazine and others). These compounds have been the subject of numerous studies due to the potential for their chemical structure modification. Over the years, the development of new compounds based on the imidazole structure has led to improved antimicrobial activity and revealed previously unknown applications for this class of drugs.

The aim of research was to synthesize a series of 11 new derivatives of 5-phenyl-2-thioxoimidazolidin-4-one differing in substituents at N-3, that has not described in the literature yet. They may exhibit antibacterial activity because of their structure.

The condensation reaction was carried out in an aqueous medium using P_4O_{10} as a catalyst, which is in line with the principles of "Green Chemistry". All reactions were conducted with minimalizing of harmful substances. [2]



Scheme 1. The reaction scheme of thiourea derivatives with phenylglyoxal.

The potential biological activity was evaluated *in silico* using the PASS Online program. The results showed that some of them exhibited a high probability of antibacterial activity up to 70%. [3]

Regardless of the type of substituent all synthesized compounds were designed to pass the Lipinski's rule and may the chance to be active after oral administration when used as drugs. [4]

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P-026

Features of *post*-transformations of Ugi bisamides based on cinnamaldehyde derivatives

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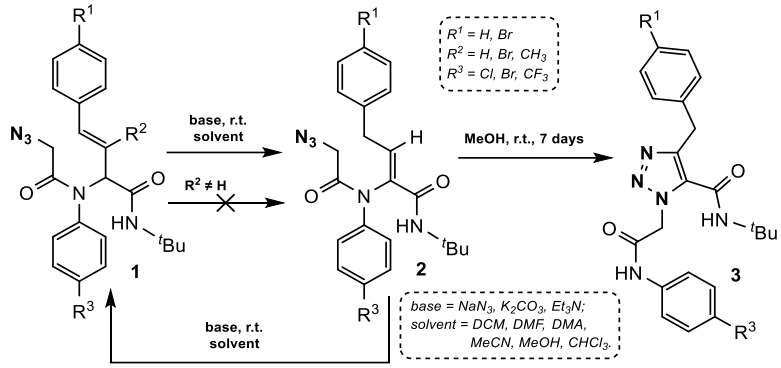
Azide-containing peptidomimetics represent versatile building blocks for a broad range of intra- and intermolecular heterocyclizations. Such scaffolds can be converted into macrocycles, hybrid molecules linked by a triazole fragment, and other classes of nitrogen-containing heterocycles with relevance in pharmaceutical chemistry and materials science.[1]

In continuation of our studies on azido-modified Ugi bisamides **1** based on cinnamaldehyde derivatives [2], we explored their base-mediated isomerization, yielding type **2** products (Scheme 1).



Scheme 1. Scheme of Ugi bisamides isomerization involving the vinyl fragment and the azido group.

The isomerization process was observed to occur spontaneously during the nucleophilic azidation of chloro-substituted Ugi bisamides [2], as well as in a controlled fashion when employing pre-synthesized azidobisamides **1**. Notably, structural isomers of type **2** were obtained under these conditions exclusively from Ugi bisamides bearing an unsubstituted α-position in the aldehyde residue (R^2 = H). In the presence of bases, a mixture of isomers **1** and **2** was formed, which could be separated due to their markedly different solubility in ethers. The isomerization resulted in the loss of the stereogenic centre at the tertiary carbon atom and the shift of the C=C bond, features that clearly distinguish the compounds of types **1** and **2** in NMR spectra. Exposing isomers **2** to analogous basic conditions also yielded mixtures of **1** and **2** (Scheme 1). In contrast, prolonged stirring of isomers **2** in methanol at room temperature led to the formation of a third isomeric form, **3**, which is tentatively considered to be the product of azide-alkene cycloaddition followed by C-N bond cleavage (Scheme 1). The structures and purity of all compounds were confirmed by ^{1}H and ^{13}C NMR spectroscopy, LC-MS (ESI), HPLC (UV), and single-crystal XRD (for each isomer type).

Acknowledgement

The authors thank the National Academy of Sciences of Ukraine for financial support and all brave defenders of Ukraine who allow us to continue scientific work.

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P-027

Synthesis of morpholine-2,5-diones by tandem of azido-Ugi and Ugi reactions

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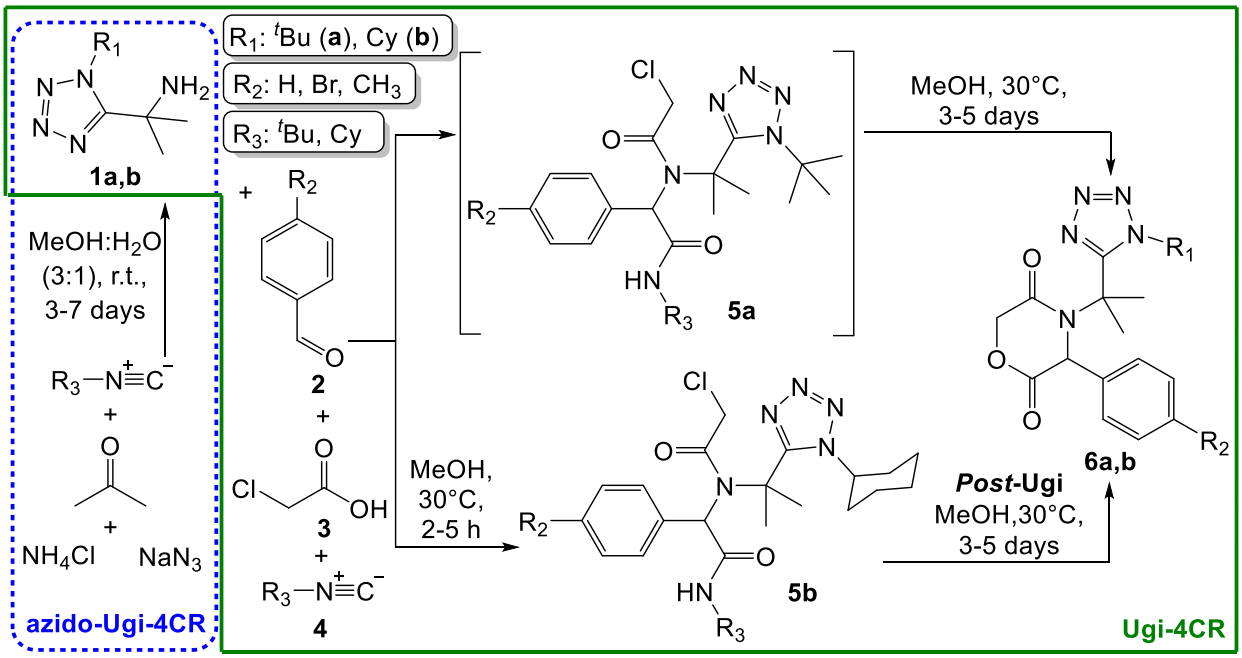
The sequential combination of the four-component azido-Ugi reaction with other isocyanide multicomponent reactions is promising [1], as it leads to the formation of long-chain peptidomimetics. Using a known method [2], by the azido-Ugi-4CR reaction, we synthesised amine components **1a**,**b** by the azido-Ugi-4CR reaction for further introduction into the Ugi-4CR (Scheme 1).



Scheme 1. Synthesis of morpholine-2,5-diones **6a**,**b**

When *α*-aminomethyltetrazole **1a** was used in Ugi-4CR instead of the classical Ugi bisamides **5a**, unexpected morpholine-2,5-dione derivatives **6a** were isolated. It is worth mentioning that only traces of the corresponding bisamides **5a** were detected by LC-MS during the reaction.[3]

By replacing the amine component in the Ugi-4CR reaction with **1b**, the bisamides **5b** could be isolated and identified. As part of further study, *post*-Ugi reactions were carried out on these objects **5b**, which led to the formation of morpholine-2,5-diones **6b**.

Acknowledgement

The authors thank the National Academy of Sciences of Ukraine for financial support and all brave defenders of Ukraine who allow us to continue scientific work.

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P-028

Antipseudomonal Activity and Toxicity of Ammonium Conjugated Derivatives of Nalidixic Acid Based on Natural Compounds

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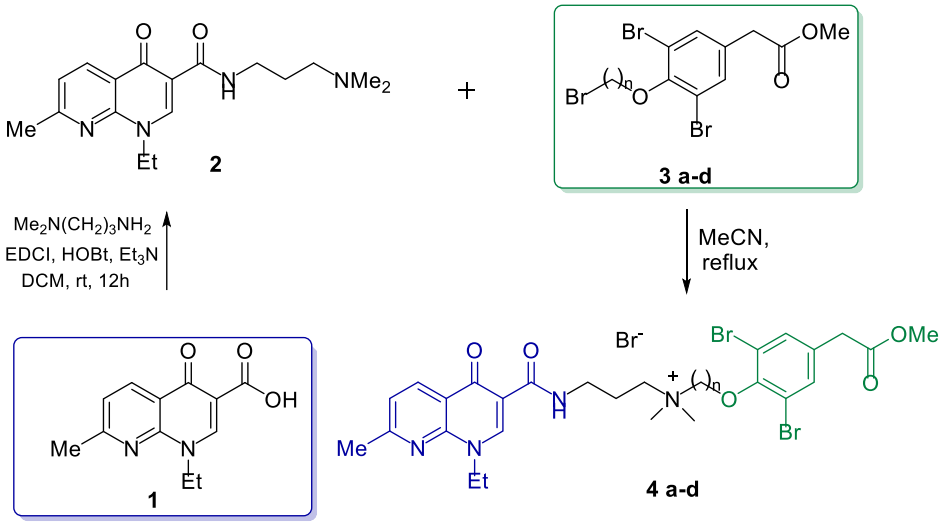
Pseudomonas aeruginosa *(P. aeruginosa*) is a common hospital pathogen well known for its ability to form biofilms that are resistant to many antibiotics. Quinolones are synthetic antibacterial agents widely used to treat a variety of biofilm-associated infections. The first quinolone antibiotic to make it to the market was nalidixic acid, active primarily against gram-negative bacteria. Although its use was discontinued, the conjugates of nalidixic acid are studied as new antibacterial agents with potentially improved properties and higher efficacy.

In line with the previous studies on new antimicrobials with antibiofilm activity [1], ammonium compounds **4a-d** were synthesized by conjugation of nalidixic acid **1** with a bromotyrosine alkaloid derivative. Quaternization of compound **2** with bromoalkoxy-substituted derivatives **3a-d** of the marine product methyl (3,5-dibromo-4-hydroxyphenyl)acetate afforded target ammonium salts **4a-d** (Scheme 1).



3, 4 **a** n= 6, **b** n= 8, **c** n= 10, **d** n= 12.

Scheme 1. Synthesis of targeted conjugated derivatives **4a-d**.

The antibacterial and antibiofilm activity of the synthesized compounds **4a-d** was studied against the *P. aeruginosa* PA01 strain by the broth dilution method. The compounds exhibited antibacterial activity with MIC values ranging from 4 to 32 μg/mL. Among them, derivatives **4b** and **4c** were found to be the most active (MIC = 4 μg/mL). In addition, **4b-d** demonstrated strong inhibition of *P. aeruginosa* PA01 biofilm formation at a concentration of 8.0 μg/mL (almost 100%).

The results of acute toxicity studies on *Daphnia magna* showed that the LC_{50} values of the conjugates **4a-d** were in the range of 3.89-13.90 mg/L. According to Passino and Smith's classification, compounds **4a** and **4b** are slightly toxic, while compounds **4c** and **4d** are moderately toxic.

Acknowledgement
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P-029

Synthesis and potential biological activity of new derivatives of 2,2-dimethyl-4-(4*H*-1,2,4-triazol-3-yl)butanoic acid

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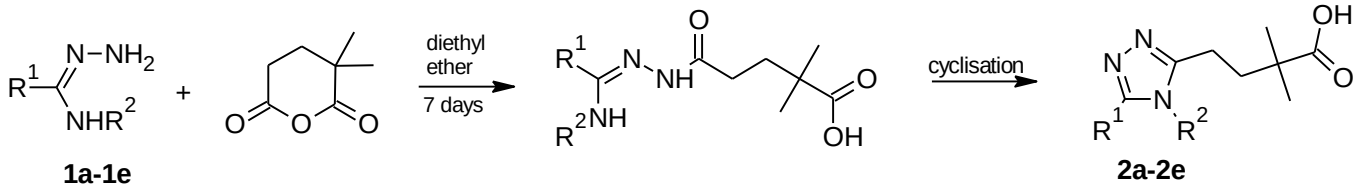
The quest for new drugs effective in the treatment of civilization diseases, caused by, among others, an unhealthy diet and insufficient physical activity, is a significant challenge for modern pharmacotherapy. The main line of cholesterol-lowering drugs are statins, which are widely used to prevent cardiovascular disease. In the search for new agents that could beneficially affect lipid metabolism, new 1,2,4-triazole derivatives containing a molecular fragment obtained by fusion of moieties present in atorvastatin and simvastatin were designed.

A series of compounds **2a-2e** were obtained by reaction of N^3-substituted amidrazones **1a-1e** with 2,2-dimethylglutaric anhydride (Scheme 1). The structure of the new compounds was determined by ^{1}H NMR, ^{13}C NMR and HRMS spectroscopic methods. Additionally, single crystal X-ray diffraction was used to confirm the position of the methyl groups in the side chain of the compound **2a**.

Toxicity of compounds **2a-2e** was assessed using the online tool ProTox 3.0 [1,2], and their potential biological activity was evaluated by online PASS (Prediction Activity Spectra for Substances) software [3].

All compounds **2a-2e** showed very low predicted acute toxicity (2000–2500 mg/kg). In addition, derivatives **2a-2e** meet the assumptions of the Lipinski and Veber rule, which means that they are characterized by very good bioavailability indicators and the possibility of good absorption after oral administration.

According to the PASS calculations, all compounds can be regulators of lipid metabolism, with the most effective compounds containing a phenyl or 4-pyridyl substituent in the R^1 position. Additionally, these compounds may beneficially stimulate kidney function. Additionally, compounds **2a**, **2c** and **2d** may be cholesterol antagonists. These premises indicate the need for further studies on the biological activity of compounds **2a-2e** in vitro.



Scheme 1. The synthesis of compounds **2a-2e**.

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P-030

Cisplatin derivatives and their complexes with PAMAM dendrimers – a way to improve efficacy of chemotherapy in vitro

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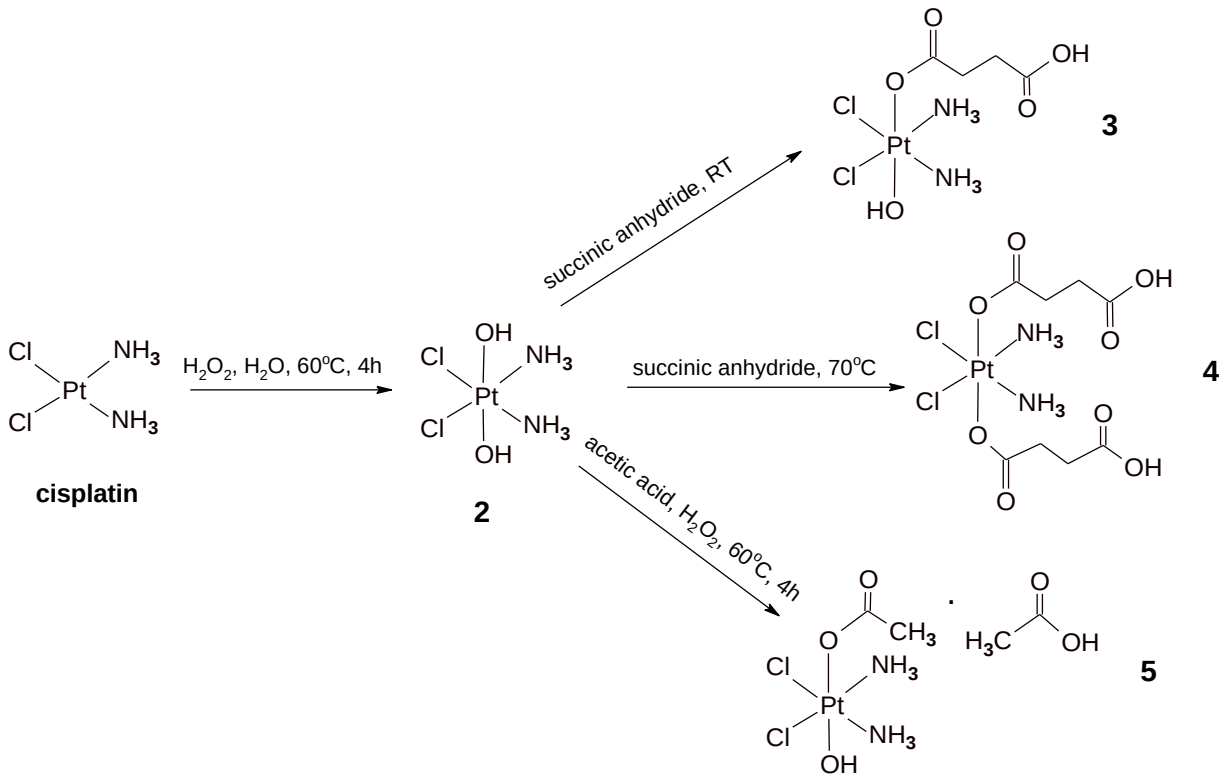
Breast and cervical cancers pose a significant public health burden, with incidence rates rising in recent decades. Cisplatin is a key drug in the treatment of various malignancies. However, its use is limited by significant challenges, such as low selectivity, drug resistance, recurrence, and poor prognosis. Therefore, there is a need for more selective and effective anticancer drugs [1].

We investigated the cytotoxicity and mechanisms of action of three cisplatin derivatives **2-5** (Scheme 1) as well as their complexes with generation 2 polyamidoamine (PAMAM) dendrimers on cancer cell lines (HeLa and MCF-7) and one non-cancer cell line (HMEC-1). The results showed that the complexes exhibited comparable or superior cytotoxicity to cisplatin and greater selectivity for cancer cells.



Scheme 1. Scheme of synthesis of oxoplatin **2**, carboxylatoplatinum(IV) complex **3**, dicarboxylatoplatinum(IV) complex **4** and hydroxyl(acetoxy)cisplatin acetic acid complex **5**.

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P-031

Multicomponent reactions of *α*-ketoglutaric acid

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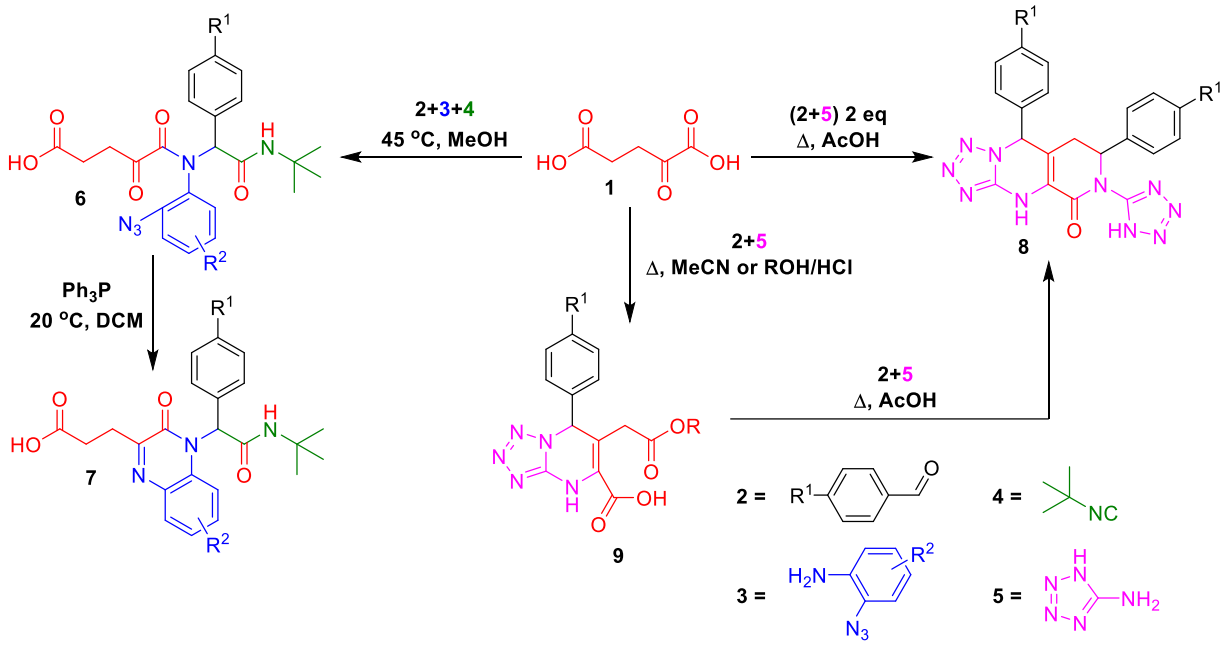
Multicomponent reactions are important tools for the synthesis of structurally complex polyfunctional organic compounds with significantly lower resource consumption and chemical waste compared to classical linear synthesis strategies [1]. An interesting and still little researched reagent for multicomponent reactions is *α*-ketoglutaric acid, which is a dibasic keto acid which plays an important role in many biochemical processes [2].

In the present work, we studied a tandem combination of Ugi/aza-Wittig reactions with *α*-ketoglutaric acid **1**, aromatic aldehydes **2**, *ortho*-azidoanilines **3** and *tert*-butyl isocyanide **4**, which led to the formation of quinoxalinone derivatives **7** by intramolecular cyclization of intermediate peptidomimetics **6**.



The interaction of *α*-ketoglutaric acid **1**, aldehydes **2** and 5-aminotetrazole **5** led to unexpected results: Boiling in acetic acid yielded the products of a tandem Biginelli/Castagnoli-Cushman/decarboxylation reaction – tetrahydropyridopyrimidinones **8**. When this interaction was carried out in an acetonitrile or alcohol medium in the presence of a catalytic amount of hydrochloric acid, a three-component reaction occurred with the formation of dihydropyrimidine derivatives – acids or corresponding esters **9**. Subsequently, the acids **9** could be cyclized to the compounds **8** by the Castagnoli-Cushman/decarboxylation reaction in acetic acid.

Acknowledgement

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P-032

Synthesis of chiral bisoxazoline ligands incorporating aza-aromatic ring and their activity in the metal catalyzed enatioselective nitroaldol reaction.

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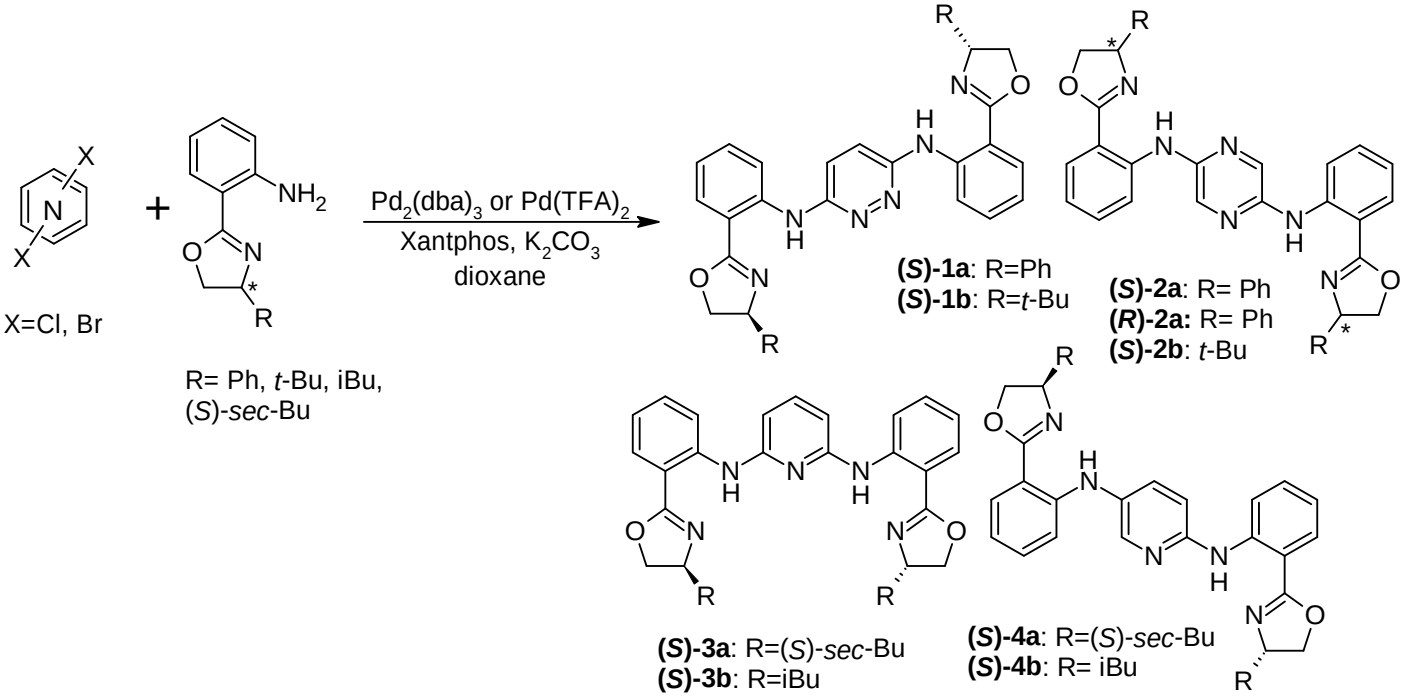
Chiral oxazoline derivatives have developed into one of the most successful ligand classes for asymmetric catalysis due to their modular nature, stability, and applicability in a wide range of asymmetric transformations.[1] Furthermore, the oxazoline ring can be easily performed from, commercially available enantiomerically pure aminoalcohols.[2,3] Among the diverse range of oxazoline ligands, C_2-symmetric bisoxazolines have gained significant attention in coordination chemistry and in asymmetric catalysis.[4] Our particular interest was the synthesis and activity of C_2-symmetric bisoxazoline ligands **(*S*)-1a-(*S*)-3b** that can simultaneously bind to two metal centers. Synthesis and investigation of C_1-symmetric bisoxazolines **(*S*)-4a** and **(*S*)-4b** that belong to the less explored group of oxazoline ligands [5] were also carried out. The synthetic approach involves the Pd-catalyzed *N*-arylation of dihalogenated pyridine, pyridazine and pyrazine with 2-(aminophenyl)oxazolines, which were obtained by the Lewis acid-catalyzed condensation of 2-aminobenzonitrile and enantiopure aminoalcohols. The catalytic activity of the thus obtained ligands was tested in the enantioselective nitroaldol reaction. In reactions catalyzed by copper, appropriate *β*-nitro alcohols were formed in good yields and moderate to good enantioselectivity.



Scheme 1. Synthesis of bisoxazoline ligands containing aza-aryl ring by Buchwald-Hartwig reaction

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P-033

Divergent hetero-[8+*n*] higher order cycloadditions of tropothione and enals catalyzed by *N*-heterocyclic carbenes

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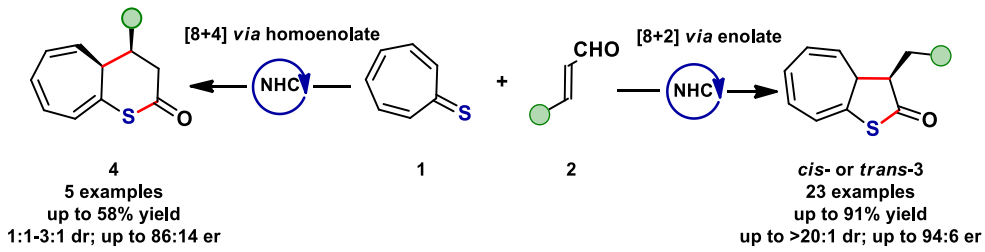
Cycloaddition reactions constitute a powerful tool for the construction of diverse carbo- and heterocyclic scaffolds from acyclic precursors.[1] The Diels-Alder reaction and 1,3-dipolar cycloadditions are the most prominent examples and they are very well recognized.[2,3] Transformations involving more than 6π-electrons overall are described as higher-order cycloadditions and they continue to be a dynamic and developing area of research providing valuable access to unique, chiral building blocks, especially when integrated with advanced principles of asymmetric organocatalysis.[4] Among various organocatalysts, N-heterocyclic carbenes stand out as highly effective tools, offering a versatile activation strategy that unlocks access to a broad range of non-classical reactivities.[5]

In this project, the divergent asymmetric NHC-catalyzed [8+*n*] higher-order cycloadditions using tropothione (**1**) as an electron-poor 8π-component and α,β-unsaturated aldehydes **2** were presented.[6] The base-dependent selectivity of the synthetic approach allowed obtaining heterocyclic products **3** and **4** bearing either γ- or δ-thiolactone rings with high enantioselectivity. The impact of base on NHC intermediate isomerization was explained by DFT studies. The diastereodivergency of the methodology was confirmed with both diastereomers ***cis*-** or ***trans*-3** being easy to isolate with very good results.



Scheme 1. [8+*n*]-Cycloadditions of tropothione (**1**) and α,β-unsaturated aldehyde **2**.

Acknowledgement

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P-034

Amine-Promoted Phosphine Substitution in $CpFe(CO)_2I$ Complexes

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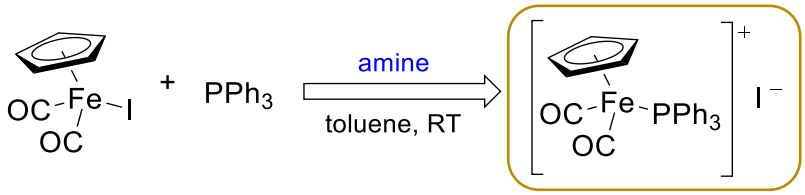
We have discovered that amines play a key role in accelerating the iodide substitution in $CpFe(CO)_2I$ (Cp = η^5-cyclopentadienyl) with phosphorus ligands, facilitating the synthesis of novel complexes that are otherwise inaccessible without the presence of amines. In a reaction between equimolar amounts of $CpFe(CO)_2I$ and triphenylphosphine in toluene containing diisopropylamine (DIPA), the complex $[CpFe(CO)_2PPh_3]^+I^-$ was produced within 5 minutes at room temperature, yielding 72%, and increasing to 90% after 24 hours. Analogous reactions employing bisphosphines such as 1,3-bis(diphenylphosphino)ethane (dppe) and 1,1′-bis(diphenylphosphino)ferrocene (dppf) were also conducted, with the products being contingent upon the reagent ratios. Furthermore, the DIPA-catalyzed reaction of $CpFe(CO)_2I$ with triethyl phosphite led to a product analogous to a Michaelis-Arbuzov rearrangement, namely $CpFe(CO)_2[P(O)(OCH_2CH_3)_2]$ [1]. To elucidate the reaction mechanism, theoretical calculations of the intermolecular interactions between $CpFe(CO)_2I$ and amine molecules were performed, proposing two potential pathways to explain the formation of the observed products [2].



Scheme 1. Amine-catalyzed reaction of $CpFe(CO)_2I$ with PPh_3.

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P-035

5-Amino-1,3-oxazole derivatives and 1,3-oxazole-5-sulfonylamides as new agents against human cytomegalovirus

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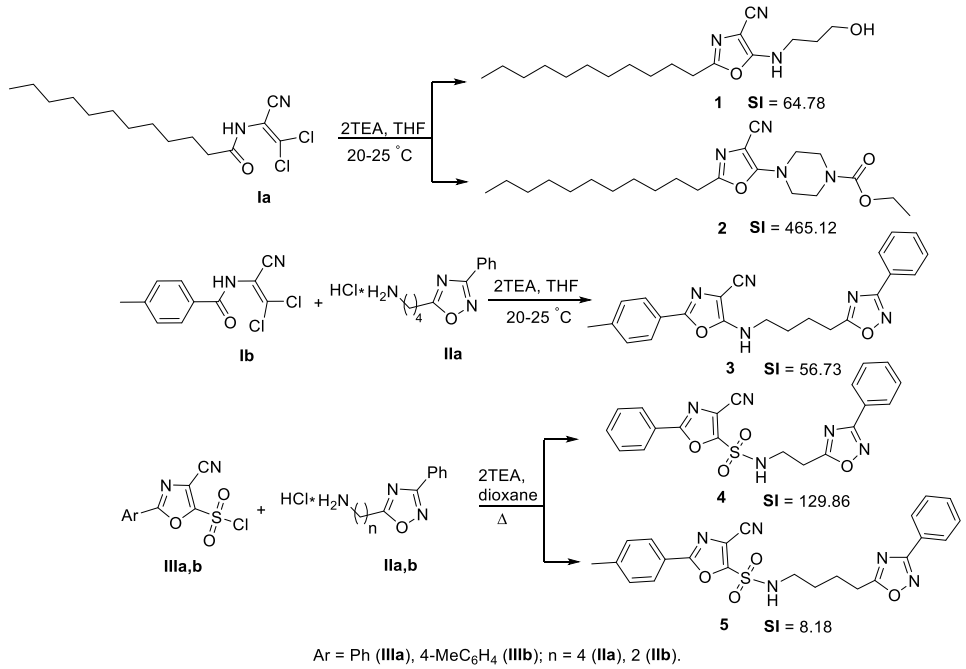
The 1,3-oxazole scaffold is a versatile structural motif commonly employed in the design of novel compounds that exhibit a broad spectrum of pharmacological activities. Oxazole derivatives have been shown to be promising antiviral agents, in particular against human cytomegalovirus (HCMV) [1]. A series of novel 1,3-oxazole derivatives **1-5** modified with amino groups (**1**, **2**), 5-amino-4-cyano-1,3-oxazole containing 1,2,4-oxadiazole (**3**) and 4-cyano-1,3-oxazole-5-sulfonylamides (**4, 5**) were synthesized starting from enamides **Ia**, **b** or 4-cyano-1,3-oxazole-5-sulfonyl chlorides **IIIa, b** (Scheme 1), fully characterized and tested for their anti-HCMV activity. Biological studies revealed that compound **2** had the highest selectivity index (SI) value (SI = 465.12), which was higher than for the reference drug ganciclovir (SI = 325.73). A favourable SI value was also obtained for compound **4** (SI = 129.86). Additionally, SI values greater than 50 were obtained for compounds **1** and **3**. Compound **5** was characterized by SI = 8.18. Test results indicate that 1,3-oxazole derivatives can be considered promising candidates in the search for new active anti-HCMV drugs.



Scheme 1. Synthesis of 4-cyano-1,3-oxazoles **1-5.**

Acknowledgement

Biological studies were financed by the Ministry of Science and Higher Education within the project POL-OPENSCREEN (no. 2024 / WK /06).

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P-036

Synthesis of 1,2,4-oxadiazole-containing 4-cyano-1,3-oxazoles

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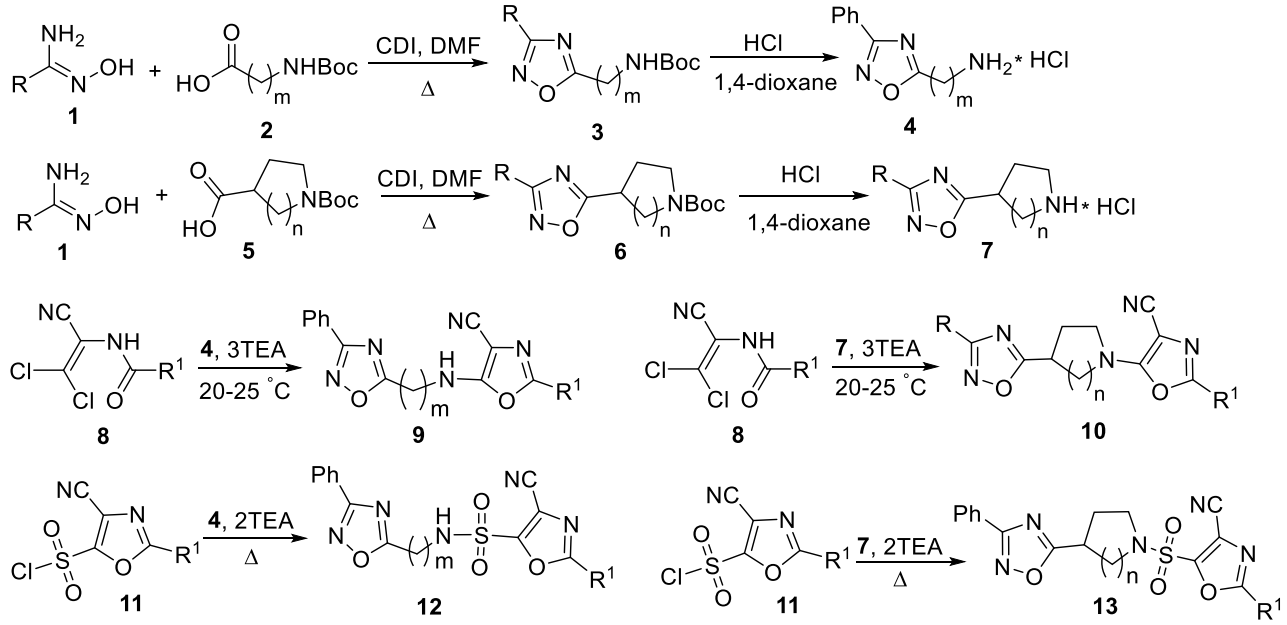
A series of novel oxazole derivatives, featuring 1,3-oxazole and 1,2,4-oxadiazole rings connected *via* an aminocarbon linker or sulfonamide group, were synthesized (Scheme 1). The interaction of amidoximes **1** and *Boc*-aminoacids **2**, **5** yielded 1,2,4-oxadiazoles **3**, **6**, which, under the action of HCl, were converted into unknown 1,2,4-oxadiazole hydrochlorides **4**, **7**. By the reaction with 2-acylamino-3,3-dichloroacrylonitriles **8** [1] or 2-aryl-4-cyano-1,3-oxazole-5-sulfonyl chlorides **11** [2], substituted 1,2,4-oxadiazole-containing 5-amino-4-cyano-1,3-oxazoles **9, 10** and 4-cyano-1,3-oxazole-5-sulfamides **12, 13** were formed.



R = C_6H_5, 3-$CH_3C_6H_4$, 4-$CH_3OC_6H_4$, 4-FC_6H_4; R^1 = C_6H_5, 4-$CH_3C_6H_4$; m = 1-7; n = 1,2,

Scheme 1. Synthesis of 5-amino-4-cyano-1,3-oxazoles and 1,3-oxazole-5-sulfamides with a 1,2,4-oxadiazole fragment.

The activity of compounds **9, 10, 12**, and **13** was evaluated for their potential anti-HCMV properties. The results of antiviral activity screening indicate that 1,3-oxazole derivatives **9**, **10, 12, 13** can be considered promising candidates in the search for new active anti-HCMV drugs.

Acknowledgement: Biological studies were financed by the Ministry of Science and Higher Education within the project POL-OPENSCREEN (no. 2024 / WK /06).

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P-037

Enantioselective synthesis of fluorinated α-hydroxy- and α-aminophosphonates via asymmetric transfer hydrogenation.

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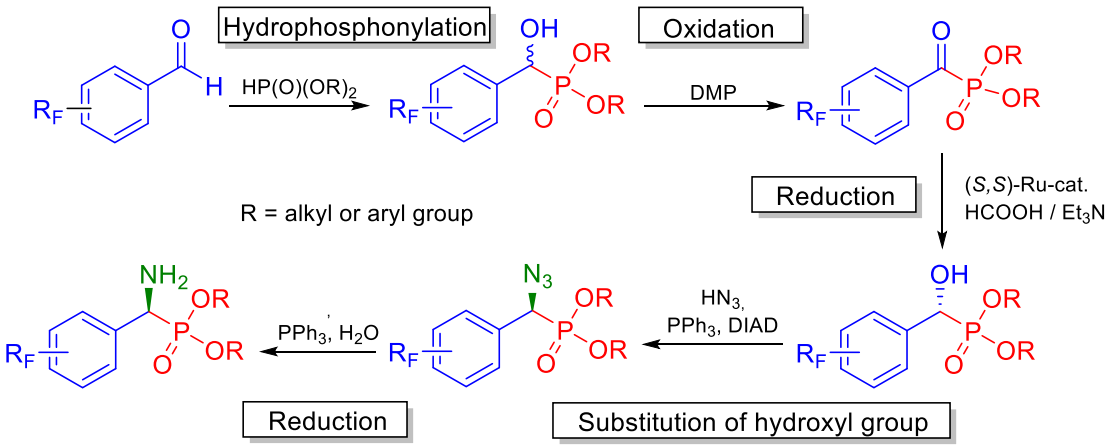
Phosphonates, and in particular α-hydroxy- and α-aminophosphonates, belong to compounds of significant importance in medicinal chemistry owing to their role as structural mimetics of amino acids and their diverse biological activities, including anticancer potential [1]. In this work, a series of novel, highly enantioenriched α-hydroxy- and α-aminophosphonates were synthesized as fluorinated analogues of phenylglycine. The synthetic route (Scheme 1) was developed using asymmetric transfer hydrogenation [2,3] as the key stereodefining step, affording α-hydroxyphosphonates in high enantiomeric excess. Subsequent transformations provided access to the corresponding α-aminophosphonates. All compounds were fully characterized by spectroscopic methods (^{1}H, ^{13}C, ^{19}F, ^{31}P NMR). In silico ADME screening (SwissADME) [4] highlighted favorable pharmacokinetic profiles, underlining their potential as biologically relevant molecules of medical importance. These findings provide a basis for further biological evaluation, with particular focus on anticancer activity.



Scheme 1. General pathway for enantioselective synthesis of α-hydroxy and α-aminophosphonates.

Acknowledgement

The authors are grateful for financial support from the Inicjatywa Doskonałości – Uczelnia Badawcza project (181/13/SNŚ/0008), the ANR (BOOSTS project, ANR-21-CE07-0034), and the Erasmus+ Programme of the European Union.

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P-038

Novel 2-amino-4,5-dihydrothiazol-4-one derivatives as selective 11β-HSD1 inhibitors

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Thiazole and dihydrothiazole derivatives are compounds that exhibit diverse biological activity. Some compounds containing a thiazole ring are known drugs with anticancer, antiviral, antiparasitic, or anti-inflammatory effects. Of particular note are Biovitrum BVT-2733, Biovitrum BVT-14225, and Amgen 2922, which are known inhibitors of 11β-hydroxysteroid dehydrogenase type 1 (11β-HSD1). This enzyme catalyzes the conversion of inactive cortisone into physiologically active cortisol. Together with its isoform - 11β-HSD2, it forms a system that regulates cortisol levels in the body. Chronic excess of cortisol in the blood can lead to, among other things, to the development of symptoms associated with hypercortisolism (Cushing's syndrome) and metabolic syndrome. Inhibition of 11β-HSD1 activity reduces cortisol levels, which may consequently result in reduced adipose tissue mass, decreased blood glucose levels in patients with type 2 diabetes, and lower total cholesterol levels [1]. The role of 11β-HSD1 in diabetes and metabolic syndrome, as well as the ongoing need for new treatments for these diseases, drive the search for new selective inhibitors of this enzyme. This may be crucial in the treatment of metabolic diseases.

Carbenoxolone is a well-known 11β-HSD1 inhibitor. However it inhibits not only 11β-HSD1 activity but also 11β-HSD2, although to a lesser extent. Inhibition of 11β-HSD2 can cause hypertension, peripheral edema, hypokalemia, and metabolic alkalosis. These adverse effects limit the clinical applications of carbenoxolone and highlight the need for new selective 11β-HSD1 inhibitors.

Among the many different groups of organic compounds tested as 11β-HSD1 inhibitors, 2-aminothiazol-4,5-dihydrothiazol-4-one derivatives are noteworthy. A series of spiro derivatives of 2-amino-4,5-dihydrothiazol-4-one, differing in the substituents on the amino group, have been synthesized and tested for their ability to inhibit 11β-HSD1 activity. Many of them demonstrate high inhibitory activity, comparable to carbenoxolone. At a concentration of 10 μM, the tested compounds inhibit 11β-HSD1 activity by a range of 48 to 94% (IC_{50} up to 40 nM). Studies on 11β-HSD2 inhibition have shown that some compounds are also more selective than carbenoxolone.

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P-039

Synthesis of new azole derivatives with potential antimicrobial activity

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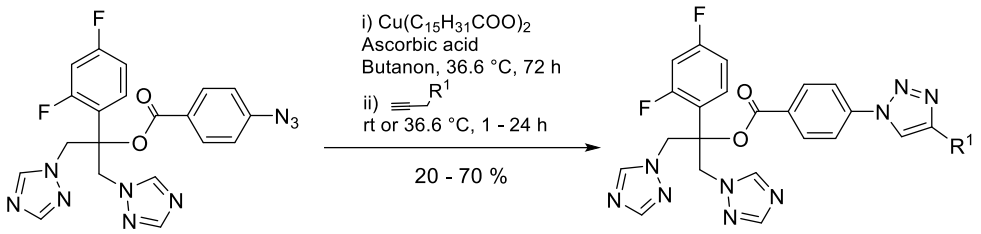
Over the past few decades, the rapid emergence of resistance among fungal pathogens has significantly reduced the clinical efficacy of commonly used antifungal drugs, including triazole derivatives such as fluconazole [1]. This phenomenon highlights the urgent need to design new antifungal molecules that could overcome resistance mechanisms and broaden the therapeutic spectrum. One promising strategy for discovering new, more active drugs is to modify known pharmacophoric structures.

The 1,2,4-triazole ring is a heterocyclic motif widely recognized for its broad spectrum of biological activity, including antifungal, antibacterial, anticancer, antiviral, and anti-inflammatory properties [2]. In the present work, we decided to utilize this pharmacophore for the structural modification of fluconazole, obtaining hybrids of these two molecules using the CuAAC reaction. Such structural hybridization can lead to compounds with a new biological profile, potentially combining or even synergistically enhancing the properties of the parent molecules. This type of hybrid compound offers a promising strategy for the discovery of new antifungal drugs with increased efficacy and the ability to address the growing problem of resistance. Selected synthesis pathways and representative conjugates will be presented.



Scheme 1. Synthesis of novel fluconazole hybrids via CuAAC reaction

Acknowledgement
The research was carried out as part of the OPUS project UMO-2019/33/B/NZ7/01608.

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P-040

Thermal analysis of paraffin–oil candles in the context of defect formation using differential scanning calorimetry (DSC)

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The purpose of the study was to evaluate how the addition of dyes and fragrance substances affects the thermal properties of paraffin candles, using differential scanning calorimetry (DSC). The research was conducted on samples containing various combinations of functional additives, reflecting the composition of decorative and aromatherapy candles. Freshly prepared samples and those subjected to an ageing process under controlled temperature conditions of 15, 25 and 40 ° C were analyzed.

DSC measurements allowed for the determination of changes in melting temperature and enthalpy, as well as the course of crystallization processes. On the basis of the analysis of the obtained results, it can be concluded that the presence of additives may significantly modify the thermal properties, indicating, among other things, unfavorable interactions between individual components. Moreover, storage conditions have a significant impact on candle stability, with 15 ° C being the least favorable temperature (Figure 1). The results obtained may serve as a basis for optimizing the composition of candles to improve their storage stability and enhance user safety.

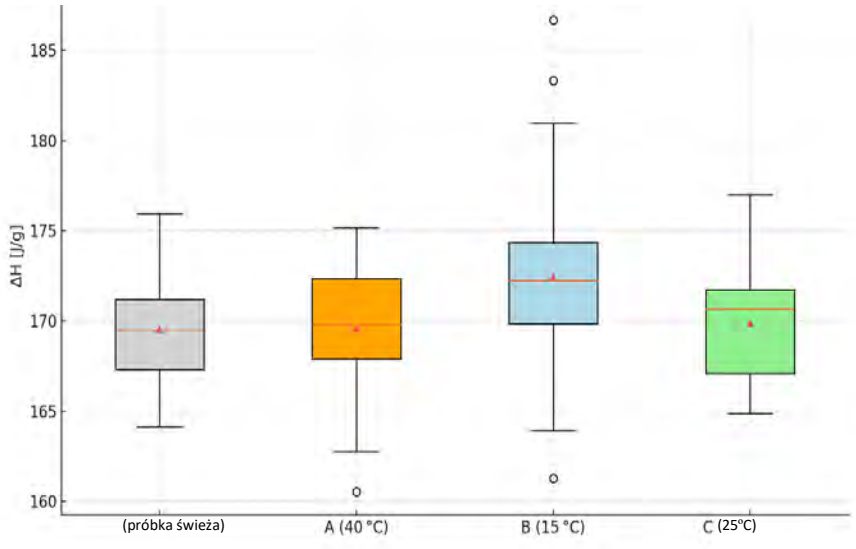

Figure 1. Comparison of the enthalpy of samples stored at different temperatures and for various periods of time.

P-041

Morpholino Nucleoside Thio- and Dithiophosphates via an Oxathiaphospholane-Based Synthetic Approach

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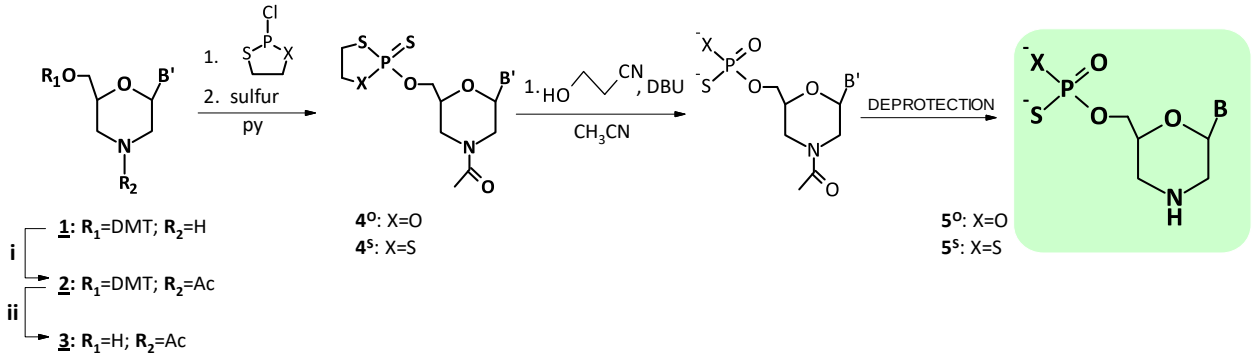
Nucleosides, nucleotides, and their analogs have diverse applications, including use as enzyme substrates or inhibitors, and as anticancer and antiviral agents, mainly targeting replication. Inside cells, they are sequentially phosphorylated to nucleoside 5′-mono-, di-, and triphosphates (NMP, NDP, NTP) by viral and cellular kinases. These compounds can inhibit enzymes involved in DNA or RNA synthesis, such as viral polymerases and kinases. Additionally, fluorescently or radiolabeled nucleotides serve as valuable probes in biochemical and molecular studies.

Here, we describe the efficient preparation of morpholino nucleoside thio- and dithiomonophosphates employing the oxathiaphospholane approach. In this methodology, suitably protected 6′-O-(2-thio)-1,3,2-oxathiaphospholane and 6′-O-(2-thio)-1,3,2-dithiaphospholane intermediates undergo nucleophilic substitution with 3-hydroxypropionitrile under DBU catalysis, yielding the corresponding **6′-O-(α-thiophosphates)** and **6′-O-(α,α-dithiophosphates)**, respectively [1, 2].



The production of modified nucleoside thiophosphate analogs remains a considerable challenge, primarily due to the complex and time-consuming purification processes involved. Nevertheless, our recent developments have greatly improved access to these intriguing and promising derivatives. The synthesized compounds exhibit low cytotoxicity toward human cells, indicating their favorable biocompatibility and potential for further biological and therapeutic applications.

Acknowledgement

This project was supported by Narodowe Centrum Nauki **2021/43/D/ST4/02433**.

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P-042

Comparison of Anticancer Activity of Free-Ribose and Acetyl-Ribose Cobalt Carbonyl Furopyrimidine Nucleosides with 5-Alkynyl Substituent

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Dicobalt hexacarbonyl 5-alkynyl furopyrimidine nucleoside analogs, with 4-alkylphenyl substituents attached at the base C-6 position, were synthesized. Attached at the C-5 position were propargyl alcohol, its methyl ether and acetate derivatives, homopropargyl alcohol, and the 4-alkylphenyl-substituted ethynyl groups. Alkyne functions were coordinated to a dicobalt hexacarbonyl unit. Those compounds were designed in the form of ribose acetyl esters and free ribose.[1,2] The cytotoxic activity of each of dicobalt modified nucleosides on cancer cells of different phenotypes was determined *in vitro*. The investigated compounds showed antiproliferative effects with median inhibitory concentration (IC_{50}) values in the ranges of 14–90 and 9–50 μM for HeLa and K562 cells, respectively. The formation of reactive oxygen species in the presence of modified nucleosides was determined in K562 cells. The results indicate that the mechanism of action for the studied compounds may be related to the induction of oxidative stress.[1,2] This report brings comparison of activity of ribose free-hydroxyl functions and acetyl esters metallo-nucleosides, a seldomly reported hybrids of furopyrimidines and dicobalt hexacarbonyl organometallic unit; component structures that proved to be extremely potent as antivirals and carbon monoxide releasing molecules (CORM), respectively.

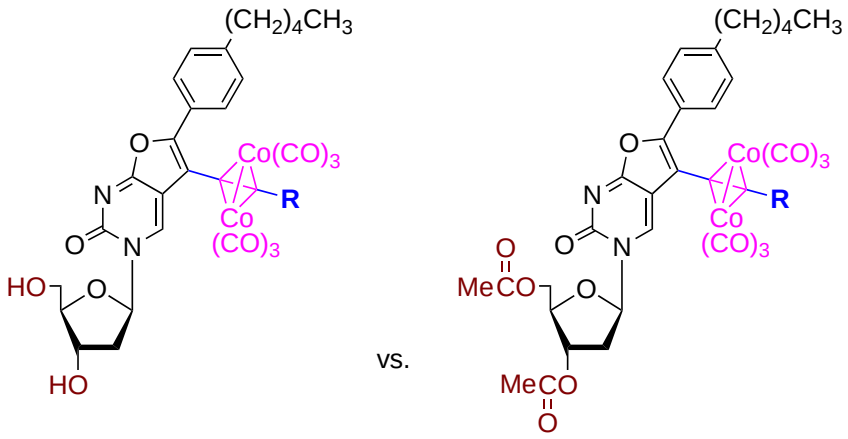

Figure 1. Nucleosides synthesized and compared in this study.

Acknowledgement
This work was supported by the Statutory Funds of CMMS PAS.

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P-043

Structurally Diverse α-Aminophosphonic Acids in the Search for New Compounds with Potential Biological Activity

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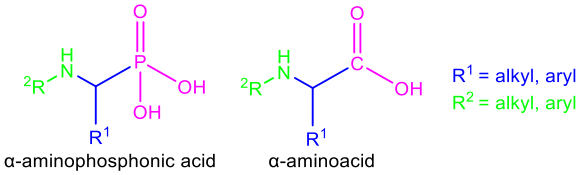
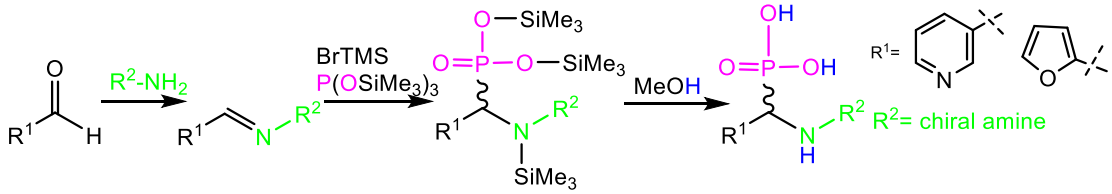
α-Aminophosphonic acids comprise a structurally diverse group of organic compounds whose common feature is the presence of a phosphonic acid group and an amine group located in the α-position relative to it. This structure makes these compounds analogues of both natural and synthetic α-aminocarboxylic acids (Scheme 1). Many α-aminophosphonic acids exhibit biological activity. Among them are compounds with anticancer, antifungal and antibacterial properties [1-4]. Therefore, α-aminophosphonic acids are considered a valuable source of potential drugs and are an interesting subject of research in the field of medicinal chemistry [5].



Scheme 1. General structure of α-aminophosphonic and α-aminocarboxylic acids.

As part of our research, new α-aminophosphonic acids containing, in addition to the phosphonate group, fluorine atoms and a heterocyclic motif were synthesised (Scheme 2) [6-7]. The combination of these three pharmacophores in a single molecule represents a new approach to α-aminophosphonic acids, which is expected to result in interesting biological properties of the compounds obtained.



Scheme 2. Strategy of the synthesis of new α-aminophosphonic acids.

Acknowledgement
The work was financed within the framework of the project "ID-UB" No. 154/39/UAM/0005.

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P-044

Reactivity of imidazolium cation complexes with carbonyl compounds in the synthesis of bisphenol derivatives in the light of quantum chemical calculations

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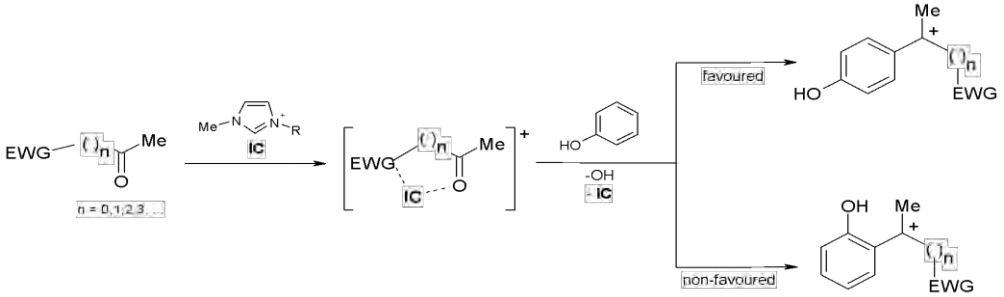
According to Domingo's terminology [1], carbonyl compound complexes with imidazolium cations should be regarded as exceptionally strong electrophiles. Their reactions with phenol, leading to the formation of bisphenols, proceed via a polar mechanism.

Kinetic studies have shown that the key stage of the reaction between electrophilic reagents and phenol is the initial electrophilic attack on the aromatic ring of phenol [2]. This process follows the mechanism of electrophilic aromatic substitution (EAS). In reactions of imidazolium-based liquids (IC), catalyzed by ionic liquid cations, benzyl cations are expected to form as intermediate products:



Scheme 1. Reaction course of electrophilic reagents and phenol under EAS mechanism

The second stage of the reaction proceeds more rapidly, and its course is governed by steric effects, which enforce substitution in the para position [3-5].

The aim of our study was twofold:
(i) to evaluate the electronic properties of selected electrophiles (derivatives of chosen carbonyl compounds) and determine how their structure influences reactivity;
(ii) based on the obtained results, to interpret the reaction pathway at the stage determining the orientation of OH groups in the final adduct.

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P-045

Condensation of Methylglyoxal with N-Substituted Thioureas: Synthesis and Biological Evaluation of Novel Imidazole Derivatives

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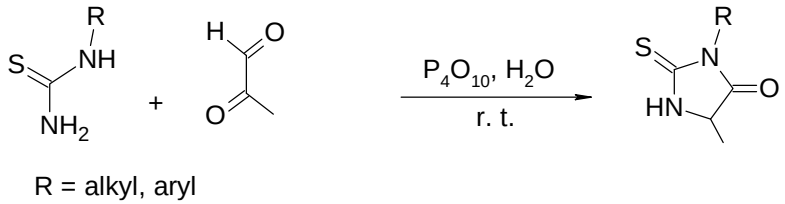
Imidazoles represent a versatile class of compounds known for their diverse biological properties, such as antibacterial, antifungal, and antiprotozoal activity. Because of the possibilities offered by modifying their chemical structure, they have been extensively investigated. Over time, structural optimization of imidazole derivatives has not only enhanced their antimicrobial potential but also uncovered new therapeutic uses within this drug family.[1] Novel modifications have made it possible to employ imidazoles as anti-inflammatory and pain-relieving agents, as well as in the treatment of cancer, viral diseases, depression, and tuberculosis.

The aim of the study was to obtain a new imidazole derivatives in the condensation reaction of thiourea derivatives with dicarbonyl compounds and to evaluate their potential biological activity and bioavailability with the aid of special computer programs (in silico methods).

A series of imidazole derivatives were synthesized in the condensation reactions of methylglyoxal with N-substituted thioureas, and their potential biological activities were evaluated. The reactions were performed in an aqueous medium with P_4O_{10} as the catalyst.[2] The obtained compounds were identified by spectroscopic methods (^1H and ^{13}C NMR, and mass spectrometry).

We obtained a new compounds- thioxoimidazolidinone derivatives with yield up to 50%. The potential biological activity was evaluated in silico using the PASS Online program. The results showed that, in terms of mechanism of action, the obtained compounds are likely to be effective inhibitors of chloride peroxidase (72% probability).[3]

Building on the positive research outcomes, additional imidazole derivatives are planned to be synthesized using various N-substituted thiourea derivatives and dicarbonyl compounds, accompanied by in vitro evaluations of their biological activity.



R = alkyl, aryl

Scheme 1. The reaction scheme of thiourea derivatives with methylglyoxal.

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P-046

Investigation of the Crystal Polymorphism of Flurbiprofen and Findings Related to its New Cocrystal Forms with Pyrazine

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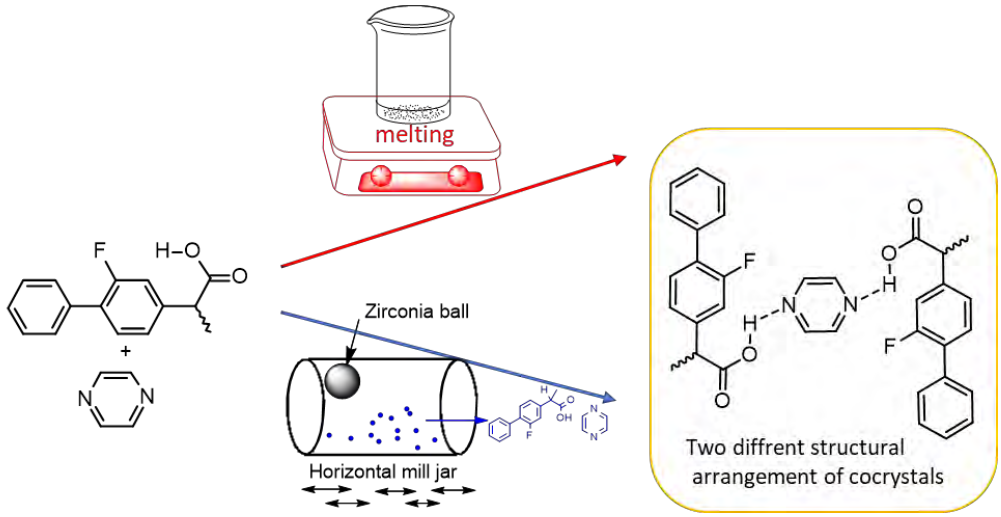
Crystal polymorphism refers to the ability of a molecule to exist in various forms, each featuring unique solid-state packing arrangements. These differences in crystal structure can result in differing chemical and physical properties, such as stability and bioactivity. Investigating the polymorphism of pharmaceuticals has become a critical goal in the pharmaceutical industry, as research indicates that different polymorphs can exhibit distinct bioactive profiles [1].

Our focus is on flurbiprofen, an active pharmaceutical ingredient known for its analgesic, antipyretic, and anti-inflammatory properties. Flurbiprofen was approved for medical use in 1987. We aimed to enhance the understanding of flurbiprofen polymorphism [2] by investigating cocrystallization processes and the subsequent release of ingredients through de-cocrystallization routes, which may lead to an alternative polymorphic structures of flurbiprofen. To achieve this, we prepared cocrystals of flurbiprofen and pyrazine and analyzed their crystalline characteristics. After the cocrystals were formed, we assessed their thermal decomposition to evaluate solid phase transitions and the potential for polymorphic changes in flurbiprofen. The appropriate cocrystals of flurbiprofen with pyrazine were obtained using two method, by melting or by dry grinding in a Retch vibrating ball mill (Scheme 1).



Scheme 1.The approach for preparing cocrystals of flurbiprofen and pyrazine

The summarized results of the cocrystal preparation, the thermal phase transition analysis, and the structure determinations will be discussed in this communication.

Acknowledgement

This work was possible due to the financial support of the Polish National Science Centre Sonata Bis project No. 2022/46/E/ST4/00392 granted to MD.

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P-047

Tuning the morphology and optical properties of phenylquinazoline thin films through oxygen to sulfur substitution

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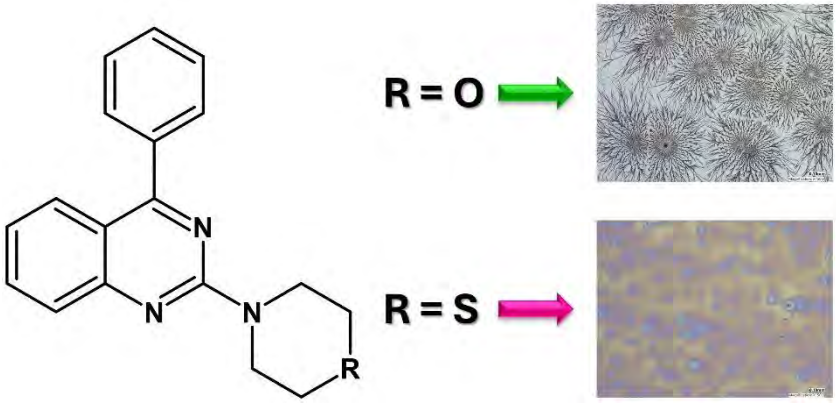
Phenylquinazolines, due to their unique photophysical features, are attracting growing attention in material science as promising building blocks for organic light-emitting diodes (OLEDs), organic photovoltaics, and related optoelectronic technologies.[1-3] Their structural adaptability, enabled by a straightforward side-group substitution, provides a versatile platform for tailoring key functional properties.

In this work, we synthesized and performed an in-depth study of two new phenylquinazoline derivatives functionalized with morpholine (**QM**) and thiomorpholine (**QTM**) moieties (Scheme 1). We systematically analyzed their absorption and emission behaviours in solution, followed by investigations of their spin-coated thin films. While both compounds displayed nearly identical photophysical characteristics in solution, the thin films exhibited strikingly different morphologies: **QM** readily crystallized and self-organized, whereas **QTM** formed predominantly amorphous films. These structural distinctions were further manifested in their functional properties. In Förster resonance energy transfer (FRET) systems, annealed **QM** films induced a substantial bathochromic emission shift when compared to **QTM** films.

Overall, our results highlight how seemingly minor, peripheral O-to-S substitution can significantly influence molecular packing, crystallinity, and functional performance in thin films of phenylquinazoline-based fluorophores.



Scheme 1. Structures of novel phenylquinazolines derivatives investigated in the study and the corresponding thin film morphologies, observed by optical microscopy.

Acknowledgement
This work was supported by the SONATA 17 project (UMO-2021/43/D/ST5/02786) financed by the National Science Centre (Poland).

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P-048

Metal Ion-Complexed Selenosteroids as Potent Agents Against Antibiotic-Resistant Bacteria

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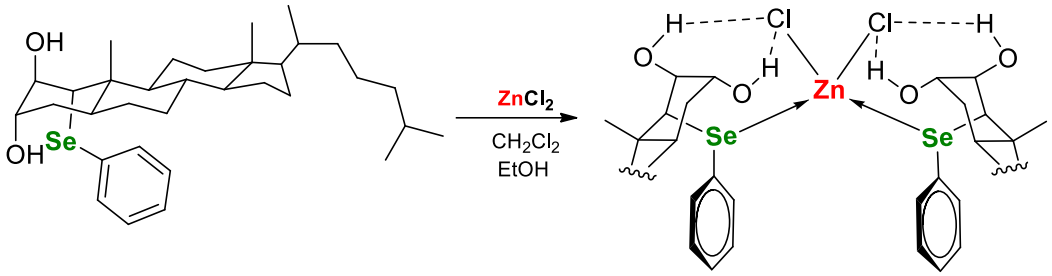
Selenosteroids (SeSt) are synthetic hybrid molecules formed by the incorporation of a selenium moiety into a steroid backbone. This structural modification can enhance the biological activities of both the steroidal and selenium components. Although SeSt compounds do not occur naturally, they have demonstrated a broad spectrum of biological properties, including glutathione peroxidase-mimetic activity, as well as antioxidant, anticancer, and antimicrobial effects.[1]

To assess their biological activity, we synthesized a novel class of metal complexes based on a steroid-derived model ligand, β-hydroxy-phenylselenide, using a straightforward and efficient synthetic protocol. The resulting compounds were thoroughly characterized by ^{1}H and ^{77}Se NMR spectroscopy, infrared (IR) spectroscopy, mass spectrometry (MS), powder X-ray diffraction, and thermogravimetric analysis (TGA).

The synthesized complexes exhibited structural variations depending on the incorporated metal ion. To confirm the proposed structures, detailed computational studies were conducted. As an example, Scheme 1 presents a plausible structure of the selenosteroid ligand complexed with Zn(II). To evaluate the bactericidal activity of these compounds, the viability of Pseudomonas aeruginosa and Staphylococcus aureus strains was assessed following incubation with the respective metal complexes.[2]



Scheme 1. Synthesis and probable structure of the complex of β-hydroxy-phenylselenide with Zn (for clarity, only the coordination center is shown).

Acknowledgement

Research equipment used to collect data on the University of Białystok was partially financed by EU funds via the projects with contract numbers: POPW.01.03.00-20-034/09-00 and POPW.01.03.00-20-004/11-00. The calculations using ORCA ver.5.0.2 were carried out in the Computer Centre of the University of Bialystok.

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P-049

Three-membered rings in the synthesis of optically pure, nitrogen-containing compounds

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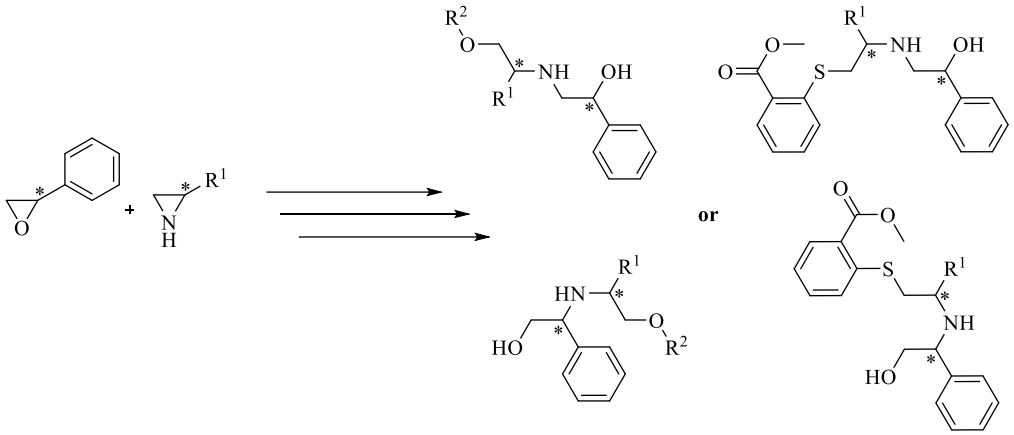
Drug resistance and the ongoing need to develop new drugs with high efficacy and minimal side effects remain key challenges of the XXI century, actively investigated by scientists worldwide. Accordingly, research is being conducted to discover new methods for synthesizing molecules with desirable biological properties.[1] Ring-opening reactions of aziridines play a crucial role in the synthesis of biologically active nitrogen-containing compounds.[2] Three-membered rings are amenable to opening reactions using various types of nucleophiles, allowing the introduction of a whole range of substituents and obtaining compounds with the expected structure and activity.[3] The regioselectivity of aziridine ring-opening reactions strongly depends on the activation of the ring. Non-activated aziridines often require prior activation by Lewis or Brönsted acids to initiate the ring-opening process. Regioselectivity is influenced by the nature of the nucleophile, the acid used, and the substituents on the aziridine ring. These factors collectively allow for precise control in synthetic applications. The site of nucleophilic attack, either at the C2 or C3 position, largely depends on the steric and electronic properties of both the nucleophile and the substituents on the aziridine ring.[2]



Scheme 1. Schematic representation of syntheses.

This project presents the synthesis of chiral ether and thioether derivatives of 1,2-aminoalcohols using selective ring opening of three-membered aziridine and oxirane rings (Scheme 1). Due to the high strain of the aziridine ring, it readily opens with sulfur nucleophiles, but the use of oxygen nucleophiles is a much more demanding task. This approach allows for the introduction of additional pharmacophoric fragments, resulting in a wide range of compounds with desired structures and favorable biological properties.

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P-050

Bienzymatic Dynamic Kinetic Resolution of Secondary Alcohols by Esterification/Racemization in Water

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Dynamic kinetic resolution (DKR) is a highly efficient method for the synthesis of optically pure compounds. However, despite its efficiency, DKR has certain limitations, including the high cost of catalysts, the necessity for anhydrous and anaerobic conditions, and the requirement for high temperatures [1-2]. To address these challenges, we have developed an alternative DKR method that utilizes enzymes in an aqueous environment [3].

We employed a variant of alcohol dehydrogenase from *Lactobacillus kefir* (Lk-ADH-Prince), which facilitates rapid racemization of substrates through a reversible sequence of oxidation-reduction reactions *via* an internal hydrogen-borrowing cascade. In parallel, we utilized recombinant acyltransferases from *Mycobacterium smegmatis*, which enable enantioselective transesterification of alcohols with 2,2,2-trifluoroethyl acetate in aqueous media, overcoming the typically unfavourable thermodynamics of such reaction systems. By integrating these two reactions into a single DKR process, we successfully synthesized a broad spectrum of optically active secondary alcohol esters with high yields (up to 87%) and excellent enantiomeric excesses (>99%), even at the 1 g scale.

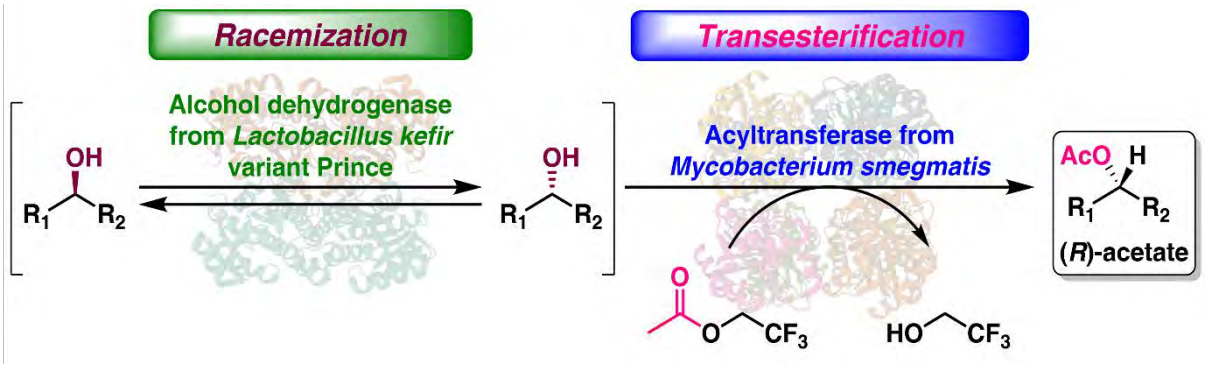

Figure 1. Dynamic kinetic resolution of secondary alcohols using two recombinant biocatalysts in an aqueous media.

Acknowledgement

This research was funded by the National Science Center (NCN) of Poland grant "OPUS 24" (Grant No. 2022/47/B/ST4/00139). Statutory support by the Faculty of Chemistry at Warsaw University of Technology (WUT) is also acknowledged. The University of Graz and the Field of Excellence BioHealth are recognized for financial support. A.R. is grateful to the IDUB project ("Scholarship Plus" program for Ph.D. students) for providing a research fellowship.

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P-051

Synthesis of optically pure amines for pharmaceutical applications

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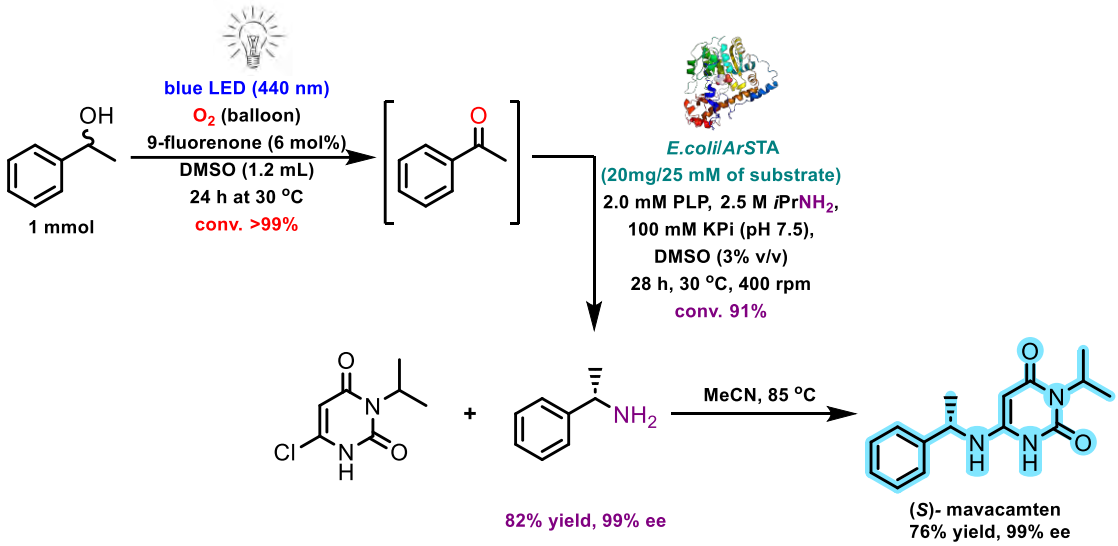
Enantiomerically pure chiral amines are essential building blocks in the synthesis of pharmaceuticals, agrochemicals and natural products, with approximately 40% of marketed drugs containing a chiral amine component [1].

Mavacamten (brand name Camzyos®) was approved by the FDA as an active pharmaceutical ingredient in 2022 for the treatment of certain classes of obstructive hypertrophic cardiomyopathy. This chiral API is an orally active cardiac myosin inhibitor whose desired pharmacological effect *in vivo* is due to its (*S*)-enantiomer. The key step of the synthesis of the drug is the preparation of optically pure (*S*)-amine followed by its functionalization with 6-chloro-3-isopropyl-pyrimidine-2,4-dione (Scheme 1) [2].



Scheme 1. Synthesis of mavacamten.

In this study, we report on a novel one-pot, two-step photo-biocatalytic synthetic procedure for the preparation of optically active amines, including (*S*)-methylbenzylamine as a key precursor in the manufacturing of mavacamten [3].

Acknowledgement

This research was funded by the National Science Center (NCN) of Poland grant "OPUS 24" (Grant No. 2022/47/B/ST4/00139). Statutory support by the Faculty of Chemistry at Warsaw University of Technology (WUT) is also acknowledged. N.A. acknowledges financial support from the IDUB project ("Scholarship Plus" program for Ph.D. students). The University of Graz and the Field of Excellence BioHealth are recognized for financial support.

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P-052

Synthesis and analysis of the energetic and structural properties of the BIT molecule

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The aim of this study was the synthesis and theoretical investigation of butane-1,4-diol diisothionate (BIT), a molecule predisposed to act as an anticancer agent intended for leukemia treatment. The currently used butane-1,4-diyl di(methanesulfonate) (Busulfan), a drug applied in leukemia therapy, exhibits poor bioavailability due to its low solubility in water.

The concept behind the synthesis of BIT was therefore to obtain a compound with anticancer properties like those of Busulfan but characterized by improved water solubility. It is assumed that the introduction of two additional hydroxymethyl groups into the Busulfan structure will lead to enhanced solubility [1–2]. The synthesis of BIT starts with the preparation of silver isothiocyanate, which subsequently reacts with 1,4-dibromobutane. The target compound, butane-1,4-diyl diisothiocyanate, was obtained with a yield of 65%.

Theoretical analysis aimed to characterize the most important structural and energetic properties of BIT using two density functional theory (DFT) approaches: M06-2X-D3/aug-cc-pVTZ and CAM-B3LYP-D3BJ/aug-cc-pVTZ. The poster will present both the theoretical results and the NMR spectra of the synthesized compound.

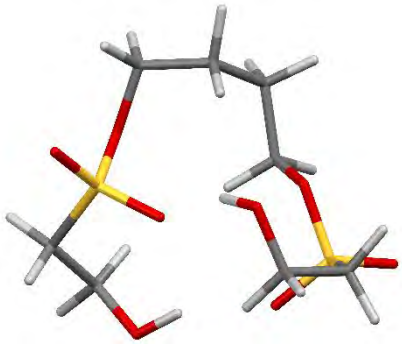

Figure 1. The most stable conformer of BIT obtained from M06-2X-D3/aug-cc-pVTZ calculations performed in water described using the PCM model.

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P-053

Synthesis and analysis of the film-forming properties of carbohydrazides

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The aim of my research was to synthesize carbohydrazides derivatives of salicylic acid.[1] Carboxylic acid hydrazides exhibit luminescence in solid state due to the presence of a large number of π double bonds in their structure. Additionally, they can form dimers through hydrogen bonds between terminal nitrogen atoms of two molecules, which enhances the phenomenon of light emission. It turns out that currently known technological device designs are increasingly using low-molecular-weight organic compounds, found in OLED displays. The rarest, due to their high radiation energy, are compounds with blue light emission. Such compounds are also highly sought after in technology, as they improve the quality, contrast, and efficiency of devices.[2] Carbohydrazides are promising candidates for use in OLED technology due to their blue emission color and the possibility of manipulating their crystal structures by adding or relocating a substituent on the aromatic ring. Therefore, I investigated the obtained compounds for use in OLED displays. To this end, I produced thin layers of the compounds on glass plates using the drop-casting method and analyzed them under a polarizing microscope.

As part of the presented work, I obtained five compounds, including: 2-hydroxybenzohydrazide, 2-hydroxy-3,5-diisopropylbenzohydrazide, 2-hydroxy-5-methoxybenzohydrazide, 2-hydroxy-5-bromobenzohydrazide, and 2-hydroxy-5-nitrobenzohydrazide (Fig. 1.). I used five different solvents to prepare the layers, allowing me to compare not only the effect of the compound's structure on the layer formation but also the effect of the solvent on this process.

Figure 1. Blue light emission of selected carbohydrazides excited by UV radiation.

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P-054

β-Carbonyl selenides with enhanced radical scavenging and anticancer potential

Magdalena Obieziurska-Fabisiak[1], Anna Laskowska[1], Agata J. Paculа-Miszewska[2], Aneta Jastrzębska[3], Angelika Długosz-Pokorska[4], Katarzyna Gach-Janczak[4], Jacek Ścianowski[1]

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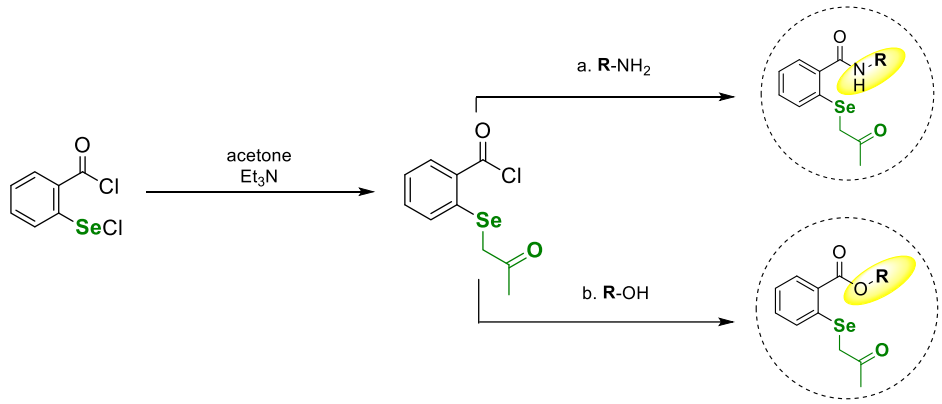
Organoselenium compounds, including selenides, diselenides, and selenols, are widely recognized for their diverse biological activities, most notably their antioxidant and anticancer properties. These effects arise largely from the intrinsic reactivity of the selenium center and its ability to mimic the catalytic functions of selenoenzymes, particularly glutathione peroxidase (GPx). In this study, a novel series of *β*-carbonyl selenides incorporating a 2-(2-oxopropyl)selanyl moiety was synthesized through efficient methodologies. [1,2] Two structural variants were prepared: a. compounds bearing *o*-amido groups substituted at nitrogen with chiral alkyl chains, and b. derivatives featuring an *o*-ester substituent at oxygen with either chiral or achiral alkyl chains. For each pair of enantiomers and diastereomers, the influence of stereochemistry on antioxidant and antiproliferative activities was systematically evaluated. The results revealed that ester substitution diminished hydrogen peroxide–scavenging capacity, yet significantly enhanced free radical neutralization and antiproliferative activity relative to the amide counterparts.



Scheme 1. Synthesis of *β*-carbonyl selenides

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P-055

Application of modern synthetic methods in the synthesis of luminescent materials

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The development of new organic luminescent compounds, particularly those exhibiting Aggregation-Induced Emission (AIE) properties, remains a significant area of scientific research [1]. This phenomenon involves compounds that show emission in the aggregated state, while their emission is minimal when dissolved in a solvent [2].

The goal of my research was to synthesize luminescent derivatives of coumarin using modern, environmentally friendly synthetic methods. Coumarin, a heterocyclic compound with biological activity and natural occurrence, serves as an excellent foundation for this type of study [3]. As a result of the reactions carried out, the obtained products exhibit luminescence in the solid state and the ability to form thin solid layers. The use of modern techniques, such as ultrasonic baths, ball milling, and microwave reactors, allowed for reduced reaction time and temperature. In particular, the application of sonication in cross-coupling reactions (e.g., Suzuki-Miyaura reaction) proved to be effective in the synthesis process, enabling the production of high-quality products in a shorter time. Additionally, it was found that the obtained compounds exhibit polymorphism, meaning their emission is dependent on the crystal form in which they occur.

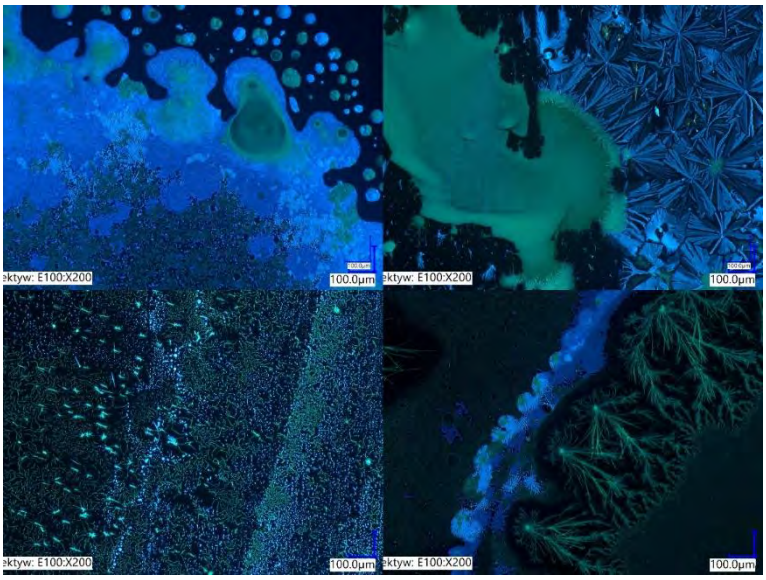

Figure 1. Thin layers obtained using fluorescence techniques, dissolved in various solvents. Images taken using the Keyence VHX7000N digital microscope.

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P-056

Antioxidant properties of co-amorphous solid dispersions of candesartan cilexetil with bioactive polyphenols

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Co-amorphization is a strategic approach to enhance solubility and bioavailability of active pharmaceutical ingredients (APIs). This pathway may lead to the development of dual-acting pharmaceutical products if an appropriate nutraceutical co-former is selected.

Our study describes shortly synthesizing co-amorphous pharmaceutical solid dispersions of poorly soluble antihypertensive drug – candesartan cilexetil (CAN-CIL) belonging to angiotensin II receptor blockers, in conjunction with polyphenols: naringenin (NAR), genistein (GEN), as co-formers. The biological properties of polyphenols include antioxidant, anticancer and anti-inflammatory effects [1].

Synthesis was performed by ball milling, reflecting the growing role of mechanochemistry in pharmaceutical sciences as a green, high-yield route to multicomponent solids [2].

In this research, we describe the antioxidant properties of starting compounds and the obtained co-amorphous products. For this purpose, the DPPH radical method was used. This method is used to assess the radical scavenging ability of the tested sample. The method quantifies radical-scavenging capacity by monitoring the decrease in absorbance at 517 nm. The conducted research will verify whether the combination of the poorly soluble API (CAN-CIL) with polyphenols (NAR, GEN) exhibits a synergistic antioxidant effect in scavenging the DPPH• radical. [3].

Scheme 1. Presentation of equipment for the mechanochemical synthesis of the obtained products (CAN-CIL with polyphenols) and the DPPH radical method.

Acknowledgement

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P-057

Synthesis and evaluation of 1,3,5-triazine derivatives as potential cholinesterase inhibitors

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Alzheimer disease (AD) is a progressive neurodegenerative disorder responsible for 60–70% of dementia cases worldwide [1, 2]. Currently, over 50 million people are affected, and this number is projected to exceed 130 million by 2050 [1, 2]. Despite extensive research, the disease remains incurable [2]. Available therapies are limited to symptomatic treatment [1, 3], but their effectiveness is limited by poor blood–brain barrier permeability and adverse effects associated with high dosing [2].

One of the hypotheses explaining the pathogenesis of AD suggests that cognitive decline – one of the main symptoms of AD – results from the degradation of acetylcholine by acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) [2, 4]. This hypothesis forms the basis for most of the symptomatic therapies currently available for AD [2].

In recent years, the potential of 1,3,5-triazines in the search for new drug candidates for AD has been investigated [2]. Since some of the reported compounds demonstrated inhibitory properties [5, 6], this research focused on the synthesis of a series of compounds structurally based on the 1,3,5-triazine scaffold modified with tryptamine, with the aim of potentially exhibiting acetylcholinesterase and/or butyrylcholinesterase inhibitory activity.

A series of seven compounds was synthesized using a three-step protocol, with the final step carried out under microwave irradiation, providing a more environmentally friendly alternative to conventional methods for the synthesis of 1,3,5-triazine derivatives [7]. Subsequently, in silico screening was conducted to predict ADME (absorption, distribution, metabolism, and excretion) properties. This included assessment of compliance with Lipinski's Rule of Five and Veber's Rules, allowing evaluation of the compounds' potential oral bioavailability [8]. Finally, the compounds were tested for their inhibitory activity against AChE and BuChE using a modified Ellman's protocol [9].

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P-058

Cerium(IV)-Catalyzed Allylic Oxidation: An Efficient Route to 4-Substituted Sulfol-2-enes

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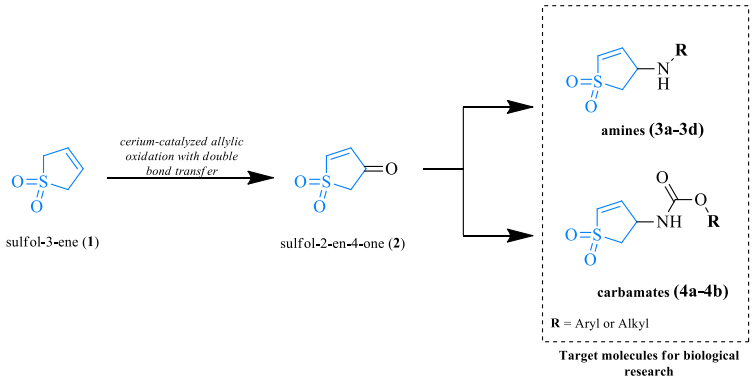
A novel cerium(IV)-catalyzed allylic oxidation protocol for the direct transformation of commercially available 3-sulfolene (**1**) to sulfol-2-en-4-one (**2**) is reported. The optimized conditions employ ceric ammonium nitrate (CAN, 0.1 equiv.) as catalyst and *tert*-butyl hydroperoxide (TBHP, 2.5 equiv.) as oxidant in aqueous medium at 70°C, delivering the desired *α,β*-unsaturated ketone in 51% isolated yield. This represents the first example of cerium(IV)-mediated allylic oxidation in the sulfolene series and proceeds under mild, operationally simple conditions without requiring inert atmosphere or rigorously anhydrous solvents. [1]

The resulting sulfol-2-en-4-one serves as a versatile electrophilic building block. Selective reduction of the carbonyl group using sodium borohydride yields sulfol-2-en-4-ol in 91% yield, which is subsequently converted to *p*-toluenesulfonate or 4-bromo derivative for nucleophilic substitution reactions. Treatment of these activated intermediates with various primary and secondary amines affords 4-amino-sulfol-2-enes (**3a**–**3d**) in moderate yields (15-59%), while reaction with isocyanates or carbamoyl chlorides provides 4-carbamate derivatives (**4a**–**4b**, 69-73% yield), (Scheme 1).



Scheme 1. Novel Ce(IV)-mediated route to bioactive 4-substituted sulfol-2-enes.

Structural optimization reveals that electron-donating substituents on the amine nucleophile enhance reaction efficiency, while sterically hindered amines require elevated temperatures (80-90°C) and extended reaction times. The methodology tolerates diverse functional groups including aliphatic amines, anilines, and heterocyclic amines, establishing a general synthetic platform for accessing 4-functionalized sulfol-2-enes from readily available starting materials. This catalytic approach significantly expands the synthetic utility of the sulfolene scaffold and provides expedient access to structurally diverse heterocyclic libraries.

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P-059

Enantio- and Diastereoselective Dearomative [4+2]-Cycloaddition of Anthracene Derivatives *via* Hydrazone Activation

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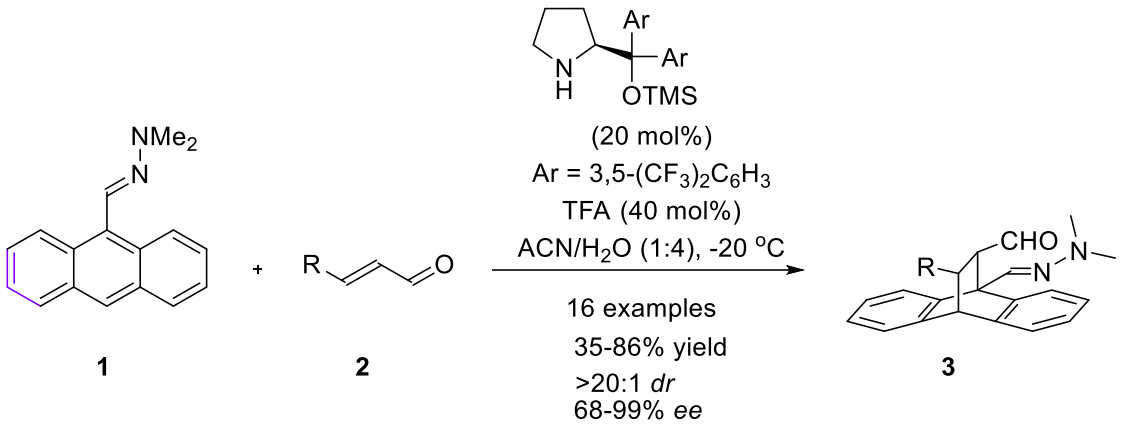
Hydrazones, as derivatives of hydrazine, exhibit the ability to induce a reactivity inversion phenomenon, as a result of which their double bond acquires a more electron-deficient character.[1] This transformation enables their reactions with a variety of olefins, contributing to the formation of new, highly complex cyclic systems.

The application of this strategy has been demonstrated in a study where the authors adapted the hydrazone approach to the dearomative asymmetric [4+2] cycloaddition of anthracene derivatives. In this approach, 9-anthracenecarbaldehyde was first converted into hydrazone **1**, while *α,β*-unsaturated aldehydes **2** were activated through the formation of iminium complexes in the aminocatalytic cycle (Scheme 1).[2] The combination of these two components resulted in an efficient and stereoselective reaction course under optimal conditions. High enantiomeric ratios and good yields of products **3** were obtained for a broad range of dienophiles.



Scheme 1. The use of a vinylogous hydrazone strategy in the synthesis of anthracene derivatives.

Acknowledgement

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P-060

New Compositions Of Bioactive Glasses: Potential Biomedical Applications.

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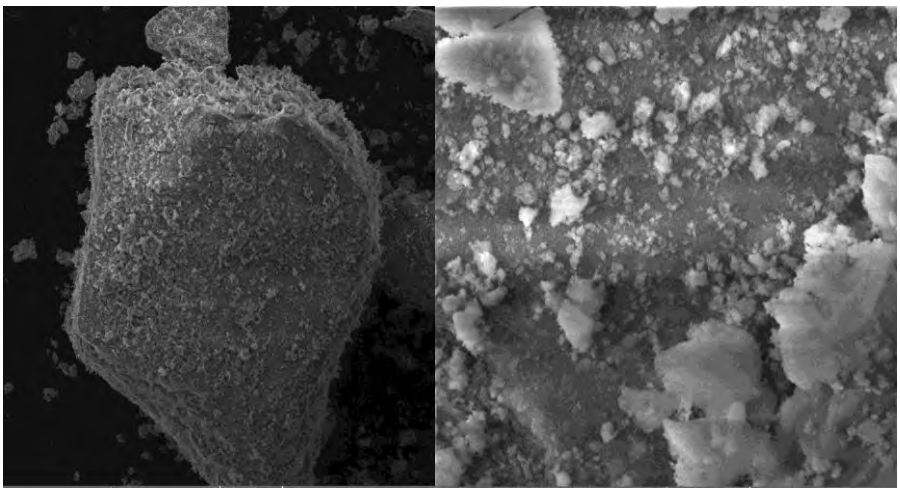
Bioactive glasses, due to their properties of interaction with biological tissues, constitute a promising class of biomaterials that have been used in many biomedical fields, such as implantology, tissue regeneration and drug delivery. In this study, we present a new composition of bioactive glass developedusing the sol-gel technique [1-4].

Our new composition of bioactive glass has been carefully selected based on the latest achievements in the field of materials engineering. The main ingredients of this glass are classic ingredients such as silica, calcium and phosphate, which are known for their ability to initiate bioactivation processes. However we have also introduced new, innovative additives that improve the bioactivity of our material, porosity and add magnetic properties. In vitro test have shown that our bioactive glass stimulates the growth of hydroxyapatite on the material and also inside it, which is a key factor tissue regeneration.

Our work sheds new light on the possibility of using new bioactive glass compositions in biomedical applications, opening the way to further research on their potential clinical applications. The preliminary results of these experiments will be presented on our poster.



Scheme 1. SEM images of bioactive glass with the composition: 36 SiO_2–22.0 CaO–22.0 Na_2O-20 P_2O_5 after bubbling, taken at four different magnifications 200x and 5kx.

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P-061

Inhibitors for HSPA5, the Cancer-Related Protein: In Silica Modeling

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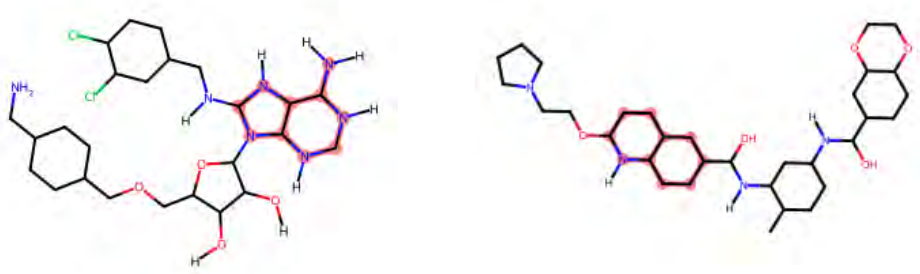
HSPA5 as the other members of the heat-shock protein family (Hsp70), is a stress-responsive chaperone that recognizes and refolds misfolded proteins [1]. Its expression is often upregulated in highly proliferative cells, linking it to multiple cancers [2]. Thus, considerable effort has been dedicated into developing small molecules that inhibit the activity of HSPA5. Although several inhibitors have shown efficacy, their limited specificity for HSPA5 reduces their suitability as anticancer agents.

In this project, we employed molecular dynamics simulation to characterize interactions that stabilize protein–ligand binding between HSPA5 and two known Hsp70-family inhibitors, VER-15508 [3] and Cct251236 [4]. From the molecular perspective, we identified residues currently engaged in ligand binding as well as new potential hotspots that are less conserved across the Hsp70 family. Based on these findings, we propose modifications to both ligands to achieve more potent and more selective inhibition. Our results indicate that small structural changes can substantially improve protein–ligand complementarity. Here we would like also to discuss the synthetic feasibility, chemical stability, and potential side reactions of these new compounds. On the basis of this assessment, the most promising candidates will be selected and further evaluated in cancer cell models.



Scheme 1. Structure of original HSPA5 inhibitors, VER-155008 (left) and Cct251236 (right).

Acknowledgement

The work is supported by the National Science Centre, Poland, under research project NCN OPUS-25 (2023/49/B/ST4/03288)

Computational resources were provided by Poland's high-performance Infrastructure PLGrid ACK Cyfronet within computational grant no plgcbmmchb01.

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P-062

Design and synthesis of new 2-(((tetrahydrofuran-2-yl)methyl)amino)thiazol-4(5*H*)-one derivatives as potent inhibitors of 11β-hydroxysteroid dehydrogenase type 1

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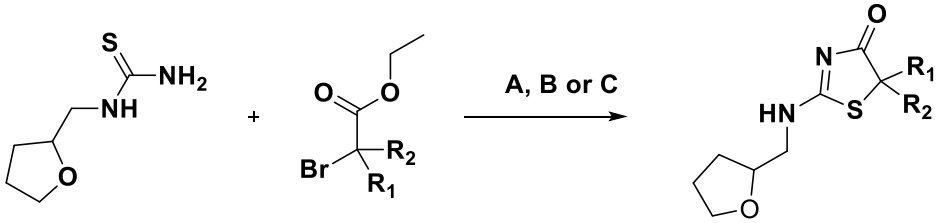
11β-Hydroxysteroid dehydrogenase type 1 (11β-HSD1) is an NADPH-dependent oxidoreductase that is predominantly expressed in adipose tissue, liver, muscle, brain, inflammatory cells and gonads [1]. Together with the type 2 isoform, it is a key enzyme responsible for the intracellular regulation of cortisol levels in the human body. Dysregulation of 11β-HSD1 activity is associated with the occurrence of Alzheimer's disease, depressive disorders, osteoporosis, cancer, and diseases related to metabolic syndrome [2]. Therefore, new 11β-HSD1 inhibitors are being sought as potential therapeutic avenues for these diseases.



Scheme 1. General synthesis of 2-aminothiazol-4(5*H*)-one derivatives. Reagent and conditions: procedure A - EtOH, microwave heating (I - 155-160ºC; II - 160-165 ºC); procedure B - EtOH, DIPEA, reflux; C - EtOH, DIPEA, microwave heating (90-110ºC).

During research on selective 11β-HSD1 inhibitors, a QSAR model was developed, which enabled the identification of potential structures of new potent pseudothiohydantoin derivatives as potential inhibitors of this enzyme [3]. Based on the obtained results, nine new derivatives of 2-(((tetrahydrofuran-2-yl)methyl)amino)thiazol-4(5*H*)-one were designed and synthesized. The target derivatives were obtained in good yields and high purity, and their structures were confirmed by MS, ^{1}H and ^{13}C NMR analyses. The next stage of the research is planned to evaluate the inhibitory activity against 11β-hydroxysteroid dehydrogenase type 1.

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P-063

Stereoconvergent Photo-Biocatalytic Sequential Cascade from Racemic Carboxylic Acids to Optically Enriched *Prim*-Amines by Harnessing Transaminases and Visible Light

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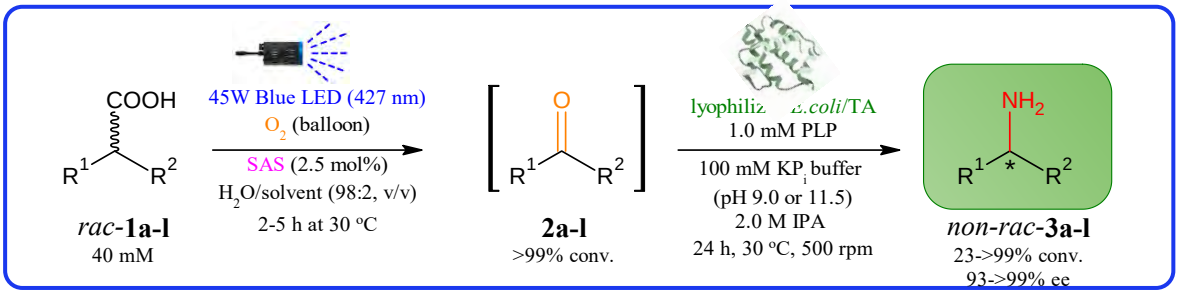
Optically active amines are common structural motifs found in a wide range of natural products, active pharmaceutical ingredients (API), and other biologically active compounds [1]. Classical methods for their synthesis typically afford moderate yields of enantiomeric products and rely on toxic reagents, catalysts, and volatile organic solvents, posing a significant threat to both the environment and human health [2]. Accordingly, the development of efficient, highly selective, economically viable, and sustainable processes for the production of optically enriched amines represents a crucial challenge and an important research direction.

In this work, we present a new method for the synthesis of optically active amines from racemic carboxylic acids, employing a two-step sequential photo-biocatalytic cascade in a "one-pot" mode that eliminates the need for isolation and purification of intermediates (**Scheme 1**).



Scheme 1. Photo-biocatalytic method for the synthesis of chiral amines from racemic carboxylic acids.

The process utilizes sodium anthraquinone-1-sulfonate (SAS) as a water-soluble, metal-free photo-organocatalyst to achieve quantitative decarboxylative oxidation (>99% conv.) of racemic aryl-alkyl carboxylic acids under blue LED irradiation (427 nm), employing molecular oxygen (O_2) as the terminal oxidant. The subsequent step employs stereocomplementary transaminases (*E. coli*/TA), which catalyze the asymmetric reductive amination of the *in situ*-generated ketones. This photo-biocatalytic strategy enabled the preparation of optically active amines with enantiomeric excesses ranging from 93% to 99.9% and up to >99% conversions after two steps. Under optimized cascade conditions, (*S*)-phenylethylamine was obtained with >99% conversion and >99% ee using a variant of (*S*)-selective transaminase from *Vibrio fluvialis*. Upscaling of the photo-biocatalytic process with 2-(naphthalen-1-yl)propanoic acid (1.0 mmol) furnished (*R*)-1-(naphthalen-1-yl)ethan-1-amine with 92% product formation, 17% isolated yield, and >99% ee.

Acknowledgement
This research was funded by the National Science Centre (NCN) of Poland grant "OPUS 24" (Grant No. 2022/47/B/ST4/00139).

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P-064

Vapor Phosphorylation of Graphene Oxide by Phosphorus Trichloride

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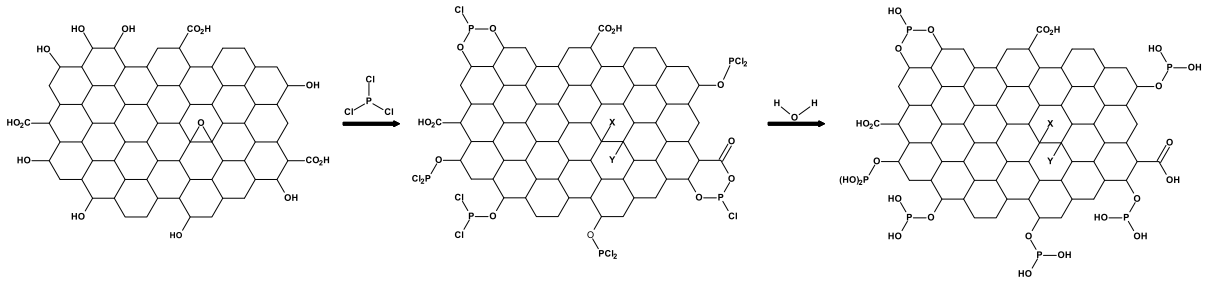
Over the past decade, graphene oxide (GO), an oxidized derivative of graphene, has been extensively used in various fields as environmental engineering, biomedicine as well as energy storage due to the presence of oxygen-containing functional groups, which provide GO with intrinsic hydrophilicity, dispersibility, superpermeability, and insulating properties. Furthermore, depending on the requirements of different applications, these groups can be modified with various functional groups to improve these characteristics [1-3]. One of them is phosphorylation - the relatively virgin domain [4,5].

In this communication we focused on a synthesis of graphene-phosphates (III) by exposing graphene oxide to phosphorus trichloride (PCl3) vapors [6]. The graphene-O-dichlorophosphines (G-O-PCl2) intermediary formed, were hydrolyzed to graphene-O-hydrogen phosphate (P(III)) (G-O-P(O)(H)(OH)) (Scheme 1) which were characterized by SEM, ATR-FTIR, FAAS, and by antimicrobial tests against Escherichia coli and Staphylococcus aureus.



Scheme 1. Phosphorylation of graphene oxide and its subsequent hydrolysis to graphene-O-hydrogen phosphate (simplified form)

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P-065

Quantitative and qualitative analysis of sulforaphane present in cruciferous vegetables using LC-MS technique

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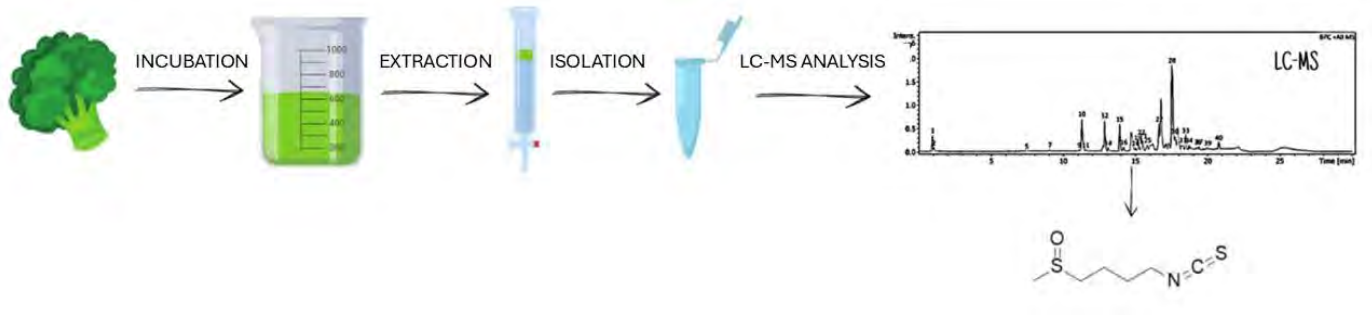
Isothiocyanates (ITCs) are an important class of biologically active compounds that have been the focus of research for many years. They are found in cruciferous vegetables (including Brussels sprouts, radishes, broccoli, or horseradish) and are formed as a result of a reaction of glucosinolates with myrosinases.[1] Many methods used for the isolation and identification of isothiocyanates from cruciferous vegetables have been described in the literature.[2] Various analytical techniques are used for their identification, including UV-Vis spectrophotometry, Fourier transform infrared spectroscopy (FT-IR), and various chromatographic techniques: thin-layer chromatography (TLC), gas chromatography (GC), high-performance liquid chromatography (HPLC), and combined techniques. One of the most commonly used techniques is liquid chromatography coupled with mass spectrometry (LC-MS).



The aim of the project was to incubate, extract, and determine the qualitative and quantitative content of sulforaphane from cruciferous vegetables (broccoli, broccoli sprouts, radish sprouts).

The incubation and extraction processes were optimized to find the best conditions. For this purpose, the following methods were used: extraction with organic solvents, solid phase extraction and microwave radiation. Quantitative and qualitative determination was performed using liquid chromatography coupled with mass spectrometry. In addition, for identification purposes, sulforaphane was synthesized in laboratory conditions in a 6-step synthesis, which was confirmed by LC-MS.

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P-066

Synthesis of Organic Ligands of Transition Metal Complexes with Potential Anticancer and Antibacterial Activity

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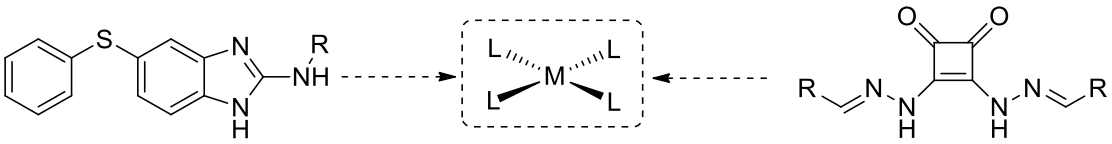
This study focuses on the synthesis and characterization of benzimidazole and squaric acid derivatives as potential ligands for transition metal ions such as Cu(II), Fe(II), and Zn(II). Due to the presence of nitrogen and oxygen donor atoms, these compounds exhibit high coordination ability, which, combined with their documented anticancer, antibacterial, and antimalarial activities, makes them promising candidates for drug design and functional materials [1–3]. Benzimidazoles, exemplified by fenbendazole, are known to form stable metal complexes that may enhance their biological activity, including anticancer effects [6]. Squaric acid derivatives, characterized by rigid planar structures and strong hydrogen-bonding capacity, serve as versatile ligands and bioisosteres, enabling modulation of stability, bioavailability, and biological profiles in the development of molecular receptors, sensors, and novel therapeutics [1,2,4,5].



Scheme 1. General formula of prepared organic ligands

The synthesis of the designed derivatives was carried out starting from proper hydrazones, squaric acid methyl ester and fenbendazole, affording the target compounds in yields ranging from 57% to 88%. The obtained derivatives were analyzed using spectroscopic techniques, including NMR and MS, which confirmed their structures and enabled purity assessment. Finally, the synthesized compounds were evaluated for their antibacterial activity.

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P-067

Synthesis of isothiocyanate-triazine conjugate as biologically active compound

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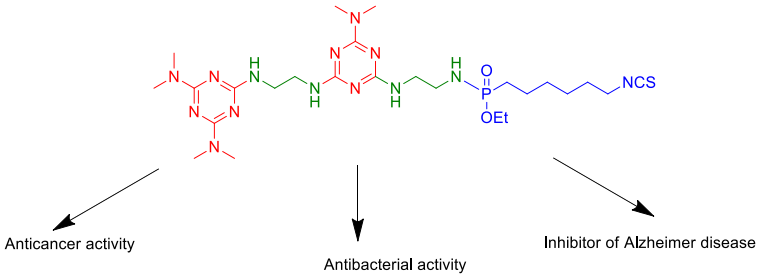
1,3,5- triazines are a group of organic compounds characterised by the presence of an aromatic ring where nitrogen atoms are located in positions 1, 3 and 5. The structure of 1,3,5-triazine allows for the substitution of three different substituents, which makes this group of organic compounds extremely interesting. The core containing a 1,3,5-triazine ring substituted with three structurally diverse substituents is present in many compounds exhibiting anticancer, antibacterial, antiviral or antimalarial properties [1]. Because of similar activities shown by phosphorus analogue of isothiocyanates (P-ITCs), conjugates which include in structure 1,3,5-triazine derivaties and P-ITCs could potentially have better biological activities than two previously mentioned groups [2-3].



Scheme 1. Structure of isothiocyanate-triazine conjugate.

The aim of the project was to synthesis an isothiocyanate-triazine conjugate consisting of two fragments of compounds with proven anti-cancer activity: 6-(isothiocyanatohexyl)phosphonate diethyl and Altretamine attached by linkers to the core of 2,4-dichloro-6-methoxy-1,3,5-triazine (DCMT).The synthesis of this conjugate required 11 reaction steps, with a total synthesis yield of 62%. The structure of the obtained compound was confirmed by ^{1}H, ^{31}P and ^{13}C NMR spectra, and its purity and mass were determined by liquid chromatography coupled with mass spectrometry. The obtained isothiocyanate-triazine conjugate was tested for its antibacterial properties on *E. coli* and *S. aureus* strains, for its anticancer properties, and as an inhibitor of Alzheimer's disease.

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P-068

Oxa- and dithiaphospholane adenosine monomers as precursors of phosphorothioate analogs of Nicotinamide Adenine Dinucleotide (NAD^+)

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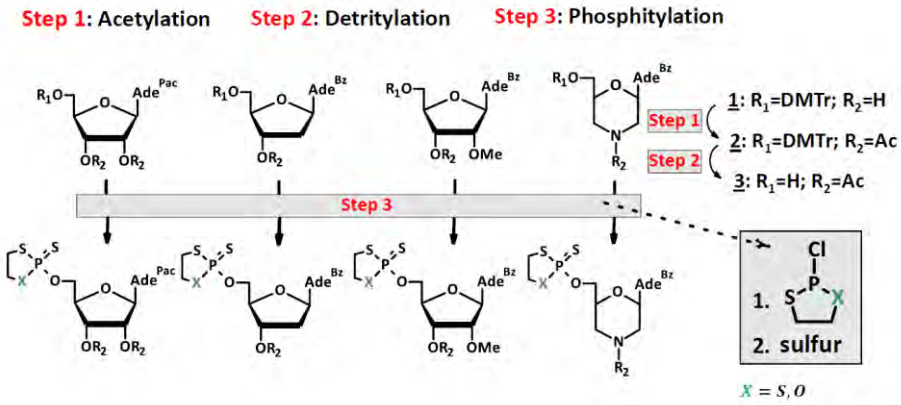
In our project, we carried out the synthesis of a series of modified nucleoside monomers, including both **oxa-** (**OTP**) and **dithiaphospholane** (**DTP**) derivatives. We developed optimized synthetic conditions and isolation procedures for these compounds. The scope of our research included the preparation of appropriately protected adenosine-derived nucleosides in morpholino, ribo-, deoxy-, and 2'-O-methyl forms, followed by their conversion into oxa- (OTP) and dithiaphospholane (DTP) monomers.



Scheme 1. Scope of our research: Synthesis of oxa- and dithiaphospholane adenosine-derived monomers.

The monomer synthesis involved three main steps: acetylation, detritylation, and phosphitylation. Protected nucleosides were first acetylated with acetic anhydride, then detritylated using dichloroacetic acid in methylene chloride. Finally, phosphitylation under anhydrous conditions was carried out using either 2-chloro-1,3,2-oxathiaphospholane, yielding OTP monomers as P-diastereomer mixtures, or 2-chloro-1,3,2-dithiaphospholane, producing the corresponding DTP monomers.

The obtained monomeric units will serve as key precursors for the synthesis of phosphorothioate analogs of nicotinamide adenine dinucleotide (NAD^+) with potential PARP inhibitory activity. Additionally, some of the synthesized compounds (morpholino analogues) were successfully applied in a previously initiated project (see Weronika Stepniak's abstract), where we converted them into the corresponding morpholino nucleoside 6'-O-(α-thiophosphates) and 6'-O-(α,α-dithiophosphates) [1].

Acknowledgement

This project was supported by Narodowe Centrum Nauki **2021/43/D/ST4/02433**.

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P-069

PET degradation by natural and synthetic cutinase-like enzymes

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The project investigates the activity of natural bacterial enzymes in PET degradation. Growing number of synthetic mutants has been also analyzed to identify relations between protein structure, composition and functionality. Rapid industrial development combined with high consumerism and poor waste management results in a large amount of non-compostable by-products of anthropogenic activity. One of them is PolyEthylene Terephthalate (PET), commonly used as a material for plastic bottles, textiles and many others. Despite its high abundance, there is no efficient strategy to counteract post-consumer PET waste accumulation [1]. In this context, more attention has been drawn to the PET-degrading enzymes found in bacteria and fungi. The recent study showed that there is a plentitude of potentially active enzymes, especially from a cutinase-like protein group [2]. Despite their different origins and sequence differences, they exhibit much similarity in structure with only small changes around a catalytic site. However, those changes result in variability of their activity against PET polymeric chains. Here, we enrolled bioinformatic tools to investigate the relations between small structural and compositional changes and efficiency in PET-degradation. Our techniques range from static analysis of crystal data structures to molecular docking performed for single-point mutants up to the molecular dynamics simulations which shed light on the subtle conformational transitions over time. The results so far indicate that enhancement in an enzyme activity originates from a delicate balance between enzyme-substrate binding affinity, an accessibility of the active center and the conformational flexibility around a binding pocket. Especially critical changes are visible as the conversion from natural cutinase into PETase requires protein reorganization to interact efficiently with a structurally different substrate. The activity-flexibility relation indicates the glove-hand enzymatic model where the more active natural PETases are the cutinases with lower substrate specificity.

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P-070

N-Aminomorpholino Phosphorothioates via Solid-Phase Oxathiaphospholane Chemistry

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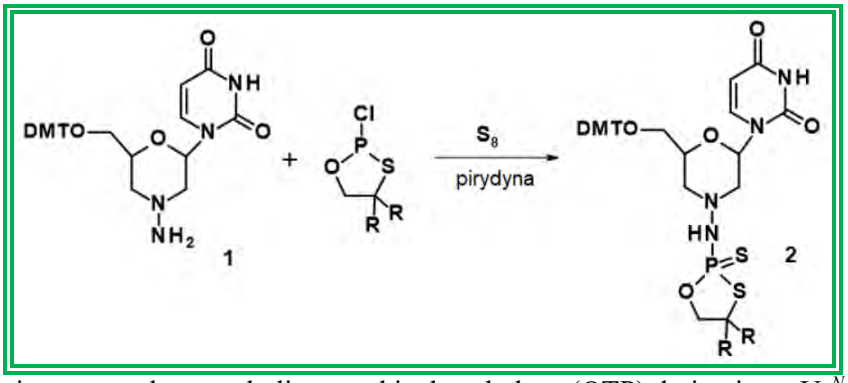
We present the application of the oxathiaphospholane method for the synthesis of novel P-stereodefined phosphorothioate *N*-modified morpholino analogs, showcasing its potential for creating therapeutically relevant compounds. Synthesis of morpholino nucleosides were performed according to the published protocols [1, 2]. Briefly, 5'-*O*-dimethoxytrityl uridine was oxidatively converted in the acyclic dialdehyde derivatives, followed by a reductive amination-cyclization reaction. Morpholino nucleosides were transformed into *N*-(2-thio-1,3,2-oxathiaphospholane) derivatives using a reported protocol [3]. Additionally, we provide valuable structural insights into their stereochemistry, including a detailed analysis of stereochemical configurations. We also report on the enzymatic stability of these compounds in 10% (v/v) fetal bovine serum (FBS), thereby mimicking in vivo conditions. These findings pave the way for further exploration of P-stereodefined nucleic acid analogs in molecular medicine and gene therapy applications.



Scheme 1. The synthetic route to the morpholino oxathiaphospholane (OTP) derivative mU-^{N}OTP (**2**). Description: DMT=dimetoxytrityl; R,R=H or -$(CH_2)_5$-.

This proposal aims to expand the library of diastereomerically pure probes with N-modified morpholine moiety available to biochemists and biologists in the hope of future applications in medicine.

Acknowledgement
This project was supported by Narodowe Centrum Nauki **2021/43/D/ST4/02433**.

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P-071

Broadband Dielectric Spectroscopy Coupled with Density Functional Theory Calculations as a Tool for Tracking Molecular Dynamics in Crown Ethers

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Crown ethers represent a unique class of cyclic polyethers whose conformational flexibility and ion-binding properties make them relevant in supramolecular chemistry, catalysis, materials science, and drug delivery.[1,2] Understanding their molecular dynamics is therefore crucial for correlating structural features with functional behavior. In our approach, we combine broadband dielectric spectroscopy (BDS) with density functional theory (DFT) calculations to investigate the relaxation processes and microscopic mechanisms that govern molecular motions in selected crown ethers and crown-like compounds. Broadband dielectric measurements spanning wide frequency, pressure, and temperature ranges provide direct insight into phase stability and molecular dynamics under diverse thermodynamic conditions, covering timescales from nanoseconds to hundreds of seconds. Complementary DFT simulations focusing on the potential energy surface analysis enables the assignment of the observed dielectric processes to specific molecular reorientations and conformational transitions, offering a molecular-level interpretation of the experimental spectra. Together, the integrated experimental–theoretical approach demonstrates that BDS, supported by DFT calculations, constitutes a powerful tool for tracking dynamic changes in flexible macrocyclic systems. The methodology presented here not only advances fundamental understanding of crown ether dynamics but also establishes a framework applicable to broader classes of supramolecular hosts and functional heterocyclic materials.

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P-072

Benzimidazole derivatives in coordination chemistry: Cu(II), Zn(II), Co(II) complexes, spectroscopic characterization and in silico assessment of pharmacokinetic properties.

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Benzimidazole is a molecule composed of a benzene ring and an imidazole ring in which nitrogen atoms provide the ability to form hydrogen bonds and coordinate with metal ions, making it a privileged scaffold in drug and coordination chemistry [1-3]. From a chemical structural perspective, the N-1/C-2 and 5-6/4-7 positions are most frequently modified, and these substitutions modulate the acid-base, lipophilicity, and donor-acceptor N profile, influencing the chelating capacity and pharmacological properties of benzimidazole derivatives. Benzimidazole derivatives are the core of many clinical drugs and preclinical candidates with a broad spectrum of activity, including antimicrobial, antiviral, antifungal, anticancer, anti-inflammatory, and antidiabetic activities, as widely documented in recent reviews. As ligands in coordination chemistry, benzimidazoles and their derivatives form stable complexes with transition ions, and this complexation often enhances biological activity against free ligands, including cancer cells and microorganisms. Coordination compounds of benzimidazole derivatives are being investigated as potential anticancer drugs, antimicrobial agents, and as functional materials, including coordination polymers with selective CO_2 sorption, which combines pharmacochemistry with materials science. [1,2] The synthetic accessibility of the core and the possibility of precise modification of coordination sites make benzimidazole derivatives and their metal complexes a promising platform for the design of selective ligands, bioactive complexes, and porous coordination materials with medical and technological applications [1-3].

The aim of the presented research was the synthesis and characterization of a series of new coordination compounds of selected metal ions (Cu(II), Zn(II), Co(II)) with benzimidazole derivatives (methyl (6-(phenylthio)-1H-benzo[d]imidazol-2-yl)carbamate, 6-(phenylthio)-1H-benzo[d]imidazol-2-amine, (E)-2-(((6-(phenylthio)-1H-benzo[d]imidazol-2-yl)imino)methyl)phenol). They were characterized using techniques such as Elemental Analysis (EA), Atomic Absorption Spectrometry (ASA), Fourier-Transform Infrared Spectroscopy (FTIR) and UV-Vis spectroscopy. As an introduction to biological research, the pharmacokinetic profile of ligands was analyzed using in silico methods, including ADME and molecular docking, which allows for the prediction of the preferred position of the ligand after binding to the macromolecule.

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P-073

Histamine H3/H4 receptor ligands — Synthesis, structural and pharmacological properties

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The H3R and H4R receptors are G protein-coupled receptors (GPCRs) that play a key role in regulating various physiological processes, making them promising therapeutic targets. The H3R receptor is primarily found in the central nervous system, where it modulates the release of neurotransmitters, including histamine and dopamine. Because of its role in cognitive function, sleep-wake cycles, and appetite regulation, the H3R receptor is a potential target for treating neurological and psychiatric disorders [1]. H3R receptor's reverse agonist/antagonist (pitolisant) has recently been approved for use in treating narcolepsy (Wakix®) [2]. In contrast, the recently discovered H4R receptor modulates the immune system and regulates inflammatory responses, making it a promising target for immune disorders such as allergies and autoimmune diseases [3][4].

In this study, we present research results on a new group of H3R/H4R ligands containing a pyrimidine, pyrido[2,3-d]pyrimidine, or 4,5,6,7-tetrahydro-2*H*-pyrazolo[4,3-c]pyridine scaffold, among other things. The designed structures were initially docked to two known 3D structures of the H4 receptor. Only structures with accepted *in silico* predicted binding parameters were selected for synthesis and *in vitro* verification.

We designed and carried out the synthesis of new ligands, isolated and purified the intermediate and then final compounds. Their structures were confirmed by using NMR and HRMS techniques. Then, compounds were subjected to preliminary biological tests (cytotoxicity and radioligand binding assays) to evaluate their potential as H3R/H4R ligands.

Funding
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P-074

Unsymmetrical Derivatives Of Terephthalic Acid as Minimal Fluorophores

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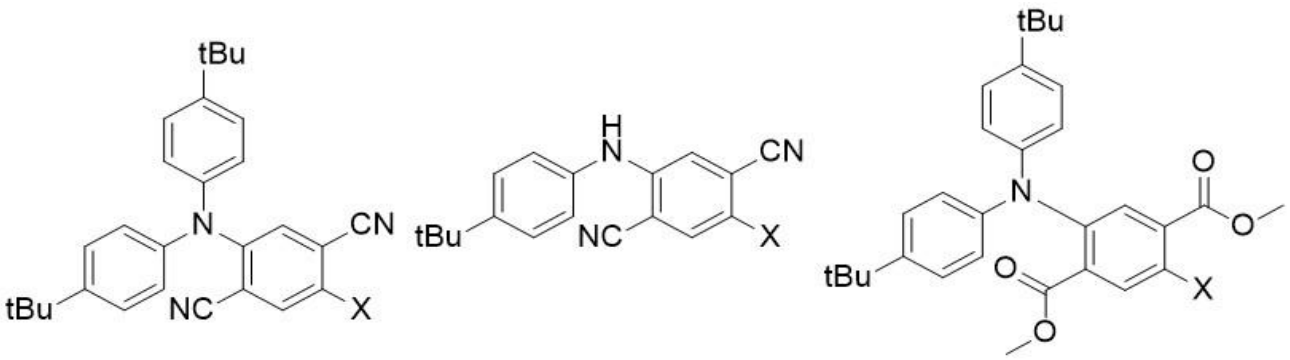
Single-benzene-fluorophores (SBFs) are a relatively new concept in the design of fluorescent materials [1]. SBFs, also known as 'minimal fluorophores', stand out amongst other luminophores due to their low molecular weights, simple structures, feasible preparation, and high quantum yields of emission in the solid state.

While the investigation of minimal fluorophores has so far been limited to symmetrical structures, it has been hypothesized [2] that unsymmetrical derivatives may exhibit distinct properties. In this work we utilize simple Pd-catalyzed coupling reactions to obtain a library of unsymmetrical derivatives of dimethyl terephthalate and terephthalonitrile. All of the synthesized compounds contain either a secondary or a tertiary amine as the donor group and benzyl, thioether, sulfone or phosphine oxide as the varying substituent

Photophysical characterization of the investigated compounds revealed that they exhibit fluorescence with good to excellent quantum yields in the solid state, phosphorescence, and aggregation induced emission effect.



Scheme 1. General Structures of the investigated compounds

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P-075

Functionalization of pyrene amides and thioamides by *ortho*-lithiation reaction

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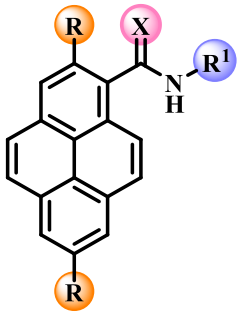
Pyrene-1-carboxamides are easily available compounds known for their photophysical behavior in both solution and solid state. Considering the increasing current interest in the development of synthetic pyrene chemistry, we became interested in exploring its synthetic potential.

Our studies revealed that *N*-tert-butylpyrene-1-carboxamide undergoes regioselective deprotonative lithiation at the C2 position, offering a promising route toward the development of novel, highly emissive pyrenyl-based fluorophores [1-4].

In 2003, Murai [5] reported that treating *N*-benzyl thioamide with butyllithium, followed by quenching with ethyl iodide, resulted in a mixture of products due to competing benzylic and *ortho*-directed lithiation pathways.



1

X O, S R H, *tert*-Bu R1 *tert*-Bu, Bn

The communication will present methods of modification of compound **1** by the *ortho*-lithiation reaction and the photophysical properties of the obtained products.

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P-076

Structures of multicomponent crystals containing trithiocyanuric acid – the impact of light conditions on the crystallization process

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Trithiocyanuric acid (TTCA) is a derivative of 1,3,5-triazine exhibiting three-fold symmetry[1] and containing three proton-donor groups (N–H) and three proton-acceptor groups (C=S).[2] The presence of these functional groups gives the molecule a strong capacity to bind heavy metal ions.[3]

The primary objective of my research was to investigate the effect of electromagnetic radiation on the crystallization process of trithiocyanuric acid systems with diazines. As a result of the experiments, four new co-crystals were obtained, which are not deposited in the Cambridge Structural Database (CSD).[4] (Fig. 1). Furthermore, it was found that light exposure conditions significantly affect the crystallization process, leading to the formation of different crystal structures from the same compounds.

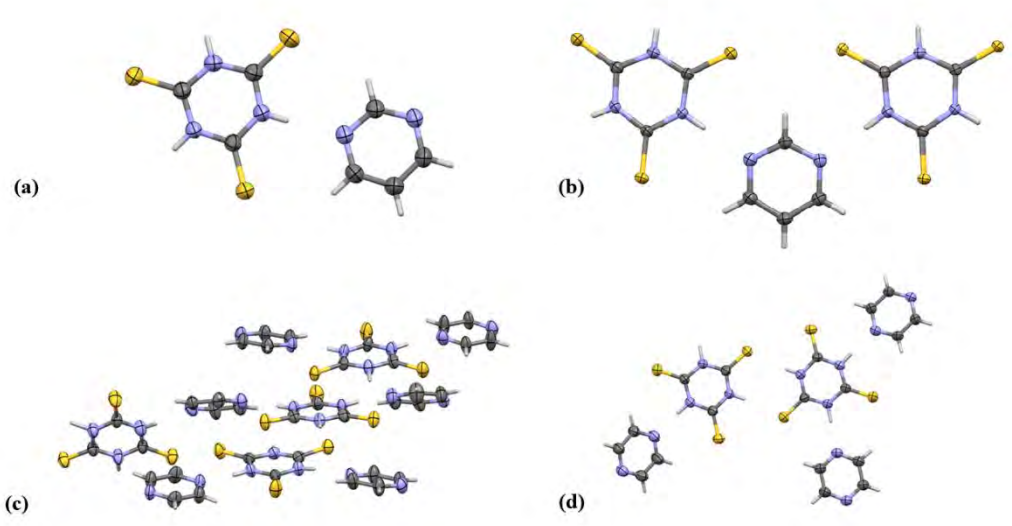

Figure 1. The diagram illustrates the molecular arrangement in the co-crystal structures of trithiocyanuric acid with pyrimidine (a, b) and pyrazine (c, d), obtained under visible light irradiation (a, c) and darkroom conditions (b, d), respectively.

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P-077

Photochemical method for obtaining Fe(III) *β*-diketonates. Synthesis and biological studies

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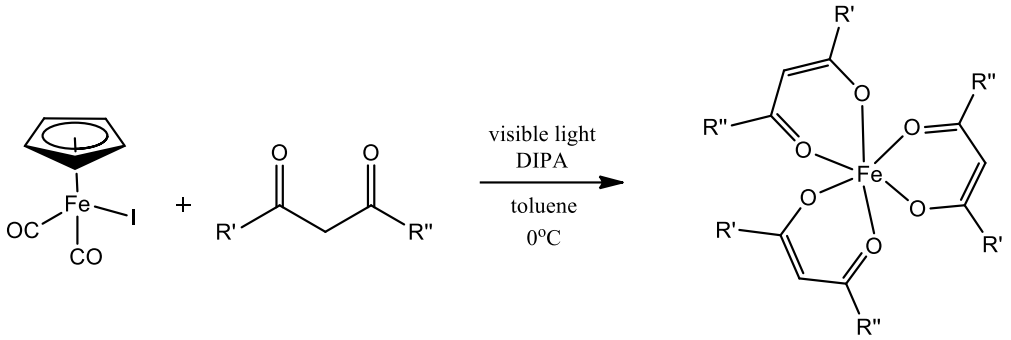
Complexes containing metals have garnered significant interest due to their unique physicochemical, photochemical and electrochemical properties. In recent years, there has been an important increase in the applications of metal complexes in medicinal chemistry to treat many diseases, including cancer [1]. One of the best-known metal complexes is cisplatin. Cisplatin is currently the first-line therapy or the second-line therapy for ovarian cancer, testicular cancer, head and neck cancer, and small-cell lung cancer [2].

The main objective of the research presented was to develop effective and efficient procedures for obtaining metal tris(acetonates) (3) in the photochemical reaction of $CpFe(CO)_2I$ (**1**) with *β*-diketones (**2**). The metal tris(acetonates) were obtained by irradiation with visible light of an argon-saturated solution of **1** and **2** and diisopropylamine (DIPA), in toluene at 0°C. [3] In this study, we also examined the compatibility and effectiveness against selected normal and cancer cell lines of metal tris(acetonates). Cytotoxicity evaluations against normal (RBCs, CD-1079sk) and cancerous (MCF-7, HeLa and SKOV-3) cell lines were performed using spectrophotometric methods (hemolysis assay and MTTT assay).



1 **2a-n** **3a-n**

Scheme 1. Photochemical reaction of $CpFe(CO)_2I$ with *β*-diketones

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P-078

From chemistry to photophysics: R-N-(*click*)$_2$-bridged nucleosides as novel building blocks for nucleic acids

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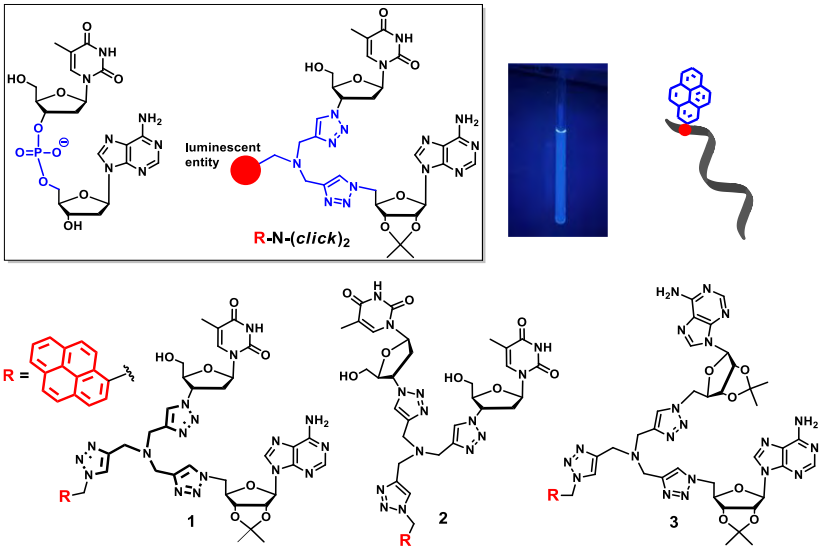
Modified nucleic acids are increasingly important tools for medicinal and other applications. Progress in this field strongly depends on advancement in synthetic chemistry which delivers suitably designed building blocks for activity-specific oligonucleotides synthesis. As synthetic chemists we contribute to this global effort by developing modified nucleosides labelled with easily detectable entities (luminescent, IR and redox-active).[1] Poster presents chemistry and luminescent properties of nucleic acid components with R-$CH_2N(CH_2)_2$-triazole bridge (abbreviated as **„R-N-(*click*)$_2$"**) substituting natural phosphodiester linkage. In particular, it features the representatives of this group with R = pyrenyl moiety (**1**-**3**).[2] Previous examples of the **„R-N-(*click*)$_2$"** nucleosides comprised the rhenium carbonyl (phosphorescent and IR-active) and ferrocene-containing (redox-active) compounds. Compound **1** was conjugated to model oligonucleotide and localization of **1**-**3** was studied in human MCF-7 cancer cells with confocal microscopy.



Scheme 1. Structures of 1,2,3-triazole-linked nucleosides **1** – **3**.

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P-079

Shikimic Acid: A Natural Key to Sustainable Antimicrobials

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Shikimic acid, a key intermediate of the shikimate pathway, is a plant-derived metabolite with growing relevance as a sustainable bioactive resource. Traditionally sourced from *Illicium verum* (star anise), shikimic acid can also be extracted from diverse, underutilized botanical materials and obtained through eco-efficient biotechnological routes. [1] This work highlights recent advances in extraction, biosynthesis, and derivatization of shikimic acid, emphasizing its antimicrobial potential against bacterial and fungal pathogens, including drug-resistant strains. The compound's mechanisms of action include membrane disruption, modulation of biofilm formation, and synergistic enhancement of conventional antibiotics. [2] In addition, the versatility of shikimic acid as a scaffold for novel derivatives underscores its value in drug discovery. By integrating chemical, biological, and technological perspectives, this work positions shikimic acid as a model example of plant-based bioactives that can be harnessed from sustainable and alternative sources. Finally, current knowledge gaps and future directions are discussed, including optimization of recovery from renewable sources, valorization of agricultural residues, and expansion of therapeutic applications, thereby contributing to the sustainable development of novel antimicrobial agents.

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P-080

Synthesis and characterization of new bio-inspired organic luminophores with potential chiroptical properties

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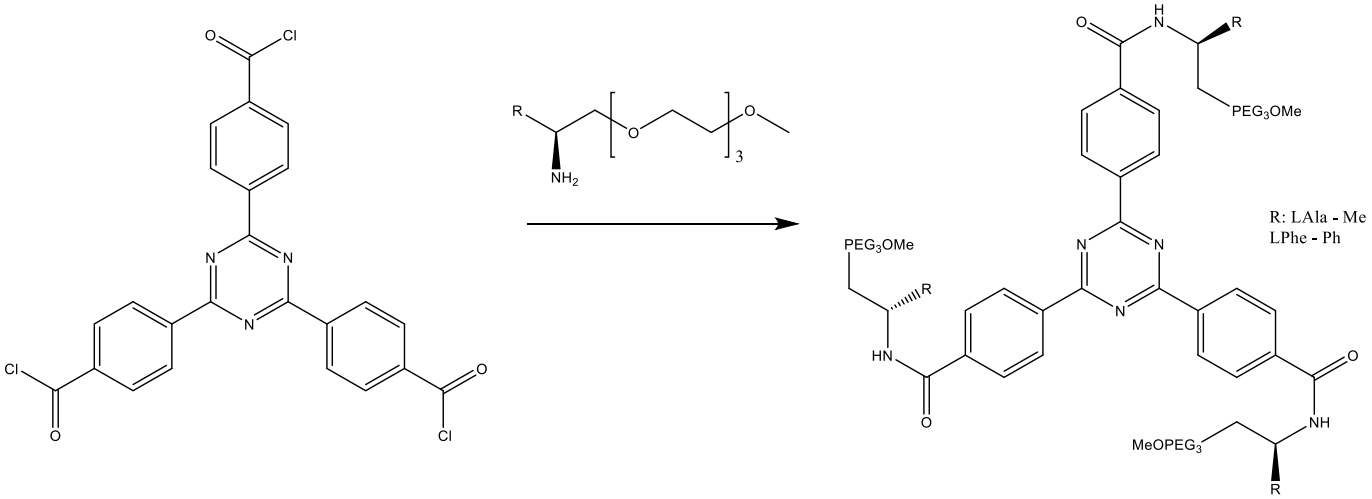
It is well known that changes in intermolecular interactions of chiral compounds often lead to changes in their circular dichroism (CD) spectra.[1] As a result, CD spectroscopy is an effective tool for monitoring molecular self-assembly processes. One group of molecules notorious for their self-assembly capabilities are derivatives of 1,3,5-triphenylbenzene. For example 4,4′,4"-s-Triazine-2,4,6-triyl-tribenzoic acid (H_3TATB) combines π-stacking with hydrogen bond formation, thus it has been used extensively as a component of organic frameworks.[2] In spite of that, reports on chiral derivatives of H_3TATB are scarce. In frame of that, we have designed and synthesized amino acid based derivatives of H_3TATB with polyethylene glycol (PEG_3) side chains.

Enantiomerically pure L-Ala and L-Phe compounds were obtained following the synthetic procedure displayed in Scheme 1. After conducting solubility tests of the new compounds in a number of solvents their optical properties were studied with the use of UV-vis absorption and photoluminescence (PL) spectroscopy. Both compounds show very similar absorption properties with maximum absorption around 290 nm and photoluminescence with two maxima (around 430 nm and 500 nm) which relative intensity depends on the solvent. The latter suggests strong self-assembly dependency on the chemical environment. Preliminary CD measurements were also carried out and yielded promising results, not only is CD signal present, the shape of the spectra suggests dependance of the self-assembly process on solvent properties. Thermally controlled NMR measurements were also carried out yielding interesting results, wherein the shape and number of ^{1}H signals in aromatic range (7,5 – 8,5 ppm) changes significantly with temperature, suggesting changes in intermolecular interactions. Further CD studies in solution are in progress and solid state studies are planned, as well as synthesis of H_3TATB derivatives bearing different types of amino acids.



Scheme 1. Synthesis of H_3TATB derivatives

Acknowledgement
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P-081

Multicomponent Crystal Structures Containing 4-Mercaptopyridine

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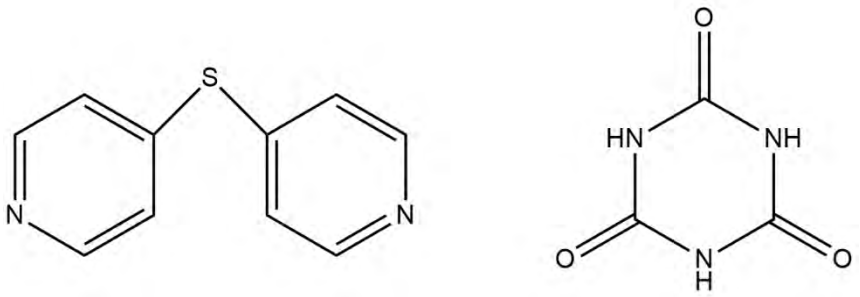
Cocrystallization of cyanuric acid with 4-mercaptopyridine offers a clear example of how small organic molecules can assemble into diverse crystal structures. 4-Mercaptopyridine, an aromatic thiol often used as a probe in surface-enhanced Raman spectroscopy (SERS) [1–3], contains both a thiol and a pyridyl group. These functional groups allow it to engage in different types of noncovalent interactions, which is why the compound also finds use in optics, sensors, and photovoltaic devices. Cyanuric acid (1,3,5-triazine-2,4,6-triol) is a nitrogen-containing heterocycle employed as a polymer precursor. It can adopt tautomeric forms, which increases its ability to adapt structurally and participate in supramolecular assemblies.

When crystallization was carried out under controlled conditions—exposure to UV light followed by storage in the dark—three different cocrystals were obtained, including a polymorphic form. All phases were stabilized by intermolecular interactions, with hydrogen bonding acting as the key organizing element. The occurrence of several crystalline forms highlights the conformational diversity of the studied molecules and the strong impact of external factors such as light on the assembly process.



Scheme 1. Scheme of di(pyridin-4-yl)sulfane and cyanuric acid molecules

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P-082

Target-Oriented Synthesis of *N*-(Arylalkyl)-3,4-Dihydroquinazolin-2-amines as Promising Acetylcholinesterase Inhibitors

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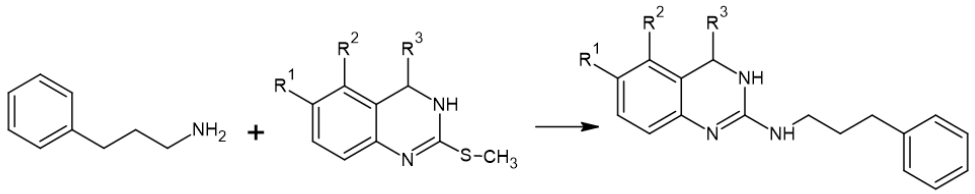
The aging demographic and the rising incidence of neurodegenerative disorders, including amyotrophic lateral sclerosis, underscore the necessity for potent acetylcholinesterase (AChE) inhibitors. [1] By inhibiting the enzyme that degrades acetylcholine, these drugs elevate its concentration in the brain, thereby improving cognitive functions that are impaired. [2] Quinazolines demonstrate pronounced efficacy as AChE inhibitors, as their molecular structure facilitates robust interaction with the enzyme's active site, leading to increased acetylcholine concentrations in synapses. [3]

As part of the study, new 3,4-dihydroquinazolin-2-amine derivatives with arylalkyl substituents at position 2 were synthesized. The synthesis involved 3-phenylpropylamine and derivatives of 2-(methylsulfanyl)-3,4-dihydroquinazoline (Scheme 1.), with triethylamine (TEA) used as an organic base. The reactions were carried out using a solvent-free approach, in line with green chemistry principles. The structures of the resulting compounds were characterized by LC-MS, and they are now scheduled for subsequent biological evaluation.



Scheme 1. Schematic diagram of the synthesis. $R^1 = CF_3$, R^2 = Cl, or CH_3, or F, $R^3 = CH_3$

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P-083

New 5-HT$_6$ receptor ligands from the *N*-(3,4-dihydroquinazolin-2-yl)naphthalene-1-sulfonamide group as a potential anticancer therapy

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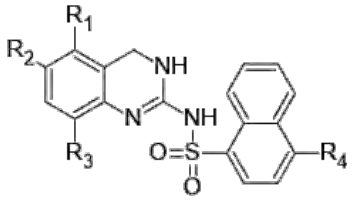
The 5-HT$_6$ receptor, a subtype of serotonin receptors, plays a significant role in the pathogenesis of central nervous system tumors.[1] Glioblastoma multiforme, one of the most frequently diagnosed and simultaneously most aggressive central nervous system tumors, continues to pose a therapeutic challenge due to the limited effectiveness of current treatment methods.[2,3,4]

In response to the need for more effective and selective therapies, a new series of low-basicity 5-HT$_6$ receptor ligands based on the structure of *N*-(3,4-dihydroquinazolin-2-yl)naphtalene-1-sulfonamides was developed. The conducted studies included synthesis and detailed structural characterization of the compounds using analytical techniques such as UPLC-MS, ^{1}H and ^{13}C NMR spectroscopy and FT-IR, as well as melting point determinations, confirming the high purity and stability of the obtained substances. The biological activity of the synthesized ligands was evaluated in vitro on glioma (U87MG) and astrocytoma (1321N1) cell lines through antiproliferative (MTT) assays, and receptor affinity was assessed using radioligand binding assays, enabling the determination of their therapeutic potential.[5]

Furthermore, to increase the efficiency of compound synthesis and ensure compliance with sustainable development principles, a new, effective sonochemical method was developed for synthesizing the unsubstituted *N*-(3,4-dihydroquinazolin-2-yl)naphtalene-1-sulfonamide molecule. The application of ultrasound enhanced the efficiency of the synthesis process and reduced the consumption of reagents and energy, fitting an eco-friendly model for the production of potential drugs.



Scheme 1. Structure of the obtained derivatives.
Substituent distribution: R_1 = Cl or H, R_2 = Cl or H, R_3 = Cl or H, R_4 = Cl or H.

Acknowledgement

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P-084

Structure-activity relationship of the thiosemicarbazone-based complexes with anticancer and antimicrobial properties

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A series of twelve thiosemicarbazones containing both chlorophenyl- (at the N1 end) and benzylidene moiety (at the N4 end of the thiosemicarbazone scaffold) bearing 4-bromo-, 3,4-dichloro- or 3,4-dimethoxy- substituents, and 24 of their Cu(II), Pd(II) complexes were synthesized and characterized physicochemically and biologically. The newly synthesized compounds were thoroughly examined using single crystal X-ray diffraction (SC-XRD), mass spectrometry (MS), Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-Vis), and were tested for anticancer and antimicrobial activity against three melanoma cell lines and a panel of Gram-negative and Gram-positive bacteria. It was confirmed by SC-XRD and MS that the complexes adopt four-coordinate, square planar geometry with ML_2 stoichiometry (where M = Cu(II) or Pd(II); L = deprotonated ligand molecule). While the parent ligands were not prominently cytotoxic, several complexes containing 3,4-dimethoxybenzylidene- and 4-bromobenzylidene- motifs showed increased activity against melanoma cells. The two most potent and selective complexes, namely **Cu(b-TSC)$_2$** and **Pd(dm-TSC-pCl)$_2$** were selected for further anticancer mechanism of action studies. Additionally, **Cu(b-TSC)$_2$** retained its activity in vemurafenib-resistant SK-MEL-28 and A-375 cells. Generally, the introduction of phenyl- instead of chlorophenyl- substituent at the N1 end, and 3,4-dimethoxybenzylidene- substituent at the N4 end positively influenced anticancer activity. On the other hand, the choice of substituent had less impact on antimicrobial properties, which were rather strain-dependent. Interestingly, one complex, namely **Cu(b-TSC)$_2$** exhibited activity towards all five tested strains. Additionally, the structure-activity relationship is further analyzed and discussed.

Acknowledgement
The full article covering our findings was recently published as a preprint at the Chemrxiv preprint server. [1]

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P-085

Guanylation of Amines Catalysed by Hydrogen Chloride: Scope and Mechanistic Investigation

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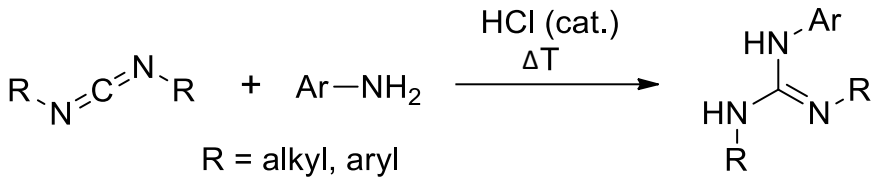
Guanidines are a popular class of organic molecules, which nowadays find many industrial applications (sweeteners, rubber additives, fertilizers, pharmaceuticals…) as well as uses in chemistry as basic/nucleophilic reagents or catalysts, polymerization initiators, recognition agents or precursors to guanidinium cations, which serve as building blocks in non-linear optical (NLO) materials.[1,2]

The central CN_3 moiety allows up to five-fold substitution, offering considerable steric and electronic variability of the target molecule. However, synthetic pathways leading to desired products often suffer from problems such as limited range of substrates/products, hardly obtainable guanylating agents, or sensitive, expensive, or toxic catalysts.[1,2,3]

The most atom-economic pathway, a direct addition of amines onto a cumulated system of N=C=N bonds of carbodiimides, has not been widely used due to a variety of reasons mentioned above. Here we utilize this approach into a simple, universal method for the synthesis of trisubstituted guanidines (Scheme 1). The reaction was catalysed using hydrogen chloride, making the process cheap, metal-free and simple. Thorough mechanistic investigations (supported by theoretical experiments), revealing a non-traditional mechanism, will be discussed.



Scheme 1. General reaction conditions for guanylation of aromatic amines.

Acknowledgement
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P-086

Highly Stereoselective (3+2) Cycloadditions of Levoglucosenone (LGO) with the *in situ*–Generated, Reactive Thiocarbonyl Ylides (*S*-Methanides) Derived from Tetrasubstituted 3-Thioxocyclobutanone

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(LGO) (**1**) belongs to the group of bio-renewable carbohydrate derivatives which is available as an enantiopure substance by the H_2SO_4 catalyzed pyrolysis of cellulose (ca. 10% yield, 95% purity), and the recently reported, optimized procedure allows its preparation as enantiopure substance (98% chemical purity). Due to the presence of an activated C=C bond, LGO is a superior candidate for exploration in cycloaddition reactions leading to optically active, polycylic heterocycles. Notably, cycloadditions typically occur in a stereoselective manner from the less hindered *exo*-face of the LGO skeleton. In a series of our recent publications, reactions of LGO (**1**) with tropothione ((8+2) cycloaddition) [2], fluorinated nitrile imines (1,3-dipolar cycloadditions) [3], and thiochalcones (*hetero*-Diels-Alder reactions) [4], have been reported.

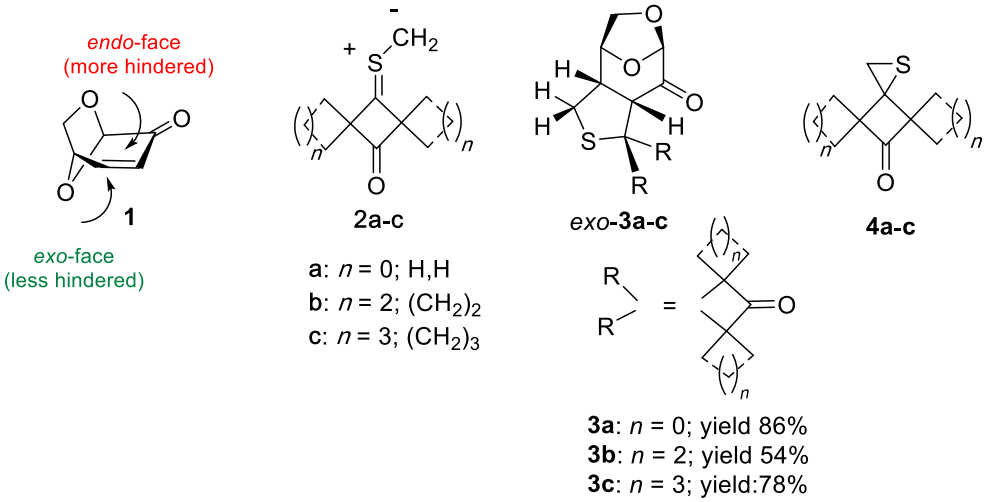

Figure. Levoglucosenone (LGO) (**1**); thiocarbonyl ylides **2a**–**c**; the (3+2) cycloadducts *exo*-**3a**–**c**, and thiirane **4a**–**c**.

In this communication (3+2) cycloadditions of the reactive thiocarbonyl ylides **2** with LGO (**1**) will be presented. Trapping experiments were carried out in THF at 45 °C (for **2a**) in toluene at 65 °C (for **2b** and **2c**) starting with LGO (**1**) and the corresponding precursor of **2** used in a molar ratio 1:3. Polycylic tetrahydrothiophenes were obtained as anticipated *exo*-(3+2) cycloadducts in a regioselective manner in reactions with **2a** and **2b** in moderate yields. In all cases thiiranes **4a**–**c** were found as side products formed in the competitive ring closure of the intermediate thiocarbonyl *S*-methanides **2**.

The stereochemical structures of cycloadducts *exo*-**3a**–**b** were elucidated by means of spectroscopic methods and finally proved by X-ray measurements.

Acknowledgements

We thank Professor Marcin Palusiak (University of Łódź) for the single crystal X-ray analysis of *exo*-cycloadduct **3b**.

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P-087

Unexpected Course of the Reaction of Methoxyallene with Dialkyl 2-Arylcyclopropane-1,1-Dicarboxylates (D-A Cyclopropanes); Dual Catalytic Activity of Scandium Triflate $Sc(OTf)_3$

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In recent years, rapidly growing interest on new applications of so, called D-A cyclopropanes of type **1** (dialkyl 2-arylcyclopropane-1,1-dicarboxylates) in organic synthesis, aimed at the preparation of multi-functionalized, cyclic (carbo- and heterocyclic) as well as acyclic compounds, have been observed [1]. Typically, their reactions with diverse nucleophilic reagents occur in the presence of an activating Lewis acid such as $AlCl_3$, $FeCl_3$, $GaCl_3$, $NiCl_2$, etc. Recently, scandium triflate $Sc(OTf)_3$ has found numerous applications as a shelf stable, low-cost and non-hygroscopic salt acting in catalytic amounts as an activating Lewis acid.

The Lewis acid catalyzed reactions of D-A cyclopropanes with activated ethylenes are known to produce carbocyclic products [1a]. For example, the Lewis acid catalyzed reactions of differently substituted allenes with D-A cyclopropanes, leading to carbocyclic five- and six-membered products *via* annulation pathways have recently been reported [3]. However, reactions of D-A cyclopropanes with methoxyallene have not yet described. On the other hand, methoxyallene (**2**) is considered as a prominent representative of allenes and its numerous applications as an unique building block in organic synthesis are well documented [2].

In this communication we report on attempted reaction of D-A cyclopropanes **1** with methoxyallene (**2**) performed in the presence of catalytic amounts of scandium triflate $Sc(OTf)_3$. Reactions were performed in CH_2Cl_2 solutions at room temperature and unexpectedly led to compounds **3** which could be isolated by chromatography in moderate yield (30-40 %). In addition, chromatographic separation of crude product mixtures led to isolation of a polymeric material. A separate experiment demonstrated that the latter is rapidly formed from methoxyallene (**2**) upon treatment with cat. amounts of $Sc(OTf)_3$.

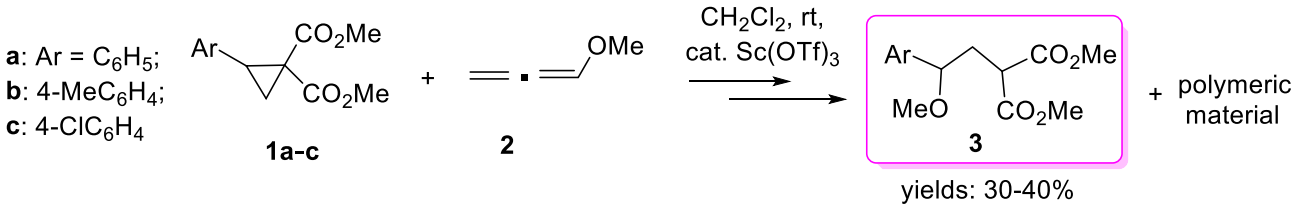

Figure. D-A Cycloproanes **1**, methoxyallene (**2**), and 3-aryl-3-methoxypropane 1,1-dicarboxylates **3** formed as unexpected products of the $Sc(OTf)_3$ catalyzed reaction of **1** with **2**.

Notably, experiments performed with three-fold mol. ratio **2** (allene):**1** (cyclopropane) resulted in a remarkable enhancement of isolated yields of adducts **3**. Some of adducts **3** are known as products of the ring opening of the corresponding D-A cyclopropanes of type **1** with MeOH in the presence of a Lewis acid, *e.g.* gallium chloride $GaCl_3$ [4].

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P-088

Synthesis and characterization of 2,8-Diphenylbenzo[1,2-*b*:4,5-*b*']bis[*b*]benzothiophene

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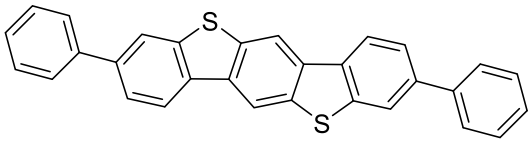
The development of novel organic semiconductors is a rapidly growing area of research in organic electronics.[1] π-Conjugated heteroacenes have attracted significant attention due to their promising performance as active materials in optoelectronic devices, including organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic photovoltaic cells (OPVs).[2] In particular, they have been extensively explored in OFETs due to their structural similarity to oligoacenes, such as pentacene, one of the best organic semiconductors for OFETs.[3] Among these compounds, benzo[1,2-*b*:4,5-*b'*]bis[*b*]benzothiophene (**BBBT**) derivatives[4] constitute an interesting class due to their chemical stability, charge-transport capabilities, rigid planar structures, and extended π-systems, which promote efficient π–π stacking and favorable molecular packing.

From the synthetic point of view, efficient strategies for the preparation of the highly extended analogues possessing more than four aromatic rings are limited. Herein, we present the synthesis, theoretical calculations, and physicochemical characterization of 2,8-diphenylbenzo[1,2-*b*:4,5-*b*']bis[*b*]benzothiophene (**2,8-diPh-BBBT**) (Scheme 1) as a potential candidate for organic electronic applications.



Scheme 1. Structure of 2,8-diphenylbenzo[1,2-*b*:4,5-*b*']bis[*b*]benzothiophene (**2,8-diPh-BBBT**).

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P-089

Chiral organophosphates compounds as chiral auxiliaries in organic synthesis

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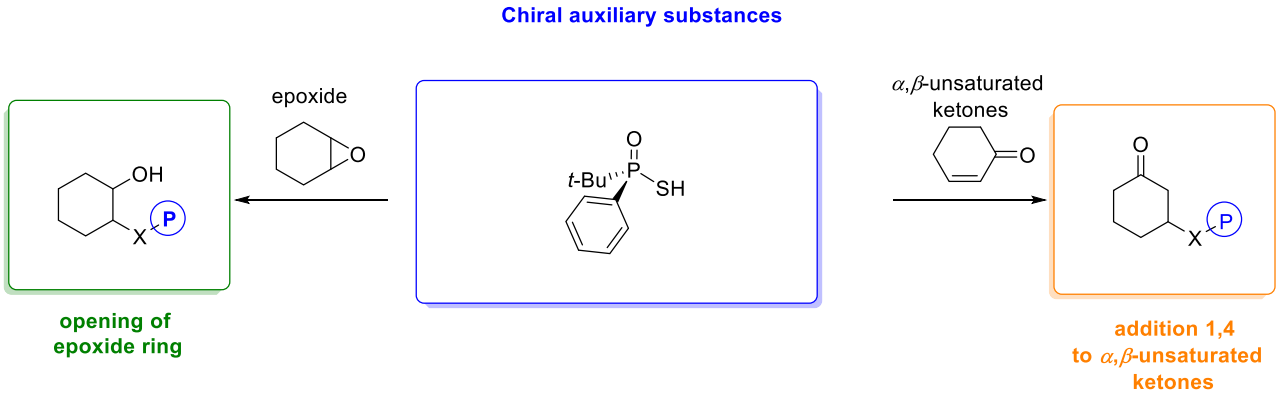
An important issue in modern asymmetric synthesis is the search for readily available and efficient chiral auxiliaries that can be temporarily incorporated into an organic molecule to control the stereochemical outcome of a reaction. Despite the existence of a rich library of compounds employed as chiral auxiliaries, further research aimed at developing new, more versatile and cost-effective systems remains highly significant for the advancement of synthetic organic chemistry [1-2].

As part of our ongoing studies, we are focusing on the optimization of stereocontrolled reactions of organophosphorus compounds serving as chiral auxiliaries. An optically active *t*-butyl(phenyl)-phosphinothioic **1** acid has been tested as a chiral auxiliary in the following reactions (Scheme 1):

a) 1,4-addition reactions to *α,β*-unsaturated ketones, and

b) epoxide ring-opening reactions.

The study includes an analysis of the influence of solvents, temperature, the number of reagent equivalents used, and the presence of an amine on the course of the reaction. The obtained results provide a basis for further research on the design of new chiral organophosphorus compounds with enhanced stereocatalytic activity and a broader range of synthetic applications.



Scheme 1.

Acknowledgement

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P-090

Ditopic ligands for metal complexes: azinium derivatives of *closo*-decaborate anion

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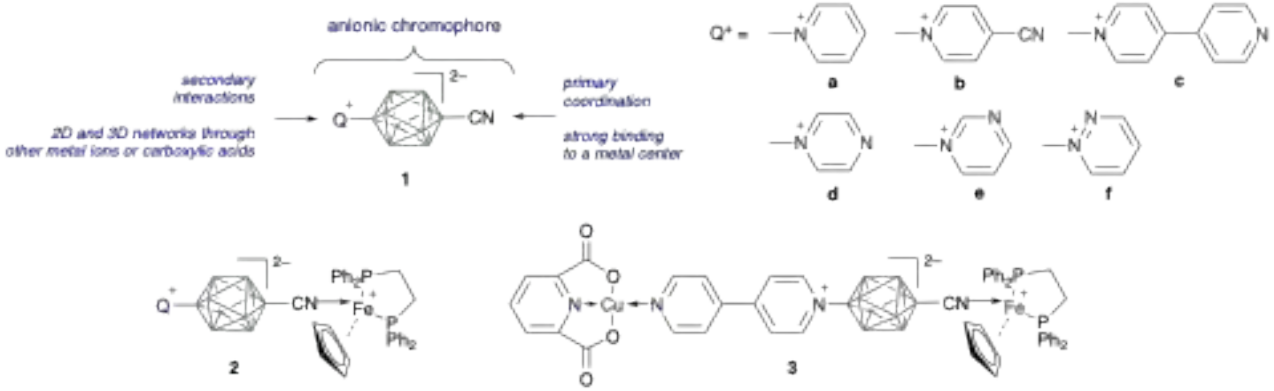
The electronic and steric properties of carboranes[1] and *closo*-boranes are attractive factors in designing functional ligands[2] for transition metal complexes acting as catalysts, luminescent materials, molecular objects, functional grids or MOFs (metal-organic frameworks). The latter materials typically use homoditopic carborane carboxylic acids as ligands. Among closo-boranes, the [*closo*-$B_{10}H_{10}$]$^{2-}$ anion is exceptional due to its D_{4d} symmetry and high lying HOMO with large amplitudes at the apical (1 and 10) positions.[3] Despite these features, it has received little attention as a structural element of functional ligands.

Herein, we present a new class of rigid, photoactive heteroditopic anionic ligands **1** based on the 1,10-disubstituted [*closo*-$B_{10}H_{10}$]$^{2-}$ anion as a step toward functional coordinational networks. The design includes two apical substituents, a metal coordinating cyano group and an azinium (Q^+ = pyridinium, 4-cyanopyridinium, 4,4′-bipyridynium, pyrazinium, pyrimidinium, and pyridazinium), which provides a secondary binding site (Scheme 1). Two of the ligands were converted to (η5-Cp)(dppe)Fe complexes **2** and one of them was used to obtain a heterodinuclear complex **3** with Cu(pdc)(H_2O)$_3$ to demonstrate the ditopic function of the ligand. The derivatives are characterized with spectroscopic (UV, IR, and NMR), electrochemical and single-crystal XRD methods, while all experimental data are augmented with DFT results.



Scheme 1. Structures of ligands **1a-f**, mononuclear complexes **2**, and heterodinuclear complex **3**.

Acknowledgement

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P-091

Synthesis of Novel 4-Phosphorylated Derivatives of 5-Mercapto-1,3-Oxazole as Potential Anticancer Agents

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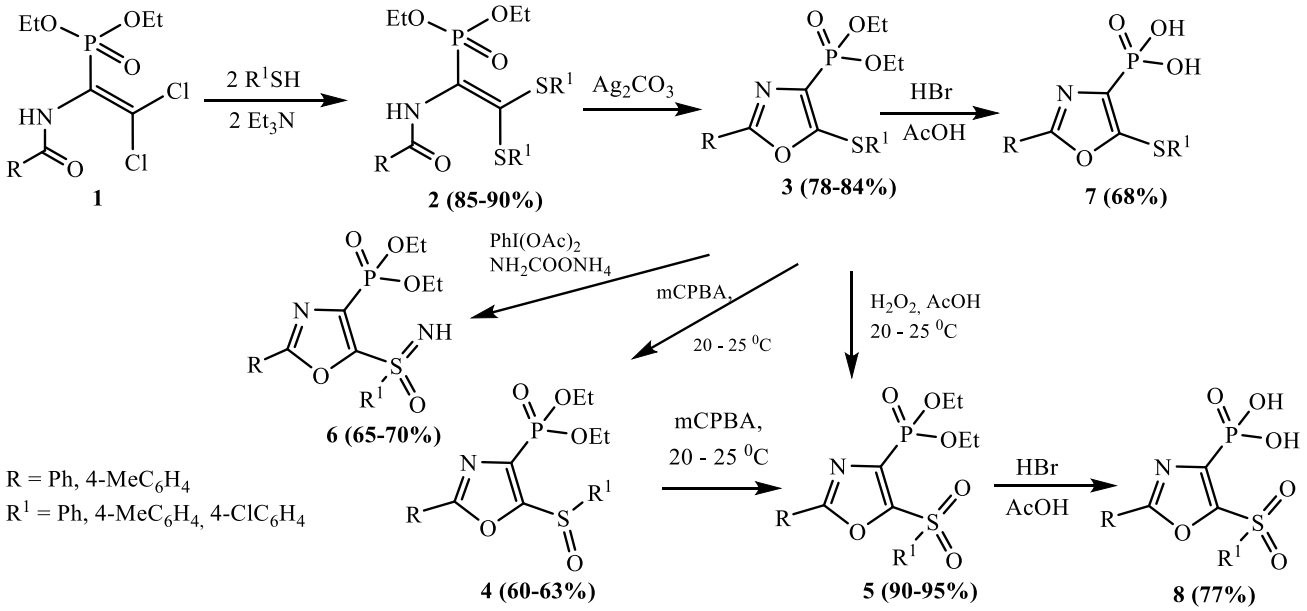
Cancer is a leading cause of death worldwide, with about 20 million new cases and 9.7 million deaths in 2022. Chemotherapy remains central to treatment but faces challenges of low selectivity and resistance. Since 1,3-oxazole derivatives exhibit strong antitumor activity, creating new compounds based on this scaffold is a promising approach in medicinal chemistry.

For the synthesis of 4-phosphorylated 5-mercapto-1,3-oxazoles, a convenient preparative approach was employed. The reaction involved the treatment of diethyl esters of 1-acylamino-2,2-dichloroethenylphosphonic acid **1** with an excess of thiophenol in the presence of triethylamine under an inert atmosphere, followed by treatment with silver carbonate, affording 4-phosphorylated 5-mercapto-1,3-oxazoles **3** in high yield.

The interaction of compound **3** with an equimolar amount of *m*-chloroperbenzoic acid afforded previously undescribed sulfoxides **4**, which were further oxidised in the presence of excess oxidant to yield sulfones **5**. Treatment of compound **3** with excess 35% hydrogen peroxide in acetic acid also provided sulfones **5**. Oxidation with iodobenzene diacetate in the presence of ammonium carbamate gave rise to sulfonimides **6**. Finally, hydrolysis of the corresponding diesters **3** or **5** with hydrogen bromide in anhydrous acetic acid produced the corresponding phosphonic acids (**7** and **8**).



Scheme 1. Synthesis of novel 4-phosphorylated 5-mercapto-1,3-oxazoles

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P-092

Copolymerization of elemental sulfur with carbonyl and thiocarbonyl comonomers using the inverse vulcanization method

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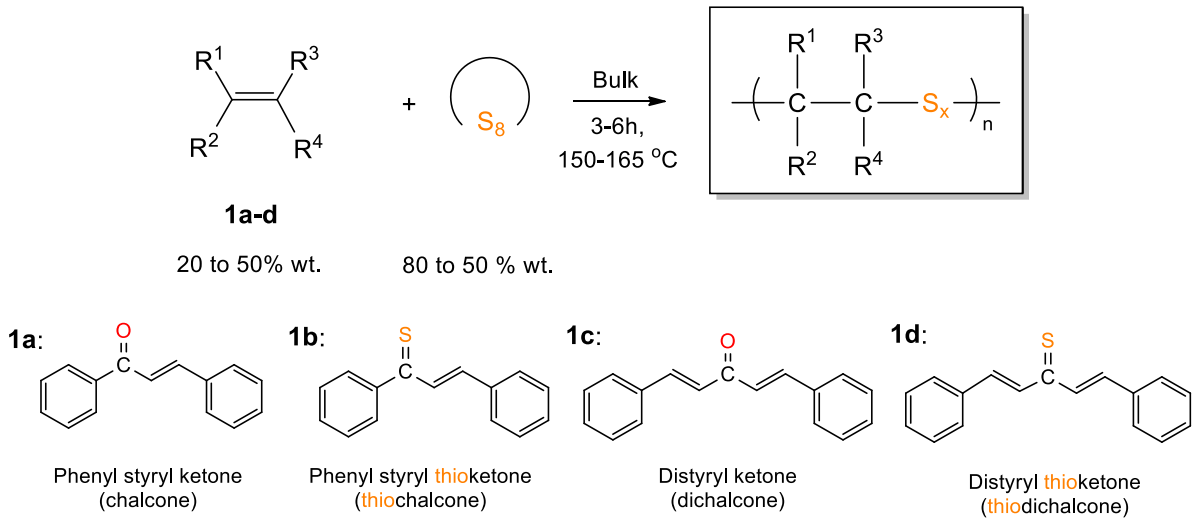
With waste sulfur production continuing to rise (over 90% of the 78 million tons produced in 2020 resulted from petroleum refining processes [1]), there is increasing interest in converting this byproduct into valuable sulfur-based materials. Polymers that incorporate sulfur atoms directly into their backbone, known as polysulfides, are especially appealing. This is due to sulfur's distinctive ability to form bonds with itself, creating sulfur bridges that offer a powerful means of controlling and customizing the structure and properties of these materials [2].

One of the well-known method of obtaining sulfur-containing polymers is the so-called „inverse vulcanization". The main idea behind this method is to use the ability of elemental sulfur to spontaneously activate as a result of thermolysis of S-S bonds at temperatures above its melting point (preferably 140-180°C), thus producing sulfur diradicals and their subsequent reaction with unsaturated monomers in the sulfur melt, without the use of solvents or initiators [2].

Herein, we report our results of the copolymerization reactions of selected (phenyl)-(di)styryl (thio)ketones **1a-d** with elemental sulfur (S_8) producing novel sulfur-rich polymers (**Scheme 1**) [3]. Characterization of the reaction products and their application as a rubber's multifunctional additives, investigating both their effect on the crosslinking process and their compatibilizing effect on the elastomer matrix with silica filler, will be discussed.



Scheme 1. General scheme of copolymerization process of (phenyl)-(di)styryl (thio)ketones **1a-d** with elemental sulfur (S_8) leading to novel sulfur-rich polymers [3].

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P-093

Ring-Fused [1,2,4]Triazinyl Radicals: Synthesis and Properties of π-Conjugated Open-Shell Systems

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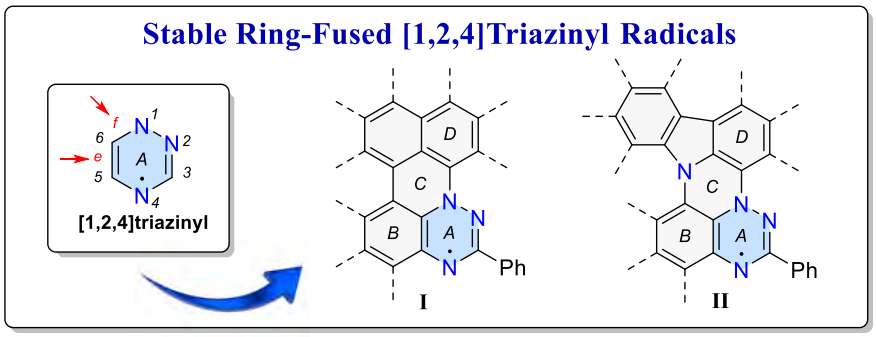
The design of persistent organic radicals represents a key strategy in the development of next-generation molecular materials for organic electronics and spin-based technologies. Particularly appealing are large polycyclic aromatic hydrocarbons (LPAHs) hosting delocalized spins, which exhibit remarkable magnetic responses, tunable redox behavior, and distinctive optoelectronic characteristics.

In this context, [1,2,4]triazin-4-yl radicals have emerged as an exceptionally robust class of open-shell species, accessible through four complementary synthetic pathways recently established by our group [1–4]. These advances not only facilitated the preparation of diverse derivatives but also extended the family of paramagnetic nanographenes with relevance for data storage and quantum information processing [5–7].

Here we report two novel LPAH architectures in which the triazinyl motif is fused to the aromatic backbone via annulation at the e and f edges. The resulting systems—perylene-type I and N-peri-annulated II planar Blatter radicals—were synthesized and thoroughly investigated. Their structures and properties were elucidated by X-ray diffraction, UV–vis absorption and EPR spectroscopies, electrochemical studies, and magnetic measurements. Experimental findings are further supported by density functional theory (DFT) calculations, offering a detailed picture of their π-conjugated open-shell nature.



Acknowledgement
This study was supported by the National Science Centre (NCN grant no. 2022/47/D/ST4/03462).

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P-094

Electronic and Structural Modulation of Blatter Radicals by Sulfur Oxidation

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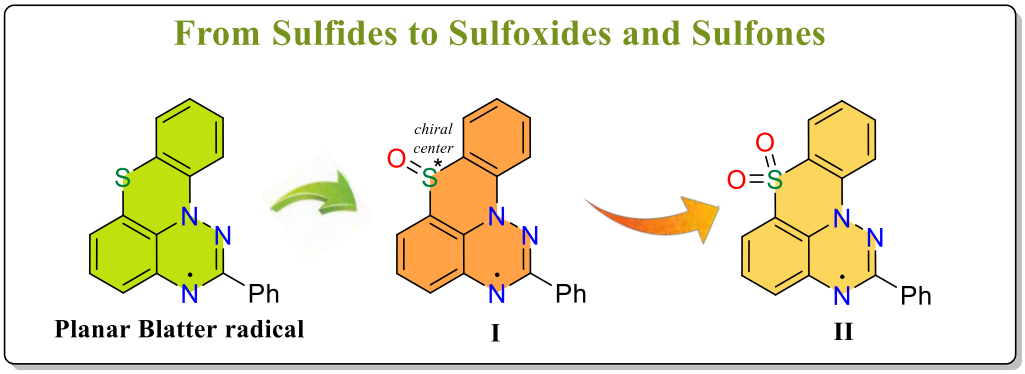
Stable organic radicals are of increasing interest in materials science due to their open-shell electronic structures, which enable unique optical, electrochemical, and magnetic properties. Among them, planar Blatter radicals are notable for their high stability and efficient spin delocalization, making them promising candidates for molecular electronics and spintronics [1-3].

In this project, we focus on the sulfur functionalization of Blatter radicals [4] through controlled oxidation of thioaryl substituents to sulfoxides **I** and sulfones **II**. This modification offers a versatile approach to tune electronic distribution and intermolecular interactions, while introducing new functionalities. Notably, sulfoxides are chiral at sulfur, allowing the preparation and resolution of enantiopure radicals—an unexplored direction in Blatter radical chemistry. The synthesis of these derivatives builds on established synthetic protocols [5] followed by selective oxidations. Their properties are probed using a combination of advanced techniques: EPR to map spin distribution, UV–Vis spectroscopy to monitor optical changes, cyclic voltammetry to study redox modulation, and X-ray diffraction to resolve structural effects of oxidation. In addition, chiral HPLC separation provides access to individual enantiomers of sulfoxides.



Scheme 1. Stepwise oxidation of thioaryl-substituted planar Blatter radical to sulfoxide and sulfone derivatives.

Acknowledgement

This study was supported by the National Science Centre (NCN grant no. 2022/47/D/ST4/03462).

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P-095

Cycloadditions vs. Nucleophilic Additions in Reactions of Lepidiline-Derived Imidazole-2-thiones with Trifluoroacetonitrile Imines

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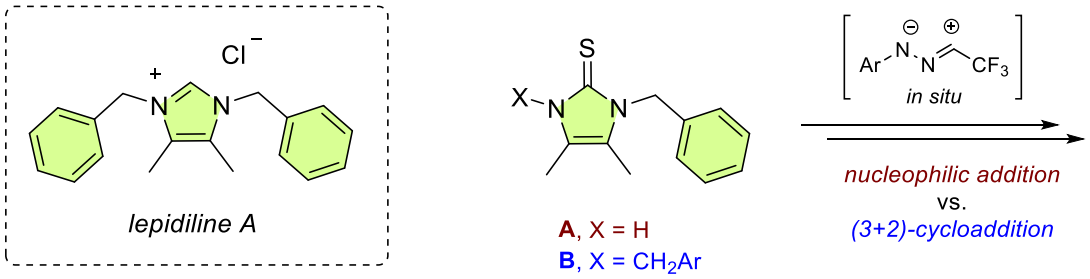
Naturally occurring 1,3-dibenzylated 4,5-dimethylimidazoliums known as lepidilines as well as their various synthetic analogues exhibit promising biological activity, including anticancer effects.[1,2] In continuation of our quest towards fluorinated lepidiline-inspired systems for cytotoxicity studies, two series of imidazole-2(3*H*)-thiones were prepared and examined in reactions with trifluoroacetonitrile imines recognized as versatile 1,3-dipolar building blocks for preparation of numerous nitrogen heterocycles.[3,4] Here, we report on excellent chemoselectivity observed in reactions with enolisable (**A**) and non-enolisable imidazole-2-thiones (**B**) with title nitrile imines, leading either to acylic hydrazonothioates or spiro [1,3,4-thiadiazole-5,2'-imidazoles], respectively.[5] Notably, ^{13}C NMR analyses of the obtained products revealed chemical shifts of the *C*-(CF_3) atom as useful probe to differentiate the open-chain hydrazonothioates (δ = 112–120), common 2,3-dihydro-1,3,4-thiadiazoles (δ = 130–145), and more strained spiro-1,3,4-thiadiazole derivatives (δ = 166–170).



Scheme 1. Structures of *lepidiline A* and the studied imidazole-2(3*H*)-thiones **A** and **B**.

Acknowledgement
Financial support by the University of Lodz in the framework of IDUB grants (WKP; #5/ODW/DGB/2022, MJ; #14/IGB/2024) is acknowledged.

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P-096

Electroorganocatalytic asymmetric synthesis of 2-phenyl-1,2,3,4-tetrahydroisoquinoline derivatives

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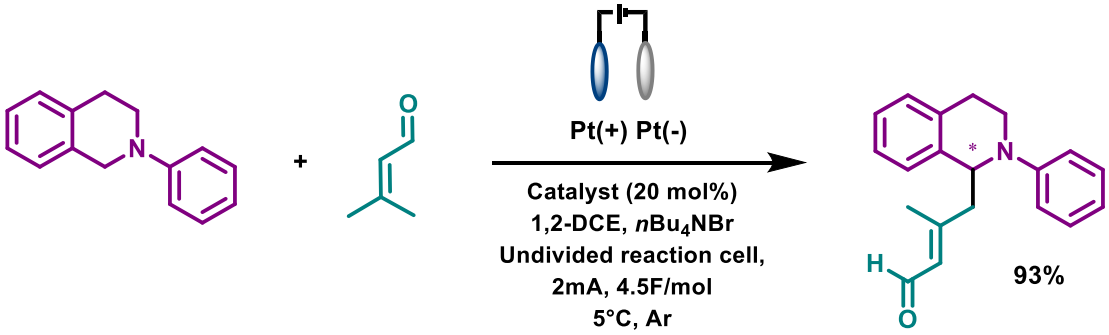
In response to the increasing costs and time requirements associated with the development of new pharmaceuticals, growing attention has been directed toward designing alternative synthetic strategies for privileged molecular scaffolds such as quinoline. Quinoline derivatives exhibit a broad spectrum of biological activities and are applied in the treatment of malaria, schizophrenia, asthma, neurodegenerative disorders, and various types of cancer. Among sustainable synthetic approaches, electrochemical methods have emerged as promising tools enabling selective functionalization of organic frameworks under mild and environmentally benign conditions.

In this study, an electro-organocatalytic approach for the synthesis of 2-phenyl-1,2,3,4-tetrahydroisoquinoline derivatives was developed, employing 2-phenyl-1,2,3,4-tetrahydroisoquinoline and 3-methylbut-2-enal as model substrates. Optimization of key electrochemical parameters – such as current density, electrolysis duration, type of catalyst, solvent, and electrolyte – resulted in the formation of the target product with a high yield of 93%. These results demonstrate the efficiency of α-C-H bond functionalization in cyclic tertiary amines via electrochemical activation. The developed method provides an efficient, selective, and environmentally sustainable tool for the synthesis of compounds with potential biological and pharmacological relevance.



Scheme 1. Scheme of a model electroorganocatalytic reaction.

Acknowledgement

The research was funded by the National Science Centre under the Sonata Bis program UMO-2022/46/E/ST4/00338.

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P-097

Electroogranocatalytic dicycloaddition of hydroquinone with α,β-unsaturated aldehydes

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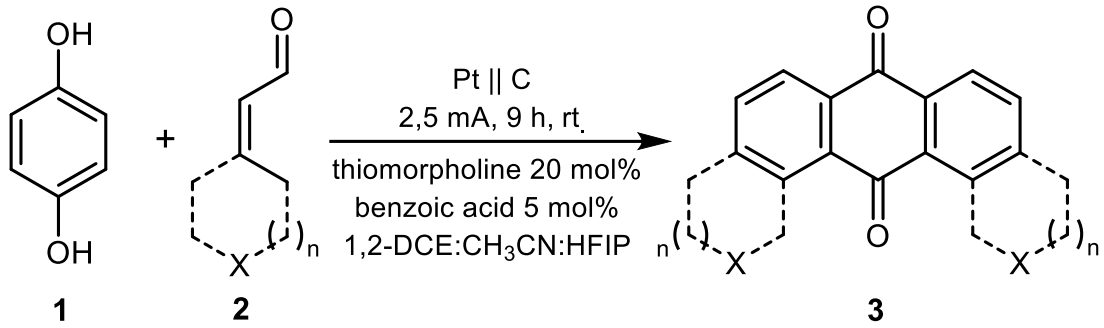
Hydroquinone, like other quinones, is a versatile precursor in organic chemistry. For this reason, quinones are often used for the synthesis of various polycyclic systems [1]. One of those structural motifs is the structure of anthraquinones, which is characterised by significant biological activity, ranging from antibiotic to anticancer properties [2]. Conventional methods of anthraquinone synthesis have numerous limitations, such as multi-step processes, the use of elevated temperatures, and the use of strong oxidants in stoichiometric ratios [3]. In contrast, electrochemical methods are a more sustainable and environmentally friendly alternative that eliminates the need for hazardous chemical reagents [4]. This paper describes an electrochemically induced Diels-Alder-type dicycloaddition reaction between hydroquinone **1** and α,β-unsaturated aldehydes **2**, using thiomorpholine as a catalyst. In order to develop an optimised protocol, a series of experiments were conducted to evaluate key reaction parameters, such as catalyst type and concentration, substrate molar ratios, type of solvent, and electrolyte composition. The developed method is an effective way to synthesise structurally diverse anthraquinones.



Scheme 1. General scheme of the electroorganocatalytic reaction of hydroquinone **1** with α,β-unsaturated aldehydes **2**.

Acknowledgement
This work was financed by a Sonata Bis grant from the National Science Centre (UMO-2022/46/E/ST4/00338).

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P-098

Selenium-derivatized methionines in protein structures

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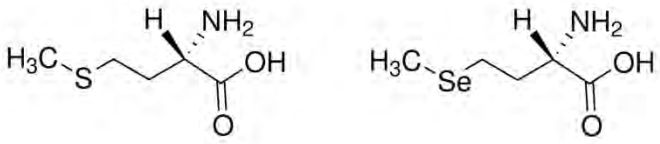
It is widely reported, that the replacement of methionines with selenomethionines, usually does not affect protein properties such as folding. [1-3] Therefore, the native, (S-Met)-containing, proteins, are frequently derivatized with selenium to facilitate the structure solution process. After successful determination of the Se-derivatized protein structure, the obtained Se-Met containing coordinate set is then used as a starting model for structure solution and refinement of the native, S-Met, data. This approach has been utilized, for example, in the X-ray structure determination of 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase. [4]

Handling selenomethionines (Se-Met) in protein structures primarily involves expressing proteins in host cells that are metabolically engineered to incorporate it in place of methionine, using a minimal medium supplemented with Se-Met. Then, crystallization of these (Se-Met)-derivatized proteins allows for experimental phasing using techniques such as Multi-Wavelength Anomalous Diffraction (MAD) or Single-Wavelength Anomalous Diffraction (SAD) to solve the protein structure. In refinement, (Se-Met)'s unique scattering properties are utilized to identify selenium sites, which are then used to generate experimental electron density maps for phase determination and model building, ultimately yielding the final crystal structure.

In the Protein Data Bank, we can find X-ray structures which were determined from selenium-derivatized proteins, but the deposited coordinates, to our surprise, contain native methionines. [5] The problem is likely due to not complete substitution of native methionines with selenomethionines. When the crystal grows from such sample, and later is subjected for X-ray analysis, it may show partial presence of native sulfur.



Scheme 1. L-Methionine (S-Met), and L-Selenomethionine (Se-Met)

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P-099

Electrophilic selenium species: probing reactivity toward thiols, amino acids, and protein

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Selenium-containing compounds have attracted significant attention due to their bioactive properties and ability to modulate redox-sensitive pathways, including the KEAP1–Nrf2 signaling axis[1,2]. Oxidative or covalent modifications of cysteine residues in KEAP1 prevent its interaction with Nrf2, leading to activation of cytoprotective genes[3]. In this study, we investigated the reactivity of electrophilic selenium species, including unsaturated selenones and selenoxides, toward model thiols and GSH, selected amino acids, and albumin, to elucidate mechanistic aspects and selectivity determinants. Using ^{1}H, ^{13}C, and ^{77}Se NMR spectroscopy, complemented by mass spectrometry, we characterized reaction products, proposed reaction pathways, and assessed structural factors influencing reactivity and stability. Reactivity studies confirmed preferential thiol modification, while hydroxyl-containing residues such as serine and tyrosine were largely unreactive. Protein interaction assays with albumin highlighted selective binding and the influence of molecular structure on stability. Preliminary biological evaluations, including cell viability and gene expression analyses, indicated that selected compounds may modulate redox-sensitive pathways, illustrating their potential biological relevance. These findings provide a mechanistic understanding of selenium–thiol interactions, emphasize the role of electrophilicity in controlling selectivity, and support the rational design of organoselenium derivatives with both chemical and biological significance.

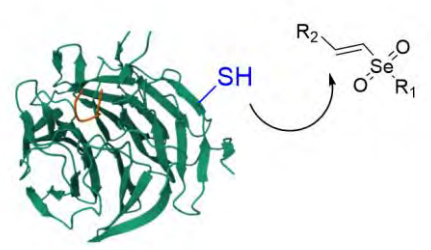

Figure 1.

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P-100

Addition of Potentially Bioactive α-Aminophosphonates to Acetylenic Derivatives

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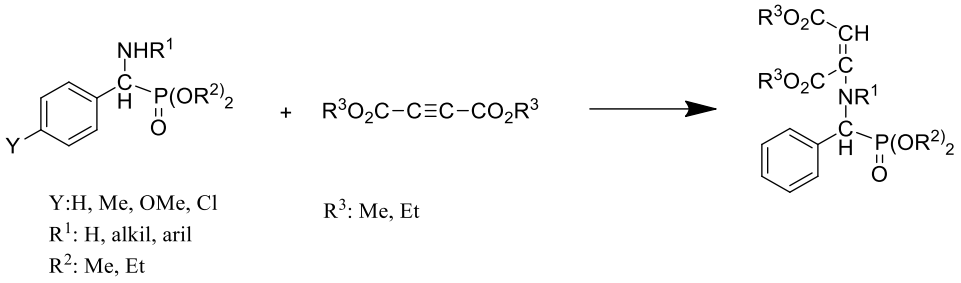
α-Aminophosphonates represent an important class of organophosphorus compounds due to their structural analogy to α-amino acids and their broad spectrum of biological activities. Numerous members of this family have demonstrated antibiotic, antiviral, anti-inflammatory, antihypertensive, and anticancer properties, highlighting their pharmaceutical and agrochemical significance.

The present work aimed to build on and refine synthetic approaches previously developed in our research group, with the goal of preparing novel α-aminophosphonate derivatives with potential biological relevance. Using modified Kabachnik–Fields-type reactions, a series of N-alkyl- and N-aryl-substituted α-aminophosphonates, as well as derivatives containing a terminal amino group (–NH_2), were successfully synthesized under optimized conditions. These compounds represent valuable framework for further structural modifications and biological evaluation. Subsequently, the synthesized α-aminophosphonates were subjected to addition reactions with dialkyl acetylenedicarboxylates (DAADs), leading to the formation of new adducts incorporating both phosphonate and acetylenic functionalities. These transformations were performed under mild conditions, and the resulting products were isolated and characterized using standard spectroscopic methods (^{1}H, ^{13}C, and ^{31}P NMR).



Y:H, Me, OMe, Cl
R^1: H, alkil, aril
R^2: Me, Et

R^3: Me, Et

Scheme 1. Reaction of α-aminophosphonate derivatives with acetylenic compounds

Acknowledgement

The author gratefully acknowledges the guidance of Dr. György Keglevich and the support of the Research Group of Environmentally Friendly and Organophosphorus Chemistry

P-101

Access to close- and open-winged fluorinated organometallic hybrids derived from pyrrolo[3,2-*c*]pyrazole

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Fluorinated *N*-heterocycles constitute privileged structural units in pharmacology, agrochemistry, and advanced functional materials chemistry, and in this group, 3-CF_3-pyrazole unit is of special importance [1]. Among the synthetic methods reported for the synthesis of the latter scaffold, remarkable attention is paid to protocols employing readily available 1,3-dipolar trifluoroacetonitrile imines and suitable dipolarophiles as reaction partners [2]. In our continuing work towards biologically active fluoroorganics, we have designed organometallic hybrids based on pyrrolo[3,2-*c*]pyrazole, a system featuring structural elements of several well-known bioactive compounds i.e. 1,4-diaryl-3-CF_3-pyrazoles (COX inhibitors), pyrrolo-pyrazoles (anti-inflammatory, anticancer), and redox-active metallocenes. To get insight into structure–biological activity relationships (SAR) dictated by the nature of substituents and functional groups (R/Ar) in the devised materials, the general approach for the synthesis of bent-core (**A**; closed-winged) and planarized (**B**; open-winged) products was developed [3]. Results on mechano- and photochemical methods applied for the preparation of title hybrids will be presented.

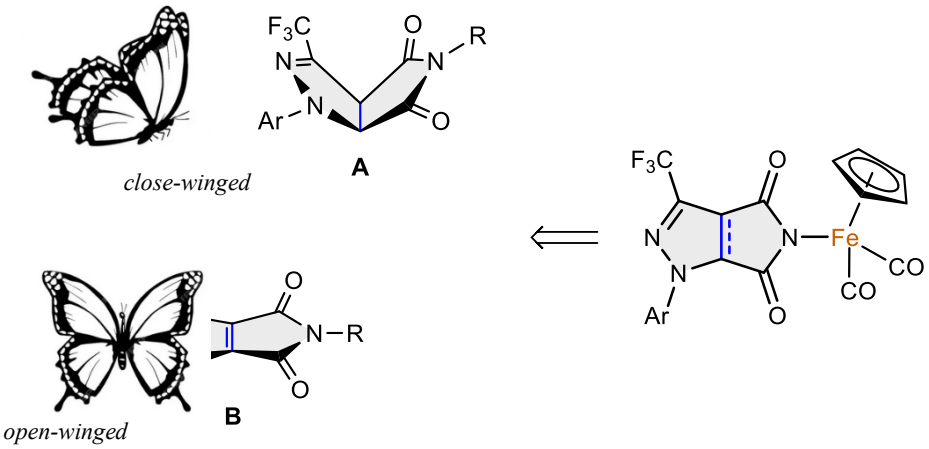

Figure 1. General structures of the devised hybrids.

Acknowledgement
This research was funded by the IDUB grant no. 19/IGB/2024.

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P-102

Mechanistic insights into Smiles rearrangement of trifluoroacetohydrazonyl esters

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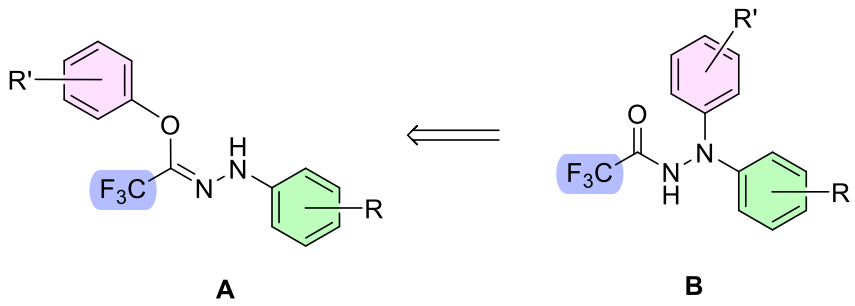
There is increasing interest in the chemistry and biological relevance of *N*',*N*'-diarylacylhydrazides recognized as promising drug candidates and agrochemicals [1]. The first report on CF_3-functionalized hydrazides diarylated at the terminal N atom is dated back to late 80', and the mentioned materials were identified as suitable precursors for generation of the respective, fairly stable hydrazonyl radicals [2]. Even though the introduction of fluoroalkyl groups into organic molecules is well known to remarkably tune their physio-chemical and biological character, little progress have been made in the synthesis and applications of CF_3-hydrazides.

In continuation of our study on the chemistry of reactive fluorinated intermediates [3], we turned attention to hydrazonyl esters **A** considered attractive building blocks for the Smiles-type rearrangements. Here we report straightforward access to unsymmetrical *N*',*N*'-diaryltrifluoroacetohydrazides (**B**) based on a two-step protocol comprising trapping of the *in situ*-generated CF_3-nitrile imine with phenolate, followed by thermal rearrangement of **A**. Molecular mechanism and scope of the proposed synthetic protocol were evaluated on the basis of the DFT calculations.



Scheme 1. Structures of intermediates **A** and the target CF_3-acylhydrazides **B**.

Acknowledgements

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P-103

Electrochemical α-functionalization of 2-phenyl-1,2,3,4-tetrahydroisoquinoline derivatives

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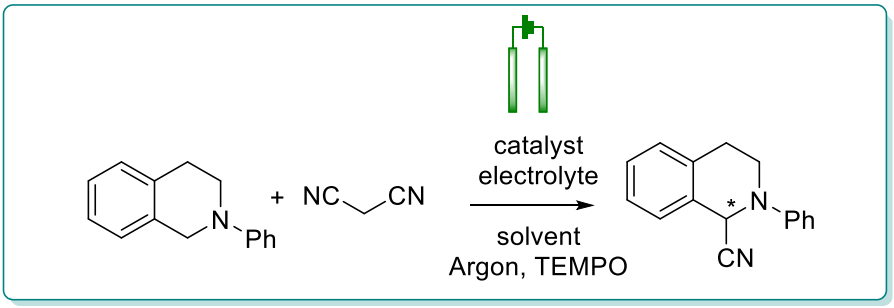
In our research team, we have recently been trying to increase the potential of organocatalysis by using a tool such as electrochemistry. [1] Electrosynthesis is modern, ecological and economic technique, following the increasing emphasis on green chemistry principles. The 1,2,3,4-tetrahydroisoquinoline ring is present in many natural alkaloids, bioactive molecules and commercial pharmaceuticals. Its derivatives have diverse biological activities, such as antifungal, antiviral, anticancer and antimalarial properties. [2] The aim of the present research was to optimize the electrochemical synthesis of tetrahydroisoquinoline derivatives. During the course of this study, a systematic investigation of various parameters — including the choice of electrolyte, solvent, current conditions, and organocatalysts — was undertaken to evaluate the feasibility of obtaining an enantiomerically enriched product. In the subsequent phase of the work, efforts will be focused on exploring the scope and limitations of the developed synthetic methodology.



Scheme 1. Model reaction.

Acknowledgement

The project was financially supported by the National Science Centre Poland within the Sonata Bis programme UMO-2022/46/E/ST4/00338.

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P-104

Synthesis and physicochemical studies of new benzotriazinyl diradicals

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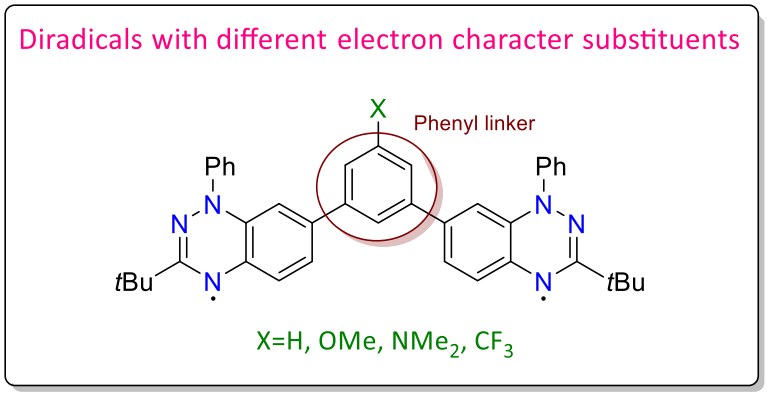
In recent years, the rapid development of molecular electronics and the growing demand for advanced functional materials have drawn researchers' attention to compounds with open-shell electronic structures. In particular, stable Blatter radicals and their derivatives – benzotriazinyl diradicals – have attracted considerable interest due to their unique physicochemical properties [1]. The presence of two unpaired electrons localized on different atoms means that these diradicals can exist in both singlet and triplet states, giving rise to ferro- or antiferromagnetic interactions. Such features make them promising functional components for modern material technologies [2].

The aim of this work was to synthesize new benzotriazinyl diradical derivatives linked via a phenylene bridge bearing substituents with varying donor–acceptor characteristics (Scheme 1). The desired bibenzotriazine precursors were obtained from benzo[1,2,4]triazines through a Stille coupling reaction and subsequently converted into the target diradicals by treatment with PhLi. The results of the syntheses and the optimization of reaction conditions will be presented in the poster.



Scheme 1. Benzotriazinyl diradicals linked by a phenylene bridge with substituents of varying electronic character.

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P-105

Calculations of n→π* and π→π* transition energies for dihetaryl ketones and thioketones

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Dihetaryl ketones and thioketones are useful building blocks for the synthesis of diverse (hetero)organic products.[1] Although dihetaryl (thio)ketones have attracted much attention over the past several years, the experimental and theoretical exploration of their molecular properties is still rather limited.[2] In particular, the theoretical characterization of their molecular properties related to optical spectra has been missing so far.

This study has been motivated by the aforementioned lack of theoretical studies on the photophysical properties of dihetaryl (thio)ketones.[3] Filling this gap was achieved by performing quantum chemical computations for a series of symmetrical dihetaryl ketones and their thiocarbonyl analogs. The n→π* and π→π* transition energies were calculated to elucidate how the hetaryl groups affect these transition energies. Trends in these transition energies for the thioketones were compared with the results obtained for the parent ketones. The effect of solvents on these trends was also analyzed.

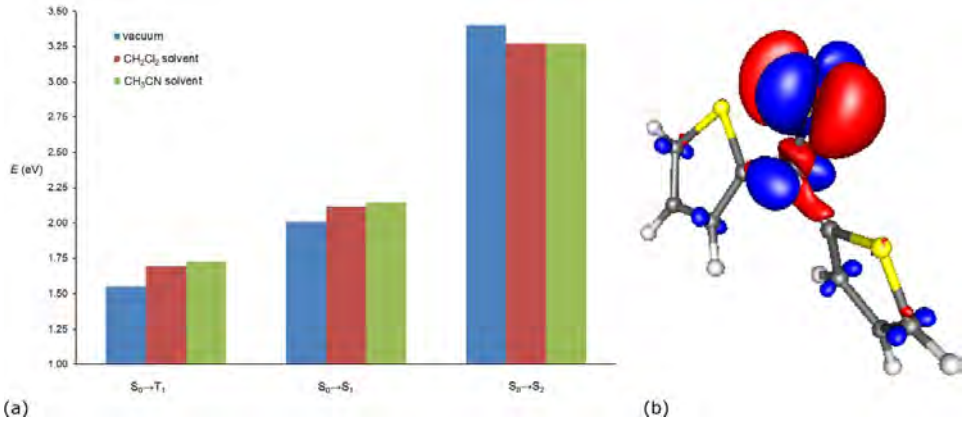

Figure 1. (a) Energies of three low-energy transitions for bis(2-thienyl)methanethione in various media. (b) Electron density difference between the ground state and the first singlet excited state of this thioketone.

Acknowledgement

The author acknowledges Polish high-performance computing infrastructure PLGrid (ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018475.

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P-106

Theoretical and Statistical Insights into the Role of Tryptophan in Ligand-Receptor Complexes

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Tryptophan (Trp) residues are critical contributors to ligand-receptor (L-R) stabilization via π-π stacking, cation-π interactions, hydrogen bonding, and hydrophobic contacts. Owing to their distinctive chemical properties, Trp residues often mediate molecular recognition and help regulate conformational states within receptor binding sites [1-3].

Expanding on these observations, a comprehensive theoretical survey of the Protein Data Bank (PDB) was carried out to quantify the occurrence, geometry, and interaction profiles of Trp residues in ligand-receptor complexes. Statistical analyses across diverse protein families revealed preferred binding environments and recurring interaction patterns involving tryptophan residues. Selected representative complexes were further analysed to characterize typical spatial arrangements and bonding tendencies. To further probe Trp-mediated interactions, a focused analysis of the 5-HT_2 receptor family was performed to investigate ligand-receptor distances and angular parameters, providing insight into the structural determinants of Trp-mediated interactions within G protein-coupled receptors. This integrative theoretical and statistical approach delineates the structural significance of tryptophan in receptor-ligand recognition and may facilitate rational design of ligands optimized for Trp-rich binding sites.

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P-107

The Friedel–Crafts acylation of ferrocene and pyrene with unprotected amino and hydroxy acids

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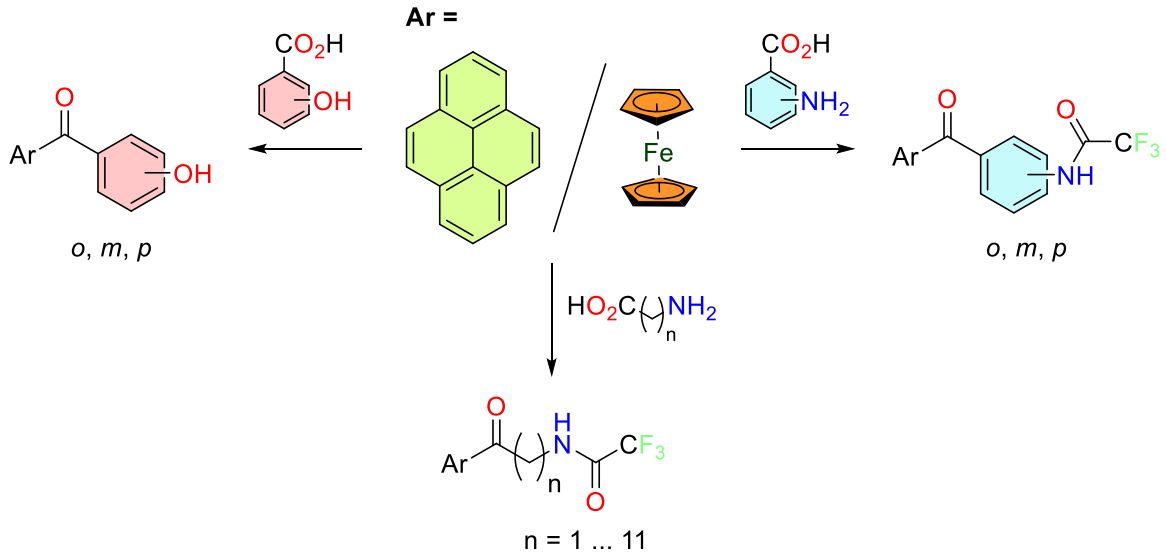
Both aminoketones and hydroxyaryl ketones play an important role in organic chemistry – as building blocks in organic synthesis and active compounds in medicinal chemistry.[1, 2]

Herein, we report the first synthesis of various types of ketones by the direct acylation of electron-rich arenes (ferrocene and pyrene) with unprotected amino and hydroxy acids (Scheme 1). The acylation is achieved using a trifluoroacetic anhydride/triflic acid system, previously used for the functionalization of ferrocene and pyrene with carboxylic acids.[3, 4]

We postulate a mechanism that includes the *in situ* protection and subsequent conversion of the substrates to reactive *N*-trifluoroacetamide mixed anhydride species. Protonated by triflic acid, these generate appropriate carbocations, which attack the electron-rich arenes to form *N*-trifluoroacetyl amidoketones or hydroxyaryl ketones.[5]

Both ferrocenyl and pyrenyl ketones can be used as versatile building blocks for the synthesis of more complex compounds, such as molecular probes or optoelectronic materials. Additionally, some of the pyrenyl amidoketones exhibit mechanofluorochromic properties.



Scheme 1. Acylation of ferrocene and pyrene to the corresponding amino and hydroxyaryl ketones.

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P-108

Functionalization of ferrocene with amino and hydroxybenzoic acids via the Friedel–Crafts type acylation

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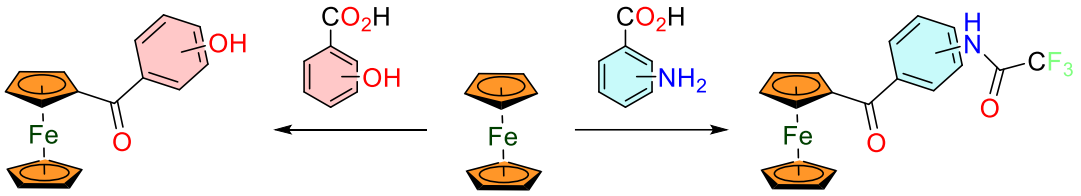
Ferrocene is an organometallic compound that has attracted continuous interest in both organic and inorganic chemistry for almost fifty years. Its stability, reactivity, and unique electrochemical properties make it an important compound for research. One of its key features is the ability to modify its redox potential by introducing electron-donating or electron-withdrawing substituents. Because of these properties, ferrocene is widely used as a building block for electrochemical probes, biomolecules, and new functional materials.[1] Developing new methods for its functionalization therefore remains an important research goal.

This report summarizes our studies on the synthesis of new ferrocene derivatives through Friedel–Crafts-type acylation. Using a method developed in our group that employs in situ protected aliphatic amino acids as acylating agents [2], we obtained a series of ferrocenyl ketones derived from ferrocene and amino- or hydroxybenzoic acids (Scheme 1). These compounds were further modified to produce new redox-active, water-soluble ferrocene derivatives. Such compounds may find potential applications, for example, in redox-flow batteries, which currently represent one of the most promising technologies for energy storage.[3]



Scheme 1. Functionalization of ferrocene with amino and hydroxybenzoic acids.

Acknowledgement
The research was funded by the University of Lodz Student Research Grant – 2025 Edition.

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P-109

Proton-Coupled Electron Transfer Processes in the incorporation of primary alkyl radicals

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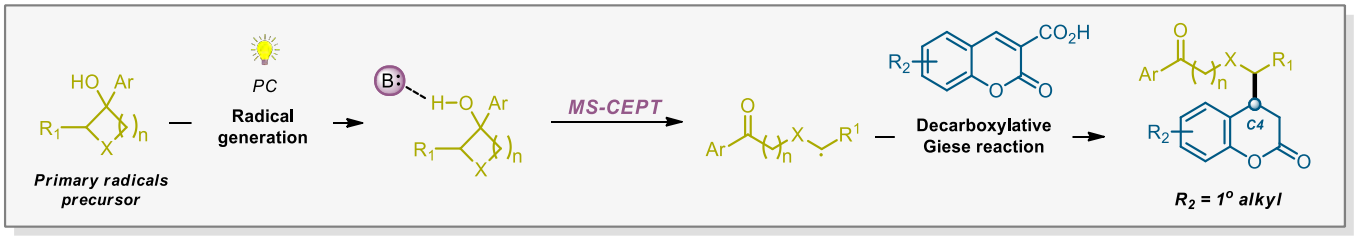
Chroman-2-ones and their derivatives have attracted considerable scientific attention due to their wide range of biological activities, spanning from basic antibacterial effects to potent anticancer properties. Numerous studies have described photocatalytic strategies for constructing molecules based on the chroman-2-one framework; however, most of these methods focus on functionalization at both the C-3 and C-4 positions.[1] In contrast, achieving selective modification solely at the C-4 position while retaining a free C-3 site remains a challenging synthetic task. In our earlier work, we introduced two photocatalytic decarboxylative methods that enabled selective substitution at the C-4 position under reductive conditions, leaving the C-3 position unaltered.[2,3] These protocols utilize a decarboxylative mechanism, where the carboxyl group at C-3 acts as a temporary activating group that can be removed without additional steps. While these methods were the first general approaches for such scaffolds, their applicability was limited to aryl and secondary or tertiary alkyl radicals, as they were incompatible with primary radicals. To address this limitation, we adopted a proton-coupled electron transfer (PCET) approach. This strategy involves the formation of a hydrogen bond between the substrate and a suitable Brønsted acid or base before the single electron transfer step (Scheme 1). Drawing inspiration from previous work, we applied this concept under mild photocatalytic multi-site concerted electron–proton transfer (MS-CEPT) conditions. This methodology provides a solution to two persistent challenges: introducing primary alkyl groups into coumarin frameworks and developing a general route to C-4-substituted chroman-2-ones with an unmodified C-3 position.



Scheme 1. Synthesis of C4-substituted chroman-2-ones

Acknowledgement

The presented research is part of a project funded under the NCN Preludium program (project no. 2023/49/N/ST5/03396).

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P-110

Design and Synthesis of π-Conjugated Polycyclic Benzotriazinyl Radicals

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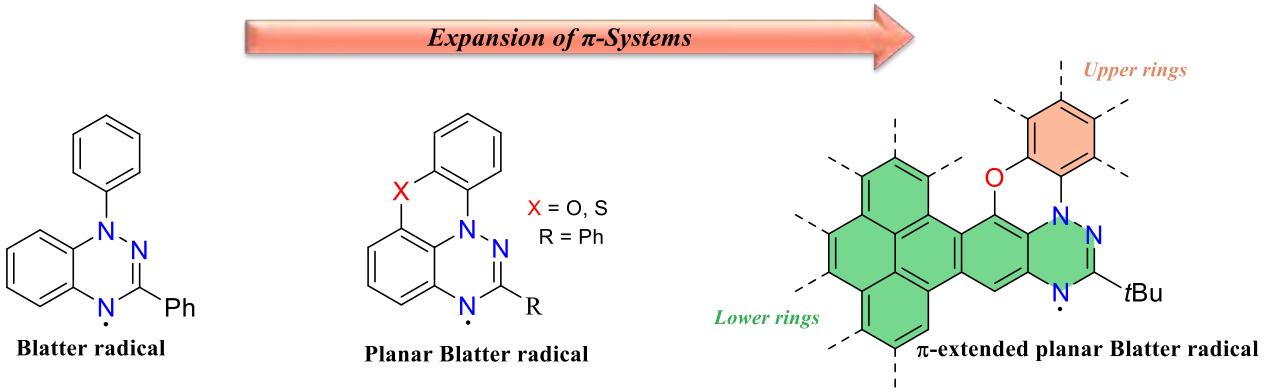
The Blatter radical and its planar derivatives (Scheme 1) [1, 2] are key structural motifs in prototypical paramagnetic materials. They exhibit many interesting properties, such as broad absorption in the visible range, low excitation energies, a narrow electrochemical window, and paramagnetic behaviour. Moreover, they show remarkable stability despite their open-shell structure. These properties make benzotriazinyl radicals potentially useful in molecular electronics, for example, in semiconductors, energy storage systems, and spintronic devices [3].

Triazinyl radicals owe their stability to π-delocalization of the spin density and the π* character of their singly occupied molecular orbital. Previous research focused on increasing π-delocalization by expanding the upper ring system, which was expected to enhance stability [4]. However, this work revealed that modifications on this side of the molecule have a relatively small effect on spin delocalization. Preliminary DFT calculations indicate that expansion of the lower rings has a greater impact on delocalization. For this purpose, polycyclic aromatic hydrocarbons (PAHs) can be incorporated into the structure of planar benzotriazinyl radicals. PAHs are interesting molecules with tunable optical and electrochemical properties, which are highly valuable in materials science [5].

The goal of this work is to obtain a new class of polycyclic aromatic hydrocarbons containing a benzotriazinyl unit for potential applications in organic electronics and to investigate their magnetic and electronic properties. The poster will present the synthetic route toward the desired materials as well as computational studies.



Scheme 1. Systematic expansion of π-systems in benzo[*e*][1,2,4]triazinyl radicals.

Acknowledgement

This work was funded by the NCN, under the SONATA grant no. 2022/47/D/ST4/03462. Computational resources were provided by the PLGrid infrastructure, grant no. PLG/2025/018596.

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P-111

Phosphonate Analogs of Sulforaphane containing isoselenocyanate moiety

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Isothiocyanates (ITCs) are an important class of biologically active heterocumulenes that have been the focus of research for many years. They are found in cruciferous vegetables (including Brussels sprouts, radishes, broccoli, or horseradish) and are formed as a result of a reaction of glucosinolates with myrosinases. Despite, the that ITCs are mainly used in organic synthesis as substrates for the synthesis of heterocyclic compounds, their anti-cancer, and anti-bacterial properties have made them a popular target of many research groups.[1]

Attempts, to synthesize a series of the unknown, phosphonate sulforaphane analogs bearing isoselenocyanate moiety, in place of the isothiocyanate group, will be presented.

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P-112

New chiral P=N derivatives of phosphaadamantane (PTA) – synthesis and application

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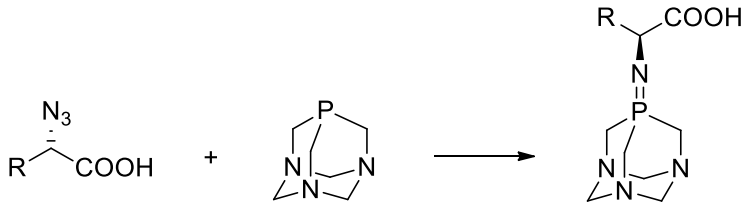
In spite of many attempts made by a high number of scientists to find chiral catalysts able to control the stereoselectivity of various reactions, the search for new reaction space continues. One of the interesting new concept is the Asymmetric Counteranion-directed Catalysis (ACDC). ACDC is a type of enantioselective catalysis, where the chirality, which is responsible for enantioselectivity of the chemical transformation is located in a chiral anion, which is accompanied by an achiral cationic species.

In an earlier review, Mahlau and List defined and discussed the application of this methodology.[1] They referred to their preparation of a large number of potential catalysts simply by combining secondary amines with binol-derived phosphoric acids. In most cases very large, complicated structures of the chiral anions were developed, basing mainly on the axially chiral binaphthyl moiety. Since their syntheses require time-consuming and sophisticated procedures leading to a large amount of waste, we have decided to check whether the use of simple, easily available and relatively cheap, compounds would fulfill the requirements to be the ACDC catalysts. As a basis, we have chosen analogues of PTA, decorated with enantiomeric aminoacid residues which will serve as a source of chiral anions.

To achieve this we initially synthesized these analogues via the Staudinger–type reaction between phosphine PTA and the corresponding azides derived from various aminoacids (Scheme 1). The resulting phosphimines were first examined as organocatalysts in selected asymmetric reactions.



Scheme 1. Synthesis of PTA-P-imines.

The results will be discussed.

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P-113

Environmentally benign, one-pot chemoenzymatic process for the synthesis of alkenes in aqueous medium.

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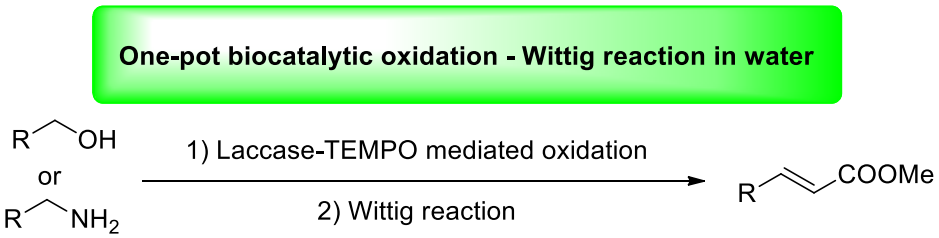
In this communication we present a one-pot, two step, environmentally benign, chemoenzymatic process for the synthesis of alkenes from alcohols or amines. The whole process is conducted in aqueous medium. It is based on application of laccase mediated alcohol or amine oxidation in presence of TEMPO as mediator, and subsequent, "on water" Wittig reaction. [1, 2]

The process can be considered as "green" because of the following advantages: a) no need of purification of the intermediate products, b) application of water as green solvent and an enzyme-laccase as natural catalyst c) application of molecular oxygen as final oxidant d) formation of water as a by-product of the oxidation step.



Scheme 1. General reaction scheme.

Acknowledgement
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P-114

Synthesis of selected ^{18}O-labeled sulfinyl derivatives

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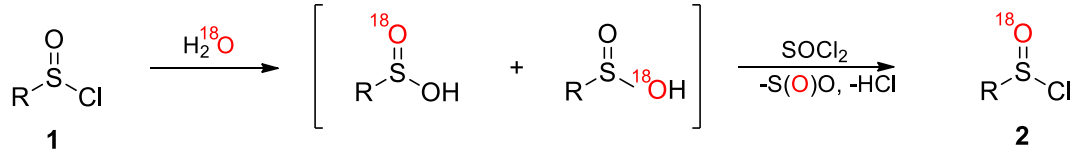
Substrates containing ^{18}O oxygen isotopes adjacent to reactive centers in their structures are excellent model compounds for explaining the mechanisms of the reactions being studied. If such structures are also optically active, this allows for the demonstration of the stereochemical pathway [1].

Sulfinyl chlorides are precursors to sulfinyl compounds. They are obtained by classical methods by chlorination of sulfenyl substrates with chlorine in the presence of acetic anhydride as an oxygen donor [2]. Isotopically ^{18}O-labeled sulfinyl chloride was obtained by chlorination of disulfide with thionyl chloride in the presence of isotopically ^{18}O-labeled hexamethyldisiloxane as an ^{18}O oxygen donor and chloride ion acceptor. This method is effective only for the methyl derivative.[3]

Sulfinyl chlorides labeled with the oxygen isotope ^{18}O were obtained according to the equation below.

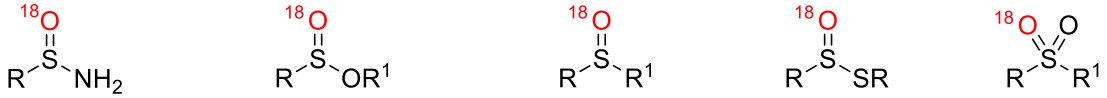


1 **2**

R= *i*-Pr, *t*-Bu

Scheme 1.

They are substrates in the synthesis of isotopically labeled with oxygen ^{18}O: sulfinamides **3**, sulfinates **4**, sulfoxides **5**, thiosulfinates **6**, and sulfones **7**.



3 **4** **5** **6** **7**

3: R= *t*-Bu **4**: R= *i*-Pr, R^1= Np **5**, **6**, **7**: R=alkyl, R^1= aryl

Scheme 2.

Two example of the use of sulfinyl derivatives labeled with oxygen isotope ^{18}O will be presented:

1. Racemic *t*-butanesulfinamide **3** in the reaction with 2-chloro-1,3,2-oxathiaphospholane **8**
2. Optically active *O*-neopentyl-*i*-propanesulfinate **4** in the synthesis and hydrolysis of chiral dialkoxysulfonium salt (metoxy-neopentoxy-*i*-propanesulfonium trifluorometenesulfonate) **9** [4].

8 **9**

Scheme 3.

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P-115

Quality Assessment of greener APIs: Spectral and Thermal Analysis of Antipoxviral Drug Tecovirimat Synthesized using environmentally-friendly approach

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Orthopoxviruses are a group of viruses responsible for highly contagious and deadly diseases such as smallpox and monkeypox [1], which sharp increase in the last decade has been observed in Africa in Europe. To prevent their spread all over the world [2], the development of potent antiviral drugs to combat Orthopoxvirus infection is of paramount importance.

A response to the Orthopoxvirus threat is the antiviral drug tecovirimat (SIGA Technologies), which in 2018 has been approved by the Food and Drug Administration and European Medicines Agency for the treatment of smallpox and monkeypox infections.

Currently, intensive efforts are being directed toward optimizing the synthesis of tecovirimat to ensure broader accessibility [3,4]. In this context, we developed a fast and sustainable synthesis of tecovirimat using environmentally friendly methods, specifically by reducing the usage of organic solvents and avoiding high temperature conditions.

Herein, we present the identification and quality assessment of tecovirimat obtained by green chemistry approach and compare them to those of tecovirimat synthesized using traditional in-solution method. For this purpose, modern analytical techniques such as 2D NMR, qNMR and Differential Scanning Calorimetry (DSC) was used to confirm the structure, purity and the presence of organic solvent residues. Results indicate that our developed sustainable protocol enables to obtain the proper isomer of tecovirimat in high quality.

The study supports the advantages to develop safer, more efficient, and environmentally-friendly approach for the synthesis of antiviral agent against Orthopoxvirus infections.

Acknowledgements
The project is financially supported by the Polish Ministry of Science and Higher Education under the program entitled “Studenckie koła naukowe tworzą innowacje” (grant number SKN/SP/602501/2024).

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P-116

Solution- and solid-state fluorescence of *N*-ethoxycarbonylthiophene imine-fused polycyclic arenes

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Heterocycle-fused polycyclic arenes have attracted increasing interest over the last decades as materials or material precursors for optoelectronic and photovoltaic applications. [1-3]

We have reported the synthesis of a series of polycyclic aromatic thioamide S-oxides containing an ester function at nitrogen and their unexpected cyclization under strongly acidic conditions to extended thiophene imine-fused π-systems. Most of the synthesized compounds, featuring (*N*-ethoxycarbonyl)-2-iminothiophene-fused polycyclic arene moieties, are fluorescent both in solution and in the solid state. [4]

Herein we present the results of a more comprehensive study of the photophysical properties of a series of such compounds **1**-**6** (Figure 1). The study encompasses investigations into solvent effects, time-resolved solution fluorescence, solid-state fluorescence and (TD-)DFT calculations.

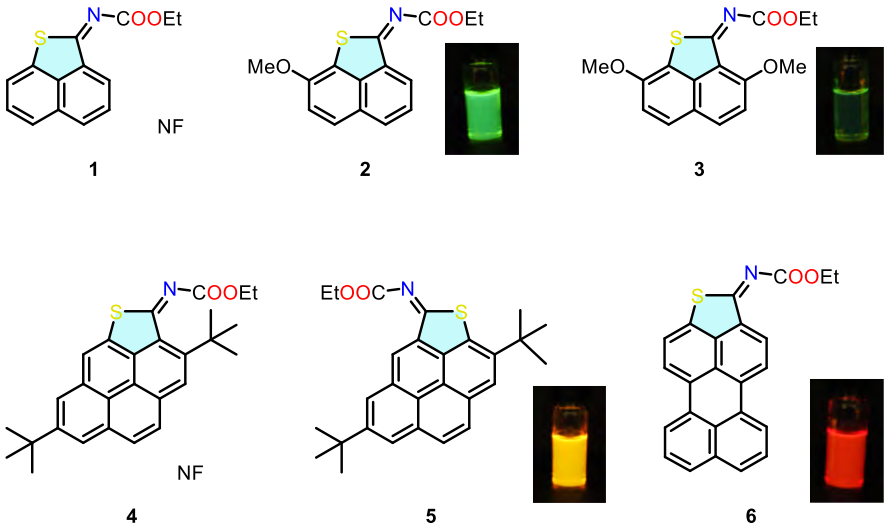

Figure 1. Structure of the heterocycles studied. The photographs depict the fluorescence of their CH_2Cl_2 solutions under UV light illumination. Compounds **1** and **4** exhibit ΦF < 0.01 and are considered non-fluorescent (NF).

Acknowledgement

This research was funded by the University of Lodz, grant number 10/WNnS/2023

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P-117

Novel Pyrene derivatives: synthesis and photophysical properties

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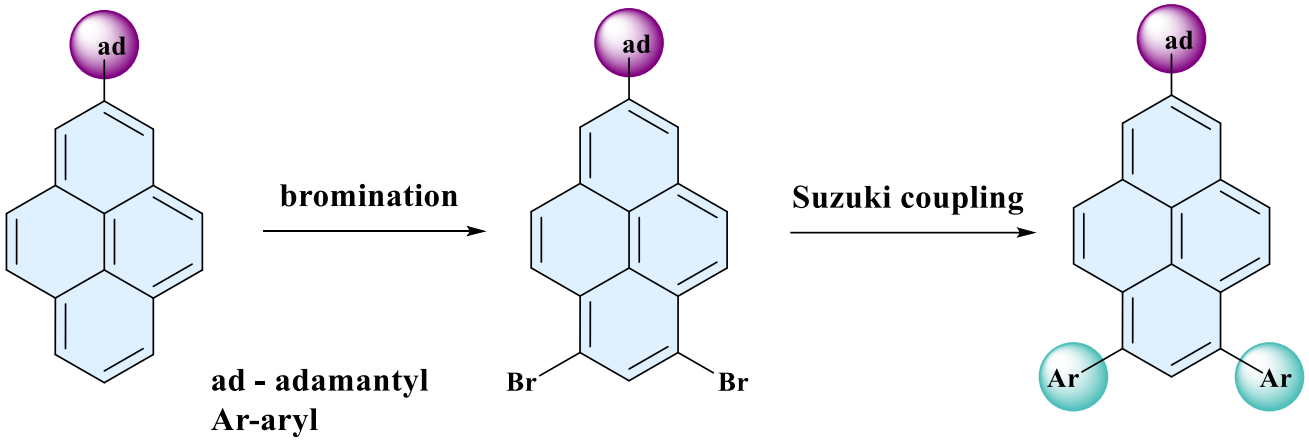
Fluorescent compounds play a key role in many areas of science and technology. They have found applications as biomolecular markers, in the production of reflective road paints, and in the fabrication of organic light-emitting diodes (OLEDs). Among them, pyrene and its derivatives are particularly useful due to their remarkable photophysical properties, such as high fluorescence quantum yields, long fluorescence lifetimes, and excellent thermal and photochemical stability. Moreover, the emissive properties of pyrene derivatives can be finely tuned through various chemical transformations, including electrophilic substitution, oxidation reactions, and transition-metal-catalyzed processes. Of special interest are the "Y"-shaped pyrene derivatives, which have found applications in optoelectronic devices.[1] One of the methods enabling the synthesis of such fluorophores is the Suzuki-Miyaura coupling of halogenopyrenes with appropriate boronic acids.

Recently, we have reported a new class of fluorophores, including 2-adamantylpyrene.[2] In this communication, we present further modifications of this compound leading to "Y"-type emitters with an extended π-electron system (**Scheme 1**).

Additionally, we discuss the results of the photophysical studies performed for the obtained 7-adamantyl-1,3-diarylpyrenes.



Scheme 1. Synthesis of novel pyrene derivatives.

Acknowledgement
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P-118

New methods of labelling biomolecules with fluorescent and organometallic labels and their spectroscopic detection

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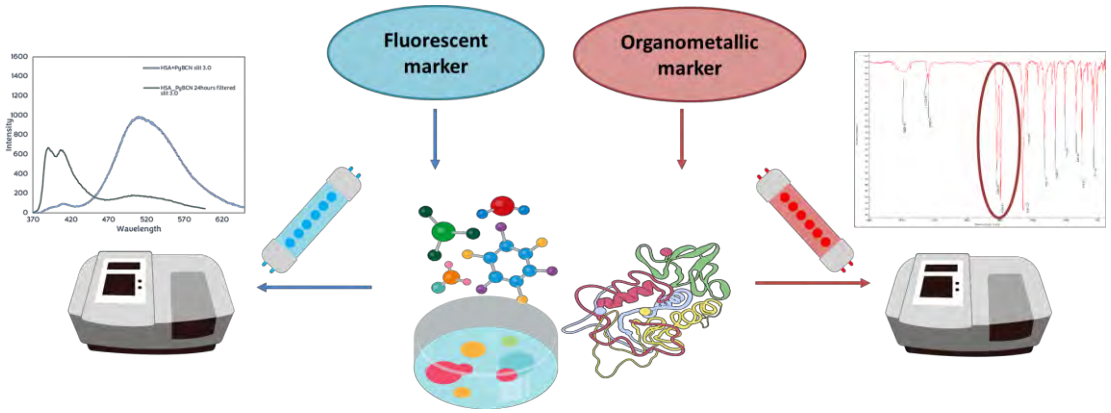
The ability to selectively form chemical bonds in a biological environment has long been a target of research for chemists interested in the modifications biological material. Modifications such as stapling or the use of bioorthogonal chemistry allow scientists to monitor processes occurring in living cells or to track the progress of therapy.

Bioorganometallic chemistry has developed rapidly and evolved along with the medicinal chemistry of inorganic, metal-based drugs. The specific properties of organometallic complexes enable their use in various branches of biology and medicine and they are used as anticancer, antibacterial, and antimalarial agents.[1] Fluorescent compounds are widely used as an invaluable tool for diagnostics, medical biology and biochemistry. The presence of a fluorescent or metal carbonyl moiety in biomolecule structure enables easy detection using spectroscopic methods. Properly designed synthetic molecules introduced into cells can be used as sensors or markers, but also constitute an element of targeted therapy (e.g. therapeutic peptides and proteins).[2]

In this communication, we would like to present a strategy for introducing fluorescent markers (containing a pyrene fluorophore) and metallocarbonyl markers ($CpFe(CO)_2(\eta^1$-imidato) derivatives) into biomolecules. Furthermore, we describe studies of markers' photophysical properties with spectroscopic methods. The ease of detection enables the use of obtained labels for imaging biochemical processes occurring in living cells.



Scheme 1. Detecting modified biomolecules with fluorescent and IR spectroscopy.

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P-119

Aggregation of Small Molecules: Computational Warning for Drug Designers

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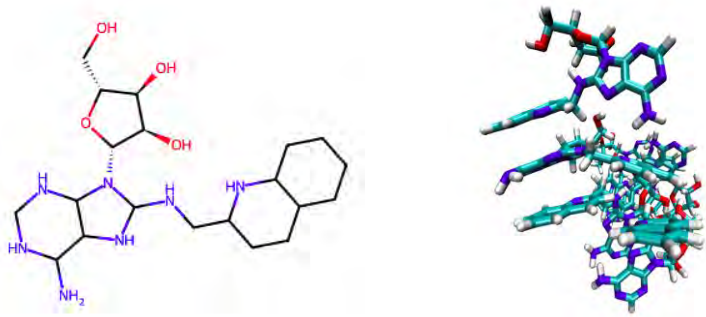
Medical treatment of human diseases often utilizes small molecules which can penetrate the cell and bind to a specific protein, influencing its activity. Often ligand binding is facilitated by various types of interactions, including hydrogen bonds, aromatic stacking or hydrophobic attraction. Hence, the potential drug candidates are usually modified with many groups capable to form weak contacts with a target.

Here, we take a closer look at an effective inhibitor of Heat-Shock Protein (Hsp70) family, VER-15508, and its derivatives, such as S10, which have been proved experimentally as an efficient competitors of ADP/ATP molecules blocking the ATP-dependent chaperon activity of Hsp70s [1]. Looking into the molecular mechanism, the computational studies reveal that the binding process competes with the ligand self-association. The abundance of aromatic groups enables the intermolecular π-stacking within VER-15508 or S10 molecules. Those π-conjugated aggregates can still bind to the protein at various places on the surface, however, those surface binding sites are much less specific and they are potentially indistinguishable between cellular macromolecules. Such aggregation might be very dangerous, eventually leading to various side effects in human body.

The computational results give directions for further experimental tests and validation. In this presentation we want to present the problem within the organic chemistry community and to discuss its significance in the view of validation using experimental methods which can be considered to optimize further drug design procedure.



Scheme 1. Structure of a the S10 molecule in monomeric state (left) and its aggregate (right).

Acknowledgement

The work is supported by the National Science Centre, Poland, under research project NCN OPUS-25 (2023/49/B/ST4/03288)

Computational resources were provided by Poland's high-performance Infrastructure PLGrid ACK Cyfronet within computational grant no plgcbmmchb01.

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P-120

Application of Supramolecular Asymmetric Catalysis in the Dearomative Michael Addition of 5-substituted-2(3*H*)-furanones to nitro-group-activated benzofurans

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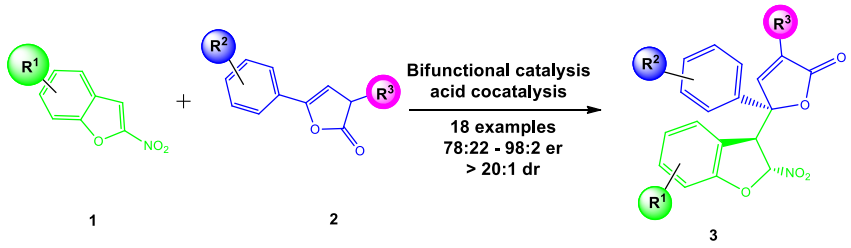
The synthesis of oxygen-containing heterocycles, such as furan, benzofuran, and γ-lactones, is of significant importance due to their broad applications in medicinal chemistry.[1,2] In this context, supramolecular catalysis has emerged as a promising alternative to classical asymmetric catalysis. The success of such an approach relies on the self-assembly of the catalyst and the reaction transition state under the reaction conditions.[3]

In this work, an enantioselective, dearomative Michael addition of nitro-activated benzofurans was developed. The approach involved the addition of 5-substituted 2(3H)-furanones to electronically activated heteroarenes, yielding 2,3-dihydrobenzofuran derivatives (**Scheme 1**.).

The research focused on the optimization of reaction conditions, which enabled the attainment of high yields and selectivity. The developed method exhibits a broad substrate scope, and DFT calculations confirmed the crucial role of weak intermolecular interactions, which facilitate the spontaneous organization of the system and govern the stereoselectivity of the reaction.



Scheme 1. Synthetic strategy toward 2,3-dihydrobenzofuran derivatives

Acknowledgement

This project was financed by the Local Government of the Lodzkie Region (grant number: 54/OPP/ 2023).

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P-121

Antimicrobial activity of copper(II) and zinc(II) complexes of fluoroquinolone antibiotic

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N-heterocyclic compounds, due to their unique structure, are often used to obtain metal complexes (1). Literature data indicate, that metal based complexes of already known drugs show comparable antimicrobial activity to parent drug and additionally can contribute to overcoming the antimicrobial resistance (2,3). In the presented studies the copper(II) and zinc(II) complexes of 1-cyclopropyl-6-fluoro-7-((1S,4S)-3-methyl-3,6-diazabicyclo[2.2.1]heptan-6-yl)-4-oxoquinoline-3-carboxylic acid, crucial fluoroquinolone antibiotic, were synthetized. The complexes were characterized by ^{1}H NMR, ^{19}F NMR and IR spectroscopy, ESI-MS spectrometry and elemental analysis. The fluoroquinolone acts as bidentate ligand coordinated through the oxygen atom of the deprotonated carboxylic group and the carbonyl oxygen atom of pyridone part of ligand, forming a stable six-membered ring. Antimicrobial activity of described compounds were determined against selected Gram-positive and Gram-negative bacteria in accordance with the CLSI standards. The obtained results indicate that synthetized metal base complexes effectively inhibit the growth of teste microorganisms and have the potential to be used as antibacterial agents.

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P-122

Iodinated Heptamethine Cyanine Dyes as Near-Infrared Photosensitizers for Antimicrobial Photodynamic Therapy

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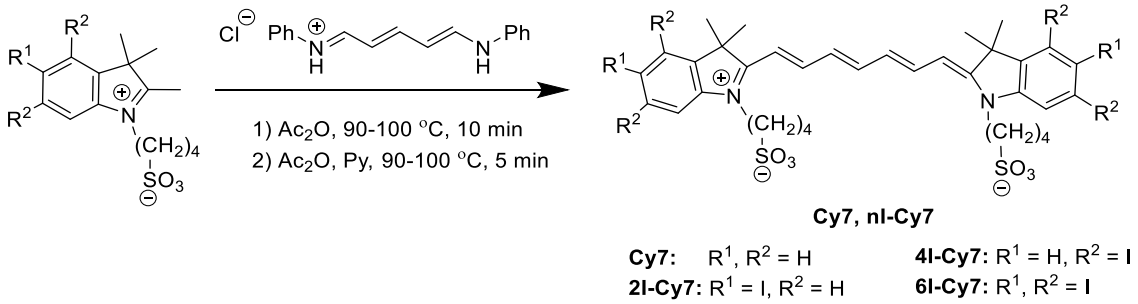
The rapid spread of antibiotic-resistant bacteria necessitates new therapeutic strategies such as antimicrobial photodynamic therapy (APDT), which employs light-activated organic photosensitizers (PS) to generate cytotoxic species. While porphyrin-based PS dominate clinical use, they are inefficient in the therapeutic near-infrared (NIR) region. In contrast, cyanine dyes strongly absorb light in the NIR but typically exhibit low phototoxicity. Recent studies have shown that introduction of iodine atoms into cyanine chromophores significantly enhances their photodynamic activity.

In this work, we synthesized a series of heptamethine cyanine dyes **nI-Cy7** with sulfonic solubilizing groups and varying numbers of iodine atoms, and evaluated the effect of the substituents on photodynamic inactivation of Gram-positive (*S. aureus*) and Gram-negative (*E. coli*) bacteria. Spectral and photophysical properties of **nI-Cy7** as well as their photodynamic efficacy were examined in comparison with non-iodinated **Cy7** and non-sulfonated commercial dye **HITC**.

The **nI-Cy7** dyes were synthesized according to Scheme 1. They absorb and emit in the near-IR region (740–796 nm) with high extinction coefficients (210,000–260,000 M^{-1} cm^{-1}). Aggregation was not observed in methanol at concentrations up to 5 μM. The quantum yields of singlet oxygen generation (Φ_Δ) increase with the number of iodine atoms in the order: **Cy7** ~ **HITC** < **2I-Cy7** ≈ **4I-Cy7** < **6I-Cy7**.



Scheme 1. Synthesis of iodinated heptamethine cyanine dyes.

All dyes exhibited negligible dark cytotoxicity against both *S. aureus* and *E. coli* at concentrations up to 100 μM. The tetraiodinated **4I-Cy7** showed pronounced phototoxicity toward Gram-positive (at 50 μM) and Gram-negative (at 100 μM) bacteria, whereas the diiodinated analogue **2I-Cy7** has reduced activity against *S. aureus* and no activity against *E. coli*, likely due to its higher solubility which diminishes effective interaction with bacterial cells. Notably, there was no significant difference in activity between tetra- and hexaiodinated derivatives (**4I-Cy7** and **6I-Cy7**) at either light dose of 50 J/cm² or 100 J/cm².

Overall, this study illustrates effective molecular design and structure-property insights enabling strong phototoxic performance of the next-generation polymethine photosensitizers.

Acknowledgement
This research was supported by National Academy of Sciences of Ukraine (project No. 0125U000603).

P-123

Sterically Controlled Template-Assisted Macrocyclization of Hemisquaraine Rotaxanes: Synthesis, Characterization, and DFT Calculations

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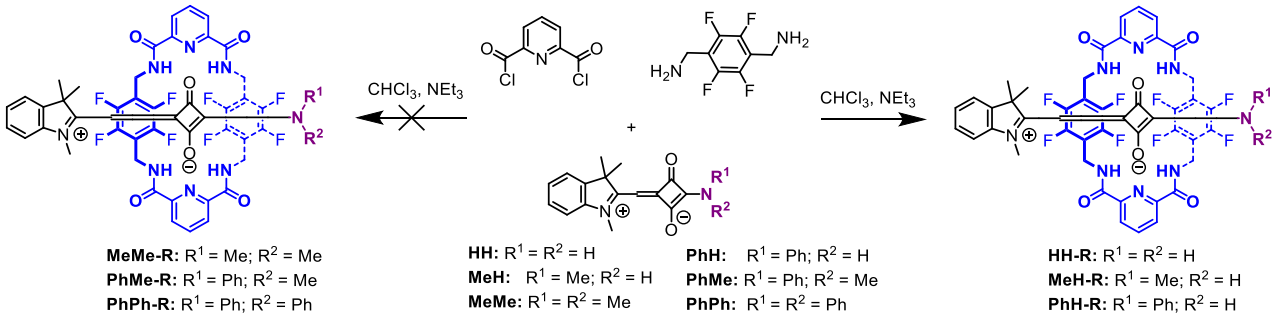
Rotaxane-type encapsulation of organic chromophores offers an effective means to tune fluorescence, enhance photostability, and protect reactive molecular cores. Among these systems, squaraine-based rotaxanes are particularly promising because squaraine dyes exhibit intense and narrow absorption bands, high molar absorptivity, and strong fluorescence across the visible–NIR range. Yet, their susceptibility to nucleophilic attack, aggregation-induced quenching, and limited photostability still restrict broader use. Encapsulation within supramolecular hosts such as tetralactam macrocycles helps overcome these drawbacks.

Recently, we reported the synthesis of a series of hemisquaraine dyes that display pronounced spectral shifts and fluorescence modulation in response to environmental changes [1]. Building on these findings, in this work we investigated their integration into mechanically interlocked architectures through an oxocyclobutenolate template-assisted macrocyclization (Scheme 1).



Scheme 1. Synthesis of hemisquaraine rotaxanes.

Hemisquaraine dyes with primary (**HH**) and secondary (**MeH**, **PhH**) amino groups successfully formed rotaxanes, whereas bulky tertiary derivatives (**MeMe**, **PhMe**, **PhPh**) did not. Encapsulation resulted in red-shifted absorption and emission bands in $CHCl_3$ and up to 7.9-fold higher fluorescence quantum yields, indicating enhanced rigidity and reduced non-radiative decay. DFT calculations confirmed the thermodynamic favorability of all rotaxanes, while reaction-path simulations showed that bulky tertiary substituents introduce longer approach distances and kinetic barriers (>7 kcal/mol) that prevent macrocycle closure. These theoretical results corroborate the experimental data and elucidate how steric hindrance governs the outcome of template-assisted macrocyclization.

Acknowledgement

This work was supported by the National Research Foundation of Ukraine, project No. 2023.05/0003 "Development of new materials based on supramolecular systems for biomedical and veterinary applications".

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P-124

PROTAC-Based Modulation of GGTase-II: A Novel Strategy for Targeting Protein Prenylation

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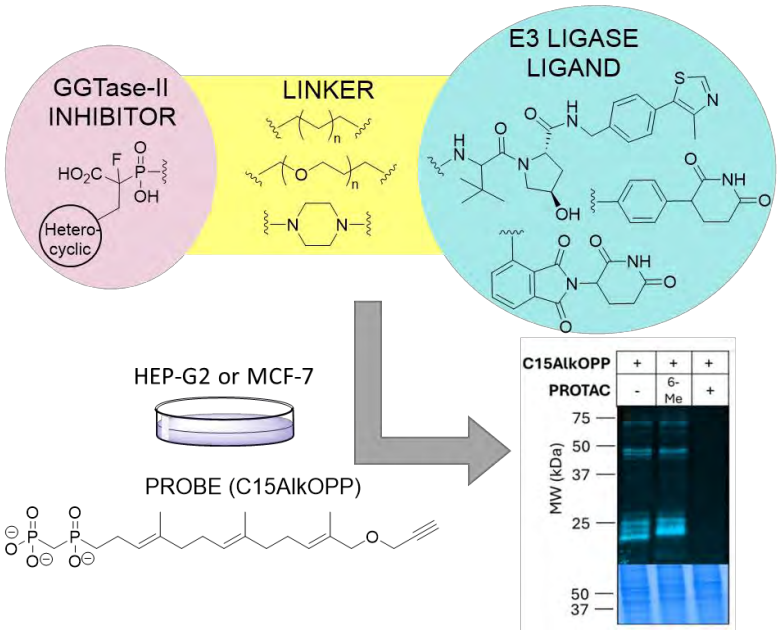
Rab geranylgeranyltransferase (GGTase-II, RGGT) catalyzes the post-translational modification of eukaryotic Rab GTPases (Rab proteins). Abnormal activity of various prenylated Rab proteins has been implicated in several diseases, including cancer, neurodegenerative disorders, and infections. Therefore, modulators of GGTase-II activity are considered a promising platform for the development of therapeutic agents and tools for studying Rab-mediated pathologies [1].

In this study, we designed a novel class of GGTase-II modulators based on the PROTAC strategy, which involves recruiting the cellular proteasome to degrade the target protein. Over 35 compounds were synthesized, each combining selected GGTase-II inhibitor with different E3 ligase ligands, through diverse linkers. The biological activity of all new compounds was evaluated *in vitro* using an isoprenoid diphosphate probe (C15AlkOPP, Scheme 1) [2]. Two compounds significantly reduced the prenylation of various proteins. The identities of the affected proteins will be determined through proteomic studies.



Scheme 1.

Acknowledgement

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P-125

Synthesis, crystal structure and anticancer activity of a novel copper(II) complexes with a coumarin derivatives containing a histamine and pyridine moiety

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Coumarins, derivatives are a large class of oxygen-bearing heterocyclic compounds, ubiquitously present in plants as secondary metabolites. [1] Coumarins can be substituted at various sites of their base structure and scaffold serves as the basis for their numerous physiological activities e.i.: anticoagulant, anticancer, antimicrobial, anti-inflamatory and neuroprotective activities. [2]

Their metal-chelating ability facilitates the formation of coordination complexes that often display enhanced biological efficacy. [3] Among transition metals, copper(II) plays a key role in numerous enzymatic, and has attracted considerable interest for its potential antitumor applications. [4]

Chromane-2,4-dione derivatives, structurally related to coumarins, are versatile scaffolds in medicinal chemistry due to their synthetic flexibility and capacity to interact with a range of biological targets. [5] Coumarin-based molecules conjugated with heterocyclic moieties containing nitrogen and oxygen/sulfur donor chelating sites have shown significant pharmacological activities, including anticancer, antibacterial, and anti-inflammatory effects. [2]

In this study, we synthesized a series of novel coumarin (chromane-2,4-dione) derivatives bearing histamine and pyridine substituents, along with their corresponding copper(II) complexes. The primary objective was to synthesize and characterize these new coordination compounds and to assess their potential anticancer activity. The obtained results highlight the relevance of metal coordination in modulating the biological activity of coumarin derivatives and support further exploration of such complexes as promising candidates for anticancer drug development.

Acknowledgement

This work was supported by Grant No. 503/3-066-02/503-31-001 from the Medical University of Lodz, Poland.

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P-126

Design, Synthesis, and Biological Evaluation of Novel 1,2,4-Triazole-Based Schiff Bases with Anticancer Activity Against Colorectal Cancer Cells

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Colorectal cancer (CRC) remains one of the most prevalent malignancies and a leading cause of cancer-related mortality worldwide [1]. Despite advances in diagnostics and therapeutic strategies, treatment outcomes for advanced CRC are still unsatisfactory, primarily due to the development of drug resistance, tumor heterogeneity, and adverse effects of conventional therapies [2]. These challenges highlight the need for novel chemotherapeutic agents with improved efficacy and selectivity [3].

Nitrogen-containing heterocycles, particularly triazoles, represent a valuable class of pharmacophores in modern drug design owing to their chemical stability, favorable pharmacokinetic properties, and broad biological activity. In recent years, 1,2,4-triazole derivatives have demonstrated promising anticancer potential, including activity against colorectal cancer cell lines. Building on these findings, we designed and synthesized a series of new Schiff base derivatives derived from 4-amino-5-(3-fluorophenyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione and 4-amino-5-(3-methoxyphenyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione.

The obtained compounds were subjected to preliminary *in vitro* screening against DLD-1 and HT-29 CRC cell lines. Three derivatives (RO1, RO4, and RO21) exhibited significant cytotoxic activity, prompting further biological evaluation using a zebrafish xenograft model with human CRC cells. The results confirm the potential of triazole-based Schiff bases as promising scaffolds for the development of new antitumor agents targeting colorectal cancer.

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P-127

Conjugate additions of selected nucleophiles to trifluoromethylated Michael acceptors

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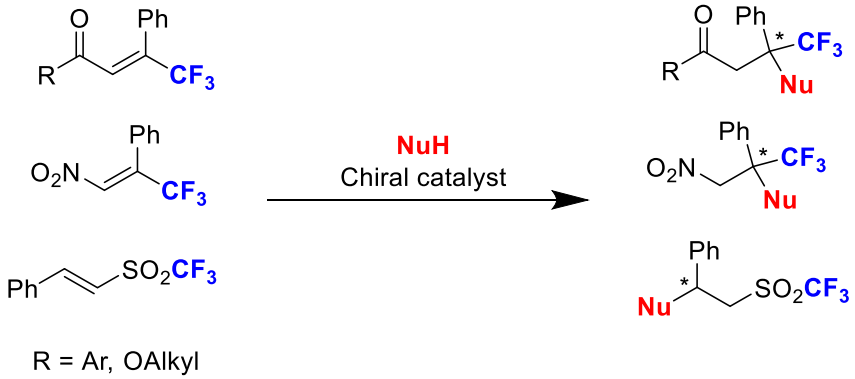
The trifluoromethyl group significantly influences the properties of organic compounds and has become an important structural motif of many drugs [1] and compounds of other applications. The increasing *importance of organic molecules containing trifluoromethyl group in* medicinal chemistry,[2] agrochemistry,[3] and material sciences[4] *stimulate the development* of new synthetic methods in this area. In particular, catalytic reactions affording enantiomerically enriched *compounds* with *quaternary* stereogenic centers *containing* trifluoromethyl group are still challenging for organic synthetic chemists.[5]

In our research, we focused on Michael addition reactions to *β*-trifluoromethyl *β*,*β*-disubstituted *α*,*β*-unsaturated carbonyl compounds (mainly ketones and esters), *β*-CF_3 nitrostyrenes and *β*-aryl *α*,*β*-unsaturated triflones (Scheme 1). Preliminary studies on the addition of selected C-nucleophiles (e.g. indoles, 2-aminofuran derivative, anthrone, nitromethane, cyanide), oxygen (alcohols, oximes) and phosphorus (H-phosphonates) nucleophiles to the mentioned acceptors, in both racemic and enantioselective variants, were conducted, leading to novel trifluoromethyl compounds. In our studies, organocatalysts as well as transition metal complexes were applied.



Scheme 1

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P-128

Synthesis and reactivity of Electron-rich 10-vertex Carborane Clusters

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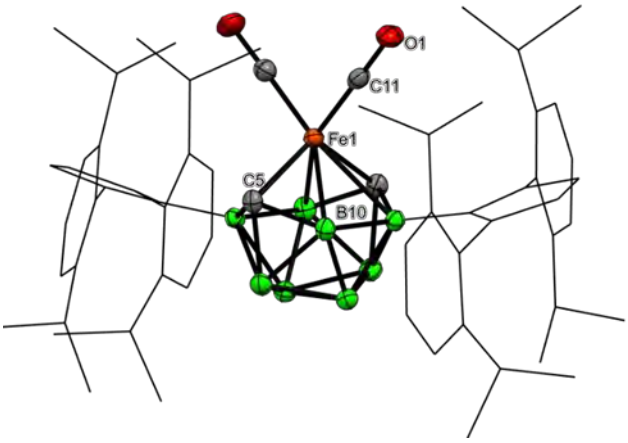
The chemistry of heteroborane clusters is a part of modern inorganic chemistry. They are based on electron-deficient two-electron multicentred bonds with the overall charge being neutral or negative. In 2021, we described the first thermally robust cationic carboranes supported by bulky N-heterocyclic carbenes, which significantly change the electron density within the cluster framework, and these compounds act as bases.1 In this work, the reactivity of 10-vertex closo-dicarbaboranes with different N-heterocyclic and mesoionic carbenes will be discussed as along with their structural rearrangements to thermodynamically stable products. The reactivity of such electron-rich clusters with various acids, transition metal complexes, and main group compounds will be presented as well.



Scheme 1. The molecular structure of [closo-(2,6-NHCDipp-1,10-C2B8H8)Fe(CO)2].

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No.	Presenting Author	Title of poster
P-001	Demchuk Oleh	*The use of Huisgen 1,3-dipolar cycloaddition in the synthesis of new conjugates with potential dual anticancer and antimicrobial properties*
P-002	Nycz Jacek	*Synthesis, Spectroscopy, and Computational Studies of Unique p-Conjugated N-Alkylated Phenazinium Salts and Their Precursors*
P-003	Demidovich Victor	*Synthesis and study of new xanthene dyes*
P-004	Młynarkiewicz Oliwia	*Synthesis and conformational studies of 1,10-N,N'-bis-(β-D-ureidolactosyl)-4,7,13-trioxa-1,10-diazacyclopentadecane*
P-005	Michałek Emilia	*Theoretical investigation of the newly synthesized lactose cryptand.*
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P-008	Cieśliński Adam	*NHC-Catalyzed Dearomative Higher-Order Cycloaddition: Access to Dihydropyrimidin-4(1H)-one Frameworks*
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P-012	Sowa Sylwia	*A new route to ethynyl(2-ethynylphenyl)phosphine oxides*
P-013	Sowa Sylwia	*Nucleophilic substitution vs ring opening – dual reactivity of benzo[b]phosphol-3-yl triflates towards alkyl Grignard reagents*
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P-017	Muzychka Oksana	*Synthesis and Structure-Activity Relationship of Pyrazino[1',2':1,5]pyrrolo[2,3-d]pyrimidines as Acetylcholinesterase Inhibitors*
P-018	Kula Karolina	*An example of the synthesis of bis-pyrazole molecular segment based on conjugated nitrodienes: DFT mechanistic study*
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