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Synthesis and Evaluation of Fluorinated Lactose-Based Glycopolymers as High-Affinity Galectin-3 Inhibitors

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The development of carbohydrate-based galectin-3 (Gal-3) inhibitors is often limited by the lack of potent and selective molecular recognition.¹ In this work, we explored selective fluorination of a lactose scaffold as a strategy to create hydrophilic glycomimetics with tunable binding properties. A series of β -lactosyl azides (**1–4**), selectively deoxyfluorinated at the 2'-, 3'-, 4'-, or 6'-position of the galactose unit, was synthesized via chemical glycosylation of a glucosyl azide acceptor with corresponding fluorinated thiogalactoside donors. These ligands were subsequently conjugated to a hydrophilic and biocompatible polyoxazoline copolymer scaffold—specifically poly(2-ethyl-2-oxazoline-co-2-but-3-ynyl-2-oxazoline)—using copper-catalyzed azide-alkyne cycloaddition (CuAAC). The resulting multivalent glycopolymers were characterized by ¹H NMR and GPC-MALS, confirming high conversion rates and narrow molecular weight distributions.

Biolayer interferometry (BLI) measurements revealed a strong positional influence of fluorination on Gal-3 recognition. Substitution at the 2'- and 3'-positions was well tolerated, yielding dissociation constants ($K_D \approx 208$ – $284 \mu\text{M}$) comparable to non-fluorinated lactose. In contrast, 4'- and 6'-fluorination resulted in a near-complete loss of binding. Upon multivalent presentation, binding affinity was markedly enhanced via the cluster glycoside effect, with the 3'-fluorinated glycopolymers showing the strongest binding with affinity in the nanomolar range ($K_D = 4.8 \text{ nM}$).

The results agree with the structural analysis of the Gal-3–lactose complex, which suggests that the 4'- and 6'-hydroxyl groups participate in key hydrogen-bonding interactions within the binding pocket. In contrast, the 2'- and 3'-hydroxyl groups are more water-exposed. Overall, our results identify 3'-fluorination as a promising modification for the design of potent, water-soluble, multivalent Gal-3 inhibitors with optimized binding properties.

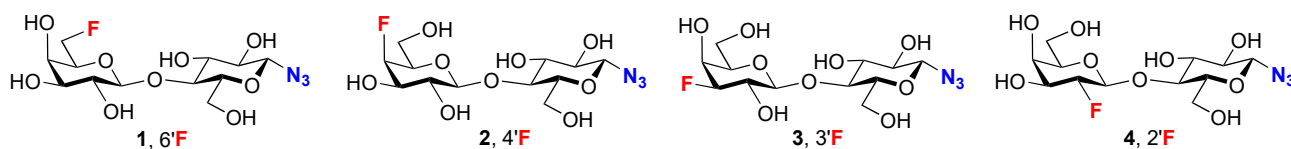


Figure 1: Structure of target fluorinated β -lactosyl azides.

Acknowledgements

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Extended Evaluation of LARCODEMS Separation Efficiency for Plastic Recycling: From Medium Density to Viscosity Effects

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The LARge COal DEnsity Medium Separator (LARCODEMS) represents a continuous density separation technology operating on the fundamental principle of the sink-float process. This method utilises a separation medium with a density precisely calibrated between those of the target particle phases, causing lighter components to float to the surface. At the same time, heavier fractions settle at the base. The LARCODEMS system utilises a dynamic vortex flow designed for continuous and efficient material processing.

In the context of the modern circular economy, the efficient separation of post-consumer plastic waste streams represents a critical challenge for subsequent high-quality recycling processes.¹ Conventional sorting methods often struggle with complex polymer mixtures, making density-based physical pre-sorting an essential step to isolate specific material fractions before advanced chemical processing.² While density separation is a well-established operation, adapting these systems for polymeric materials introduces significant complexities due to the overlapping densities of different plastics.³ Utilising the LARCODEMS device for this purpose offers a promising high-capacity alternative to traditional methods. However, achieving sharp separation in these systems requires a precise understanding of how multi-component plastic mixtures behave within the separation medium.⁴

This contribution represents a direct continuation and extended study of prior experimental work. While earlier phases focused on establishing the baseline separation efficiency as a function of medium density, the logical next step is to evaluate medium viscosity. The primary objective of this study was to assess the specific impact of viscosity on separation performance. Ultimately, the integration of both density and viscosity data serves as the foundation for developing a robust correlation to predict overall separation efficiency based on these combined transport phenomena.

Acknowledgements

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Electricity Cost and Spectral Effects of LED Lighting in *Limnospira maxima* Cultivation

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Illumination is a major operational cost in photobioreactor systems with artificial illumination for microalgae cultivation. Light-emitting diodes (LEDs) offer high photosynthetically active radiation (PAR) efficiency and various spectral output¹; however, the relationship between spectral quality, biomass productivity, pigment synthesis, and electricity consumption remains insufficiently quantified for *Limnospira maxima*.² This study evaluated the effects of six LED sources — polychromatic daylight white (DW), and warm white (WW), and monochromatic red (R), green (G), yellow (Y), and blue (B) — on biomass and pigment production under controlled cultivation conditions.

All LEDs were operated at equal photosynthetic photon flux density (PPFD = 50 ± 5 $\mu\text{mol photons/m}^2/\text{s}$). Biomass productivity, pigment content, and electricity consumption for each illumination were systematically compared. DW and WW illumination resulted in the highest biomass productivities (0.31 and 0.29 g/L/day, respectively), whereas blue light produced significantly lower biomass yields (0.03 g/L/day). Pigment contents remained relatively stable across most spectra, indicating effective photoadaptive regulation of the photosynthetic apparatus. However, substantial differences were observed in the electricity demand required to achieve equivalent PPFD. To achieve the same PPFD, the electrical power input ranged from 0.23 W for blue LEDs to 3.15 W for yellow LEDs. Energy costs per unit of biomass and pigment produced increased in the order DW < WW < R < G < B < Y.

The results demonstrate that white LEDs provide the most favorable balance between biological productivity and electrical efficiency in *L. maxima* cultivation. In contrast, yellow and blue LEDs exhibited poor electricity-to-product conversion efficiency, regardless of the electrical input. These findings highlight the importance of integrating both spectral optimization and energy-efficiency analysis when designing photobioreactor lighting systems. The presented approach provides a framework for improving the techno-economic sustainability of large-scale cyanobacterial production.

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Optimalization of Hydrodynamics and Mass Transfer in Raceway Pond Reactors for the Production of Microalga

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The cultivation of microalgae in raceway pond reactors represents a sustainable and scalable technology for CO₂ fixation and biomass production¹. Previous research in an 80 m² reactor successfully introduced a new online methodology for optimizing biomass production and removing excess O₂ that inhibits biomass growth. The methodology is based on the application of controlled air pulses to the system, resulting in efficient O₂ removal driven by concentration gradient between the air and the supersaturated liquid. However, a detailed understanding of hydrodynamics is key for further scale-up of the reactor and maximizing biomass yield². Building upon these findings, the research focuses on the scale-up and optimization to a 600 m² reactor. The aim of the research is to develop and validate strategies for optimizing hydrodynamics and O₂ stripping in this larger system to maximize biomass productivity and ensure process sustainability. This knowledge will create a base of an autonomous system, that will be able to control raceway pond reactors under different conditions such as temperature, light intensity and more.

The experiments were conducted in a pilot-scale outdoor raceway pond with an area of 600 m² and a working volume of 95 m³. The reactor is composed of three main parts – the channel, the paddlewheel, and the sump. The channel is an open section characterized by an extensive surface exposure to the atmosphere and light. The paddlewheel drives the liquid circulation, keeping the reactor homogenized, and is characterized by high turbulence. The sump is a deeper structural section of the reactor where gas-liquid exchange is enhanced via gas distributor placed at the bottom^{1,2}. The distributor was composed of 13 AFTP2100 ECOTEC diffusers. To evaluate the scale-up, the air pulsing method was tested for the same gas flow rates as in the 80 m² raceway ranging from 125 to 500 l/min, which corresponds to 0.0548 to 0.2192 cm/s of superficial gas velocity, and across various operating scenarios, such as weather changes, additional CO₂ injections, nutrient sources and more.

The results show that the current setup in the pilot-scale raceway cannot achieve the desired O₂ removal. During the experiments, the O₂ oversaturation was frequently way above 200%, which is the considered threshold between proper photosynthesis and O₂ inhibition. Data suggest that conditions such as weather and CO₂ addition have minor role in biomass growth compared to light intensity, which leads to high O₂ production and consequently to process inhibition. To address this, alternative hydrodynamic conditions are being tested to achieve efficient O₂ removal and biomass production.

Acknowledgements

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Analytical Solution for Scalar Transfer to Arrays of Arbitrarily Distributed Reactive Surface Sinks

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The transfer of scalar quantities (typically heat or mass) from a flowing fluid to a wall can be considered one of the fundamental problems of transport phenomena¹. From the fluid core, transfer occurs through the boundary layer to a delimited area, such as a reactive surface, or in other words, a sink. A wide range of fields can benefit from the findings on this topic, whether in environmental sciences, thermal engineering, or medicine.

M. A. L  v  que² laid a rigorous foundation for the above-mentioned problem by analytically describing the temperature profile above the surface of a single thermal sink. Using classical simplifying assumptions for the diffusion boundary layer located within a viscous sublayer, he found a solution for a simplified variant of the convection-diffusion equation. Building upon L  v  que solution, a successful generalization³ was achieved by considering both the region above the sink and the region of the downstream wake, which had previously resisted complete analytical solution. The essence of the derivation consisted in linking the Dirichlet and Neumann problems using the Laplace transform and specific convolution identities. This yielded integral relations for a complete description of the scalar field.

The aim of the present work is to achieve further generalization, building on the study³ that has already been carried out. We consider an array with an arbitrary number of sinks separated by non-reactive regions. Recursive relations are derived which, based on the solution for the first sink and the wake, can quantify the transfer to a general system with an arbitrary number of sinks. Two basic cases are considered: periodic and completely random. A periodic system for which a situation is recognized where the gap regions can be neglected and the array effectively behaves as a single sink, as well as a situation representing a periodic system with negligible inter-sink interactions, are discussed. Practical correlations are provided for determining both cases. A more complex constellation of sinks with entirely random distribution of the leading and trailing edges is similarly examined in terms of the effect of sink placement on the overall transfer.

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Hybrid Strategy for Diclofenac Removal: Modified Clinoptilolite Adsorption for Preconcentration and Subsequent Advanced Photo-oxidation

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This study was focused on a hybrid water treatment strategy utilizing adsorption and subsequent photodegradation. A Surface-modified zeolite adsorbent was used to capture diclofenac (DCF), a Nonsteroidal Anti-Inflammatory Drug (NSAID) and an emerging pollutant¹. The adsorption process was followed by photodegradation under UV irradiation combined with H₂O₂, or under visible light irradiation with the use of metal-free photocatalyst, graphitic carbon nitride (g-C₃N₄). The process addresses higher demands for tertiary wastewater treatment, caused by the rising concentration of drugs, pesticides and other persistent pollutants, by lowering the overall wastewater volume to be treated, while utilizing low-cost substances such as clinoptilolite and g-C₃N₄².

The adsorption of diclofenac was studied on raw and surface-functionalized clinoptilolite specifically to target hydrophobic pharmaceuticals in wastewater at pH $\approx$ 6. Clinoptilolite is a natural aluminosilicate with high specific surface area, chemical stability and regenerability. Raw clinoptilolite possesses a hydrophilic surface, which limits adsorption capacity for non-polar or weakly polar compounds³. In order to increase the affinity of diclofenac to the raw adsorbent, clinoptilolite was modified by either NaOH or tetrabutylammonium bromide (TBAB) separately and finally dual-modified in a two-step sequence, first by NaOH and then by TBAB to create hydrophobic or organophilic sites. The adsorption capacity of dual-modified clinoptilolite was improved to 26.7 mg·g⁻¹, which is 2.5 times higher than the raw material.

Diclofenac was desorbed at pH $\approx$ 9 with the use of Na₂SO₄ while achieving efficient recovery (>70%) and 20-fold preconcentration compared to the original dilute solution of DCF.

The UV/H₂O₂ degradation of DCF exceeded 96% conversion and 62% mineralization in just 30 minutes in cuvette experiments, whereas photodegradation using g-C₃N₄ and visible light reached a DCF conversion of only 45% in 240 minutes.

This proof-of-concept study of the adsorption/desorption process and subsequent photodegradation proved to be an effective and economically viable framework upon sorbent reuse, which validates the concept for future application in wastewater treatment technology.

Acknowledgements

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Ions and Particles During NPF: Long-Term Observations

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Atmospheric new particle formation (NPF) is an important source of atmospheric aerosol number concentrations. For investigating the earliest stages of NPF, atmospheric ions are important as they provide information on sub-3 nm cluster formation and growth¹. Recent work has further shown that intermediate ions (2.0 to 2.3 nm) can serve as sensitive indicators of local NPF intensity².

In this study, a three-year dataset measured by a Neutral cluster and Air Ion Spectrometer (NAIS) at the National Atmospheric Observatory Košetice (NAOK), a rural background site, was analysed to describe NPF events in the context of particle charge. Event strength was determined using nanoparticle ranking analysis, which ranks days according to the daily increase in 2.5–5 nm particle number concentration³. The ranked days were subsequently divided into percentile classes of NPF intensity, as illustrated in **Fig. 1**, showing that the characteristic NPF pattern becomes increasingly pronounced with increasing percentile rank.

Based on this classification, size-resolved diurnal patterns of negative ions, positive ions, and total particles are presented across different NPF intensity classes, together with growth-rate statistics for selected size ranges and ion polarities. These results provide a descriptive summary of the long-term NAIS observations and the behaviour of ions and particles during NPF events.

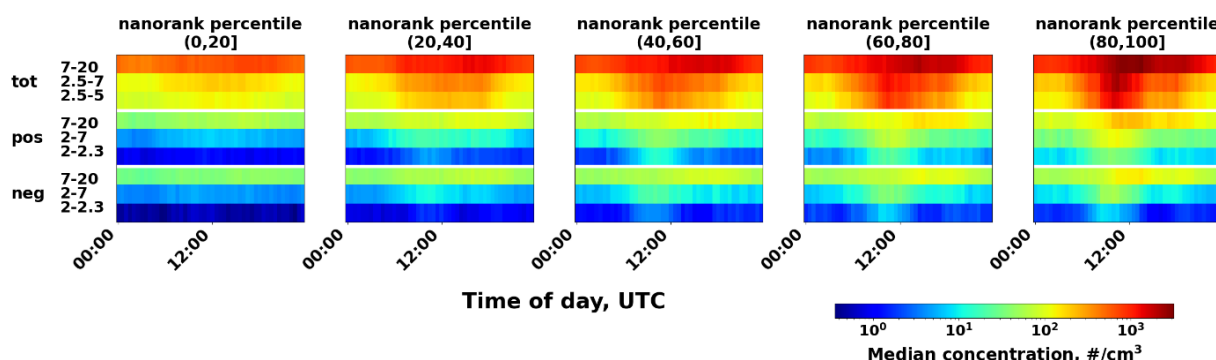


Fig. 1: Median diurnal cycle heatmaps of size-resolved negative ions, positive ions, and total particles across five rank percentile classes.

Acknowledgements

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Enantioselective Separation of DNB-Leucine Using PVDF-Based Mixed Matrix Membranes with Cinchona-Derived Selectors

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Enantiomers have the same physicochemical properties in an achiral environment. They are mirror images of each other, similarly to our left and right hands. Chirality in nature occurs in many life-important compounds, such as amino acids, carbohydrates, steroids and alkaloids. Chiral compounds can drastically impact our health as drugs, where both enantiomers might have very different therapeutic effects in our body. Enantioselective separation remains a key challenge in the production of optically pure compounds, particularly in the pharmaceutical industry. While chromatographic techniques employing chiral selectors are well established, alternative scalable approaches are highly desirable. Membrane-based separations represent a promising route due to their simplicity, continuous operation, and potential for scale-up.

In this work, enantioselective ion-exchange mixed matrix membranes (MMMs) were developed by incorporating quinidine-based chiral selectors immobilized on silica particles into polymer matrices, namely poly(vinylidene fluoride) (PVDF) and poly(ethylene-co-vinyl alcohol) (EVOH). The membranes were prepared using phase inversion techniques, enabling high particle loading and controlled membrane morphology.

The separation of N-(3,5-dinitrobenzoyl)-leucine enantiomers was studied under concentration-driven conditions alone or in combination with applied electric field. Addition of water into otherwise typically methanolic solvent led to increased retention, observed selectivity and sensitivity to electric field applied both along and against the direction of concentration-driven diffusion. Enantiomeric excess values up to 90% were achieved in a single-stage process with a decrease over time due to saturation of the chiral binding sites. It is shown that while electric field did not help to avoid the saturation completely, it can be used to increase product recovery when applied along the direction of the diffusion at a minimal expense of selectivity, while its application against the direction of the diffusion enables modulation of the retention on the chiral membrane. In all cases, the PVDF-based membranes exhibited excellent mechanical stability and regenerability in ammonium acetate methanolic solution, which enables reusability. Overall, the developed mixed matrix membranes (MMMs) integrate the advantages of mechanically robust polymer matrices with highly selective chromatographic fillers, thereby offering a promising and scalable strategy for the enantioselective separation of acidic racemates. This strategy represents a promising bridge between chromatographic and membrane-based separation techniques¹.

Acknowledgements

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Immobilization of a Rising Bubble: Role of Surfactant Structure

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Surfactants profoundly alter the hydrodynamics of gas-liquid interfaces in multiphase industrial processes (e.g., flotation, bioreactors). This study investigates the impact of non-ionic surfactants on the rise velocity and surface mobility of isolated bubbles in a stagnant liquid. The accumulation of surfactant molecules at the interface induces Marangoni stresses, shifting the boundary condition from fully mobile (free-slip) to rigid (no-slip)¹.

To evaluate the effect of molecular structure and footprint on this immobilization process, five surfactants were examined: short- to medium-chain alcohols (1-propanol, 1-pentanol, 1-octanol), and bulky surfactants (α -Terpineol and Triton X-100). Experiments were conducted across a wide concentration range using two approaches: tracking the dynamic local velocity profiles (LVP) during the bubble rise and measuring bubble properties in terminal state.

The terminal state results (Figure 1) reveal a strong dependence of interfacial mobility on the surfactant structure. For the homologous alcohols, increasing the alkyl chain length significantly reduces the concentration required for full immobilization (U_{rel}). Whereas short-chain 1-propanol requires exceptionally high bulk concentrations, bulky structures restrict interfacial mobility much more effectively. Most notably, the macromolecular Triton X-100 completely immobilizes the bubble at trace concentrations, roughly six orders of magnitude lower than 1-propanol. It is also worth noting that at very high concentrations in solution 1-propanol undergo interfacial remobilization.

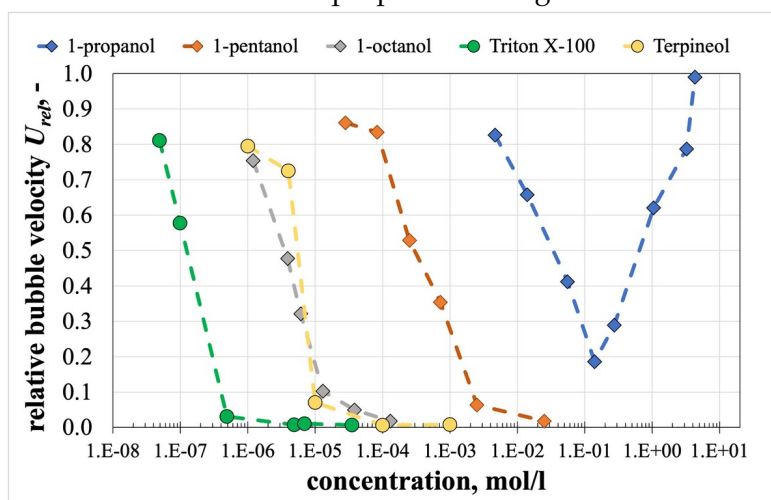


Figure 1: Relative terminal velocity (U_{rel}) as a function of bulk concentration for 1 mm bubbles. $U_{rel} = 1$ denotes a fully mobile interface, while $U_{rel} = 0$ corresponds to an immobile (rigid) surface.

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The Effect of Friction Coefficient, Agitator Speed and Secondary flows on the Process of Segregation in a Vertical Bladed Mixer

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Gravel, sand, rice or tablets, granular materials are widely used in more than a 50% of world industrial processes such as pharmacy, agriculture or food industry. Whether its packing, mixing, filling or transport, it is necessary that granular material be thoroughly mixed. One of the phenomena working mostly against the homogenization process is a segregation. Therefore, study of the granular dynamics is crucial for optimizing the industrial processes. In recent years, many studies focused on the segregation process, using either experimental or computational approach using Discrete Element method (DEM).

Segregation is occurring during manipulation with granular material due to the different material properties, such as size, shape, density or surface roughness. Despite detailed description of segregation mechanisms, unity theoretical description remains ambiguous^{1,2}.

This study examines the effects of an interplay of varying agitator speed (ranging from 15 to 480 rpm (*Revolutions per minute*)), and the inter-particle friction coefficient (ranging from 0.1 to 0.9) on the segregation process in a binary granular mixture. DEM simulations were realized in a cylindrical mixer, equipped with a two-blade agitator with a rake angle of 45°. The simulation system consisted of 37,200 glass particles. 36,800 were 2 mm in diameter and the rest were 4 mm in diameter. Analysis of DEM simulations confirmed that the friction coefficient supports the transport of the particles in both axial and radial directions, enhancing segregation processes. Examining the effects of agitator speed and its effect on the formation of the secondary flows led to the revelation of 5 segregation regimes, underlining the importance of the interplay of material properties and mixing conditions on the granular flows.

In-depth analysis was used to determine whether segregation phenomena was supported or not. A higher agitator speed led to greater surface deformation, affecting mixing conditions and, therefore, homogenization. Detailed investigation of the flow patterns was performed, and uncovered the origin of segregation changes among 5 distinct segregation regimes. These insights supported the knowledge of the segregation mechanisms and poses a potential improvement and impact on the industrial processes.

Acknowledgements

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Catalysts of Oxygen Elimination in the C-C Condensation Reaction of 1-Butanol

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The presence of oxygen heteroatoms makes the processing renewable feedstocks difficult, as they lead to equipment corrosion and reduced fuel energy value. While traditional hydrodeoxygenation (HDO) is common in treating fatty-acid-rich feeds, the oxygen-rich sources like bioalcohols make HDO impractical due to the consumption of large amount of hydrogen. Direct C-C condensation of bioalcohols including 1-butanol is a promising alternative, enabling simultaneous carbon chain extension and oxygen removal as water. Although homogeneous catalysis is already used industrially for manufacturing of fine chemicals, its extensive application is limited. Research is therefore shifting towards heterogeneous catalysis and full-scale plant modeling¹. We found the MgO/C and Sm₂O₃/C catalysts perspective and so we synthesized and characterized them both in the form of grains (0.16–0.32 mm) and extrudates (cylinders of 3.2 mm diameter and 5 mm length). This work links the experimental kinetics of 1-butanol condensation (continuous flow tube reactor, 350–400 °C, 3 bar) into higher hydrocarbons (C₇/C₈) and the model evaluation of overall process feasibility. MgO/C was proved to be highly selective toward C₈ hydrocarbons (the $2n$ pathway), whereas Sm₂O₃/C favored the formation of 4-heptanone and trances of C₇ hydrocarbons (the $2n-1$ pathway). The simulation in the Aspen Plus® successfully confirmed the scalability of the reactor measure was possible using the results of the isothermal microkinetic study. For example, 160 kg of MgO/C can catalyze reaction of 1440 kg of 1-butanol to 768 kg of C₇/C₈ products daily in whole plant model (reaction + separation). Moreover, the remarkably low specific energy demand of MgO/C catalyzed process, 0.02 MJ·kg⁻¹ of heat and 0.22 kWh·kg⁻¹ of electricity, was quantified. This low energy demand was achieved by the heat and mass recovery and thus it is two times lower than the values reported previously^{2,3} for the ethanol condensation. Transition from the lab-scale microkinetic data to lab-scale semi-pivotal data, i. e. the research over real-scale industrially used extrudates, revealed severe macro-kinetic limits. Due to internal diffusion and laminar flow in the semi-pivotal reactor, the overall efficiency factor for MgO/C extrudates was 0.48 (external 0.91, internal 0.52), while the highly active Sm₂O₃/C extrudates reached an overall factor of only 0.29 (external 0.69, internal 0.42). Consequently, the apparent activity ratio of Sm₂O₃/C, the more active catalyst, to MgO/C shrank from 2.5 to just 1.7 for the microkinetic and semi-pivotal reaction, respectively. It was also found that the formation of hot spots in the extrudates can be neglected. In conclusion, our results demonstrate the possibility of the industrial implication of both studied catalysts. Sm₂O₃/C possesses high activities while MgO/C catalyst favors the formation C₈ derivatives.

Acknowledgements

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Light Attenuation Effect on Biosynthesis of Phycocyanin in the Microalga *Galdieria Sulphuraria*; Implications for Harvest Timing

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Galdieria sulphuraria is a polyextremophilic unicellular red microalga, one of the few eukaryotic species capable of phycocyanin (PC) biosynthesis. PC is a blue tetrapyrrole based chromophorylated protein complex utilized as an accessory light harvesting mechanism associated with photosystem II. Unlike the PC commonly sourced from the cyanobacterium *Limnospira* sp., commonly known as spirulina, PC sourced from *Galdieria* sp. displays greater stability at high temperatures and low pH, making it a suitable colorant for food and beverage applications. Due to its extremophilic nature, photoautotrophic cultivation of *Galdieria* sp. requires bioreactor systems capable of sufficient heat retention and acid resistance, while maintaining high illuminated surface to volume ratio in order to fuel the photoautotrophic growth. The levels of illumination are, however, dependent on the cell density within the reactor, as the cells self-shade at high biomass concentrations. In order to capture maximum of the photosynthetically active radiation at low availability induced by self-shading, *Galdieria* increases its total intracellular content of PC as the cell density increases. This implies the existence of optimal culture density to light availability ratio, which would enable sufficient biomass productivity, while maintaining high PC content. In order to determine this ratio, an experimental cultivation in bubble column photobioreactors was carried out, measuring the total PC content and productivity throughout the growth period. The PC content was then correlated with the specific cell density at the time of sampling and used to determine the optimal cell density at constant photobioreactor diameter, incidence illumination intensity and wavelength distribution. In order to extrapolate the data to varying reactor width and incidence light intensity, a light attenuation model was employed in order to calculate specific light attenuation at different cell densities¹. Results show that there is an optimal average light intensity at which PC productivity reaches the maximum level, equating to approximately 15 $\mu\text{mol}_{\text{photons}}/\text{m}^2/\text{s}$. Our results provide a comprehensive insight into harvest timing optimization for commercial PC production in various isothermal cultivation systems with artificial controlled illumination.

Acknowledgements

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Exploiting the Carbonyl-Like Reactivity of Phosphanaphthalenes: from Electrophilic Substitution Toward Chiral Phosphaphenylene Helicenes

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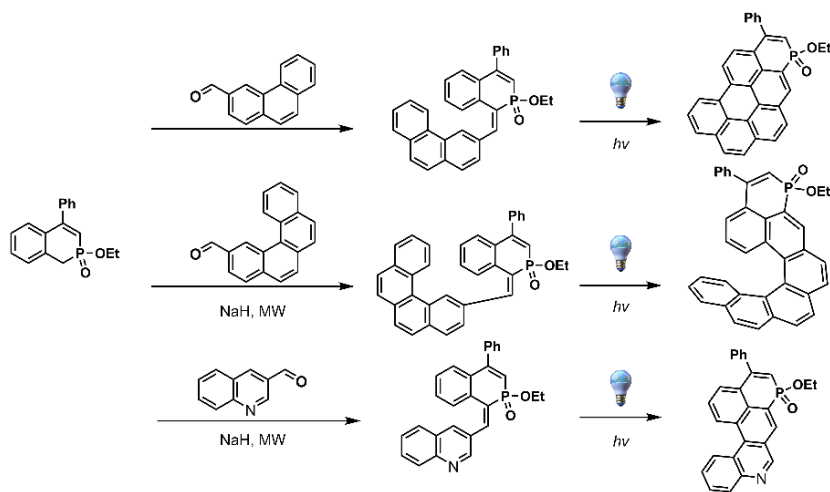
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The introduction of a phosphorus atom into a polycyclic aromatic system can significantly improve key properties, such as solubility and chemical stability, and enhance electroluminescence and ambipolar redox behavior.^{1,2} Within our research group, a robust synthetic methodology³ for phosphanaphthalene-like frameworks was previously developed and utilized for the construction of various polycyclic aromatic compounds⁴.

While further derivatization of the fundamental phosphanaphthalene skeleton typically focuses on the phosphorus center itself,⁵ highly valuable reactivities can be unlocked at the sp^3 hybridized α -carbon. This reactivity is governed by the electronic polarization induced by the adjacent $P=O$ bond, which enhances the nucleophilicity of the carbon center. Utilizing this reactivity, a diverse series of condensation products was prepared with various aldehydes. Subsequent oxidative photocyclization of the resulting stilbene-like intermediates successfully yielded the desired polycyclic aromatic frameworks. Remarkably, the final cyclization proved to be highly stereoselective, which highlights a key benefit of our approach, where the phosphorus atom acts as a built-in inducer of absolute chirality.



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Long-Term Decline in Cloud Condensation Nuclei Activation Ratio

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The cloud condensation nuclei (CCN) activation ratio is a useful indicator of the fraction of aerosol particles that can activate into cloud droplets at a given supersaturation, linking aerosol microphysical properties with potential aerosol–cloud interactions^{1,2}.

In this study, the weekly median activation ratio was analyzed from 11/2021 to 11/2025 using monthly distributions, LOcally WEighted Scatterplot Smoothing (LOWESS), Sen's slope, and Mann–Kendall trend statistics. The results show (Fig. 1) a clear, statistically significant decline in the activation ratio over the observation period. The Mann–Kendall test indicated a significant decreasing trend with $\tau = -0.57$, while Sen's slope showed a reduction of $-3.8\% \cdot \text{yri}^{-1}$ with respect to the mean activation ratio. Monthly boxplots showed pronounced short-term and seasonal variability, with median activation ratios generally ranging from about 15% to 40%, while the 95th percentile exceeded 70% in several months. Despite this variability, the LOWESS-smoothed trend decreased from approximately the mid-30% range in 2021 to near 20–25% by 2024–2025. This suggests that, over time, a smaller fraction of measured condensation nuclei activated as CCN. Such a decline may reflect changes in aerosol size distribution, chemical composition, hygroscopicity, source contributions, or atmospheric aging, all of which are known to influence CCN activity^{1,2}.

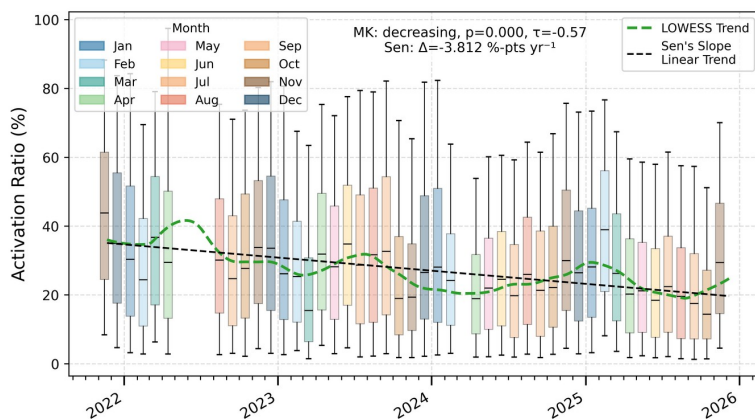


Figure 1. Monthly activation ratio distributions and trends from 11/2021 to 11/2025. Boxes represent the 25th–75th percentiles; whiskers show the 5th–95th percentiles; and medians are shown as horizontal lines. The LOWESS-smoothed trend and Sen's slope linear trend.

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What the Air Remembers: Pollution, Transformation, and a Long View

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Atmosphere represents one of the most sensitive and continuous recorders of natural and anthropogenic activities, not only as a passive medium that enables the coexistence of humans and diverse living beings, but also as a temporally stratified active archive of the varying perturbations in the Earth's environment.

Receptor sites are strategically fixed measurement stations where the ambient atmospheric composition reflects the physico-chemical characteristic features of emission sources distributed across local, regional, and continental scales¹⁻³. The ambient concentrations of chemical constituents including aerosol-phase trace metals, carbonaceous compounds, reactive trace gases and secondary inorganic aerosols measured at receptor sites serves as an imprint of industrial transitions, structural transformations, energy system shifts, the progressive adoption of emission abatement technologies, and the periodically evolving scenario in human health driven by fluctuations in air quality⁴, collectively inscribing a continuous and quantitatively interpretable history of the relationship between human society and the air it inhabits.

The work presented here systematically explores the analytical frameworks for characterising the long-term variability and directional trends of key atmospheric chemical constituents at a network of strategically selected background monitoring stations across the Czech Republic. Complementing the chemical trend analysis, the study employs meteorological and trajectory-based approaches to delineate the relative contributions of possible emission pathways, regional and long-range transport of atmospheric pollutants across oceanic-continental boundaries.

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Online Ice Nucleation Particles Measurement in the Central European Rural Background

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Atmospheric aerosols (AA) have significant impacts on Earth's climate and weather as they contribute to cloud formation and define cloud properties (albedo, lifetime, and hydrometeor production)¹. Depending on physical and chemical properties, certain AAs allow the formation of ice crystals in the atmosphere, these are called Ice Nucleation Particles (INP), while some AAs are prone to create water droplets (Cloud Condensation Nuclei (CCN)). The ratio between INP and CCN, the solid fraction, is of crucial importance, challenging to measure, and thus one of the major blind spots in climate models affecting climate sensitivity uncertainties².

Different parameterizations can be used to retrieve INP concentrations from simple aerosol measurements. It can be done from empirical aerosol number concentration³, or from aerosol surface area and ice-active site density parameterization⁴. However, those parameterizations rely on INP samples, often analysed from filters or laboratory experiments conducted for a specific type of aerosols.

Thanks to the Portable Ice Nucleation Experiment (PINE, Bilfinger) installed since August 2025 at the National Atmospheric Observatory Kosetice (NAOK), Czech Republic (49.573°N 15.080°E), a central European rural background measurement site, we measure online INP concentration at temperatures between -25 and -10 °C every 5 °C and a temporal resolution of 123 min.

With continuous measurements from 27th July 2025 until the end of February 2026, we find a decrease in INP concentration by 70 to 50% between summer and winter for the lowest and warmest measurement temperatures, respectively. We also find a significant impact of air mass origin on INP concentration at -25 and -20 °C, with higher concentrations observed for continental air masses from Western and Eastern Europe compared to Atlantic and Arctic air masses.

We compare online INP measurements with parameterized INP concentration from 12 different formulas built for different aerosol populations; we thus recalibrate their constant parameters for our continental climate measurement site.

The 10% worst parameterized INP concentration of each parameterization tends to converge more than the 10% best parameterized concentrations. The period with the best agreement between measured and parameterized INP concentrations is characterized by the highest total particle number concentration. On the other hand, the overestimation periods are typical for the lowest particle number concentration, combined with the highest coarse-to-fine particle ratio, indicating that too much emphasis is given to coarse particles while the ice nucleation ability of fine particles is underestimated.

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Thermodynamic Analysis of Nickel Speciation in Nitric Acid, Methanesulfonic Acid, and Glycine Leaching Systems

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The thermodynamic behavior of nickel in nitric acid (HNO_3), methanesulfonic acid (MSA)¹, and glycine-based leaching systems was investigated using Medusa/Hydra software in order to evaluate nickel stability, complexation, and precipitation under different chemical conditions. Fraction, predominance, logarithmic concentration, solubility, and Eh–pH (Pourbaix) diagrams were constructed at 25 °C over a wide pH range using nickel concentrations derived from rejected materials generated during Solid Oxide Cell (SOC) manufacturing.

The thermodynamic analysis revealed two fundamentally different equilibrium regimes. In nitric acid systems, nitrate ions did not exhibit significant complexation with Ni^{2+} , indicating that nickel speciation is mainly governed by acid–base equilibria. Under acidic conditions, nickel remains stable as free Ni^{2+} , while increasing pH promotes hydrolysis and precipitation as $\text{Ni}(\text{OH})_2(\text{s})$, with a sharp transition occurring near pH 6. Similar behavior is expected for methanesulfonic acid due to the absence of strong Ni–MSA aqueous complexes reported in standard thermodynamic databases.

In contrast, glycine strongly modified nickel thermodynamic stability through the formation of stable aqueous complexes such as $\text{Ni}(\text{gly})^+$, $\text{Ni}(\text{gly})_2$, and predominantly $\text{Ni}(\text{gly})_3^-$. Increasing glycine concentration from 1 M to 2 M expanded the stability region of dissolved nickel species and shifted hydroxide precipitation to significantly higher pH values. The predominance and Eh–pH diagrams demonstrated that nickel stability in glycine systems depends on the combined effects of pH, redox potential, and ligand concentration, whereas nitric acid systems are primarily controlled by pH alone².

From a Gibbs free energy perspective, the diagrams identify the most thermodynamically stable nickel species under each condition, showing that ligand complexation reduces the activity of free Ni^{2+} and stabilizes nickel in solution. These results provide a thermodynamic framework for interpreting nickel leaching behavior and selecting suitable operating windows for hydrometallurgical recovery processes³.

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On-Road Remote Vehicle Emission Measurements for High-Emitter Identification

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Supervising Expert: RNDr. Petra Vondráková Pokorná, Ph. D.

Over the past decades, air quality in the Czech Republic has significantly improved. Nevertheless, air pollution remains a serious problem with proven negative impacts on human health and the environment. In urban agglomerations, where population density is highest, road traffic represents the dominant source of pollution. Traffic-related pollution includes both gaseous emissions, primarily nitrogen oxides (NO_x) and carbon monoxide (CO), and solid aerosol particles.¹ The amount of emissions produced by a specific vehicle varies significantly depending on several factors, including technical condition, age, engine type, current operating conditions, and driving style and traffic fluency.²

The aim of this work was to test the capability of an experimental measurement setup to serve as a reliable method for the remote identification of high-emitting vehicles directly in real-world traffic. These high-emitters contribute disproportionately to total traffic emissions, and their early detection is crucial for effectively improving urban air quality.³

A measurement campaign was conducted at a barrier gate at the parking lot of the Czech University of Life Sciences, Prague. This location was deliberately selected for the experiment: the presence of the barrier ensured that every passing vehicle had to come to a complete stop at the gate and subsequently accelerate. This controlled driving maneuver standardized the measurement conditions and allowed for a more relevant comparison of the emission plumes of individual vehicles under engine load, when emission production typically increases rapidly.² The sampling of air containing emissions from passing vehicles was carried out simultaneously at two independent sampling sites. The first sampling point was located directly in the roadway below the level of the car exhausts. From here, the gas sample was drawn through a carbon tube into a mobile laboratory housed in a van. Inside the mobile laboratory, the sampling line was isokinetically divided into smaller branches connected to a suite of measuring instruments for the online analysis of both gaseous and solid components. The second sampling point was located at the edge of the roadway. Here, the sample was drawn using two sampling heads directly attached to a measurement box equipped with additional instrumentation. These heads were positioned at a height of 0.75 meters above the ground and at an average distance of 1.5 meters from the exhaust axis of the passing vehicles.

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Preparation of MgO Nanofibrous Catalysts by the Electrospinning Technique for Liquid-Phase Guerbet Coupling

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The growing demand for renewable and sustainable energy resources has accelerated interest in the upgrading of lower primary bio-alcohols (e.g., bioethanol or biobutanol) into higher-value products (e.g., 2-ethylhexanol). Higher alcohols are used as sustainable fuels, solvents, and chemical intermediates¹. Among different catalytic pathways, the Guerbet reaction represents an effective transformation for converting primary alcohols (1-butanol) into β -branched dimer alcohols (2-ethylhexanol) with high atom economy through dehydrogenation, aldol condensation, and hydrogenation reactions. Homogeneous noble metal catalysts offer high selectivity but are limited by high cost and difficult separation of the catalyst from the reaction mixture².

MgO-based electrospun nanofibrous heterogeneous catalysts have emerged as a promising catalytic system due to their surface-to-volume ratio, structural tunability, and lower mass transfer resistance compared to conventional supported noble metal catalysts. Moreover, different parameters of electrospinning offer tuneable microstructural and morphological properties such as pore-size, nanofiber diameter, and microstructure, which play a crucial role in active sites, mass transfer and catalytic selectivity in Guerbet reaction.

This work focuses on the development of MgO electrospun nanofibrous catalysts, evaluating the impacts of precursor spinning solution composition and calcination temperature on their structural properties and catalytic performance in the Guerbet reaction.

The prepared catalysts are characterized using X-ray diffraction (XRD), nitrogen physisorption, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray photoelectron spectroscopy (XPS). Catalytic activity and selectivity will be evaluated in a batch reactor in the liquid phase

SEM analysis confirmed the formation of MgO nanofibers with retained nanofibrous morphology after calcination at 500 °C, 600 °C, and 700 °C.

The research presents a viable electrospinning method for developing effective bulk heterogeneous nanofibrous catalysts. It demonstrates their potential for use in liquid-phase reactions, such as Guerbet coupling.

Acknowledgements

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Recycling of Lithium-Ion Batteries: Influence of Battery Material Composition and Topology on Efficiency of Selected Recycling Processes

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Lithium-ion batteries (LiB) have become the dominant solution powering the emerging markets of mobile electronics, stationary storage, and electric vehicles. To achieve such energy densities, manufacturers have to develop complex battery chemistries including a multitude of critical raw materials (CRM) such as Ni, Mn, Co, Li oxides (NMC) and graphite¹. The new EU battery recycling regulation (2023/1542) places great emphasis on improving the overall efficiency of the recycling process to reduce dependence on imports and limit environmental damage from improper recycling. Regulation imposes stricter limits on recovery of individual CRMs by year of 2027 and 2031, respectively. However, the same manufacturing practices that enable the high energy density and reliability also create severe challenges when it comes to the LiB recycling². The current predicament is defined by a struggle between the actual capabilities of the established LiB recycling industry and the proposed limits, leaving only a few technologies that can successfully address both challenges³.

This study aims to outline how EU regulation, together with certain LiB manufacturing and recycling practices, influence the complexity, efficiency, and financial sustainability of established methods like pyrometallurgy⁴ and hydrometallurgy⁵ as well as new direct recycling methods in active development stage⁶. By doing so, it hopes to provide new valuable perspectives on the problem of LiB recycling.

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Amonia Decomposition on Heterogeneous Catalyst

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This study examines the decomposition of ammonia for hydrogen production using a nickel catalyst and its potential application in commercial microreactor systems. The aim of the work is to describe the reaction mechanism using an empirical equation that captures the processes occurring in the microreactor, and to identify the rate-limiting step in the decomposition of ammonia on the nickel catalyst¹.

The existing literature on ammonia decomposition focuses primarily on ruthenium-based catalysts, which exhibit high catalytic activity. However, their wider commercial use is limited by the high cost of this metal. For this reason, this work focuses on more economically accessible nickel catalysts. In general, for catalysts used in the decomposition of ammonia, nickel catalysts are inhibited by nitrogen, while ruthenium catalysts are inhibited by hydrogen².

The catalysts used are being developed in collaboration with RANIDO s.r.o., a company specializing in their synthesis. Experimental measurements were performed in a microreactor with a catalyst cartridge of inner diameter of 4.8 mm length 39 mm. The catalyst has been reduced in situ under flow of pure hydrogen, temperature 600 °C and pressure 6 bar. The reaction mixture at the reactor outlet was analyzed by on-line gas chromatograph. The dependence of ammonia conversion on temperature and pressure was evaluated at various space velocities (WHSV). The measurements were conducted in the temperature range of 350–600 °C, at space velocities of 3.5, 4.5, and 8.3 WHSV, and absolute pressures of 1, 3, 5, and 7 bar.

The experimental results demonstrate a significant effect of temperature on the achieved ammonia conversion that can be approximated by an Arrhenius equation. Data also reveal effect of increased pressure that decreases the ammonia conversion, even being far from equilibrium. The study also includes assessment of catalytic activity stability by a comparison of the conversions achieved under identical reaction conditions on fresh and spent catalyst.

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