1ST POLISH-ITALIAN CONFERENCE

ON CHEMISTRY, MATERIALS AND BIOMEDICINE (CMB)

BOOK OF ABSTRACTS

17-19 September 2025
Rome, Italy

1ST POLISH-ITALIAN CONFERENCE

ON CHEMISTRY, MATERIALS AND BIOMEDICINE (CMB)

Rome 2025

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Polish Academy of Sciences – Scientific Centre in Rome
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ABSTRACTS

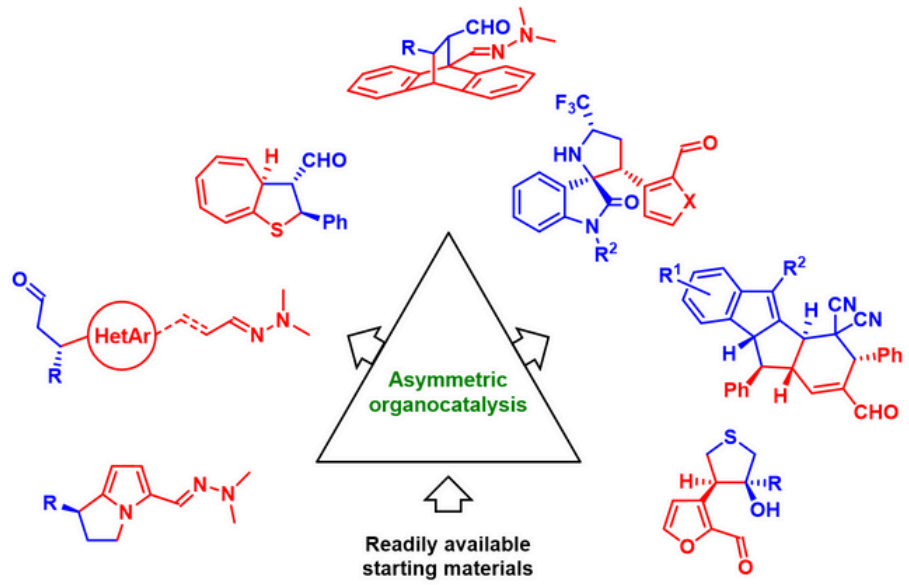
Plenary Lectures

A QUEST FOR CHEMICAL DIVERSITY – ORGANOCATALYTIC CYCLOADDITIONS, HIGHER-ORDER CYCLOADDITIONS AND BEYOND

Łukasz Albrecht
Lodz University of Technology, Institute of Organic Chemistry
Żeromskiego 116, 90-924 Łódź, Poland
email: lukasz.albrecht@p.lodz.pl

The development of enantioselective reactions where prochiral substrates are converted into enantiomerically enriched products in the presence of chiral catalyst are of great importance. Recently, asymmetric organocatalysis, where simple organic molecules are used as catalysts of various enantiodifferentiating reactions, has become a highly useful synthetic tool enabling for the efficient asymmetric induction based on diverse activation modes [1]. Within this research area, the development of novel cycloaddition reactions created new synthetic possibilities. Cycloaddition reactions constitute one of the most usable synthetic methodologies, giving access to various, interesting building blocks. The most popular [4+2] Diels--Alder and 1,3-dipolar cycloadditions are well-recognized, as different variants of these reactions already appeared in literature, including catalytic and asymmetric methodologies. Different approach in the field of cycloaddition reaction focuses on the reactions in which more than 6π take part. These processes are called higher-order cycloadditions, discovered in 70' and being currently an objective of intensive studies [2].

Herein, we report our studies on the development of new organocatalytic cycloadditions, higher-order cycloadditions and other reactions for the synthesis of biologically relevant molecules containing carbo- or heterocyclic scaffolds [3-9]. The devised approaches utilize readily available chiral organocatalysts to control stereochemical reaction outcomes.



This work was realized within grants from National Science Centre: Opus programme (2021/41/B/ST4/03385) and Sheng programme (2018/30/Q/ST5/00466).

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THE INTRIGUING WORLD OF NUCLEOAMINO ACIDS AND NUCLEOPEPTIDES: SYNTHETIC APPROACHES, NUCLEIC ACID BINDING STUDIES AND SELF-ASSEMBLING PROPERTIES

Domenica Musumeci[a,b], **Claudia Riccardi**[a], **Ettore Napolitano**[a], **Chiara Platella**[a], **Daniela Montesarchio**[a], **Moayad Ismail**[c], **Giovanni N. Roviello**[b]

[a] Department of Chemical Sciences, University of Napoli Federico II, 80126 Napoli, Italy
[b] Institute of Biostructures and Bioimaging (IBB) - CNR, 80145 Napoli, Italy
[c] Faculty of Medicine, European University, 76 Guramishvili Ave., 0141 Tbilisi, Georgia
email: domenica.musumeci@unina.it

In the last two decades, we have explored several synthetic conjugates composed of nucleobases inserted on amino acid or peptide backbones (namely nucleoamino acids and nucleopeptides, respectively; **Figure 1**) finding in many cases interesting properties – including binding to specific biomolecular targets (e.g. nucleic acids) or formation of supramolecular network through self-assembly – that make them useful tools in both therapeutic (e.g. antigéne/antisense strategies, drug delivery, etc.) and diagnostic applications as well as in the field of novel nanomaterials development [1-5].

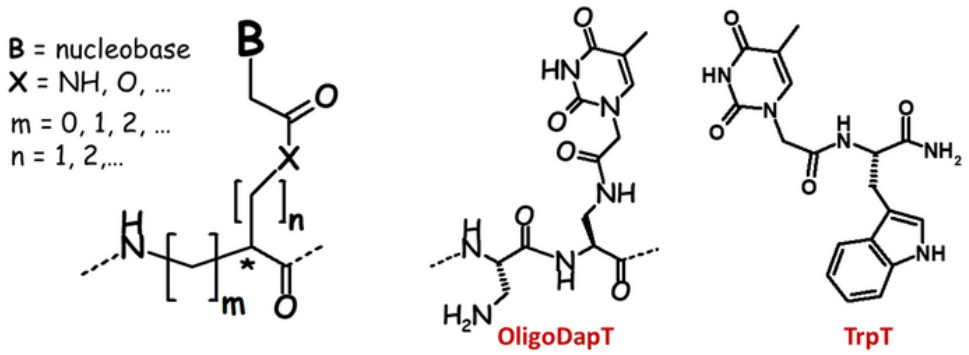

Figure 1. Generic structure of a nucleopeptide composed of a (α-, β-, γ-, δ-)peptide backbone on which nucleobases are anchored through a suitable linker (left). Examples of a homothymine nucleopeptide with a L-diaminopropanoic acid-based backbone (middle) and of a nucleoamino acid based of L-tryptophan (right)

Here, different synthetic approaches for the preparation of nucleoamino acids/nucleopeptides, their characterization, the investigation of their nucleic acid binding ability, by mainly exploiting CD and UV spectroscopy, as well as their self--assembling properties, explored essentially by DLS and fluorescence techniques, will be presented.

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NEW FLUOROPHORES AND NOBLE METAL NANOCLUSTERS AS TWO-PHOTON PROBES FOR AMYLOID IMAGING

Agata Hajda, Patryk Obstarczyk, Anna Pniakowska, Manuela Grelich-Mucha, Joanna Olesiak-Bańska

Institute of Advanced Materials, Wrocław University of Science and Technology
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
email: joanna.olesiak@pwr.edu.pl

Two-photon microscopy (2PM) is a powerful imaging technique that requires specialized fluorescent probes with exceptional properties. Key characteristics for these probes include near-infrared (NIR-I) emission, high fluorescence quantum yields (FQY), and large two-photon absorption cross-sections (σ_2).

Here we present how to tune optical properties of organic fluorophores and noble metal nanoclusters and improve their protein-binding properties for efficient staining and bioimaging of aggregates of misfolded proteins-amyloids.

We created a new O,N,O-coordinated organofluoroboron dye with a donor–acceptor–donor (D–A–D) structure specifically for imaging amyloids [1, 2]. The new dye outperforms similar D–A analogs and the commercial amyloid probe methoxy-X04 in terms of two-photon and fluorescent properties, showed significant advantages. Moreover, we characterized the two-photon properties of the dyes not only in solutions, but also upon binding with amyloids, which is rarely presented in the literature. These results confirm that investigated dye scaffold holds great promise for both, detecting amyloids and advanced two-photon imaging.

To expand the range of available 2P fluorophores, we also investigated atomically precise noble metal nanoclusters (NCs). We investigated silver NCs stabilized with single-stranded DNA (Ag_N-DNAs). These nanoclusters are appealing due to their high FQY in NIR range (up to 73%) and favorable two-photon properties. We characterized four different Ag_N-DNA systems, and proved that they show strong σ2 responses, emitted light in the NIR region (above 700 nm), and were water-soluble, making them exciting alternatives to traditional organic dyes for deep-tissue 2PM [3]. We investigated also gold NCs and established their excellent two-photon properties [4, 5]. NCs stabilized with functional supramolecular ligands presented NIR fluorescence and tunable hydropilicity, thus their penetration and binding in amyloid structures outperformed water-soluble nanoparticles [6, 7].

Collectively, this research introduces two distinct classes of high-performance fluorescent probes — novel organic fluorophores and noble-metal nanoclusters — which are well-suited for the demanding requirements of advanced two-photon imaging in biological and medical applications, such as amyloid detection.

The presented research was performed in collaboration with other outstanding scientists: Dr. Patryk Rybczyński and Prof. Borys Ośmiałowski (UMK, Toruń, Poland), Prof. Robert Zaleśny (PWr, Wrocław, Poland), Prof. Thomas Buergi and his group (University of Geneva, Switzerland), prof. Stacy M. Copp and her group (University of California-Irvine, USA).

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NATURAL POLYPHENOLS AS MODULATORS OF COPPER-MEDIATED AMYLOID-β AGGREGATION AND TOXICITY

Arian Kola[1], Aleksandra Hecel[2], Stefania Lamponi[1] and Daniela Valensin[1]
[1]Department of Biotechnology, Chemistry and Pharmacy, University of Siena, 53100 Siena, Italy
[2]Faculty of Chemistry, University of Wrocław, 50383 Wrocław, Poland
email: daniela.valensin@unisi.it

Amyloid-β (Aβ) peptides are prone to aggregation into toxic oligomers and fibrils, processes that are closely associated with the onset and progression of neurodegenerative diseases such as Alzheimer's disease. Among the various factors influencing Aβ aggregation, copper(II) ions play a critical role by promoting structural changes in the peptide and generating reactive oxygen species through redox cycling [1-5]. Copper dysregulation contributes to oxidative stress and accelerates the formation of neurotoxic aggregates.

Our recent investigations have focused on the capacity of selected natural polyphenols and alkaloids to modulate the interaction between copper and Aβ peptides. These bioactive molecules can chelate Cu(II), limit its redox activity, and thereby inhibit metal-induced aggregation [6-9]. Moreover, their intrinsic antioxidant properties enable them to scavenge free radicals and counteract oxidative damage [10, 11]. By reducing copper-mediated toxicity and aggregation, these compounds demonstrate significant potential as multi-target agents in the context of metal-associated neurodegenerative disorders. Their dual action—metal chelation and radical scavenging—highlights a promising therapeutic strategy aimed at mitigating both the biochemical and structural components of Aβ-related neurotoxicity.

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ABSTRACTS

Oral Presentations

PLANT-DERIVED EXTRACELLULAR VESICLES FOR DRUG DELIVERY

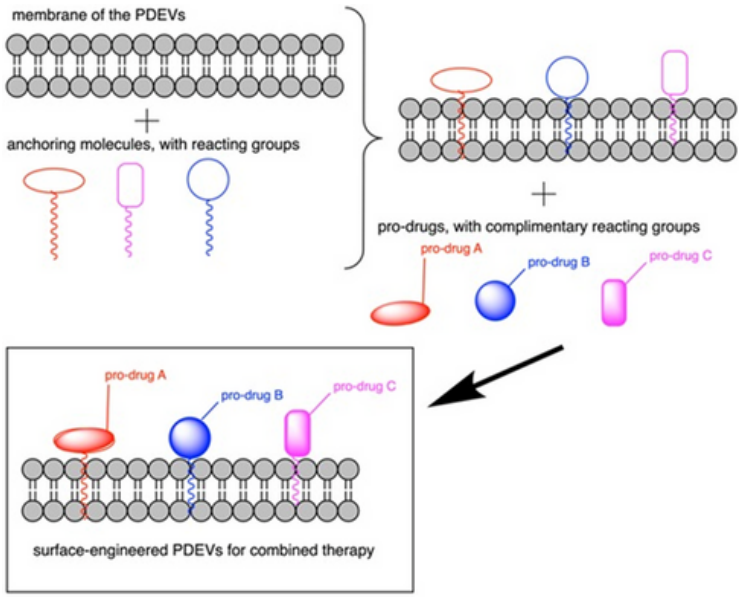
Ana García-Moreno, Miquel Barceló-Oliver
University of the Balearic Islands
Ctra. Valldemossa km 7.5, E-07122 Palma de Mallorca, Illes Balears, Spain
email: miquel.barcelo@uib.es

The scientific community has made great efforts to develop new drugs that can treat many of the diseases currently affecting us. However, it is essential to transport these drugs to their therapeutic targets. Various strategies have been developed to improve drug delivery.

Our approach of using extracellular nanovesicles for drug delivery appears to pose the fewest risks and have the fewest associated side effects.

Specifically, we have developed a method to obtain these vesicles from plant waste, enabling us to reuse it. Thus far, we have extracted suitable vesicles from orange waste (used to make juice), grape waste (from the wine industry), and *Posidonia oceanica* seaweed.

This presentation will describe our strategy of functionalizing the surfaces of these vesicles with anti-inflammatory prodrugs using click chemistry, as well as evaluate their efficacy against osteoarthritis models.



Although this strategy was initially developed for drugs, it is believed that it could also be used for molecules that enhance specificity, detection, and theranostic approaches. In this sense, thanks to our project, we increased the payload capacity of the vesicles: in addition to the interior load, we can access the entire surface of the vesicles, which also allows for their use before they even penetrate cells (e.g., on membrane receptors).

DEVELOPING OF NEW ARTIFICIAL PSEUDOENZYMES BASED ON SPYTAG/SPYCATCHER ANCHORED ON BACTERIA SURFACE FOR HYDROGEN PRODUCTION

Valentina Borghesani[a], Marianna Vescovi[a], Chiara Bottoni[a], Gloria Spagnoli[a], Federico Droghetti[b], Mirco Natali[b], Angelo Bolchi[a], Matteo Tegoni[a]

[a] Department of Chemistry, Life Sciences, and Environmental Sustainability, University of Parma, Italy
[b] Department of Chemical and Pharmaceutical Sciences, University of Ferrara, Italy
email: valentina.borghesani@unipr.it

Metalloproteins promote some of the most complex biomolecular processes in nature. The design of artificial metal binding sites or catalytic sites on proteins is often challenging. The protein we used is Spy, an artificial protein redesigned for its use as protein conjugation tool. Spy is made by two components that spontaneously quick recombine: the protein SpyCatcher (SC) and the peptide SpyTag (ca.15 residues) [1].

We are currently developing artificial metalloenzymes incorporating diverse functional groups, ranging from metal binding sites for redox catalysis to luminescent dyes for bioimaging and energy transfer. Here we will discuss two types of artificial metalloproteins for photocatalytic hydrogen production based on Co(II) or Ni(II) metallopeptides.

We previously demonstrated that introducing an ATCUN (Amino Terminal Cu and Ni binding) site at the N-terminus of ST we can selectively bind Cu(II) and the binding at SpyCatcher occurred only upon the addition of a second equivalent of Cu(II).[2] Based on this knowledge, a new series of Co-ATCUN SpyTag has been developed. The metallopeptides (CoST) were characterized by UV-visible spectrophotometry. The CoST and the reconstituted metalloproteins (SC/CoST) were tested for the catalytic reduction of aqueous H^+ into gaseous H_2 using $Ru(bpy)_3$ as the photosensitizer and ascorbate as the sacrificial reductant. The systems we have studied not only signed a milestone in metalloenzyme development, but also highlight how to exploit the side chain of Lysine residue, even if not directly involved in Co(II)/Co(III) coordination, impacts the catalytic activity.

We have studied also a system based on the minimalist two-nickel peptide (NB) developed by Nanda[3], bearing the NB sequence upstream the SpyTag sequence (NBST). We demonstrated that this NBST and the corresponding reconstituted Spy protein acted as catalyst in the photochemical production of molecular hydrogen.

Finally, performance of both systems have been tested when ST/SC is anchored on bacteria (E.Coli) surface, demonstrating that the catalytic activity can be (at least in part) retain.

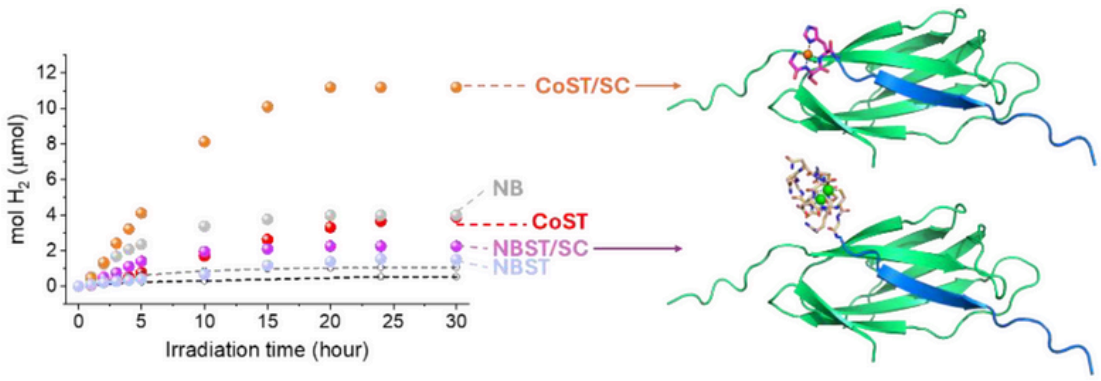


Figure: Left: Plot of µmol of produced H_2 as a function of irradiation time (at 460 nm) for a system containing CoST/SC (in orange) or di-nickel NBST/SC Spy protein (in purple).

Project "Artificial enzymes for the photocatalytic production of hydrogen in photosynthetic bacteria" National Recovery and Resilience Plan (NRRP), M2 C2 Inv. 3.5 funded by the European Union – NextGenerationEU. Project RSH2A_000009, C.D. 445 29/12/2022 Italian Ministry of Environment and Energy Security. Project of National Interest (PRIN) 2022 prot. 2022RCRWE5 - Italian Ministry of University and Research (MUR).

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INTERPLAY BETWEEN HEMIN AND NEURONAL PEPTIDES RELEVANT TO NEURODEGENERATIVE DISEASES

Simone Dell'Acqua, Chiara Bacchella, Silvia De Caro, Stefania Nicolis, Luigi Casella, Enrico Monzani
Dipartimento di Chimica, Università degli Studi di Pavia, Italy
email: simone.dellacqua@unipv.it

Heme is essential for many physiological processes, acting as a prosthetic group of proteins and enzymes involved in oxygen transport, electron transfer, enzymatic reactions that requires O2 activation.[1] On the other hand, free heme is highly toxic because of its potential oxidizing and nitrating properties. For this reason, heme homeostasis dysregulation can contribute to several pathologies such as neurodegenerative diseases, vascular disorders, cancer, or severe hemolysis and is also relevant under conditions of heavy heme release occurring, e.g. on traumatic brain injury.[2]

Our research group investigated the binding and reactivity of ferric heme (hemin) and peptide fragments of proteins involved in neurodegeneration. For instances, histidine residues present in amyloid beta (Aβ), tau protein and prion protein allow hemin coordination with moderate affinity.[3-7] The peroxidase-like activity of the hemin-prion peptide complexes and hemin-induced aggregation were also evaluated. Giving to the importance that reactive nitrogen species (RNS) has on neurodegeneration, we have extended our interest on nitrative reaction promoted by hemin-Aβ16 complex.[8]

We are also extending the previous study of hemin-Aβ interaction to related metal-macrocyclic complexes with similar capability to interact with Aβ peptide. Our current interest thus focuses on expanded metalloporphyrins known as texaphyrins, which capable of deactivating ROS and RNS. Mn-texaphyrin has been probed to drastically reduce the oxidation and nitration of Aβ.[9]

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SELECTIVE FORMATION OF SILVER-MEDIATED X-AGI-T BASE PAIRS IN DNA DUPLEXES

Carmen López-Chamorro[1], Antonio Pérez-Romero[1], Alicia Domínguez-Martín[1], Uroš Javornik[2], Oscar Palacios[3], Janez Plavec[2], Miguel A. Galindo[1]

[1]Departament Inorganic Chemistry, University of Granada, 18071 Granada, Spain
[2]Slovenian NMR Center, National Institute of Chemistry and Faculty of Chemistry and Chemical Technology, University of Ljubljana, SI-1000 Ljubljana, Slovenia
[3]Departament de Química, Facultat de Ciències, Universitat Autònoma de Barcelona, Cerdanyola del Vallès 08193, Spain
email: adominguez@ugr.es

The development of predictable metal-DNA assemblies represents a transformative advancement in DNA-based nanotechnology, offering a versatile platform for designing novel functional materials with enhanced stability, tunable properties, and broad applicability. CD spectroscopy, NMR spectroscopy, and ESI-MS were used to evaluate the formation of Watson–Crick silver-modified 7deazaAdenine$_{15}$-Ag$_{15}$-T$_{15}$ systems. The preferential formation of alternative silver–metalated base pairs involving 7-deaza-purines in duplexes, without intentional mismatches, was successfully achieved [1]. Moreover, it was demonstrated that these heterobase pairs are preferentially formed over homobase pairs such as X-AgI-X and T-AgI-T, thus reinforcing structural stability and preserving the Watson–Crick organization within 7-deaza-DNA duplexes (Figure 1).

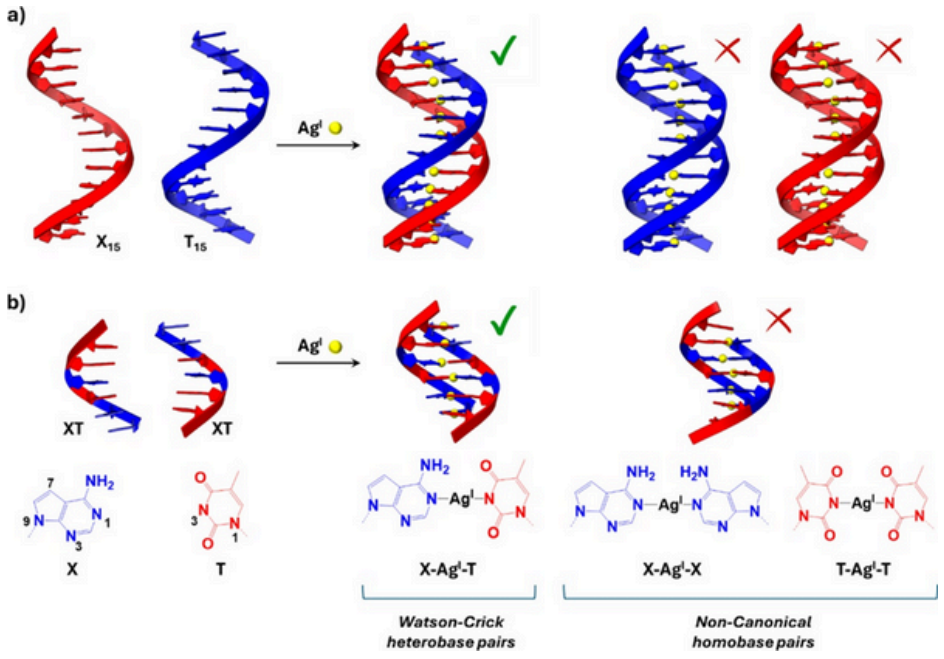

Figure 1. Scheme of the reaction between oligonucleotides containing X (7-Deazaadenine) and T (Thymine) bases with Ag^I ions, potentially leading to the formation of Duplexes comprising X-Ag^I-T heterobase Pairs and X-Ag^I-X or T-Ag^I-T homobase Pairs. These interactions may occur through (a) strand displacement or (b) strand slippage events.

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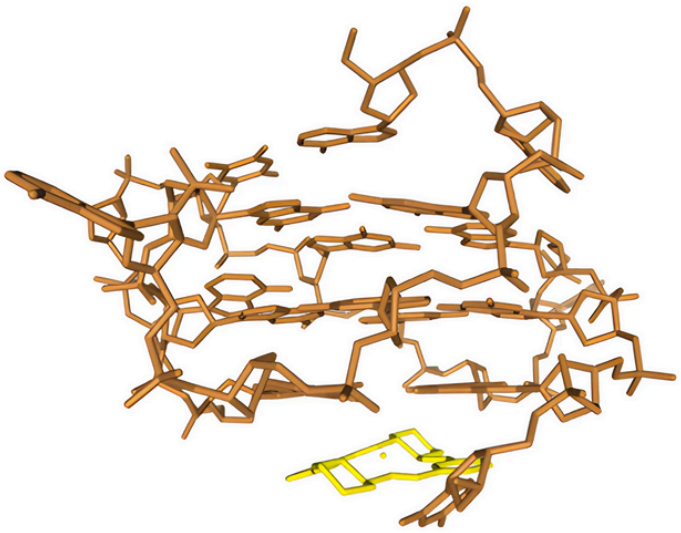
LANTHANUM(III) AND DYSPROSIUM(III) HEXAAZA MACROCYCLES REVISITED: ENHANCED STABILIZATION OF G-QUADRUPLEX DNA

Ernest Ewert[a], Dawid Marcinkowski[a], Izabela Pospieszna-Markiewicz[a], Zbigniew Hnatejko[a], Maciej Kubicki[a], Ewelina Wieczorek-Szweda[a], Violetta Patroniak[a], Giovanni N. Roviello[b], Marta Fik-Jaskółka[a]

[a]Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
[b] Institute of Biostructures and Bioimaging, Italian National Council for Research (IBB CNR), Area di Ricerca site and Headquarters, Via Pietro Castellino 111, 80131 Naples, Italy
email: marta.fik@amu.edu.pl

We synthesized and structurally characterized two 18-membered hexaaza macrocyclic complexes, $[LaL]^{3+}$ and $[DyL]^{3+}$, obtained via lanthanide-templated reactions. Their interactions with G-quadruplex (G4)-forming sequences (Tel26, Tel22, Pu22) were examined in detail. $[LaL]^{3+}$ stabilized G4 structures more effectively than $[DyL]^{3+}$, with negligible effects on duplex DNA. In particular, $[LaL]^{3+}$ showed pronounced stabilization of both telomeric and oncogene promoter G4s, displaying especially high affinity for Tel26. The selective G4 targeting is attributed to the macrocycle's architecture and accessible axial coordination sites, while the diffuse electron density of La^{3+} enables specific interactions, including coordination to the O6 atom of G15 in the central channel of the hTERT G4. These results highlight unique structure–function relationships in lanthanide macrocycles and provide a rare complement to prior studies on lanthanide–DNA interactions.



Pose view of macrocyclic complex $[LaL]^{3+}$ attached to the terminal quartet of G4 at the 3' end of DNA.

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COPPER UPTAKE AND METALLOPHORE-MEDIATED TRANSPORT IN PATHOGENIC BACTERIA

Aleksandra Hecel[1], Arian Kola[2], Daniela Valensin[2], Danuta Witkowska[3], Henryk Kozłowski[1,3], Magdalena Rowińska-Żyrek[1]

[1] University of Wrocław, Faculty of Chemistry, 50383 Wrocław, Poland
[2] University of Siena, Department of Biotechnology, Chemistry and Pharmacy, 53100 Siena, Italy
[3] University of Opole, Institute of Health Sciences, 45060 Opole, Poland
email: aleksandra.hecel2@uwr.edu.pl

Transition metal ions are essential elements for many pathogens. These nutrients play significant structural and catalytic roles in numerous biological processes. The growing interest in metallophores, metal-chelating molecules excreted by pathogens to efficiently bind specific metal ions, and their interactions with corresponding transmembrane transporters is a consequence of the dramatic rise in antimicrobial resistance [1].

To thrive within the host and outcompete commensal microbes, pathogenic bacteria must tightly regulate metal ion acquisition and distribution via specific transport systems [2-4]. Bacterial copper transport mechanisms are particularly diverse compared to those in eukaryotes, with some systems restricted to specific bacterial groups or species. While copper import in bacteria has been less studied, the outer membrane transporter OprC has been identified as a key player in this process. OprC facilitates copper uptake through a unique CxxxM-HxM metal-binding site. The interaction between metallophore CopM and OprC has been extensively studied. We identified two metal-binding sites in CopM, with MxxHH and MHxxH motifs, both capable of binding Cu(II). At pH 7, the MxxHH motif shows the highest affinity for Cu(II), suggesting that it binds copper more tightly than the CxxxM-HxM site in OprC. This indicates that CopM likely transports copper into the cell alongside the metal through OprC [5].

Copper homeostasis in bacteria is further regulated by metal-sensing transcriptional repressors, such as CopY. Found exclusively in Gram-positive bacteria, CopY coordinates Cu(I) via a conserved C-terminal CxCxxxCxC motif. Due to the presence of polyCys motif in the sequence, it is highly probable that this protein can binds more than one Cu(I) ions. Interestingly, in E. hirae, when copper availability is low, CopY preferentially binds Zn(II), forms a dimer and activates the promoter of copYZAB operon [6]. Moreover, CopY also interacts with chaperone CopZ, which is rather unique and not demonstrated for other Cu(I)-sensing transcriptional regulators.

Effective acquisition of metal ions is crucial for the survival and virulence of many pathogens, thus maintaining metal homeostasis is a critical process that must be precisely coordinated by them. Elucidating these metal transport pathways in bacteria offers promising strategies to disrupt bacterial physiology and could play a

significant role in overcoming antimicrobial resistance by targeting microbial metal uptake systems with new therapeutic interventions.

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ARTIFICIAL INTELLIGENCE IN CHEMISTRY: DESIGNING MOLECULES WITH DESIRED PROPERTIES

Damian Nowak, Rafał Bachorz, Marcin Hoffmann
Faculty of Chemistry, Adam Mickiewicz University in Poznań
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
e-mail: mmh@amu.edu.pl

The recent development of artificial intelligence (AI) has profoundly changed the approach to designing novel chemical entities. One of the key applications of AI in chemistry is the prediction and generation of molecular structures with desired biological or physicochemical properties, such as protein-binding affinity, solubility, or metabolic stability [1,2]. This presentation highlights current methods of data-driven molecule generation, with particular attention to biologically active compounds exhibiting cytoprotective activity toward cell membranes. Generative neural models, including encoder–decoder architectures and variational approaches, were employed to propose and prioritize new compounds capable of stabilizing erythrocyte membranes — viewed as dynamic lipid–aqueous phase boundaries [2,3]. Key descriptors such as lipophilicity, polarizability, and hydrogen-bonding capacity were used to identify molecules that improve membrane integrity and reduce susceptibility to osmotic stress. Computationally generated candidates were evaluated using machine learning models trained to predict biochemical effects on model lipid membranes and erythrocyte behavior. Beyond cytoprotection, the talk will briefly discuss AI-assisted prediction of enantioselectivity in asymmetric epoxidation reactions catalyzed by metal complexes [4,5]. Here, deep-learning models combining molecular descriptors with experimental enantiomeric excess data illustrate the growing role of AI not only in drug design but also in physical organic chemistry and phase-boundary phenomena. Finally, we address current limitations — most notably, limited availability of large, high-quality chemical datasets, the need for greater interpretability of predictive models, and the importance of synergistic integration with quantum-chemical computations and experimental data. Altogether, AI emerges as a powerful tool for accelerating molecular discovery in both biomedical and physical chemistry contexts.

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CAGE-LIKE FUNCTIONALIZED SILSESQUIOXANES: MULTIFUNCTIONAL BUILDING BLOCKS FOR BIOMEDICINE

Łukasz John
Faculty of Chemistry, University of Wrocław
14 F. Joliot-Curie, 50-383 Wrocław, Poland
e-mail: lukasz.john@uwr.edu.pl

Silsesquioxanes constitute a sophisticated class of organosilicon compounds characterized by the empirical formula $RSiO_{3/2}$, where "R" denotes a hydrogen atom or various reactive or inert organic groups. Among the diverse structural motifs within this family, particular attention has been drawn to double-decker (DDSQ) silsesquioxanes (Fig. 1) and polyhedral oligomeric silsesquioxanes (POSS). These architecturally unique molecules have attracted significant interest due to their promising properties and wide-ranging potential in both fundamental and applied research.

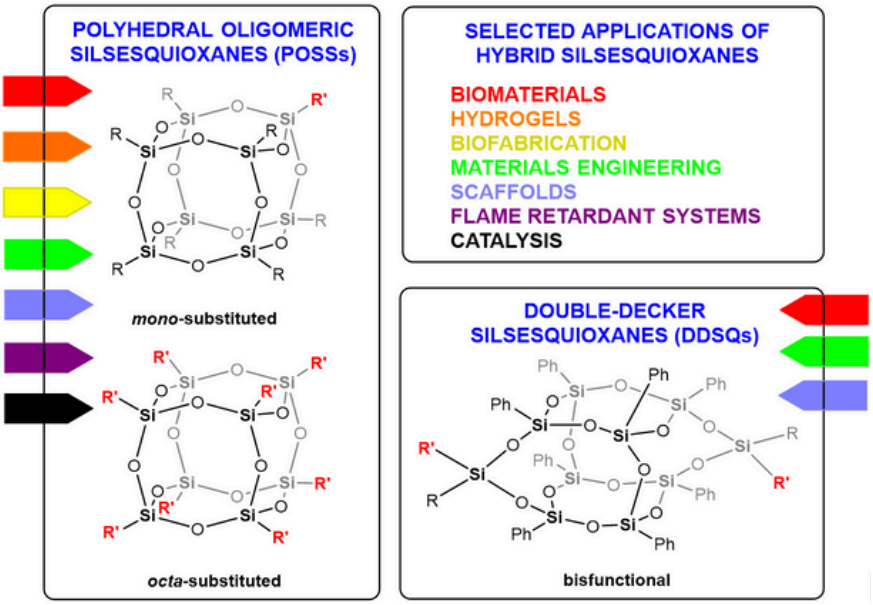

Figure 1. Representative structures of cage-like silsesquioxanes.

The hallmark of these compounds is their intrinsic hybrid character, arising from the combination of an inorganic siloxane core with customizable organic functionalities at the periphery. This dual nature enables versatile chemical modifications and tailors them for a broad spectrum of advanced applications.

In this presentation, I will showcase the recent advances from our research group involving functionalized POSS and DDSQ systems. Emphasis will be placed on their interdisciplinary applications, spanning from biomaterials science [1-3], through the design of innovative organic materials [4–6], to coordination chemistry frameworks [7,8]. These examples will illustrate how the hybrid architecture of silsesquioxanes can be strategically exploited in cutting-edge material development.

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ADSORPTION OF PROTEINS AND PEPTIDES AT THE LIQUID-LIQUID INTERFACE

Julia Maciejewska-Komorowska[a], Angelika Holzinger[a], Shayon Bhattacharya[b], Magdalena Wiloch[a], Damien W. M. Arrigan[c], Martin Jönsson-Niedziółka[a]

[a] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

[b] Department of Physics, SSPC the SFI Research Centre for Pharmaceuticals, Bernal Institute, University of Limerick, V94 T9PX, Ireland.

[c] Curtin Institute for Functional Molecules and Interfaces, School of Molecular and Life Sciences, Curtin University, GPO Box U1987, Perth, Western Australia, 6845, Australia

email: martinj@ichf.edu.pl

Electrochemical processes at the interface between two immiscible electrolyte solutions (ITIES) are studied because of their implication in practical applications like ion extraction, phase-transfer catalysis, and electroanalysis [1], but also because the liquid|liquid interface is a simple model system that mimics processes at biological interfaces [2].

In this work, we investigate the electrochemical behaviour of proteins and peptides by ion-transfer voltammetry at the ITIES. In the first instance, we use an array of microinterfaces, with a gelled organic phase, comprising a glass membrane with 100 micropores in the shape of truncated cone (\ /). The application of this type of measurement makes it possible to detect analytes at picomolar concentrations [3].

Haemoglobin is the main oxygen-carrying protein in mammal blood. It has previously been studied at the μITIES [4], but here we show that it is possible to distinguish between the various oxygenated and deoxygenated forms of the protein by their behaviour at the ITIES. This is a clear demonstration of the possibilities to use the organogel-μITIES for studies of complex biomolecule interactions.

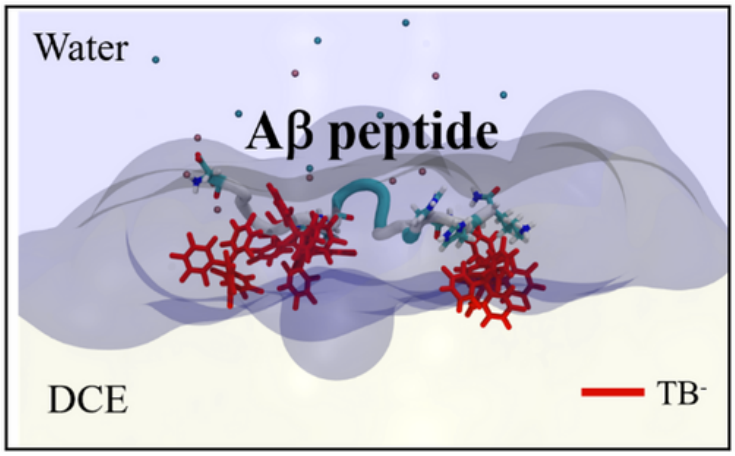

Figure 1. Representative snapshot of the MD simulation showing the interaction of the Aβ peptide with tetrakis(pentafluorophenyl)borate (TB^-) as anion of the organic electrolyte at the water-DCE interface.

However, the interaction between a protein and the ITIES is very complex, so to simplify the system, we also studied amyloid-β (Aβ) peptides with short amino acid sequences and their corresponding Cu(II) complexes at a water/1,2-dichloroethane (DCE) interface. Electrochemical data were complemented by molecular dynamics (MD) simulations, enabling a molecular-level understanding of peptide adsorption at the liquid-liquid interface. We believe that this combination of methods of investigating peptides at the ITIES can lead to a deeper understanding of the adsorption behaviour of more complex molecules such as proteins.

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STRUCTURAL AND FUNCTIONAL CHARACTERIZATION OF METALLOPORPHYRINOID–AMYLOID B INTERACTIONS

Arian Kola[a) b)], Valerio Ciccone[a)], Matteo Tegoni[c)], Simone Dell'Acqua[d)], Lucia Mobidelli[a)], Daniela Valensin[b)]

[a)]Department of Life Science, University of Siena, Via Aldo Moro 2, 53100 Siena, Italy
[b)]Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Via Aldo Moro 2, 53100 Siena, Italy
[c)]Department of Chemistry, Life Sciences and Environmental Sustainability, University of Parma, Parco Area delle Scienze 17/A, 43124 Parma, Italy
[d)]Department of Chemistry, University of Pavia, Via Taramelli 12, 27100 Pavia, Italy
e-mail: arian.kola@unisi.it

In complex biological systems, reactive oxygen and nitrogen species (ROS/RNS) are not merely by-products of metabolism, but play pivotal roles in signaling, immune responses, and the regulation of numerous physiological functions at both cellular and systemic levels [1,2]. Their delicate balance is maintained largely through metal-based redox systems, among which heme is a central player, known for its dual ability to activate dioxygen and to scavenge excess ROS/RNS. In recent years, attention has increasingly turned to synthetic analogues of heme, especially porphyrinoids with modified macrocyclic structures such as contracted corroles (COR) and expanded texaphyrins (TEX) [3–8]. These macrocycles, when complexed with redox-active metal ions, exhibit unique catalytic and electronic properties that make them promising tools for redox modulation.

In this study, we explored the redox behavior and biological potential of newly synthesized water-soluble COR- and TEX-based metal complexes, focusing on their ability to regulate ROS/RNS and interact with neurodegeneration-related targets. In particular, these compounds were evaluated for their affinity toward amyloid beta (Aβ) peptides, whose aggregation and associated oxidative stress are key features of Alzheimer's disease. Notably, complexes such as Mn-TEX and Fe-COR have previously demonstrated the ability to inhibit Aβ aggregation and ROS formation [6].

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PEPTIDOMIMETICS AND PEPTIDE CONJUGATES – A CHALLENGE FOR COSMECEUTICAL AND PHARMACEUTICAL INDUSTRY

Rafał Latajka
Wrocław University of Science and Technology, Department of Bioorganic Chemistry
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
e-mail: rafal.latajka@pwr.edu.pl

Peptides have a wide range of functions, which underpins a large number of potential applications, ranging from active pharmaceutical ingredients to innovative nanomaterials. Peptide conjugation is a strategy used to expand their utility in various fields including medicine and diagnostics. Conjugating peptides to a wide range of molecules, could improve their stability, immunogenicity, targeting capabilities, as well as design useful research tools. On the other hand, interest in peptidomimetics is connected with the fact that they are synthetic molecules designed to mimic the structure and function of peptides or proteins, but with improved properties like stability and bioavailability, making them valuable in drug discovery.

During the lecture it will be presented results of our collaboration with colleagues from University of Florence in this area of investigations – starting from peptidomimetics in cosmeceutical and pharmaceutical interest, ending in peptide conjugates as inhibitors of enzymes [1-5].

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METAL ION–PEPTIDE INTERACTIONS: EFFECTS ON THE STRUCTURE AND CHEMISTRY OF COSMETIC AND BIOLOGICALLY ACTIVE PEPTIDES

Francesca Nutti[1], Fosca Errante[1], Anna Kloska[2], Jakub Brzeski[3], Robert Wieczorek[4], Dariusz Wyrzykowski[3], Anna Maria Papini[1], Joanna Makowska[3]

[1]Interdepartmental Research Unit of Peptide and Protein Chemistry and Biology, Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 13, 50019 Sesto Fiorentino, Italy
[2]Faculty of Biology, University of Gdańsk, Wita Stwosza 59, 80-308 Gdańsk, Poland
[3]Faculty of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland
[4]Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
e-mail: joanna.makowska@ug.edu.pl

This study investigates the interactions between selected derivatives of cosmetic peptides (*Argireline* and *Eyeseryl*) and fragments of the human antimicrobial peptide LL-37 with divalent metal ions Cu(II), Zn(II), and Mn(II). The aim was to evaluate how these interactions influence the structural, chemical, and potential functional properties of the peptides. For the cosmetic peptides, a specific chemical modification was introduced, which significantly improved their Cu(II)transport-related characteristics, suggesting enhanced bioavailability and potential efficacy in topical applications. In the case of LL-37 fragments, binding with metal ions was confirmed through spectroscopic and analytical techniques. It was proved, that these interactions did not induce cytotoxic effects, indicating the safety of the resulting complexes. Moreover, the findings suggest that metal coordination may influence the antimicrobial potential of LL-37 derivatives, opening possibilities for designing new peptide-based agents with tunable biological activity. The results provide a foundation for future development of multifunctional peptide-metal systems for biomedical and cosmetic applications.

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BIOINSPIRED METAL–LIGAND COORDINATION COMPOUNDS AS SELECTIVE AGENTS AGAINST DRUG-RESISTANT CELLS AND PATHOGENS

Agnieszka Chylewska[1], Aleksandra M. Dąbrowska[1], Mateusz Kowalik[1], Sandra Brzeska[1], Paulina Nowicka[1], Magdalena Stasiuk[1], Natalia Żukowska[1], Jakub Brzeski[1], Aleksandra Ciesielska[1], Dawid Dębowski[1], Mariusz Makowski[1]

[1]University of Gdańsk, Faculty of Chemistry
W. Stwosza 63, 80-309 Gdańsk, Poland
e-mail: mariusz.makowski@ug.edu.pl

The rise of antimicrobial resistance (AMR) and the growing burden of cancer, particularly drug-resistant and late-stage malignancies, pose urgent challenges to modern medicine. Conventional small-molecule therapeutics are increasingly ineffective, and the stagnation in new antibiotic classes exacerbates this crisis. In this context, coordination compounds of transition metal ions with organic or inorganic ligands have emerged as promising candidates because of their ability to interact with unique biological targets and offer novel mechanisms of action.

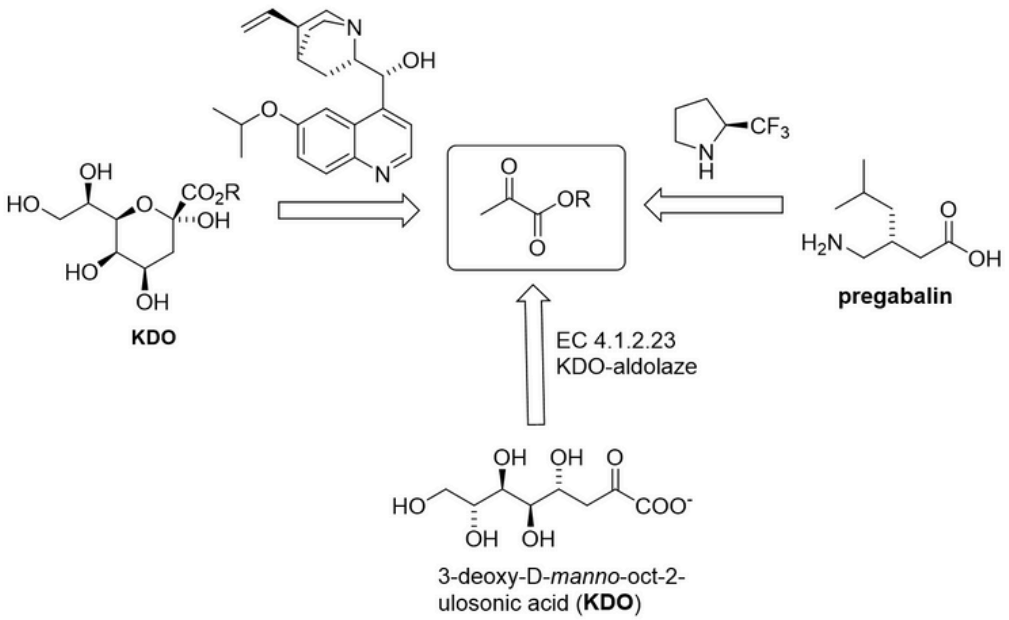
In our recent study, we have explored the therapeutic potential of Rh(III), Ru(III), and Ir(III) coordination compounds bearing bioactive sulfonamide ligands. The Rh(III) bipyridyl sulfonamide complex exhibited selective cytotoxicity toward breast cancer cells (SKBr3) while sparing non-malignant epithelial cells (HB2), and impaired mitochondrial function, as well as disrupted Rac1/VASP signaling pathways.

Moreover, we observed promising selectivity for cadmium(II) compounds coordinated to carboxyimidazole-based ligands. These coordination compounds exhibited distinct biological profiles and warrant further investigation as possible antimicrobial agents. Interestingly, preliminary results also indicate that these chemical connections exhibit selective antifungal activity. This presentation highlights our structure–activity relationship findings and mechanistic insights that support the continued exploration of d-block metal coordination compounds in the context of drug-resistant diseases.

BIOMIMETIC ORGANOCATALYTIC REACTIONS OF PYRUVATE

Jacek Młynarski
Institute of Organic Chemistry, Polish Academy of Sciences
Kasprzaka 44/52, 01-224 Warsaw, Poland
e-mail: jacek.mlynarski@icho.edu.pl

Despite the significant role of pyruvic acid and phosphoenolpyruvate (PEP) in biotransformations,[1] the use of pyruvates as substrates in asymmetric catalysis remained limited for many years, with only a few examples of narrow practical relevance. Moreover, although numerous enzymes activate pyruvic acid via an enamine-based mechanism, analogous transformations have not been successfully reproduced using organocatalysts [2]. Only recently has organocatalysis been effectively applied to the biomimetic synthesis of natural and bioactive compounds from pyruvic acid esters [3]. In this lecture, selected examples will be presented demonstrating the use of both established and newly developed organocatalysts in the synthesis of ulosonic acids and g-aminobutyric acid (GABA) derivatives [4].



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UNCOVERING METABOLIC ALTERATIONS IN COGNITIVE DECLINE: FOCUS ON THE ASTROCYTE-NEURON LACTATE SHUTTLE

Natalia Pudełko-Malik[1], Dominika Drulis-Fajdasz[2], Agnieszka Gizak[2], Piotr Młynarz[1], Dariusz Rakus[2]

[1] Department of Biochemistry, Molecular Biology and Biotechnology, Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370, Wrocław, Poland
[2] Department of Molecular Physiology and Neurobiology, University of Wrocław, Sienkiewicza 21, Wrocław, 50-335, Poland
e-mail: dariusz.rakus@uwr.edu.pl; piotr.mlynarz@pwr.edu.pl

Aging is a complex process marked by progressive functional degeneration at both cellular and organ levels, particularly in the brain. This degeneration leads to reduced synaptic plasticity and cognitive decline. Recent hypotheses suggest that disruptions in energy metabolism, specifically involving the astrocyte-neuron lactate shuttle (ANLS), underlie these cognitive deficits. The ANLS mechanism suggests that astrocytes metabolize glucose to lactate, which is then transported to neurons as their primary energy source.

Current research primarily using young animal models has highlighted the importance of metabolic processes in synaptic activity. However, there is limited understanding of ANLS in the context of aging. Studies on older animals (2-year-old mice and rats) have shown that inhibiting glycogen breakdown can improve memory consolidation, suggesting changes in metabolic homeostasis with aging[1].

Our study utilized metabolomics to investigate metabolic changes in specific brain regions associated with different types of memory (hippocampus, cerebral cortex, and cerebellum) as well as other organs (liver, heart, and skeletal muscles). The findings provide a comprehensive view of metabolism about ANLS and age-related physiological changes across the mouse organism.

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THE MULTIFUNCTIONALITY OF SELF-ASSEMBLING COPPER(II) SUPRAMOLECULAR SYSTEMS BASED ON IMINE LIGANDS

Daria Nowicka, Karol Garbaczewski, Adam Gorczyński, Teresa Łuczak, Maciej Kubicki, Violetta Patroniak

Adam Mickiewicz University
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
e-mail: d.nowicka@amu.edu.pl

Imine ligands and their complexation products are commonly employed systems due to their facile synthesis and versatile application in coordination chemistry[1]. Careful design, well-defined ligand backbone structure and supramolecular interactions such as hydrogen bonds or coordination bonds with d-block metal ions result in the synthesis of coordination systems that have diverse applications in many areas of science, such as biomimetic activity[2] (oxidative O-demethylase) or electrochemical properties[3] (ability to detect neurotransmitters). The former, oxidative O-demethylase biomimetics, will lead to the development of alternative methods that will break the C-O-C bond in a simple and environmentally friendly manner, a feasible strategy using appropriate imine ligands[2]. The latter, on the other hand, are of particular interest, as they could contribute to controlling content of neurotransmitters in living organisms, which will enable faster detection of neurodegenerative diseases (Parkinson's disease, Alzheimer's disease, Tourette syndrome, schizophrenia)[3,4] so could help in solve some of the global problems.

Herein, a set of multifunctional copper(II)-based imine coordination compounds with a variety of supramolecular structures will be presented with applications in the fields of biomimetics (oxidative O-demethylation) and electrochemistry (neurotransmitter sensor).

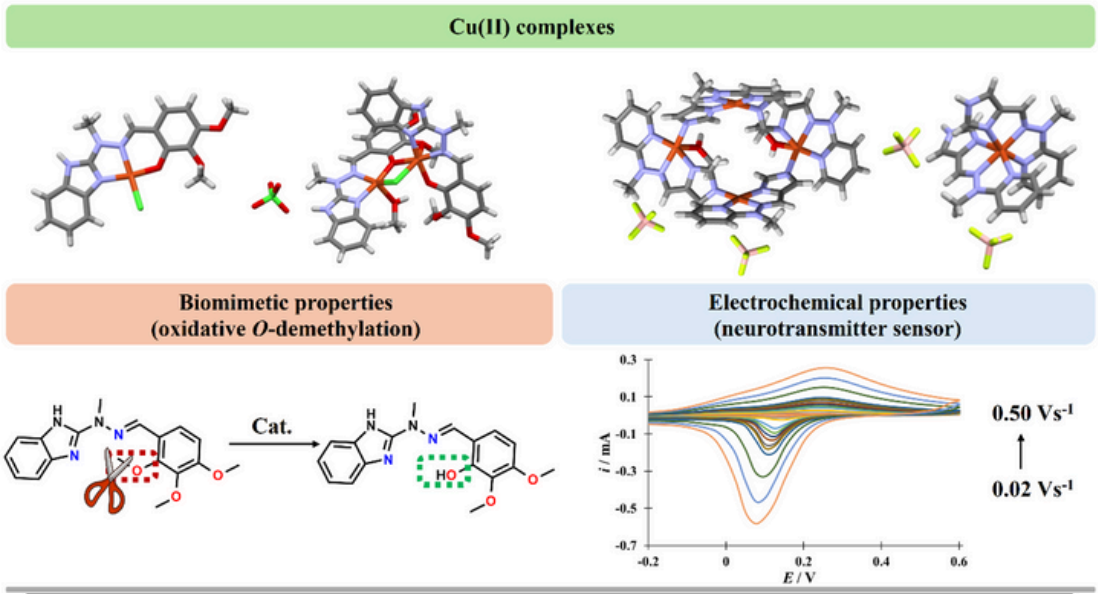

Figure. Schematic presentation of structures of copper(II) supramolecular complexes with biomimetic and electrochemical properties.

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ENGINEERING INTERACTIONS TO TAILOR NANOMATERIALS FOR ANTIMICROBIAL AND ANTIVIRAL APPLICATIONS: FROM SURFACE ENGINEERING TO SELECTIVE BIOCONTROL

Jan Paczesny
Institute of Physical Chemistry PAN
Kasprzaka 44/52, 01-224 Warsaw, Poland
e-mail: jpaczesny@ichf.edu.pl

The increasing threat of microbial contamination and the limitations of conventional disinfection methods have intensified interest in multifunctional nanocomposite materials with tunable antimicrobial and antiviral properties. Our recent research explores the synthesis and interfacial design of nanomaterials capable of selectively inactivating pathogenic bacteria and bacteriophages while minimizing harm to beneficial microorganisms and mammalian cells.

We investigate systems ranging from surface-engineered metal oxide coatings to mixed-ligand and natural compounds, each tailored to exploit specific physicochemical mechanisms, such as redox activity, nanostructure-induced membrane disruption, and selective photoprotection. Through controlled synthesis conditions, including variation of ligand chemistry, dopants, or reaction additives, we demonstrate how material composition and surface architecture influence biological interactions at the nanoscale.

These materials exhibit broad-spectrum efficacy, stability, and biocompatibility, with potential applications in bioprocess protection, medical devices, and food and water safety. This work underscores the role of rational material design in creating next-generation antimicrobial nanocomposites and highlights the importance of integrating surface science with biological performance criteria.

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REDOX CHANGES IN CARBO-/HETEROCYCLIC 3D SKELETONS

Miłosz Pawlicki
Faculty of Chemistry, Jagiellonian University
Gronostajowa 2, 30387 Kraków, Poland
e-mail: pawlicki@chemia.uj.edu.pl

Extended delocalisation within p-conjugated carbon skeletons remains a key aspect allowing an extraction from unsaturated hydrocarbons the properties and behaviours unavailable for other type of organic compounds e.g., extremely efficient absorption of the visible light that can be easily tuned towards red region of the spectrum. The need for a strict control of the achieved properties always requires a precise structural design followed by a synthetic approach leading to obtaining a skeleton with proper connectivity and planned substitution. It allows for stabilisation of uncommon oxidation or spin states that substantially influence the recorded behaviour. All changes relying on the redox modulation incorporate into the conjugated p-system a defect responsible for a globalisation of the delocalisation eventually leading to global diatropic current, but also introduce an open-shell character correlated with a radical formation in single-electron processes. The radical states entrapped in the p-conjugated systems show increased stability correlated with the extended delocalisation. It leads to formation of relatively stable radicals because of redox modifications and their enhanced stability opens a set of possible application in several fields because of, among the others, their optical properties with usually bathochromically shifted absorption and emission.

In the three-dimensional structures (3D motifs) the change of oxidation state can be followed by deep conformational dynamic opening a possibility of having the global diatropic conjugation,[1] but also can lead to stabilisation of a radical state[2]. The separate possibility is correlated with the macrocyclic effect of conjugation which, mostly because of their designed construction allows a globalisation of the conjugation in the frames of available p-cloud,[1] but also open the venues for stabilisation of the open-shell states as doublet with one unpaired electron[2,3], or incorporation of two unpaired electrons in diradicaloid systems with potential singlet/triplet equilibrium[4,5] .

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TRANSITION METAL BIOAVAILABILITY AND COORDINATION IN MICROBIAL DEFENSE AND VIRAL INVASION

Massimiliano F. Peana
Department of Chemical, Physical, Mathematical and Natural Sciences, University of Sassari
Via Vienna 2, 07100 Sassari, Italy
e-mail: peana@uniss.it

Transition metal ions, iron, manganese, zinc, and copper, are essential cofactors in microbial and viral systems, where they regulate enzymatic catalysis, oxidative stress responses, and host interactions. Their coordination chemistry governs critical biological outcomes.

In *Escherichia coli*, the FeoB transporter exemplifies competitive uptake of Fe(II), Mn(II), and Zn(II), with ligand-specific preferences that support survival in nutrient-depleted or oxidative environments [1,2]. These preferences underscore how trace metals shape bacterial metabolic adaptability.

The extremophile *Deinococcus radiodurans* offers a model of Mn-based oxidative stress tolerance, accumulating Mn(II)-antioxidant complexes that preserve protein integrity and sustain DNA repair enzymes. This mechanism provides insights into natural radioprotection, with translational potential in anti-aging and cancer therapy [3-5].

In viral systems, metal ions are increasingly recognized as modulators of host-pathogen dynamics. The ACE2 receptor, exploited by SARS-CoV-2, contains histidine- and carboxylate-rich sites that bind Zn(II) and Cu(II), potentially altering receptor conformation and viral binding efficiency [6].
This presentation will delve into the coordination chemistry of metal ions in microbial and viral systems, emphasizing spectroscopic and potentiometric approaches used to unravel these interactions. The findings shed light on the fundamental bioinorganic mechanisms at play and point to promising strategies for therapeutic innovation in infectious disease control and oxidative stress mitigation.

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PHOSPHA-FLUOROPHENYLGLYCINES, SYNTHESIZED AS POTENTIAL INHIBITORS OF HUMAN UROKINASE PLASMINOGEN ACTIVATOR AND EVALUATED FOR THEIR ANTICANCER ACTIVITY

Karolina Ciesielska[1], Dariusz Wawrzyniak[2], Grzegorz Dutkiewicz[1], Maciej Kubicki[1], Wojciech Jankowski[1], Marcin Hoffmann[1], Karol Kamel[2], Tatiana Da Ros[3], Katarzyna Rolle[2], Donata Pluskota-Karwatka[1]

[1]Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
[2]Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań, Poland
[3]Universita degli Studi di Trieste, Piazzale Europa 1, 34127 Trieste, Italy
e-mail: donatap@amu.edu.pl

Phosphonate analogues of α-amino acids offer broad opportunities in medicinal chemistry, while fluorine is well known for fine-tuning the properties of organic molecules. In our newly designed α-aminophosphonates (Fig. 1) we merge these two pharmacophores — the phosphonate group and fluorine atoms — within a single scaffold. The compounds were synthesised by a diastereoselective hydrophosphonylation of imines that were generated through an environmentally friendly mechanochemical protocol [1].

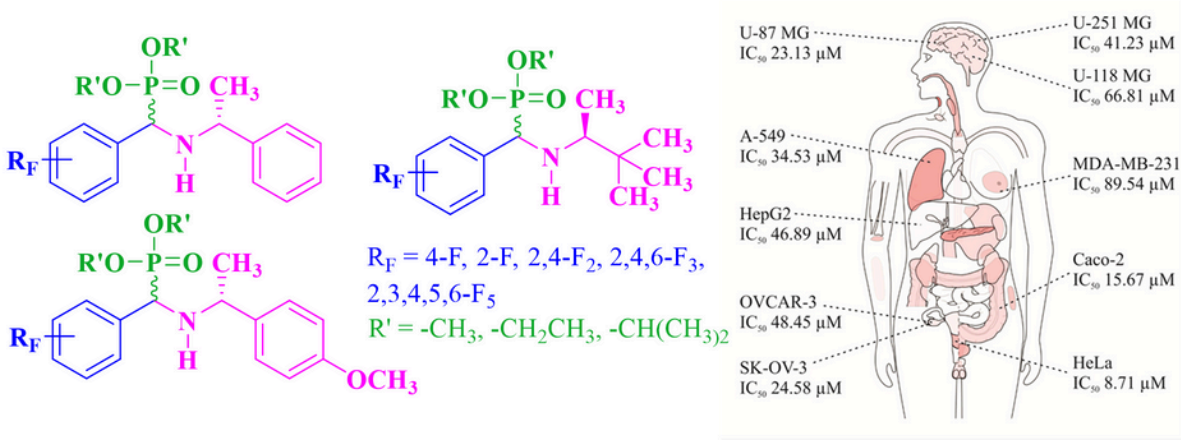

Figure 1. General structure of the synthesised α-aminophosphonates and mean IC_{50} values obtained in studies of their cytotoxicity.

The SwissADME analysis indicated a favourable pharmacological profile for the synthesised compounds and highlighted their ability to interact with proteases. Screening against ten human cancer cell lines from different organs (Fig. 1) showed that most of the tested molecules exhibited greater activity and selectivity than 5-fluoro-2′-deoxyuridine, the reference drug [2]. Molecular docking revealed strong binding of one α -aminophosphonate to the urokinase-type plasminogen activator (uPA), suggesting anti-metastatic potential. These findings position the synthesised α-aminophosphonates as promising scaffolds for developing anti-tumour therapies targeting cancers with elevated uPA expression. Our results also demonstrate that fluorinated α-aminophosphonates can be used to functionalise carbon nanotubes, yielding new materials with attractive properties [3].

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NOVEL ADVANCED SUPRAMOLECULAR SYNTHONS BASED ON COMBINED SETS OF MOLECULAR MULTISITE ANION RECEPTORS

Dorota Głosz[1,2], Aleksandra Żabińska[1], Martyna Dyczkowska[1], Joachim Grzybowski[1], Monika Srebro-Hooper[1], James G. M. Hooper[1], Tadeusz M. Muzioł[3], Robert Podgajny[1]

[1] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland
[2] Doctoral School of Exact and Natural Sciences, Jagiellonian University, Lojasiewicza 11, 30-348 Krakow, Poland
[3] Faculty of Chemistry, Nicolaus Copernicus University in Toruń, 87-100 Toruń, Poland
e-mail: robert.podgajny@uj.edu.pl

Search for the artificial anion transport channels are important from the standpoint of replacement for malfunctioned ion transport systems in living organisms [1]. In this context, studies on multicomponent molecular architectures provide insight into molecular aggregation and recognition of dominant supramolecular synthons along with the overall interaction hierarchy. Based on our previous results [2] and inspired by other teams, [3] we present herein an emerging library of multicomponent systems involving combined sets of multisite anion receptors and simple organic-inorganic salts (Fig. 1a). The A-type coformers bearing resorcinol (1,3-dihydroxobenzene) function(s) can bind anions via hydrogen bonds, while the π-acidic $HAT(CN)_6$ (1,4,5,8,9,12-hexaazatriphenylene; **B**) attracts anions through anion···π interactions. The resulting ternary aggregates [koformer-**A**][koformer-**B**][anion]$_2$ are glued by fundamental interactions inherent in binary adducts [koformer-**A**][anion]$_2$ (H-bonds) [koformer-**B**][anion]$_2$ (anion···π), and [koformer-**A**][koformer-**B**] (π···π) (Fig. 1b).

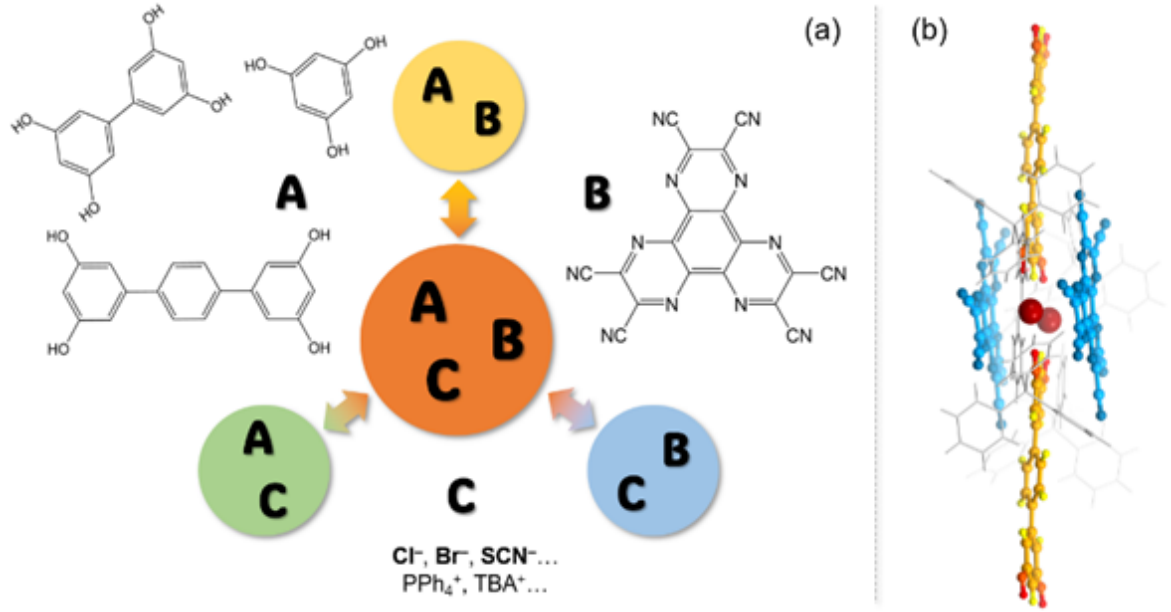

Figure 1. (a) An image of the emerging library of multicomponent supramolecular systems combining hydrogen-bonds, anion···π and π···π interactions. **(b)** The example of composed synthon in crystalline $[PPh_4][rez3][HAT(CN)_6][Br]_2 \cdot 2MeCN$

The underlying synthons are supported by secondary interactions involving cations and solvent molecules. The consistent information set on the above systems was acquired by structural (sc-XRD), spectroscopic (UV-Vis; ^{1}H, ^{13}C, ^{81}Br NMR), and computational (gas phase DTF, TD-DFT, periodic conditions DFT) studies [4].

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METAL-HISTIDINE COMPLEXES, THE PILLAR OF A THIRTY-YEAR COLLABORATION BETWEEN FERRARA AND WROCŁAW UNIVERSITIES

Maurizio Remelli
Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara
via L. Borsari 46, 44121 Ferrara, Italy
e-mail: maurizio.remelli@unife.it

The imidazole ring of histidine (His) serves as one of the most significant metal-binding sites in peptides and proteins. Its intermediate pK_a value (≈ 6.5) ensures that the imidazole nitrogen is only partially deprotonated at physiological pH, making it readily available for metal ion coordination. Furthermore, the tautomeric protonation equilibrium between the two nitrogen atoms of its imidazole ring provides His with additional flexibility in adapting to diverse metal-complex geometries. This flexibility enhances its efficiency as a primary anchoring site for metal complexation.

The position of histidine within a peptide has a profound impact on the stability and geometry of the resulting metal complex. Additionally, depending on the identity of adjacent residues, complexation often extends beyond His once metal ions are anchored to it. This progression can move toward either the N- or C-terminus based on the relative strength of newly formed interactions.

It is also important to note that many proteins harbor multiple histidine domains, which are highly conserved across various species despite the exact biological role remaining unclear. Nonetheless, these conserved His sequences confer exceptional metal-binding properties to the proteins they reside in, properties that have been harnessed in techniques like Immobilized-Metal Affinity Chromatography (IMAC) for protein purification.

Research into the thermodynamic properties of metal binding in His-containing peptides has been the central focus of collaboration between our team at the University of Ferrara and the Bioinorganic and Biomedical Chemistry group led by Henryk Kozłowski at the University of Wrocław, recently evolved to the Biological Inorganic Chemistry Group, led by Elżbieta Gumienna-Kontecka and the Biologically Active Metallopeptides Research Group headed by Magda Rowińska-Żyrek. Over nearly three decades of joint efforts, this partnership has produced significant discoveries and about 40 scientific papers.

In addition, an Erasmus agreement has been established and several students of any level have been exchanged between the two University. Morever, an International Ph.D. Program Agreement has been signed in 2017 and renewed in 2022, with the main objective to manage jointly procedures to award Ph.D. degrees and jointly run a Ph.D. research Programme in Chemical Sciences.

EXPLORING SYNTHETIC AMINO ACIDS FOR BIOMEDICAL APPLICATIONS

Hayarpi Simonyan [1], Tatevik Sargsyan[1,2], Lala Stepanyan[2], Monika Israyelyan[2], Kristina Hovsepyan[2], Mohammad Mahdi Asaadi[3], Rosanna Palumbo[4], Giovanni N. Roviello[4], Pasqualina Liana Scognamiglio[5]

[1]Yerevan State University, 1 Alex Manoogian Str., 0025 Yerevan, Armenia
[2]Scientific and Production Center "Armbiotechnology", NAS RA, 14 Gyurjyan Str., 0056 Yerevan, Armenia
[3]University of Naples Federico II, Via Tommaso De Amicis 95, 80131 Naples, Italy
[4]Institute of Biostructures and Bioimaging, National Research Council (IBB-CNR), Via Pietro Castellino 111, 80131 Naples, Italy
[5]University of Basilicata, Via dell'Ateneo Lucano 10, 85100 Potenza, Italy
email: pasqualina.scognamiglio@unibas.it

This work explores the structural properties and the biomedical potential of novel synthetic non-proteinogenic amino acids. Their ability to interact with biomolecular targets and form supramolecular assemblies was assessed through spectroscopic, microscopic, and computational approaches. Circular dichroism spectroscopy revealed that these amino acids can bind proteins and significantly influence their secondary structure, particularly enhancing α-helical content. Additionally, one of the compounds demonstrated selective binding to G-quadruplex DNA, suggesting potential in nucleic acid targeting for anticancer strategies. Dynamic light scattering (DLS) and scanning electron microscopy (SEM) analyses showed that these amino acids are capable of self-assembling into nanoscale to micrometric aggregates (Figure 1).

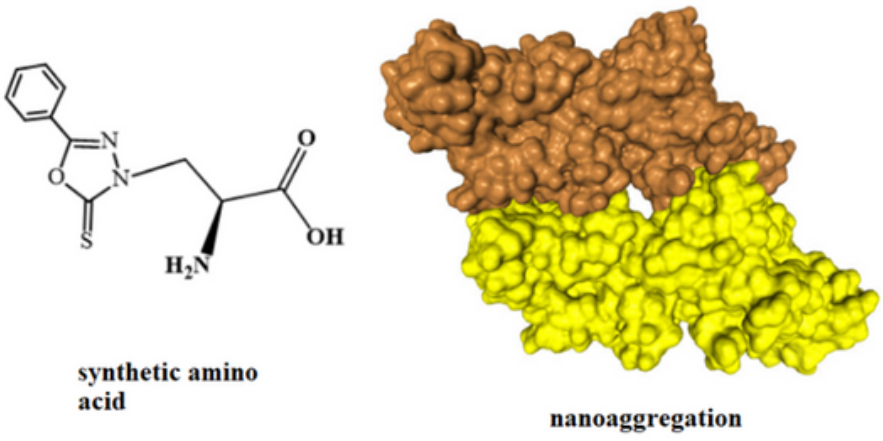

Figure 1. One of the derivatives employed in our study and an example of their nanoaggregates.

These aggregates exhibited structural features suitable for encapsulating small bioactive molecules, such as curcumin, indicating a promising role in targeted drug delivery.

Cell viability assays on human fibroblasts confirmed the biocompatibility of the derivatives, with some variants also promoting cell proliferation, highlighting their potential in tissue regeneration and scaffold development.

Overall, this study highlights the structural versatility and functional promise of synthetic amino acids as molecular tools for biomedicine, combining protein and DNA interaction capabilities with self-assembly behavior and cellular compatibility.

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MERCURY LEVELS IN BIOLOGICAL SAMPLES OF WOMEN WITH AND WITHOUT BREAST CANCER: CORRELATION AND RISK ASSESSMENT

Joanna Słowik[1], Barbara S. Radecka[2], Joanna Tomiczek-Szwiec[3,4], Patryk Zając[5], Mariusz Kubus[6], Mariusz Głowacki[7], Danuta Witkowska[1]

[1]Institute of Health Sciences, University of Opole, 45-060 Opole, Poland
[2]Department of Oncology, Institute of Medical Sciences, University of Opole, 45-040 Opole, Poland
[3]Department of Biology and Genetics, Institute of Medical Sciences, University of Opole, Oleska 48, 45-052 Opole, Poland
[4]Clinical Department of Oncological Gynecology at the Oncology Centre in Opole, 45-061 Opole, Poland
[5]Department of Clinical Biochemistry and Laboratory Diagnostics, Institute of Medical Sciences, University of Opole, Poland
[6]Centre of Education and Mathematics Applications, Opole University of Technology, 45-758 Opole, Poland
[7]Institute of Environmental Engineering and Biotechnology, University of Opole, Kard. B. Kominka 6a, 45-032, Opole, Poland
e-mail: joanna.slowik@uni.opole.pl

Heavy metals, including mercury, are commonly found in the human environment, food, cosmetics, and dietary supplements [1,2]. These elements may exert harmful effects on human health, including mutagenic activity that can contribute to carcinogenesis[3,4]. Mercury exposure has also been associated with nonspecific symptoms such as fatigue, cognitive impairment, and neurodegenerative disorders [5]. Mercury is divalent metalloestrogen that may activate estrogen receptor alpha (ERα), induce the expression of estrogen-responsive genes, and promote the proliferation of breast cancer cells, particularly in the MCF-7 cell line [6]. Although present in both normal and cancerous breast tissues, mercury may contribute to carcinogenesis by interacting synergistically with other toxic metals, potentially driving genetic mutations and tumor progression.

The objective of this study was to investigate the potential association between mercury exposure and the risk of developing breast cancer. In a retrospective study, mercury levels were measured in biological samples from women diagnosed with breast cancer (n = 25) and compared with a control group of healthy women without a history of cancer (n = 42). In the control group, mercury levels were assessed in both hair and nail samples. In the breast cancer group, only nail samples were analyzed. Mercury concentration was measured using the AMA 254 analyzer. Correlations between mercury concentrations in hair and nails were also examined. The study did not reveal elevated mercury concentrations in biological materials from the oncology group. However, other noteworthy associations were identified.

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ANTIMICROBIAL PEPTIDOMIMETICS BASED ON SALIVARY PEPTIDES –A COMPARISON OF STABILITY, STRUCTURE, COORDINATION CHEMISTRY AND ANTIMICROBIAL ACTIVITY

Klaudia Szarszoń[1], Arian Kola[2], Tomasz Janek[3], Fabio Zobi[4], Robert Wieczorek[1], Daniela Valensin[2], Joanna Wątły[1]

[1] Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
[2] Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Via A. Moro 2, 53100 Siena, Italy
[3] Department of Biotechnology and Food Microbiology, Wrocław University of Environmental and Life Sciences, Chełmońskiego 37, 51-630 Wrocław, Poland
[4] Department of Chemistry, Fribourg University, Chemin Du Musée 9, 1700 Fribourg, Switzerland
email: klaudia.szarszon@uwr.edu.pl

Salivary mucin, MUC7, involved in the body's innate immune defense, is naturally cleaved into peptide fragments in saliva, some of which exhibit potent antimicrobial activity[1]. However, their therapeutic potential is limited by rapid enzymatic degradation. To overcome this challenge, a native MUC7-derived peptide was chemically modified using D-amino acids and a *retro-inverso* strategy to enhance its stability without compromising its function[2].

Given the known role of metal ions in modulating antimicrobial peptides [3], we explored the coordination chemistry and biological activity of both native and modified MUC7 fragments with Cu(II) and Zn(II) ions. A comprehensive suite of experimental and computational techniques - including potentiometric titrations, UV-Vis, circular dichroism (CD), EPR, NMR spectroscopy, mass spectrometry, and DFT calculations, were employed to characterize metal binding, peptide and complex structure, and thermodynamic stability of complexes.

Our findings reveal that the standard substitution of L-amino acids with D-amino acids, as well as the modifications introduced by *retro-inverso* strategy, preserve the peptides' secondary structure and antimicrobial activity, while altering significantly the thermodynamic stability of the metal complexes and proteolytic stability of the studied peptides[4,5].

Acknowledgements: The work was supported by the National Science Centre (Grant UMO-2021/41/B/ST4/02654).

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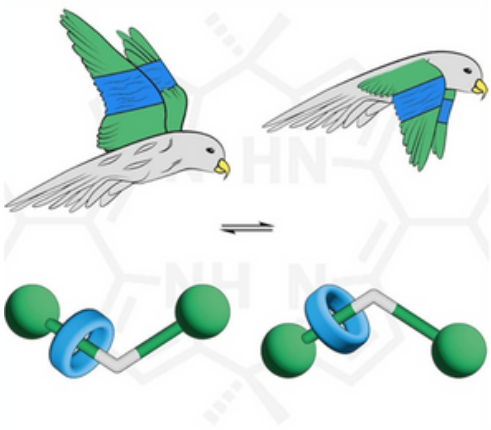
PYRROLE-BASED MECHANICALLY INTERLOCKED MOLECULES: DYNAMICS, TAUTOMERISM, CHIRALITY

Bartosz Szyszko
Uniwersytet Wrocławski
F. Joliot-Curie St. 14, 50-383 Wrocław, Poland
email: bartosz.szyszko@uwr.edu.pl

Mechanically interlocked molecules (MIMs) represent a unique class of supra-molecular systems characterized by the presence of a mechanical bond, with rotaxanes and catenanes serving as prototypical examples[1]. This talk will focus on two fundamental aspects of mechanically interlocked pyrrole-based MIMs. First, it will explore the use of the diiminopyrrole motif in subcomponent self-assembly[2-4], to construct molecular knots and links that exhibit intramolecular dynamics facilitated by the fluxionality of coordinated metal centers. Furthermore, the discussion will highlight how the introduction of more complex pyrrole-derived building blocks enables the synthesis of mechanically interlocked porphyrinoids, offering new avenues for functional molecular design. The second part of the talk will discuss a new class rotaxanes incorporating dipyrro-methane stoppers designed to construct dynamic MIMs5. A key focus will be on the discovery and characterization of a new mode of molecular motion, referred to as fluttering, which is reminiscent of butterfly wing flapping.

The multimodal motion can be precisely modulated using simple acid-base chemistry, providing a versatile platform for designing stimuli-responsive molecules. The higher-order calix[4]phyrin-based mechanically interlocked molecules will also be discussed, further expanding the structural and functional diversity of these systems[6]. Eventually, it will be demonstrated how the molecular editing of an achiral [2]rotaxane comprising a pyrrole ring allows it to transform into the mechanically planar chiral species7.



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FORMATION OF POLYMERS LAYERS FOR ELECTROCHROMIC APPLICATIONS BY ON-SUBSTRATE POLYMERIZATION METHODS

Monika Wałęsa-Chorab
Departament of Chemistry, Adam Mickiewicz University
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
e-mail: mchorab@amu.edu.pl

Electrochromism is defined as the capability of the material to changes of its optical properties (color change) in response to an external electric stimulus. New absorption bands at different parts of the visible or near infrared regions are generated by switching between different redox states[1]. Electrochromic compounds are widely used as active materials in many device types, such as e-papers, smart windows and mirrors, and dynamic camouflage technologies. For the construction of electrochromic devices electroactive material must be deposited onto electrode as a thin film. Solution processable materials, when used as electroactive layers are often miscible with electrolyte gel what results in limited device lifetime, poor device performance, localized color defects and poor color contrast[2]. The best way to obtain non soluble electrochromic layer is formation of the thin film by polymerization of solution processable monomers directly on an electrode surface.

There are few different ways of obtaining of stable thin films of polymers for electrochromic uses directly onto an electrode surface including photo-polymerization[3], electropolymerization[4] or polycondensation of complementary monomers. New materials obtained by on-substrate polymerization methods will be presented and their electrochromic properties will be discussed.

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TRANSITION METAL VS. ORGANOCATALYZED HYDROMETALLATION REACTIONS

Jędrzej Walkowiak, Jakub Szyling, Tomasz Sokolnicki, Paweł Huninik, Barbara Krupa, Konrad Stęsik, Aleksandra Szymańska, Adrian Franczyk, Kinga Stefanowska

Adam Mickiewicz University, Center for Advanced Technologies
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
e-mail: jedrzejw@amu.edu.pl

Organoboron and organosilicon compounds are key reagents in modern organic chemistry due to their high stability, low toxicity, and unique reactivity [1]. While transition metal (TM)-catalyzed processes still dominate this field, catalysts based on main group elements or organocatalysts are increasingly gaining importance. Notably, these alternative catalytic approaches often lead to different products compared to conventional TM-catalyzed hydrometallation reactions.

Our research focuses on highly selective methods for the synthesis of organoboron and organosilicon compounds, based on hydrometallation of olefins, alkynes, conjugated 1,3-diynes, carbonyl compounds, imines, and nitriles [1-7]. The communication will discuss the new methods for the functionalization of these compounds using practical and straightforward catalytic systems based on TM and organocatalysts. We will demonstrate that the appropriate selection of readily available catalysts can significantly influence or alter the regio- and stereo-selectivity of the process. The application of the obtained products in the synthesis of valuable compounds and active pharmaceutical ingredients (APIs) will be also discussed [1-7].

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DEVELOPMENT OF NOVEL PEPTIDE-MIMETIC COMPOUNDS AS POTENTIAL ANTICANCER AGENTS: A COLLABORATIVE POLISH-ITALIAN-ARMENIAN STUDY

Danuta Witkowska[1], Giovanni N. Roviello[2], Agnieszka Rombel-Bryzek[3], Paweł Lenartowicz[4] and Hayarpi Simonyan[5]

[1]Institute of Health Sciences, University of Opole, 45-060 Opole, Poland
[2] Institute of Biostructure and Bioimaging, CNR, 80134, Naples, Italy
[3] Institute of Medical Sciences, University of Opole, 45-052 Opole, Poland
[4] Institute of Chemistry, University of Opole, 45-052 Opole, Poland.
[5]Institute of Pharmacy, Yerevan State University, 0025, Yerevan, Armenia
e-mail: danuta.witkowska@uni.opole.pl

The search for effective anticancer drugs has been ongoing for decades. While many potential therapeutic candidates have been identified, the search for effective anticancer therapeutics remains a major challenge in biomedical research[1]. Although numerous candidate compounds show promising anticancer activity, their clinical applicability is often limited by significant toxicity to healthy human cells and organs[2]. To overcome this limitation, we have designed a novel series of compounds structurally inspired by natural short peptides.

These peptide-mimetic compounds are intended to inhibit the bifunctional purine biosynthesis protein ATIC by disrupting its dimerization, thereby suppressing pathological cell proliferation. This approach specifically targets cancer cells, which exhibit a heightened reliance on *de novo* purine synthesis[3], as well as cells involved in proliferative arterial disease[4].

The initial series of compounds underwent molecular docking studies, from which the most promising candidates were selected for chemical synthesis. Their interactions with ATIC are currently being characterized through isothermal titration calorimetry (ITC) and dynamic light scattering (DLS). In parallel, cytotoxicity assays on various cancer cell lines *in vitro* are underway to assess their therapeutic potential.

This multidisciplinary project combines the expertise of research teams from Poland (University of Opole), Italy (CNR-IBB), and Armenia (YSU) in identifying the most potent and selective peptide-mimetic inhibitors. Compounds that demonstrate favorable *in vitro* activity and biophysical properties will be advanced to *in vivo* evaluation at our partner institution (CCU, USA), using genetically engineered *Drosophila melanogaster* models that recapitulate cancer-related pathologies.

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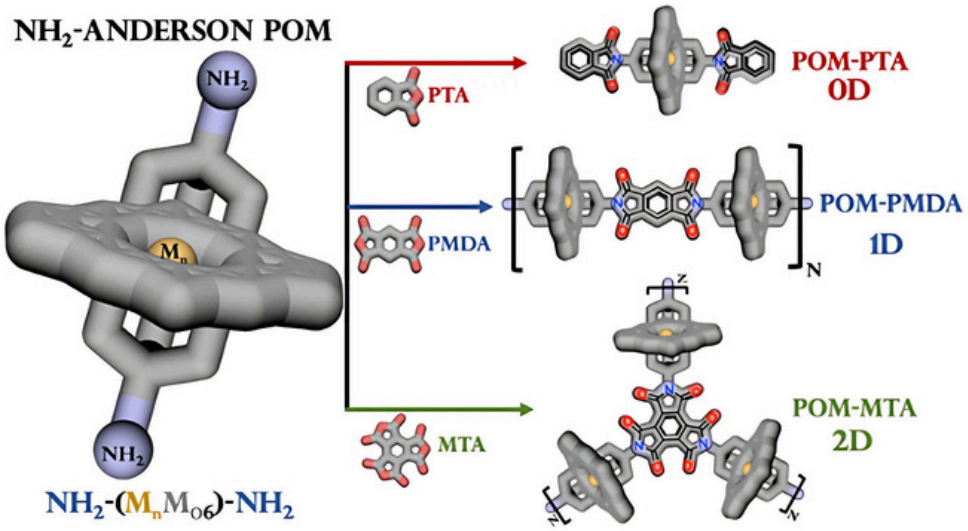
ABSTRACTS

Poster Presentations

NEW MULTIFUNCTIONAL COMPLEXES D- AND F-METAL IONS WITH SCHIFF BASES AND POM

Violetta Patroniak
Adam Mickiewicz University
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
email: violapat@amu.edu.pl

The synthesis of supramolecular complexes is currently one of the most explored areas of coordination chemistry due to their chemical and physical properties, unusual structures, and potential applications[1]. Characterization and study of the properties of new complexes of d- and f-metal ions are scientific goals pursued for many years by our research group. The presented topic of the talk will concern transition metal complexes with N-heterocyclic ligands and POMs, with special emphasis on their luminescent, magnetic, catalytic, photocatalytic, electrocatalytic and biological properties[2-9].



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SALEN-TYPE NICKEL(II) COMPLEXES IN DISTINCT SELECTIVE HYDROSILYLATION OF ALKENES UNDER MILD CONDITIONS

Bartłomiej Szarłan, Jakub Robaszkiewicz, Maciej Zaranek and Piotr Pawluć
Faculty of Chemistry and Centre for Advanced Technologies Adam Mickiewicz University Uniwersytetu Poznańskiego 8-10, 61-614 Poznań, Poland
email: piotrpaw@amu.edu.pl

The hydrosilylation reaction represents one of the most pivotal catalytic processes employed in the synthesis and functionalization of organosilicon compounds. Traditionally, these transformations have relied on complexes of noble metals such as platinum, rhodium, and ruthenium. However, the high cost and limited recyclability of these metals in industrial applications have prompted the search for alternative catalysts that are both more economically and environmentally sustainable. In this context, increasing attention is being directed toward catalysts based on more earth-abundant first-row transition metals (*3d*-block elements) such as iron, cobalt, and nickel [1].

In this communication, we report on the development of novel, efficient, and selective catalytic systems for the regiodivergent hydrosilylation of functionalized alkenes. These systems are based on nickel(II) complexes bearing salen-type ligands (Figure 1) in combination with alkali metal trialkylborohydrides [2].

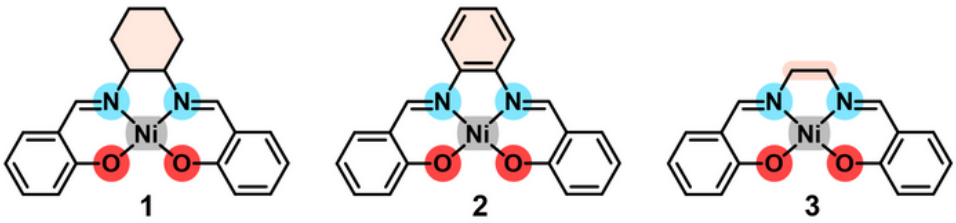

Figure 1. Nickel salen-type complexes used in our studies.

A key aspect of the research involves the optimization of experimental protocols to enhance the efficiency and selectivity of the investigated catalytic systems, alongside efforts to elucidate the underlying mechanisms of the catalytic transformations. Particular attention will be devoted to examining the influence of ligand architecture and complex structure on the catalytic performance and selectivity of nickel-based (pre)catalysts.

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FORMATION OF GRAPHENE/MNO_2 COMPOSITE ELECTRODES FOR A MICROFLUIDIC DEVICE FOR THE QUANTITATIVE DETECTION OF H_2O_2

Veronika Poltavets[a], Martin Jönsson-Niedziółka[b]

[a] Dnipro State Medical University, Vernadsky St., 9, Dnipro City, Ukraine, 49044.

[b] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

email: martinj@ichf.edu.pl ; verapolt9@gmail.com

Quantitative detection of hydrogen peroxide in biochemical processes provides important information for screening oxidative stress. Microfluidic electrochemical systems make it possible to work with microquantities of biological material and determine H_2O_2 concentrations of the order of micromoles[1]. The high selectivity and sensitivity of electrodes based on MnO_2 materials have an important influence on the process. However, manganese dioxide has some disadvantages that became apparent during the work process. Due to poor conductivity, the layer of working material must be very thin and does not allow for long-term use of the chip.

The aim of this investigation is to form a graphene/MnO_2 composite as a working electrode, which will combine high sensitivity and more stable operation of the biosensor.

During work, we used graphene from ACS MATERIAL: graphene dispersion in water 1-3 μm. The reagent was diluted in water and prepared in several solutions. The material was ultrasonicated, then a drop was applied to the glass of the ITO and kept at 300 ^{0}C for 10 minutes. The surface was examined by SEM and showed that it contains graphene with some flakes perpendicular to the surface in the form of peaks. The lower the concentration of the solution, the thinner the flakes, but they do not cover the entire surface. Therefore, the optimal method for applying a graphene substrate is sequential application of three layers of graphene from a low-concentration solution. The resulting precipitate was then electrochemically coated with MnO_2 from a sulphate electrolyte, controlling its thickness.

During measurements of the catalytic activity of the obtained graphene/MnO_2 composite, a stable analytical signal with high sensitivity was obtained.

Acknowledgements: This work was supported by the Fellowship Program from the Visegrad Fund for supporting researchers (62510049).

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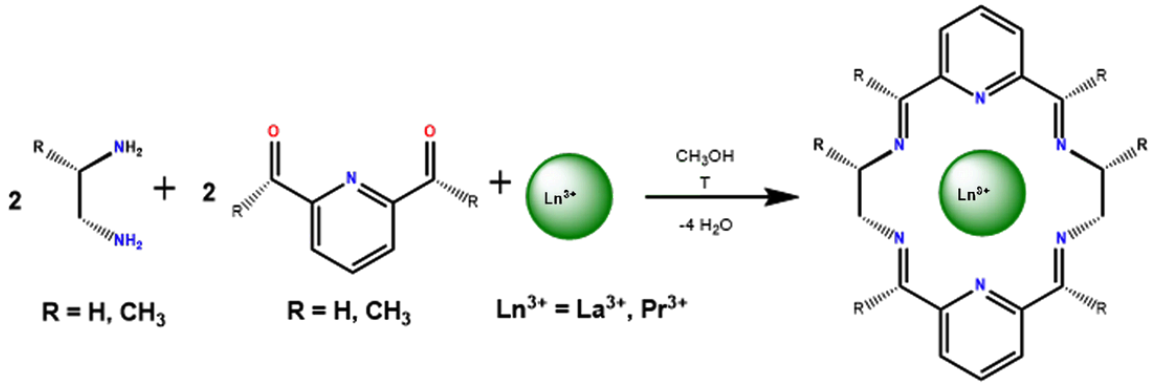
SUPRAMOLECULAR ARCHITECTURES FORMED BY SELF-ASSEMBLING N6-DONOR SCHIFF BASE LIGANDS WITH LANTHANIDE ION

Izabela Pospieszna-Markiewicz, Marta Fik-Jaskółka, Ernest Ewert, Violetta Patroniak
Adam Mickiewicz University
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
email: izap@amu.edu.pl

Q Hexadentate macrocyclic ligands containing six nitrogen donor atoms constitute highly effective chelating agents, particularly in the coordination chemistry of lanthanide ions. These ligands coordinate through all six nitrogen atoms concurrently, resulting in the formation of kinetically inert and thermodynamically stable complexes. The macrocyclic structure forces the molecule into a specific shape and increases the stability of the complex due to the macrocyclic effect. Lanthanide ions, characterized by relatively large ionic radii and a propensity for high coordination numbers, exhibit a strong affinity for hexadentate nitrogen-donor ligands. Such ligands effectively occupy the metal coordination sphere. The lanthanide complexes demonstrate significant applicability in various biomedical domains. They are extensively employed in diagnostic imaging modalities, targeted therapeutic delivery systems, and advanced bioanalytical methodologies. The unique photophysical and magnetic properties intrinsic to lanthanide ions, when stabilized by hexadentate macrocyclic ligands, facilitate sensitive detection, and real-time monitoring of biochemical and molecular events.

We report the synthesis of various Schiff base compounds containing six nitrogen donor atoms (N6). Macrocyclic complexes with lanthanide ions were obtained by templated synthesis exhibit differences in the substituent R= -H or -CH_3, present in the ketone or aldehyde substrate as well as in the diamine molecule (Scheme 1). [1,2] The synthetic conditions were modified to obtain different types of supramolecular compounds. The following substrates were used: 2,6-pyridinedicarboxyaldehyde, 2,6-diacetylpyridine, 1,2-diaminoethane, and 1,3-diaminoethane.



Scheme 1. Synthesis of different types of hexadentate macrocyclic complexes.

NEW HORIZONS IN ANTICANCER THERAPY: THE ROLE OF DIPYROMETHENE-BASED COMPLEXES

Ewelina Wieczorek-Szweda[1], Martyna Mańka[1,2], Patrycja Płócienniczak-Bywalska[3], Izabela Pospieszna-Markiewicz[1], Ernest Ewert[1], Giovanni Roviello[4], Marta Fik-Jaskółka[1], Violetta Patroniak[1]

[1] Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznanskiego 8, 61-614 Poznan, Poland

[2] Université de Strasbourg, CNRS, ISIS 8 allée Gaspard Monge, Strasbourg 67000, France

[3] Institute of Chemistry and Technical Electrochemistry, Poznan University of Technology, Berdychowo 4, 60-965 Poznan, Poland

[4] CNR, Istituto di Biostrutture e Bioimmagini – (Area di Ricerca Site and Headquarters), 80131 Napoli, Italy

email: ewelina.wieczorek-szweda@amu.edu.pl

In the present era, the objective of researchers and oncologists alike is the establishment of a comprehensive framework for the eradication of cancer, with a concomitant reduction in the toxicity of the treatment and an improvement in the quality of life of patients. The development of new DNA-binding agents helps in understanding cellular functions and exploring potential treatment for cancer-related diseases [1-3]. While dipyrromethene based ligands, particularly BODIPY derivatives, have been extensively studied for these purposes, their metal ion complexes remain unexpectedly underdeveloped in this area. To address this, a small library of new azadipyrromethene (ADPM) and dipyrromethene (DPM) complexes with zinc(II), cobalt(II) and copper(II) ions was prepared, with bromo-substituent located at the proximal terminus of the ligand (Fig. 1).

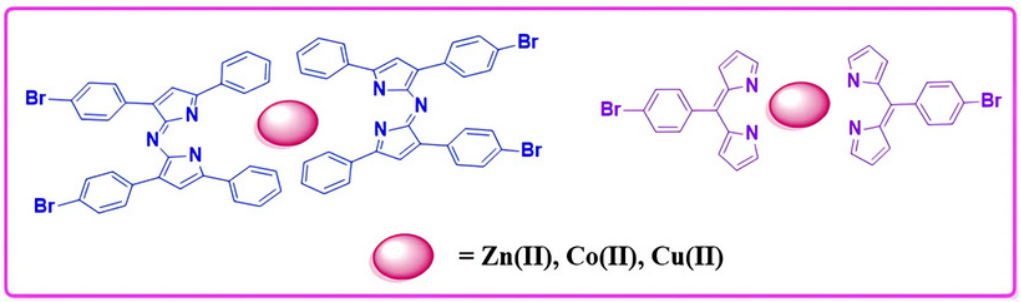


Fig 1. Synthesis of different types of hexadentate macrocyclic complexes.

Due to their structural characteristics, these compounds exhibit favorable spectroscopic, electrochemical, and photochemical properties, making them well-suited for use as anticancer agents. The development of a this novel class of metal complexes incorporating DPM and aza-DPM ligands coordinated with biologically relevant metal ions represents a promising strategy for the design of new anticancer agents.

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APPLICATION OF 3D METAL PINCER COMPLEXES IN THE SYNTHESIS OF ORGANOBORON COMPOUNDS

Grzegorz Hreczycho
Adam Mickiewicz University
Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland
e-mail: g.h@amu.edu.pl

Modern chemical synthesis places a strong emphasis on sustainability by minimizing the use and generation of hazardous substances. This is largely achieved through catalysts that activate new reaction pathways, enhancing process selectivity and enabling the use of less reactive substrates[1].

A noteworthy example of recently well-studied homogeneous catalysts is pincer 3d metal complexes. These catalysts are known for their relatively simple synthesis, high stability, activity, and selectivity in reactions such as hydrogenation, hydroboration, hydrosilylation, and bond formation[2-4]. A key feature is their tunable selectivity, which can be modified by altering reaction conditions or ligand structure.
In my communication, I will present the synthesis of organoboron compounds catalyzed by cheap pincer complexes. The presented methodology enables ligand-controlled synthesis regarding the principles of sustainable chemistry leading to a valuable group of compounds[5-7].

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AMINO ACID BASED SELF-ASSEMBLED NANOSTRUCTURES

Artur R. Stefankiewicz[1,2]

[1] Center for Advanced Technologies, Adam Mickiewicz University in Poznań, Poland
[2] Faculty of Chemistry, Adam Mickiewicz University in Poznań, Poland
e-mail: ars@amu.edu.pl

The self-assembly approach, where molecules spontaneously arrange themselves into ordered structures through non-covalent interactions, has been a subject of extensive research. Initially focused on purely synthetic or natural components, this approach is currently shifting towards incorporating hybrid building blocks that seamlessly blend synthetic and naturally occurring motifs[1-6]. This change is particularly intriguing due to the potential of adaptive materials mimicking biopolymers, which have found profound applications across biotechnology, medicine, and engineering. This presentation will highlight selected examples of the self-assembly of amino acid based component into functional nanostructures (more information at www.arsgroup.amu.edu.pl).

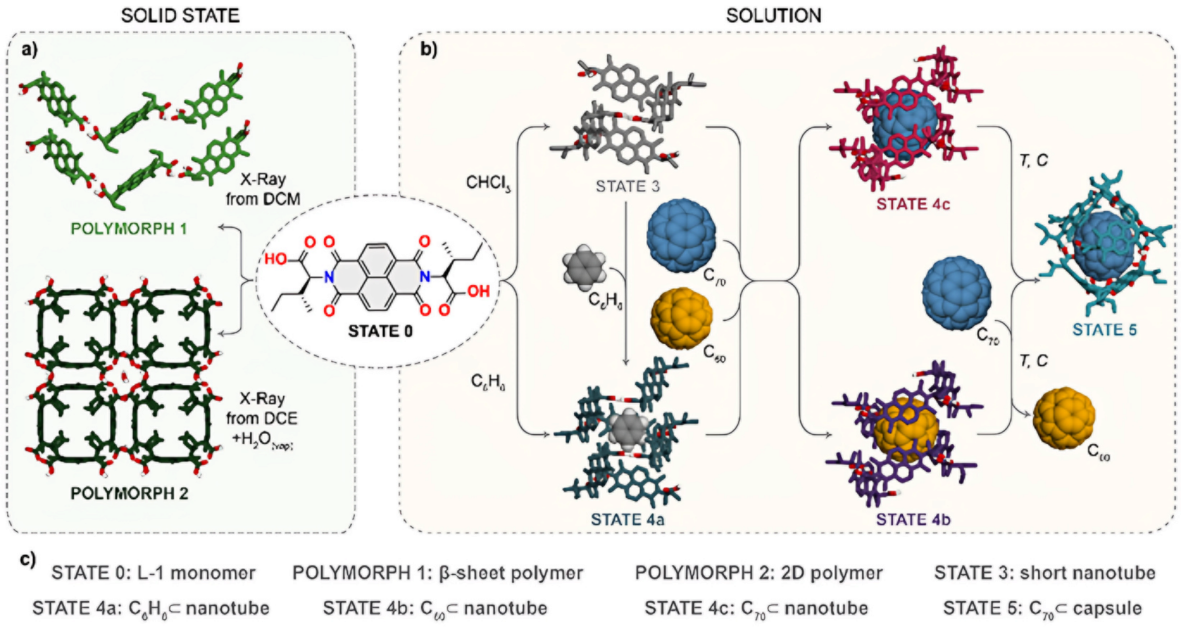

Figure 1. A structural reorganization of this artificial system into five distinct supramolecular states was accomplished, through modulation of solvent, temperature, concentration, and guest molecules.

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Javornik Uroš
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K
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Peana Massimiliano F.
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Plavec Janez
Pluskota-Karwatka Donata
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Pniakowska Anna
Podgajny Robert
Poltavets Veronika
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Remelli Maurizio
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Robaszkiewicz Jakub
Rolle Katarzyna
Rombel-Bryzek Agnieszka
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S
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Wątły Joanna
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Wieczorek-Szweda Ewelina
Wiloch Magdalena
Witkowska Danuta
Wyrzykowski Dariusz

Z
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Zaranek Maciej
Zobi Fabio

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