
8th George Olah Conference

*XXIV Conference of the George Olah
Doctoral School*

15 September 2026



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Program

EVENT VENUE: BME CH201 ROOM PUNGOR

8³⁰ Opening

ORAL PRESENTATIONS

Chairman: László Poppe

8³⁵-9¹⁰ Norbert Németh– Applications of nonlinear phenomena in chemical systems and synthesis methods especially ZIF formation – Invited lecturer, George Olah Prize winner in 2025

9¹⁰-9⁴⁵ András Kotschy – The future of drug discovery: challenges and answers – Invited lecturer from Servier Research Institute of Medicinal Chemistry

9⁴⁵-10²⁰ Ádám Csaba – From Feedstock to High-Performance Polymers – MOL's Integrated Petrochemical Value Chain – Invited lecturer from MOL Petrochemicals Co. Ltd., Polymer Asset Team Technology Leader

10²⁰-10⁴⁰ Coffee Break

Chairwoman: Emília Csiszár

10⁴⁰-11⁰⁰ Viktória Feigl – Bioleaching of critical raw materials from bauxite residue – Invited lecturer from the Department of Applied Biotechnology and Food Science

11⁰⁰-11²⁰ László Ferenc Simon – Surface wave-based multiparametric biosensors for comprehensive analysis of biomolecules – Invited lecturer from the Department of Inorganic and Analytical Chemistry

11²⁰-11⁴⁰ Péter Keglevich – Synthesis of anticancer Vinca alkaloid and flavonoid derivatives – old scaffolds, new perspectives – Invited lecturer from the Department of Organic Chemistry and Technology

11⁴⁰-12⁰⁰ Borbála Tegze – Energy transfer between upconverting nanoparticles and dye molecules in aqueous suspensions and in chitosan-based composite coatings – Invited lecturer from the Department of Physical Chemistry and Materials Science

12⁰⁰-12²⁰ Éva Pusztai– Beyond regulatory guidelines: industrial applications of tolerance intervals – Invited lecturer from the Department of Chemical and Environmental Process Engineering

12²⁰-13²⁰ Coffe Break and Poster session – 2nd floor

P01	Emanuela Cullhaj	Viscoelasticity and adhesion of hydroxypropylmethyl cellulose and chitosan films on biomimetic hydrogels.
P02	Otília Tóth	Investigating the effect of catalytically inactive dUTPase enzyme in mouse embryonic fibroblast cells
P03	Petra Kántor	Controlled hydrothermal decomposition of polymers and their composites
P04	Balázs Almási	Thiolactams to cyclic (alkyl)(amino)carbenes – catalysis of alkali metal reduction
P05	Kenéz Balázs	Development of Functionalized Bacterial Nanocellulose Membranes for the Selective Immobilization of Recombinant Enzymes
P06	Lucy Nyambura Karanja	Visible light photocatalytic activity of 2D/1D g-C ₃ N ₄ /ZnO heterostructure for efficient degradation of Rhodamine 6G, 4-Nitrophenol, and Ciprofloxacin
P07	Kese István	Synthesis and Characterization of Novel Alkylthioether-Alpha-Cyclodextrin Derivatives and Their Impact on Bacterial Biofilm Formation
P08	Daniel Mulu Mengistu	Production of Bacterial-Derived Bio-filler For Concrete Crack Bio-grouting and Sealing in Construction and Buildings
P09	Laki Anna	Comparison of Tolerance Interval Calculation Methods for Accuracy and Precision under USP <1210>
P10	Apoko S. Omondi	Mn–Cr dopant association in dilute co-doped ZnAl ₂ O ₄ revealed by combined EPR and optical spectroscopy

STUDENTS' ORAL PRESENTATIONS**Section A – CH201****Chairman: Zsolt Kelemen**

- 13²⁰-13³⁵ **Noor Al Deeb** – Quantum Chemical Insight into Catechol/o-Quinone redox cycling and O₂⁽⁻⁾ generation: The case of Estrogens
- 13³⁵-13⁵⁰ **Gao Yanhong** – B-substituted carboranes as light-emitting materials
- 13⁵⁰-14⁰⁵ **Dániel Steinsits**– Synthesis of various C3-substituted oxindoles from isatins
- 14⁰⁵-14²⁰ **Máté Gergő Benczúr** – Innovative modelling of tablet dissolution using physics-informed neural networks

14²⁰-14³⁰ Break

Section B – CH201

Chairman: **László Poppe**

- 14³⁰-14⁴⁵ **Ghazwan Saleh Ahmed** – Kinetic study for enzymatic biodiesel production from sunflower oil by interesterification reaction
- 14⁴⁵-15⁰⁰ **Szajkó Milda Blanka** – Thymidylate synthase inhibition is associated with single-stranded DNA accumulation and mutagenesis
- 15⁰⁰-15¹⁵ **Daniel Mulu Mengistu** – Production of Bacterial-Derived Bio-filler For Concrete Crack Bio-grouting and Sealing in Construction and Buildings
- 15¹⁵-15³⁰ **Judit Budai** – Optimization of the glycolysis of flexible polyurethane foams for sustainable polyol recovery
- 15³⁰-15⁴⁵ **Sameela Thachaparamban** – Measurement of local viscosity with a fluorescent molecular rotor

Abstracts of students' lectures

Quantum Chemical Insight into Catechol/o-Quinone redox cycling and $O_2^{\cdot-}$ generation: The case of Estrogens

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Long-term exposure to estrogens has been associated with an increased risk of carcinogenesis, with their oxidative metabolites proposed as key contributors to this process. Estrogen-induced carcinogenicity arises from two major pathways: direct genotoxic effects through DNA-quinone adduct formation, and the redox cycling of catechol metabolites, which generates superoxide radical anions ($O_2^{\cdot-}$) and oxidative stress. While experimental evidence supports redox cycling for certain polycyclic aromatic quinones, the capacity of estrogen-derived catechols to sustain this process under physiological conditions remains unresolved.

In this work, we developed a quantum chemical protocol to assess the redox cycling potential of nine catechol/quinone systems, including 2- and 4-hydroxylated metabolites of estrone, equilin, and equilenin, benchmarked against three reference compounds with experimentally established redox-cycling activity (β -lapachone[1], 1,4-naphthoquinone[2], and 9,10-phenanthrenequinone[3]). Acidity constants (pK_a) and standard reduction potentials (E°) were computed using density functional theory (DFT) and validated against high-accuracy LNO-CCSD(T) calculations. Kinetic barriers for electron transfer were evaluated using Marcus theory, while hydride transfer transition states were located explicitly.

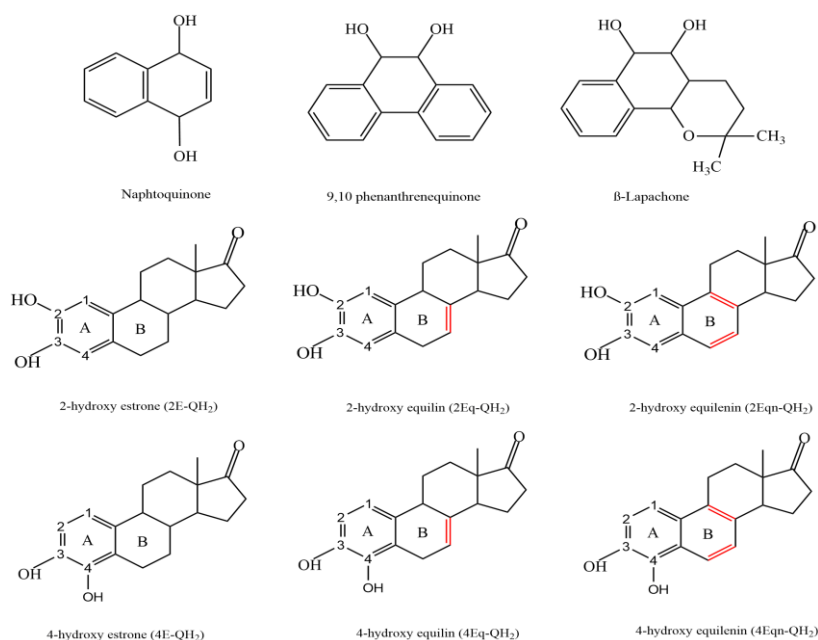


Figure 1 Structure of species with experimentally established redox-cycling: 1,4-naphthoquinone (Naph-Q), 9,10-phenanthrenequinone (Phe-Q) and β -lapachone (Beta-Q) and Structure of the studied estrogen catechols. Unsaturated bonds in ring B are shown in red.

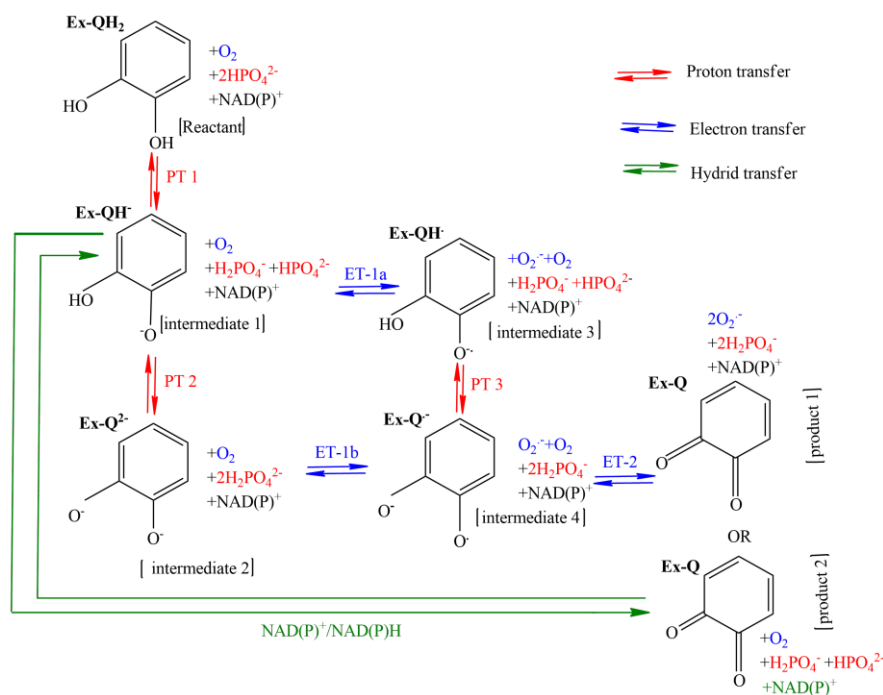


Figure 2 Elementary steps of the redox cycle. In our study we used O₂ as oxidant and the H₂PO₄⁻/HPO₄²⁻ couple as proton acceptor and donor.

The combined thermodynamic and kinetic analysis demonstrates that 4-hydroxyequilenin, which is represented in the HRT drug (**Premarin**), is the only estrogen metabolite whose redox profile closely resembles that of the reference compounds, indicating its potential to generate superoxide radical anions through continuous redox cycling. Therefore, we suggest that its concentration in pharmaceutical formulations should be carefully monitored. All other studied estrogen catechols exhibit elevated reduction potentials, pK_a values, and activation barriers inconsistent with efficient redox cycling. Furthermore, we propose the first reduction potential of the quinone and the pK_a of the catechol as rapid screening descriptors for assessing the oxidative toxicity of catechol/quinone pairs.

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- [1] L. Dunsmore *et al.*, "Controlled masking and targeted release of redox-cycling ortho-quinones via a C–C bond-cleaving 1,6-elimination," *Nat. Chem.*, vol. 14, no. 7, pp. 754–765, Jul. 2022, doi: 10.1038/s41557-022-00964-7.
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B-substituted carboranes as light-emitting materials

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o-Carborane-based fluorophores have emerged as a distinctive class of luminogenic materials owing to the unique electronic and structural characteristics of the three-dimensional carborane cage. In particular, their pronounced aggregation-induced emission (AIE) and crystallization-induced emission (CIE) behaviors have attracted considerable attention in recent years, as these phenomena provide an effective strategy for overcoming the aggregation-caused quenching commonly encountered in conventional π -conjugated fluorophores. The rigid, electron-deficient, and highly three-dimensional nature of the *o*-carborane cage enables it act as an electron acceptor while the restriction of intramolecular motions upon aggregation or crystallization can efficiently suppress nonradiative relaxation pathways. Despite the C-substituted derivatives of carboranes were deeply investigated and their properties were even reviewed several times, the number of study on the fluorescence of only B-substituted derivatives are limited. In this work, we explored whether B-functionalized *o*-carboranes could provide an alternative platform for AIE/CIE-active fluorophores.

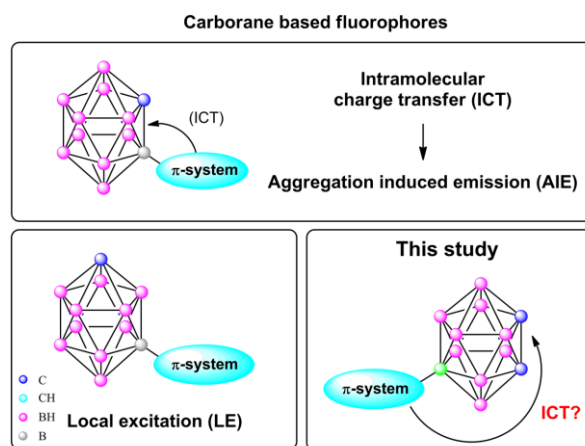


Figure 1. Short description.

A series of B-substituted *o*-carborane derivatives carboranes with different polycyclic aromatic rings with an increased number of rings, phenyl, naphthyl, phenanthrenyl and biphenyl were synthesized and characterized. Their photophysical properties were investigated in solution, aggregated states in THF/H₂O mixtures, and the solid state using UV/Vis absorption and photoluminescence spectroscopy. The compounds showed relatively weak emission in dilute solution but exhibited a slightly increase in fluorescence upon aggregation and several derivatives also displayed strong emission in the crystalline state based on the quantum yield, confirming both AIE and CIE behavior.

Overall, this study demonstrates that B-substituted *o*-carboranes can serve as AIE/CIE-active fluorophores, providing an alternative to conventional C-substituted systems. More importantly, it establishes B-functionalization as a new structural handle for tuning the solid-

state emission of carborane-based materials, thereby expanding the molecular design space for luminescent carboranes.^[1]

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Synthesis of various C3-substituted oxindoles from isatins

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Oxindoles are pharmaceutically interesting molecules due to their wide range of biological properties, including antioxidant, antimicrobial, antiviral, anticancer and central nervous system activities among others.^[1] Similarly, xanthenes also show biological activities in addition to their use as traditional and fluorescent dyes.^[2,3]

In our first research topic, we developed an efficient and simple procedure for the synthesis of 3,3-bis(hydroxyaryl)oxindoles and xanthene-based spirooxindoles. Both groups of oxindoles have been successfully synthesized in good yields using solvent-free microwave (MW)-assisted conditions and low equivalencies (*Figure 1/A*). The synthesized compounds were subjected to *in vitro* cytotoxic activity investigation on six cancer cell lines (4T1, A549, B16, HT29, HT168, HL60) and to antibacterial activity investigation on Gram-positive (*Bacillus subtilis*) bacteria.

In our second research topic, we created a fully continuous, flow procedure for the three-step reductive alkylation of isatins. The process enables the synthesis of 3-alkyloxindole directly from isatin derivatives with wide carbonyl and isatin substrate scope (*Figure 1/B*). The modularity of the method was also demonstrated with successful synthesis of the anticancer drug sunitinib.

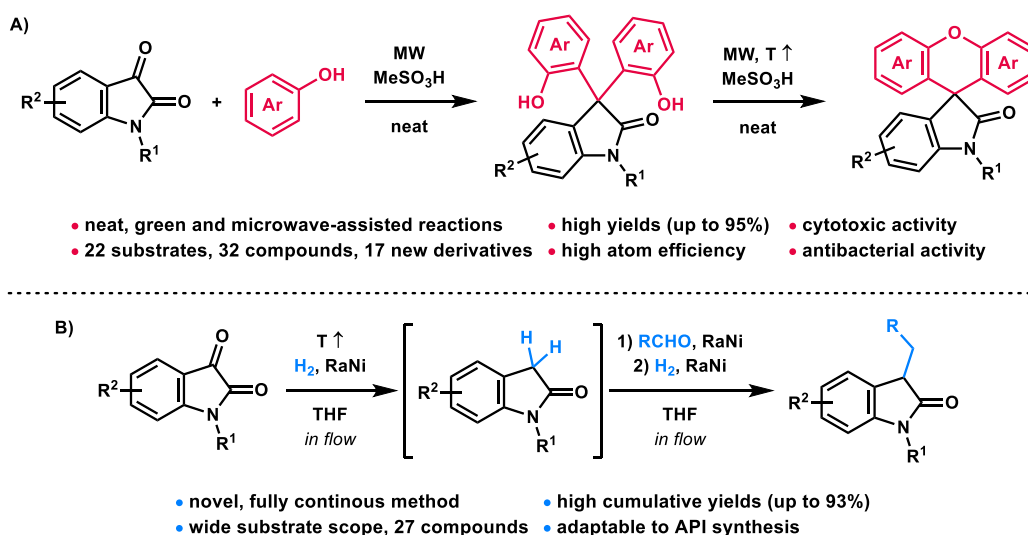


Figure 1. Transformation of isatins via Fridel–Crafts-type reaction to 3,3-bis(hydroxyaryl)oxindoles and xanthenes (A), and via reduction alkylation to 3-alkyloxindoles (B).

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Innovative modelling of tablet dissolution using physics-informed neural networks

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In recent years, the rapid advancement of digitalization has increasingly impacted - among many other fields - the pharmaceutical industry. The Pharma 4.0 paradigm is gaining importance as a key direction of industrial development, emphasizing advanced digital data processing, artificial intelligence, and automated decision support.^[1]

Advanced modeling approaches play an important role in this development, enabling the real-time usage and interpretation of large volumes of manufacturing data for the prediction of critical quality attributes. However, modeling complex pharmaceutical technology systems can present significant challenges. For instance, the modeling of tablet dissolution is a particularly complex task, as the dissolution behavior is simultaneously influenced by numerous technological and formulation parameters, including particle size, porosity, compaction pressure, and excipient composition.^[2] Conventional statistical or mechanistic models may not always accurately capture the underlying complexity of real-world processes, while purely data-driven models, such as the nowadays commonly used neural networks often require large datasets and may not provide reliable predictions across varying process conditions.

The aim of this study is to address this caveat with the development of an artificial intelligence-based model that incorporates relevant physical knowledge, in the form of differential equations. Thanks to the integrated equations, the proposed model is expected to achieve more accurate predictions and improved generalization while requiring substantially less experimental data.^[3]

Empirical mathematical models of tablet dissolution, the Noyes-Whitney and Weibull models were used to explore usage, capabilities and limitations of the method. The models built this way were capable of more accurate predictions compared to traditional neural networks, especially in the case of predictions outside the scope of the training data. Although, in order to achieve accurate predictions, nondimensionalization of the incorporated differential equations was required.

Using these mathematical models, the potential of the proposed method was further tested in situations where the incorporated equations differ from the data used for training and testing. The results indicated that the method is capable of learning the difference between the incorporated equations and the training data, however as said difference was increased, the model was losing accuracy. Therefore, it can be concluded that in order to build a neural network-based model which incorporates physical knowledge, the incorporated physics cannot have significant discrepancies to the modelled phenomenon, thus the data.

In conclusion, the proposed method has potential to take significant part in the implementation and shaping of the Pharma 4.0 paradigm, by providing a modeling approach capable of more accurate and generalizable predictions compared to neural network-based models, with more

flexibility than most mechanistic models. The flexibility of the method also lies in the freedom of choosing any mathematical model to be incorporated, allowing the modeling of complex processes such as tablet dissolution.

The project supported by the Doctoral Excellence Fellowship Programme (DKÖP_M-01-1-BME-17) is founded by the National Research Development and Innovation Fund of the Ministry of Culture and Innovation and the Budapest University of Technology and Economics. Project no. 152739 has been implemented with the support of the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the NKKP Starting_25 funding scheme.

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Kinetic study for enzymatic biodiesel production from sunflower oil by interesterification reaction

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Biodiesel is considered a good alternative to diesel fuel because of its sustainability and environmental-friendly compared to fossil fuels [1-3]. The interesterification reaction for biodiesel production has proved to be a promising reaction type, especially with enzyme catalysts, because it overcomes the problem of glycerol production and the need of its later separation and inhibition effects of glycerol in enzymes^[4,5]. In this study, biodiesel was produced from sunflower oil (used as model oil) by interesterification reaction in a batch process using Novozyme 435 as a catalyst. The reaction conditions used here were temperature (35, 50, and 65 °C) and methyl acetate to sunflower oil molar ratio (9,15, and 30) in 5 h at atmospheric pressure. The experimental results were fitted to the modified Michaelis-Menten equation with allosteric behavior (Eq.1). where V_i is the initial rate (mmol/ml.min), V_{max} is the maximum rate (mmol/ml.min), K_{mTG} and K_{mMA} are the Michaelis-Menten constants for triglyceride and methyl acetate (mmol/ml), K_i is the inhibition constant (mmol/ml), and n is the Hill exponent.

$$V_i = \frac{V_{max} * ([MethAcet][Trigly])^n}{(K_{mTG} * [MethAcet])^n * \left(1 + \frac{[MethAcet]}{K_i}\right) + (K_{mMA} * [Trigly])^n + ([MethAcet][Trigly])^n} \quad (1)$$

The predicted results obtained with the fitted parameters showed an acceptable agreement with the experimental results, as shown in Figure 1 for 50 °C. In order to increase the yield, measurements were conducted for 72 h, and the average equilibrium yield for all conditions was 65.48%.

Pressureized measurements using CO₂ were conducted as well at 50 °C, 9 MR and 72 h with different pressures (2-10 MPa) to increase the yield, and the results showed that the yield was shifted down where CO₂ has a bad effect on the enzyme activity^[6]. The results under carbon dioxide pressure are shown in Figure 2. Unfortunately, although carbon dioxide dissolution in the oil phase was supposed to decrease the viscosity and therefore enhance the reaction rate, the equilibrium conversions were significantly lower than without carbon dioxide.

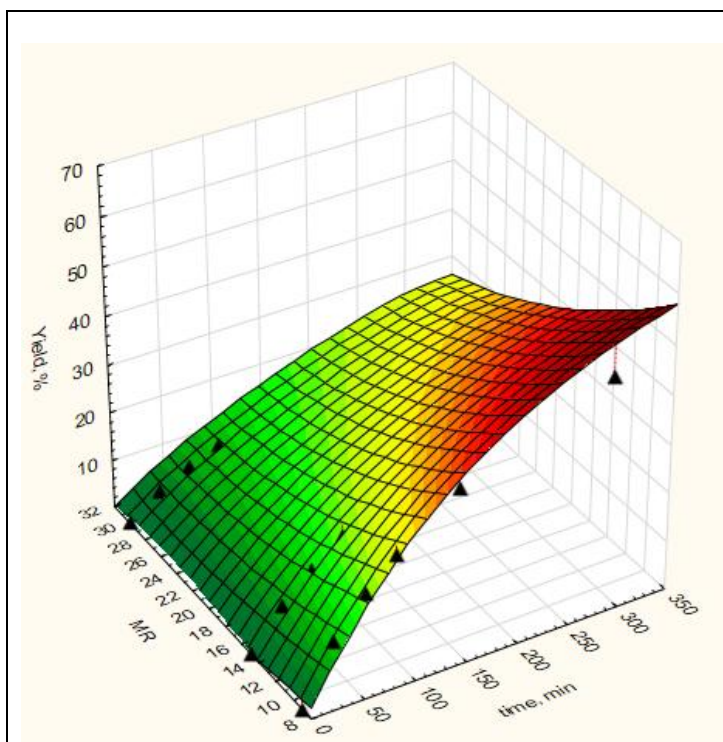


Fig. 1: Atmospheric batch measurements for enzymatic biodiesel production at 50 °C. Surface: fitting, triangle: Experimental

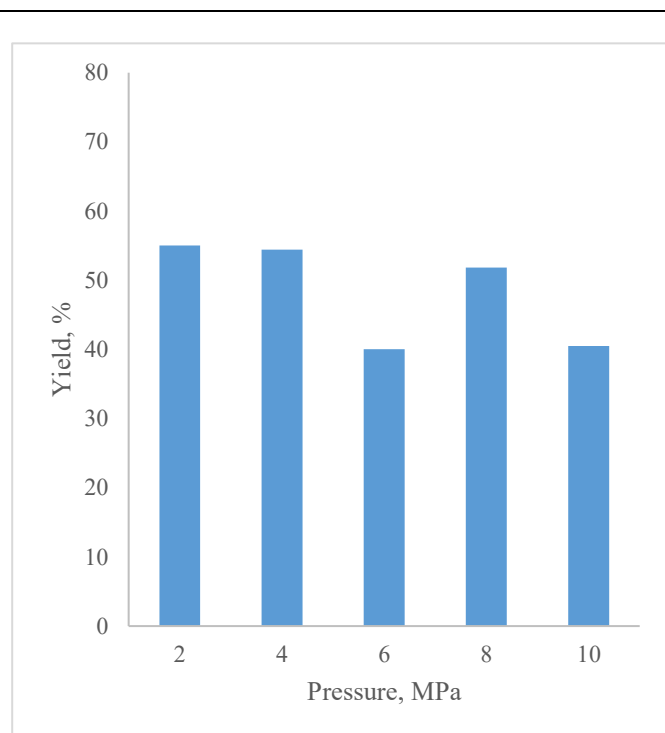


Fig. 2: Pressurized batch measurements for enzymatic biodiesel production at 50 °C, 9MR, and 72 h.

Acknowledgments

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Thymidylate synthase inhibition is associated with single-stranded DNA accumulation and mutagenesis

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Uracil is primarily known as a base of RNA; however, it can also occur in DNA. One possible source of uracil in DNA is cytosine deamination, which can occur spontaneously or be catalyzed by enzymes such as members of the APOBEC family. Since uracil is analogous to thymine in terms of base pairing, unrepaired uracil generated by cytosine deamination can lead to C-to-T transition mutations. At the same time, uracil can also be incorporated into DNA in place of thymine during DNA synthesis. This does not necessarily result in mutations by itself; however, extensive uracil incorporation can lead to genomic instability and, ultimately, cell death due to increased activity of the repair pathways responsible for uracil removal.

This mechanism is exploited by chemotherapeutic agents used in the clinic, which inhibit thymidylate synthase and thereby increase the intracellular dUTP/dTTP ratio, resulting in increased incorporation of uracil into DNA. When uracil excision is inhibited, high levels of genomic uracil can accumulate. In the present study, we investigated the effects of two thymidylate synthase-inhibiting chemotherapeutic agents, raltitrexed (RTX) and 5'-fluoro-2'-deoxyuridine (5FdUR), in a DNA-repair-inhibited colon cancer cell line. The dTTP depletion resulting from thymidylate synthase inhibition can induce replication stress and increased genomic uracil incorporation, which may ultimately lead to cell death.

We performed our experiments using the HCT116 UGI colorectal cancer cell line, which is deficient in mismatch repair and stably expresses an inhibitor of the main uracil-DNA glycosylase (UGI). As removal of uracil is inhibited, genomic uracil accumulates and its consequences can be investigated. Based on our previous results [1], the two drugs induced distinct patterns of uracil accumulation and mutagenesis, which were associated with different cellular responses. RTX treatment resulted in stronger S-phase arrest and lower cell viability than 5FdUR treatment. Moreover using whole genome sequencing, an increased frequency of C→T transitions has been detected in 5FdUR-treated cells compared with both RTX-treated and untreated samples. These mutations primarily occurred in clusters, and their mutational spectrum showed a clear similarity to the AID/APOBEC-associated SBS2 signature. These findings suggested that the increased C→T transitions observed following 5FdUR treatment may be associated with APOBEC-mediated cytosine deamination, resulting in uracil that appears as thymine after PCR and in synthesis-based sequencing methods. In the same study, qPCR analysis revealed drug-induced expression of APOBEC3 (A3) family members, including A3B, C, D, and H. A3C, A3D, and A3H showed a mild increase, with a shift towards 5FdUR, whereas A3B mRNA levels increased markedly following both RTX and 5FdUR treatment.

As single-stranded DNA (ssDNA) is a preferred substrate for APOBEC enzymes, we also investigated the presence of ssDNA in the genomes of these treated cells. Based on

immunocytochemical staining of chromatin-bound RPA, we unexpectedly observed significantly more RPA-positive cells following RTX treatment than following 5FdUR treatment. In parallel, EdU staining revealed significantly lower replication intensity in RTX-treated cells, indicating stronger replication stress. Despite the increased presence of ssDNA and APOBEC expression following RTX treatment, we did not observe a significant increase in C→T transitions. One possible explanation is that RPA provides protection against APOBEC enzymes. An alternative hypothesis was that the ssDNA regions were lost at some later stage of the experiment. Therefore, we repeated the sequencing using a library preparation strategy that also preserves single-stranded DNA.

Using the U-DNA-Seq [2] method developed by our group, we enriched the samples for DNA fragments containing uracil. The method involves adding a uracil-DNA-recognizing sensor to sonicated genomic DNA, followed by immunoprecipitation of sensor-labeled fragments using a specific antibody and subsequent sequencing of both enriched and input samples. The resulting coverage allows the identification of genomic regions enriched in uracil. Variant calling was performed on the non-treated (NT), RTX-treated, and 5FdUR-treated immunoprecipitated samples relative to the NT input samples, using both conventional and ssDNA-preserving library preparation strategies.

The results showed an increased frequency of C→T transitions in 5FdUR-treated samples even with conventional sequencing library, which was further pronounced with ssDNA-preserving sequencing. In contrast, no detectable contribution of ssDNA to the C→T transitions was observed following RTX treatment. This suggests that the RPA-bound ssDNA components in RTX-treated cells were practically not subjected to APOBEC-induced cytosine deamination. In contrast, in 5FdUR-treated cells, where RPA-positive cells were less frequent, ssDNA-preserving sequencing revealed a surprisingly high contribution of C→T transitions associated with ssDNA regions, suggesting the presence of ssDNA regions not covered by RPA, and exposed to editing enzymes such as APOBEC3s. The mutational spectra further supported APOBEC-induced cytosine deamination, particularly in 5FdUR-treated cells.

The putative ssDNA fragments lacking RPA protection may be associated with intermediates arising during later stages of DSB repair, abnormal DNA structures associated with DNA damage, or post-replicative gaps. Regarding the extent of DNA damage, our previous results demonstrated similarly increased γ H2AX signal by both treatments, which was also confirmed in the present study by immunofluorescence microscopy. In contrast, additional components of DSB repair, including 53BP1 foci and BRCA1, showed a strongly 5FdUR-selective accumulation.

Overall, our results indicate that the two thymidylate synthase-inhibiting treatments are associated with distinct patterns of replication stress, ssDNA accumulation, and mutagenesis. The C→T transitions observed following 5FdUR treatment, together with the APOBEC-associated mutational spectrum, induction of APOBEC3 expression, and the contribution of ssDNA, collectively raise the possibility of a role for APOBEC-mediated cytosine deamination in 5FdUR-induced mutagenesis. In contrast, despite substantial RPA-associated ssDNA accumulation and APOBEC induction following RTX treatment, we did not detect comparable ssDNA-associated C→T mutagenesis, suggesting that RPA-mediated protection may limit APOBEC access to ssDNA.

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Optimisation of the glycolysis of flexible polyurethane foams for sustainable polyol recovery

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Polyurethane (PU) foams are widely used in furniture, automotive and construction applications, but their end-of-life management remains a significant environmental challenge. Chemical recycling offers an attractive route for recovering valuable components from PU waste and reintegrating them into new materials. Within the ROBUST project, the chemical recycling of flexible PU foam waste is being investigated, with a focus on the utilisation of the recovered polyol in value-added polyurethane products.

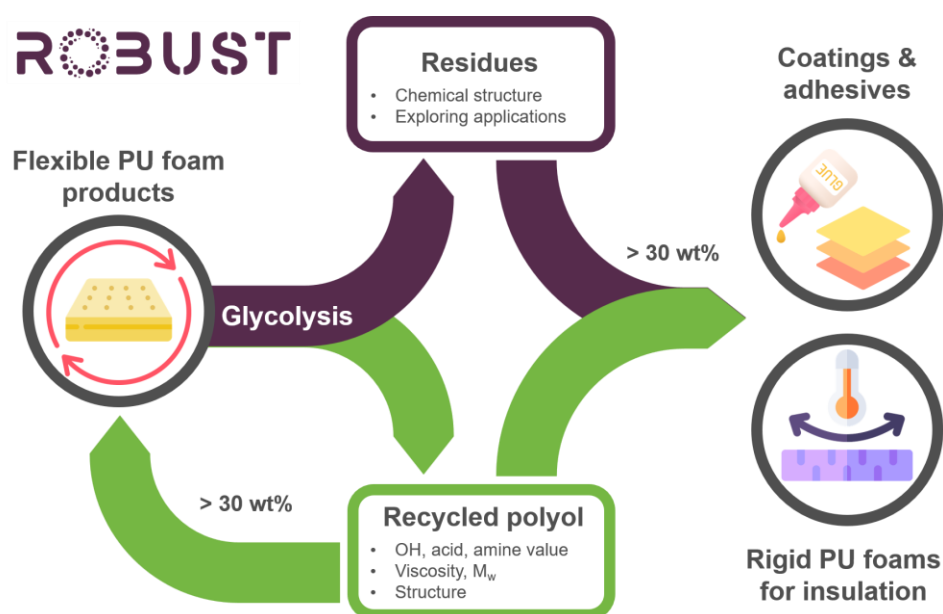


Figure 1. Project concept.

Our work focuses on the optimisation of glycolysis as a chemical recycling route. In the first stage of the study, different glycols and catalysts were screened, resulting in diethylene glycol (DEG) and potassium hydroxide (KOH) being selected as the most promising glycolysis system. In the subsequent optimisation stage, the effects of reaction temperature (180–220 °C), reaction time (1–4 h), DEG:PU ratio (1.5–4.0) and KOH concentration (0.5–2.0 wt%) were systematically investigated using a statistical design of experiments approach. Statistical analysis indicated that conditions close to the centre of the investigated parameter ranges, meaning the central point, provided the most favourable overall glycolysis performance.

The optimised process produces a phase-separated product, including a polyol-rich upper phase that can be recovered and further utilised as a raw material for the production of new polyurethane materials. Based on these results, the recovered polyol is currently being investigated in value-added applications, including rigid polyurethane foams for thermal insulation and polyurethane/urea coatings for industrial flooring.

Acknowledgement

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Adhesive behavior of polymer films on biomimetic hydrogels

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Mucoadhesive polymeric films are a promising dosage form for buccal drug delivery, enhancing bioavailability by avoiding first-pass metabolism. Despite extensive work on mucoadhesive films, the correlations between the adhesion and viscoelastic properties of single-polymer films and their mucoadhesive performance remain incompletely elucidated.

This study investigates freestanding films of hydroxypropyl methylcellulose (HPMC) and chitosan, polymers with dissimilar physicochemical properties, fabricated at two thicknesses (0.5 mm and 1 mm) via solvent casting from their aqueous solution with glycerol as a plasticizer. Four poly(vinyl alcohol) (PVA) hydrogels with different stiffness were synthesized via the freeze–thaw (FT) method (one or three FT cycles) with and without mucin as biomimetic mucosal substrates. PVA hydrogels containing mucin, the main macromolecular component of the mucus, were synthesized to assess how mucin influences the mucoadhesive interaction with the polymer films. The mechanical and viscoelastic properties of the films were characterized, as well as their adhesion is studied on the gels.

For all thicknesses, films containing HPMC and chitosan showed a decrease in storage modulus (G') upon hydration, which indicated that the hydration of the polymer network enhances chain mobility and decreases mechanical stiffness (**figure 1**). Chitosan films exhibited greater stiffness and reduced deformability compared to HPMC films; glycerol reduced stiffness and enhanced deformability in both types. Chitosan films demonstrated higher adhesion toughness than HPMC films across all four substrates, consistent with electrostatic interactions with the anionic mucin in PVA-mucin hydrogels. The stiffness of the substrate influenced the strength and work of adhesion in those films.

These findings reveal quantitative structure-property connections to support the design of mucoadhesive film formulations.

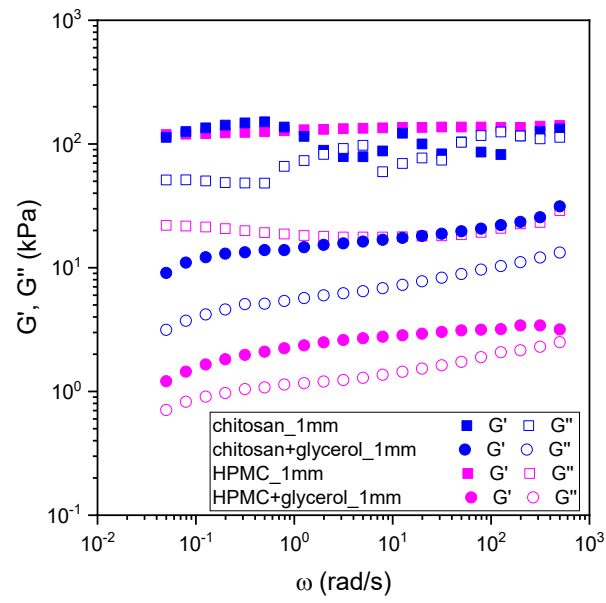


Figure 3. Frequency-dependent dynamic moduli (G' , G'') of chitosan and HPMC films with and without glycerol with a wet thickness of 1mm

Investigating the effect of catalytically inactive dUTPase enzyme in mouse embryonic fibroblast cells

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Enzyme dUTPase plays a crucial role in nucleotide metabolism by hydrolyzing deoxyuridine triphosphate (dUTP) to deoxyuridine monophosphate (dUMP)^[1]. This enzymatic activity is essential for maintaining the cellular dUTP/dTTP ratio and thereby genomic integrity. By hydrolyzing dUTP available for DNA synthesis, dUTPase prevents uracil incorporation into DNA. This is particularly important because DNA polymerases cannot discriminate between thymidine and uridine nucleotides, and an elevated dUTP/dTTP ratio can therefore lead to the misincorporation of uracil during DNA replication. Consequently, dUTPase contributes to genome integrity by preventing excessive uracil incorporation into DNA. However, uracil can also arise spontaneously through the deamination of cytosine, therefore, uracil in genomic DNA is corrected by the base excision repair (BER) pathway. Uracil-DNA glycosylases recognize and remove uracil residues, initiating BER and allowing the damaged nucleotide to be replaced; however, excessive uracil accumulation can lead to hyperactivation of BER, resulting in strand breaks and contributing to genomic instability or cell death. The importance of dUTPase is also supported by the fact that *Dut* gene knockout in mice results in early embryonic lethality^[2]. Interestingly, mice lacking both major uracil-DNA glycosylases, *Ung* and *Smug1*, are viable and fertile despite their impaired ability to remove uracil from DNA^[3]. However, our recent results demonstrated that mice with the *Ung* *-/-* *Smug1* *-/-* *Dut* *-/-* genotype also die during the early blastocyst stage, suggesting that loss of dUTPase becomes deleterious even when the major enzymes responsible for uracil repair are absent.

To determine whether the catalytic activity of dUTPase is required for cellular viability and development, we generated mouse embryonic fibroblast (MEF) cells expressing a catalytically inactive form of dUTPase in an *Ung* *-/-* *Smug1* *-/-* background. Cells were generated using the CRISPR/Cas9 cytosine base-editing (CBE) system to introduce the D100N mutation in the *Dut* gene, resulting in a catalytically inactive enzyme. Although the *Ung* *-/-* *Smug1* *-/-* D100N cells exhibited highly elevated genomic uracil levels, reduced proliferation rate, and altered dUTPase localization, they remained viable. The ability of these cells to survive despite the presence of catalytically inactive dUTPase is of particular interest, as complete deletion of the *Dut* gene causes a much more severe phenotype in mouse embryos. These findings suggest that the biological functions of dUTPase cannot be explained solely by its enzymatic activity and may include an additional function important for cellular homeostasis, genomic integrity, or embryonic development; however, the precise mechanism remains to be determined.

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Controlled hydrothermal decomposition of polymers and their composites

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The growing accumulation of thermoset polymer and composite waste requires efficient recycling technologies capable of recovering valuable organic products and reinforcing materials. Hydrothermal treatment using subcritical water offers a promising chemical recycling route, as water can simultaneously act as solvent, reactant, and reaction medium, enabling the cleavage of hydrolytically susceptible bonds without additional catalysts.^[1]

In this work, the controlled hydrothermal decomposition of different polymer systems and their glass-fiber-reinforced composites was investigated in a semi-continuous high-pressure flow setup. The studied materials included a bisphenol A-based epoxy resin, a decommissioned wind turbine blade composite, three polyurethane systems with different polyol structures, and a glass-fiber reinforced polyurethane composite. The effects of temperature and residence time on polymer decomposition and product formation were evaluated, while the liquid and solid product fractions were characterized by complementary analytical techniques.

For the DGEBA-based epoxy resin, complete conversion was achieved within 9 min at 360 °C, yielding a selective product profile dominated by three main aromatic compounds. The optimized methodology was successfully transferred to decommissioned wind turbine blade waste, resulting in efficient matrix decomposition and recovery of glass fibers with approximately 99% purity.^[2] In the case of polyurethanes, the structure of the polyol component strongly influenced hydrolysis selectivity and the recovery of the polyol-rich fraction. Up to 95.6% polyol-rich fraction recovery was achieved at 250 °C for the polyether-based polyurethane. The methodology was further extended to glass-fiber reinforced polyurethane, where efficient matrix removal was achieved while the recovered fibers retained high purity.

These results demonstrate that semi-continuous subcritical water treatment is a versatile strategy for the controlled decomposition of structurally different thermoset polymers and composite materials. The simultaneous recovery of valuable organic fractions and high-purity glass fibers highlights the potential of hydrothermal processing for obtaining circular materials from complex polymer waste streams.

Acknowledgements

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Thiolactams to Cyclic (Alkyl)(Amino)Carbenes *via* Alkali Metal Reduction

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The evolution of N-heterocyclic carbene (NHC) chemistry spans over seven decades, from the Breslow intermediate (1957) and the Wanzlick conjecture (1968) to the crystalline Arduengo carbene (1991) and NHCs' emergence as ancillary ligands in homogenous transition metal catalysis.^[1] While today they are mainly prepared by the deprotonation of the parent azolium salt, a great variety of approaches are available, one of which employs potassium to reduce cyclic thiourea derivatives, yielding imidazole-2-ylidenes.^[2] We combined this strategy with the ever-growing relevance of cyclic (alkyl)(amino)carbenes (CAACs, pioneered^[3] and extensively studied by Bertrand et al.) and theorized a new synthetic route for CAAC production from thiolactams.

My poster aims to exhibit our attempts at catalyzing the reduction to facilitate carbene generation at ambient temperatures. *In situ* stabilization of the free carbene *via* adduct formation was investigated as well as various methods for their conversion to stable azolium salts with moderate yields. *N*-alkyl substituted substrates formed an air- and moisture sensitive triethylborane adduct, which reversibly transforms into carbene, substantiating its use as precursor for the valuable ligand family.

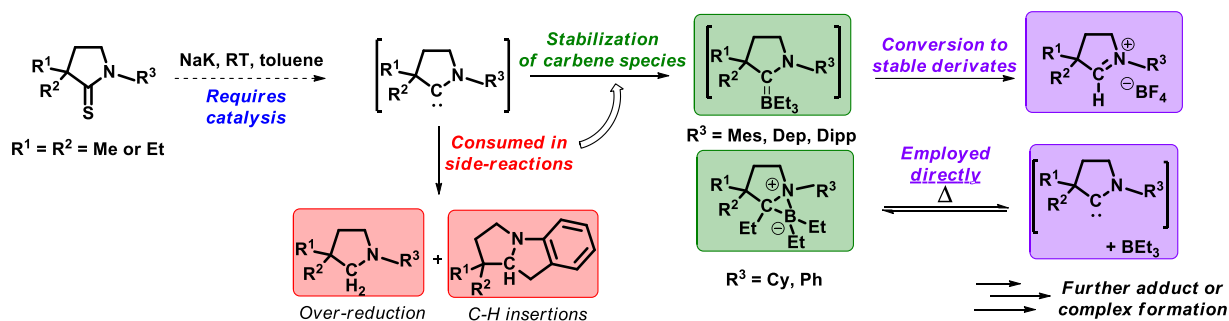


Figure 1. general considerations and results for desulfurization of thiolactams

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Development of Functionalized Bacterial Nanocellulose Membranes for the Selective Immobilization of Recombinant Enzymes

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Bacterial nanocellulose (BNC) is an attractive sustainable biopolymer with an ultrafine nanofibrillar network, high chemical purity, excellent water-holding capacity, and superior mechanical durability, which makes it a promising carrier for biocatalysis.^[1,2] While traditional immobilization relies on physical adsorption (compromised by enzyme leaching) or random covalent attachment (often inducing steric hindrance or catalytic inactivation),^[3] affinity-based oriented immobilization provides controlled biocatalyst orientation and preserves catalytic competence. Herein, an Immobilized Metal Ion Affinity (IMAC)-inspired surface engineering strategy was developed on BNC membranes to achieve oriented, stable binding of recombinant polyhistidine-tagged enzymes. Phenylalanine ammonia-lyase from *Anabaena variabilis* (AvPAL) carrying an N-terminal His₆-tag was chosen as a model biocatalyst. AvPAL is the active enzyme in PalynziqTM (pegvaliase), the only FDA-approved therapeutic for phenylketonuria (PKU), and serves as an important industrial catalyst for synthesizing unnatural aromatic amino acids.^[4,5]

BNC membranes were prepared from commercially available, food-grade nata de coco via consecutive alkaline and oxidative purifications, followed by high-shear mechanical disaggregation.^[6] Regioselective ring-opening oxidation of glucopyranose units was systematically performed using sodium periodate (NaIO₄, 0.5 eq/glucose unit) across 1, 2, 6, and 24 h to generate reactive dialdehyde groups, which were measured by copper number titrations. The activated membranes were functionalized with ethylenediamine linkers via Schiff base formation and borohydride reduction, followed by coupling with ethylenediaminetetraacetic acid (EDTA) anhydride. Transition metal ions (Ni²⁺, Co²⁺, or Fe³⁺) were subsequently coordinated to form selective-affinity docking platforms for His-tagged AvPAL (Figure 1). Surface grafting and metal coordination were verified by FT-IR spectroscopy and SEM-EDX elemental analysis.

The periodate oxidation followed a saturation curve, and the aldehyde content increased sharply up to 6 h. Single-axis tensile tests showed that oxidation and chelator modification resulted in significantly lower ($p < 0.001$) membrane tensile strength due to cleavage of the pyranose ring and disruption of interchain hydrogen bonds. Membranes oxidized for 24 h showed severe mechanical degradation, whereas 6 h oxidation preserved adequate mechanical durability and maximized the available reactive anchoring sites. All metal-charged BNC membranes were successful in capturing His₆-AvPAL: Fe³⁺-loaded membranes had the highest immobilization yield (~40%), followed by Co²⁺ and Ni²⁺ (~20–30%). All immobilized AvPAL-BNC

preparations showed a remarkable increase of the specific catalytic activity (UE up to 48,000 U g⁻¹) in the catalytic deamination of L-phenylalanine to trans-cinnamic acid in comparison to the native soluble enzyme (13,586 ± 465 U g⁻¹). Most importantly, the Ni²⁺-loaded membranes exhibited a dramatic hyperactivation >23-fold, providing an evidence that the hydrophilic surface of nanocellulose creates a favorable microenvironment to stabilize catalytically competent tetrameric conformations.

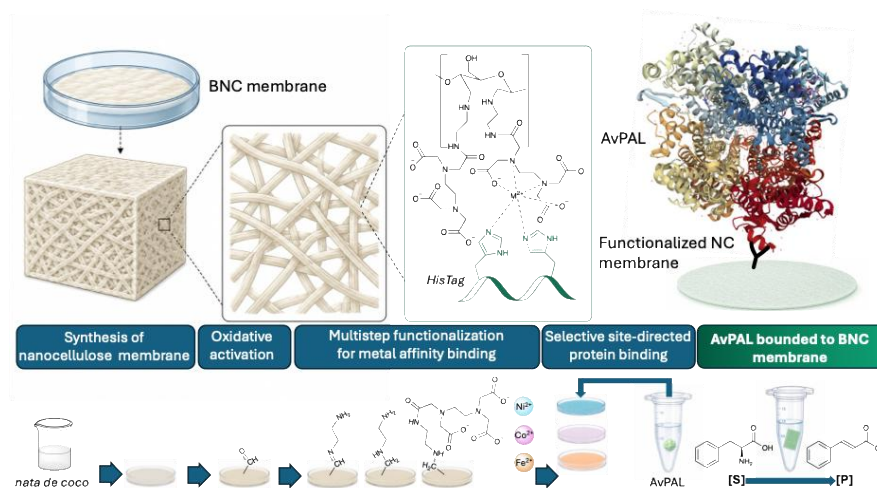


Figure 1. Schematic illustration of bacterial nanocellulose (BNC) membrane preparation from nata de coco, regioselective periodate activation, ethylenediamine-EDTA chelating linker functionalization, transition metal ion charging (Ni²⁺, Co²⁺, Fe³⁺), and selective His-tagged AvPAL immobilization.

Targeted elution experiments confirmed superior binding stability: under standard IMAC elution conditions (300 mM imidazole), no detectable enzyme detachment was observed. Even under 1 M imidazole, enzyme release remained negligible (≤6% for 1–2 h oxidized samples) and undetectable for 6–24 h preparations. AlphaFold 3-based structural modeling revealed that homotetrameric His₆-AvPAL docks preferentially through a "His₆-tag_bottom_His₆-tag" orientation. In this configuration, dual His₆-tags coordinate with surface metal ions, while polar residue clusters (notably His335/Asp336) engage the positive curvature of BNC nanofibrils in auxiliary stabilizing contacts. In conclusion, this work establishes a robust, sustainable, and highly active biocatalytic membrane system, demonstrating great potential for continuous-flow biotransformations and diagnostic biosensors.

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Visible light photocatalytic activity of 2D/1D g-C₃N₄/ZnO heterostructure for efficient degradation of Rhodamine 6G, 4-Nitrophenol, and Ciprofloxacin

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The persistent release of organic contaminants into aquatic environments has increased the demand for efficient and sustainable water-treatment technologies. Visible-light photocatalysis is a promising approach, although rapid charge-carrier recombination can limit the performance of semiconductor photocatalysts ^[1, 2]. In this work, g-C₃N₄/ZnO microrod heterostructures were prepared through the *in situ* hydrothermal growth of ZnO microrods in the presence of pre-synthesized g-C₃N₄ at 90 °C for 6 h and 120 °C for 3 h. Structural and morphological characterization confirmed the successful formation of crystalline ZnO microrods coupled with the g-C₃N₄ matrix. UV-Vis analysis showed the optical response of the heterostructures, while photoluminescence quenching and the reduced semicircular arc observed by electrochemical impedance spectroscopy indicated improved separation and interfacial transfer of photogenerated charge carriers. The photocatalytic activity was evaluated under visible-light irradiation using Rhodamine 6G (Rh 6G), 4-nitrophenol (4-NP), and ciprofloxacin (CIP) as model contaminants. The heterostructure synthesized at 90 °C for 6 h exhibited the highest activity, achieving degradation efficiencies of 87.7%, 79.8%, and 79.5% for Rh 6G, 4-NP, and CIP, respectively, with corresponding apparent rate constants of 17.2, 12.9, and 12.2 × 10⁻³ min⁻¹. Common inorganic anions inhibited CIP degradation in the order HPO₄²⁻ > SO₄²⁻ > Cl⁻ > NO₃⁻, demonstrating the influence of water-matrix constituents on photocatalytic performance. Radical trapping experiments identified •O₂⁻ as the predominant reactive species, with •OH and photogenerated holes also contributing to degradation. Together with the calculated band-edge positions, the results support a proposed direct Z-scheme charge-transfer mechanism. The optimized heterostructure retained approximately 90.8% of its initial activity after four consecutive CIP degradation cycles, while post-cycling FT-IR and XRD analyses confirmed preservation of its functional and crystalline structures. These findings demonstrate the potential of g-C₃N₄/ZnO microrod heterostructures as stable visible-light photocatalysts for the degradation of structurally diverse aqueous contaminants.

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Synthesis of Novel Alkylthioether-Alpha-Cyclodextrin Derivatives and Their Impact on Bacterial Biofilm Formation

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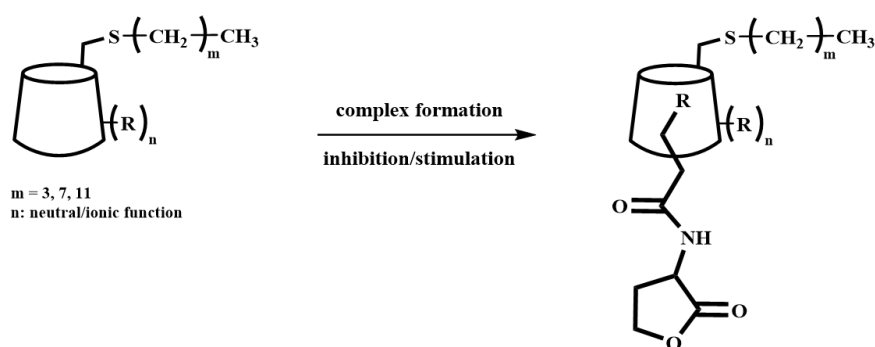
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Bacterial communication, called *Quorum Sensing* (QS) is a cell density dependent signaling process that allows the microbial population to behave as a multicellular organism in colonizing the host, forming biofilms, producing virulence factors, and thus adapting to changing environments. This communication system is based on the production and detection of extracellular signal molecules (called autoinducers), e.g. acyl-homoserine lactone type signals, (AHLs). [1] The inhibition of QS, *Quorum Quenching* (QQ) involves several different molecules and methods, which have in common, that they do not kill or exert selective pressure on the bacteria, as the conventional antibiotics do, but only prevent communication between cells. Direct modulation of this microbial communication is a new wave strategy avoiding microbial resistance; a potential tool for inhibiting QS is trapping the signal molecules. [2]

Nowadays, cyclodextrins (CDs) are widely used due to their ring structure and their ability to form inclusion complexes. According to previous studies, they can reversibly encapsulate the AHL molecules in Gram-negative bacteria, preventing them from binding to the receptors and interrupting the communication. [3,4]



The aim of the research was to develop a series of water-soluble mono-alkylthioether- α CD derivatives randomly substituted with sulfobutyl (SB), hydroxypropyl (HP), quaternary amino (QA) functional groups with high complexation rate to signal molecules and a novel synthetic approach. These derivatives were characterized using NMR techniques, HPLC-MS and CE. Furthermore, short-term microbiological study was performed with the synthesized water-soluble alkylthioether- α CD derivatives to systematically investigate the potential QS-disrupting ability and compare their effect on the biofilm formation of *Pseudomonas aeruginosa*. According to the results the contact time, the temperature and also the structure of the derivatives (length of alkyl chain, type of the substituent to improve the solubility) had a significant influence on both the viability of the cells and on the biofilm formation.

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COMPARISON OF TOLERANCE INTERVAL CALCULATION METHODS FOR ACCURACY AND PRECISION UNDER USP <1210>

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Analytical procedures are widely used in the pharmaceutical industry for the determination of the quantity of specific components. It is essential that the measurements provide reliable results. Therefore, these analytical procedures must be validated before they are used in industrial practice. During the analytical validation, it must be demonstrated that the procedure is suitable for its intended use. This is achieved by measuring known samples (validation standards), statistically analyzing the obtained measurement results, and deciding based on this, whether the validation is successful—that is, whether the analytical procedure is capable for its intended purpose. The aim of the statistical evaluation is to reach an appropriate validation decision. Guidance regarding the number of required number of measurements and the statistical evaluation of results can be found in the International Council for Harmonisation – Guideline Q2 (ICH Q2)^[1] – which harmonizes the requirements of Europe, Japan, and the United States – as well as in the United States Pharmacopeia (USP) <1210> guideline^[2].

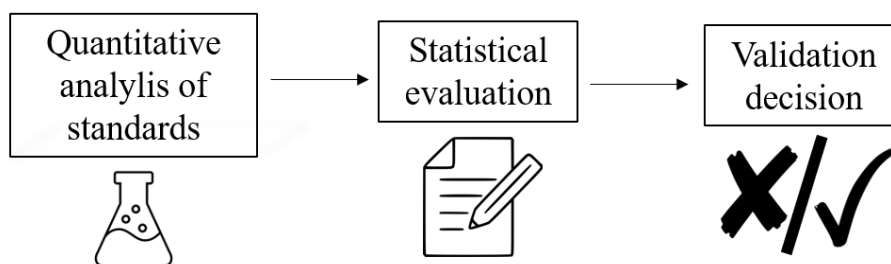


Figure 1. Main steps of analytical validation

In our work, we investigate datasets that can be described by a one-way random effects ANOVA model. In practice, this model arises, for example, when repeated experiments are conducted on different days. The number of groups and replicates is small, which is typical of analytical practice: the number of groups is either 3 or 5, the number of replicates is either 3, 6, or 10. The method for calculating tolerance intervals found in USP <1210> is theoretically inapplicable to these datasets since it does not account for the two sources of variation. However, several calculation methods applicable to datasets containing multiple sources of variation can be found in the literature. As these methods always employ some form of approximation, the boundaries of the intervals calculated by different methods may vary to a greater or lesser extent. We selected three methods that are suitable for determining the tolerance interval and that can be applied in analytical practice: Mee-Owen^[3], Beckman-Tietjen^[4], and Hoffman-Kringle^[5] methods.

We compare these methods based on coverage probabilities and make a recommendation regarding which tolerance interval calculation method should be used for datasets that can be described by a one-way random effects ANOVA model. We also demonstrate the difference

that arises when using the single-source-of-variation evaluation – also found in the USP <1210> – instead of the theoretically correct evaluation.

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Mn–Cr dopant association in dilute co-doped ZnAl₂O₄ revealed by combined EPR and optical spectroscopy

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Transition-metal-doped ZnAl₂O₄ spinel is a versatile phosphor host in which Mn and Cr occupy distinct crystallographic environments and give rise to spectrally separable colour centres. While Mn²⁺/Cr³⁺ co-doped systems are commonly discussed in terms of donor–acceptor energy transfer, the structural consequences of co-doping for the individual centres remain poorly resolved. We report a correlated optical and magnetic-resonance study of two dilute Mn/Cr co-doped ZnAl₂O₄ series prepared hydrothermally and annealed at 1100°C. Photoluminescence and excitation spectra were deconvoluted under Tanabe–Sugano constraints, and complemented by X-band EPR, Raman spectroscopy and Rietveld-refined XRD. Mn co-doping enhances the Cr³⁺ emission, with optima at 0.12 and 0.24 mol% Mn for the low- and high-Cr series respectively, although the mean dopant separation of ≈ 1.4 nm places the system far outside the resonant energy-transfer regime. The Cr³⁺ excitation spectra show no Mn-derived features; instead, the ⁴A₂→⁴T₁ band shifts stepwise to the red with the Racah parameter B falling by 10–17%, while the Cr³⁺ EPR line loses about three quarters of its intensity without any new resonance appearing. We interpret these as two independent probes of the same effect: a trigonal distortion of the CrO₆ octahedron induced by Mn incorporation on neighbouring sites. The distortion correlates with the cation inversion parameter, tracked independently through the ~ 509 cm⁻¹ T_{2g}(2) Raman mode of AlO₆ origin, indicating that antisite defects mediate the Mn–Cr exchange coupled interaction. Consistent with this, Mn is found in multiple valence and coordination environments, with emission channels at 510, 678 and 650 nm assigned to tetrahedral Mn²⁺, octahedral Mn²⁺ and Mn⁴⁺ respectively. The octahedral Mn and its charge-compensating defect lift the inversion symmetry of the Cr³⁺ site and strengthen its parity-forbidden absorption, enhancing the emission without energy transfer. EPR spin counts give a dissociation constant $K_d \approx (2-5) \times 10^{-4}$, an association free energy near $8 k_{BT}$, and a population following the law of mass action. Above a Cr-dependent Mn threshold the added Mn repartitions into EPR-silent octahedral configurations that quench both emissions.