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Unravelling the Fate and Transport of Micro and Nanoplastics in Water Treatment PlantsS. Stoll¹

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Microplastics which are increasingly detected in aquatic environments constitute a global concern due to their persistence, mobility, and potential risks regarding water resources used to produce drinking water. This presentation aims to investigate the presence of microplastics in a conventional water treatment plant used in Geneva (CH) to provide tap water for 500'000 consumers.

Microplastic concentrations, size distributions, chemical compositions in raw and treated water and removal efficiency will be discussed as well the impact of the different water treatment processes. On the other hand, nanoplastics which are expected to result from the fragmentation of microplastics (probably the most hazardous fraction) will also be discussed. In particular, adsorption to mineral surfaces, considered as one of the most important processes controlling their fate and transport in conventional water filtration systems, will be presented by considering adsorption isotherms and kinetic models.

Adsorption mechanisms, influencing physicochemical parameters (pH, natural organic matter), and adsorption capacities of the different porous media used in water treatment will be investigated using complementary techniques such as dynamic light scattering, laser Doppler velocimetry, scanning electron microscopy and turbidity measurements.

Towards Safe and Sustainable by Design: The Potential of Read-Across Microbiomes Approaches to Assess Soil Biodegradability of Chemicals

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Active pharmaceutical ingredients and agrochemicals are indispensable to modern society, yet increasing scrutiny of their environmental impact shifted the focus toward a new space of innovation: the design of small molecules that combine high performance with environmental biodegradability. While the “Safe and Sustainable by Design” (SSbD) paradigm is widely embraced, its practical implementation is hindered by one major bottleneck: the absence of rapid, high-throughput, and decision-grade testing frameworks for early-stage chemical research.

We address this gap with a disruptive read-across framework that leverages activated sludge degradation data to predict the environmental fate of chemicals in soil. Our proof-of-concept demonstrates that such read-across experiments provide high predictive accuracy for soil degradation and significantly outperform current in-silico prediction tools. By integrating these empirical metrics into the discovery phase, we enable a transition from reactive assessment to proactive molecular design. This approach transforms sustainability from an aspirational goal into a practical design criterion, establishing new standards for innovation across pharmaceutical and agrochemical industries.

Interactive Generative Modelling for Safe and Sustainable by Design Chemicals: A Case Study on Antioxidants

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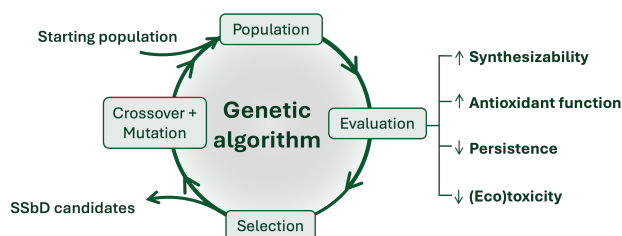
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Ensuring the safety of novel chemicals requires proactive strategies that consider environmental and health hazards already at the molecular design stage [1]. Phenolic antioxidants are widely used and increasingly considered contaminants of emerging concern, exemplifying the need for molecular (re)design that maintains function while reducing risk [2]. This work addresses this challenge by developing an interactive generative modelling framework for the de novo design of safer phenolic antioxidants aligned with Safe and Sustainable by Design (SSbD) principles.

We employ a genetic algorithm to generate and evolve molecular structures while optimizing multiple criteria spanning synthesizability, antioxidant function, environmental fate, and (eco)toxicity. Because these criteria rely on imperfect predictors, a fully automated search can exploit their weaknesses and produce high-scoring but practically unsuitable structures. To counteract this we have built a human-in-the-loop interface that enables domain experts to supervise and guide the optimization. Users can dynamically adjust objective weights and components, remove undesirable candidates and manually add new structures, integrating intuition that is otherwise difficult to capture.

The genetic algorithm efficiently identifies a diverse set of promising phenolic structures with improved predicted profiles for performance and safety. Molecular similarity analysis confirms high structural diversity among the generated molecules, which supports a broad exploration of independent structural strategies. Comparison with a curated set of antioxidants in current use shows that early generations of molecules generated by the genetic algorithm rediscover known molecules, while later generations explore increasingly novel chemical space.

This work demonstrates how generative modelling, expert interaction, and predictive hazard assessment can be integrated into a practical SSbD-oriented design workflow. It is embedded in an interdisciplinary project in which our project partners are developing experimental high-throughput methods for assessing persistence, toxicity, and degradation-product hazards. The project lays the foundation for a closed-loop design approach coupling high-throughput experimentation and generative modelling via active learning to accelerate the development of safer functional chemicals.



[1] European Commission Recommendation of 8.12.2022 establishing a European assessment framework for "safe and sustainable by design" chemicals and materials.

[2] Carolin Seller-Brison, Franziska Weissbach, Kjell Jorner, Martin Scherlinger, Kathrin Fenner, *Environmental Science & Technology Letters* **2026**, 13, 560–567.

Environmental Hazard Screening of Phenolic Antioxidants: From Persistence to *In Vitro* Toxicity Assessment for Safe-by-Design Chemical Development

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Safe-by-design principles rely heavily on hazard assessment data of chemicals in commerce. Unfortunately, such information is lacking for a wide range of substances, particularly concerning the persistence and toxicity of industrial chemicals. This project aims to address this knowledge gap by developing high-throughput screening tests to investigate the environmental hazards of synthetic antioxidants.

Synthetic antioxidants are contaminants of emerging concern due to their widespread use in various applications, including as preservatives in plastics, fire retardants, synthetic fibers, fuels, and even foods. As a result, these compounds are now frequently detected in multiple environmental matrices, including natural water bodies, sediments, air, and biota [1]. While previous studies have shown that certain synthetic antioxidants and their transformation products can exert toxic effects on living organisms, data on the environmental fate and (eco-)toxicity of most compounds within this diverse and extensive class remains limited [2].

To address this data gap, we first assessed the environmental persistence of 60 phenolic antioxidants using activated sludge biodegradation assays, alongside the development of a targeted LC-MS analytical method for the detection of a broad range of phenolic antioxidants. Activated sludge biotransformation experiments represent a higher-throughput yet robustly predictive alternative for biodegradation testing in complex environmental microbial communities, thereby enabling more efficient data collection for persistence assessment. To further optimize this approach, we integrated a full sludge suspension extraction procedure into the method, addressing the challenges associated with testing strongly sorbing antioxidants in activated sludge. Building on this, we are developing methods to couple biodegradation assays with animal-free *in vitro* bioassays to evaluate multiple cellular toxicity endpoints before and after simulated degradation [3].

Our findings will provide critical data for the environmental hazard assessment of phenolic antioxidants. Moreover, the tested workflows and optimized analytical method may eventually be integrated into the early stages of the chemical development process for emerging synthetic antioxidants, thus providing essential information for the design of safe and sustainable chemicals.

[1] Liu, R. & Mabury, S. A. *Environ. Sci. Technol.*, 2020, 54, 11706–11719.

[2] Seller-Brison, C., Weissbach, F., Jorner, K., Scheringer, M. & Fenner, K. *Environ. Sci. Technol. Lett.*, 2026, 13 (4), 560-567.

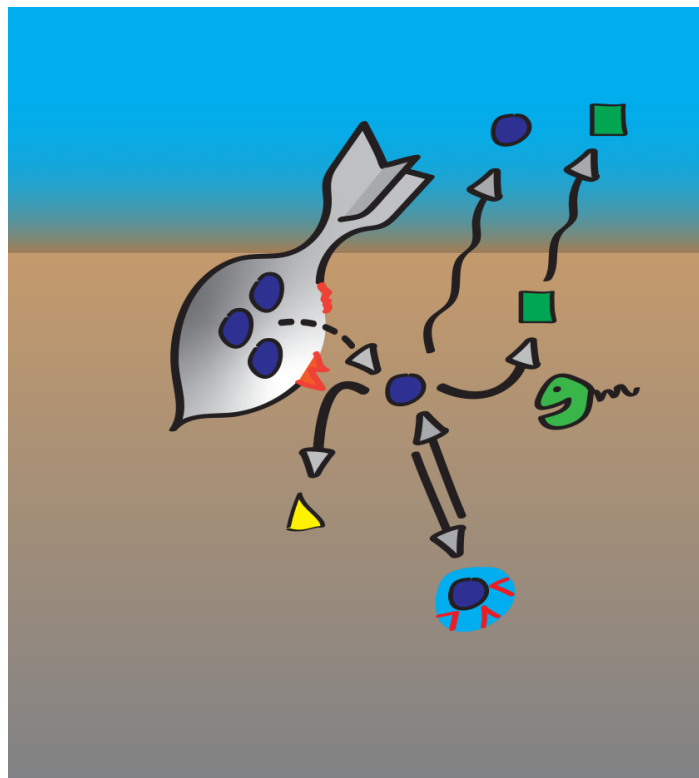
[3] Escher, B. I. et al. *Arch. Toxicol.*, 2023, 97, 1267–1283.

Revisiting Deposition of Ammunition in Swiss Lakes: from Monitoring Organic Munition Constituents to Assessing their Release and Fate

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Chemical pollution of aquatic and terrestrial environments with munition constituents (MCs) such as explosives from the legacy of military activities poses a potential risk to ecosystems and human health. The exposure assessment of the diffuse pollution originating from several hundred thousand tons of ammunition dumped worldwide into aquatic environments during the 20th century was, however, impeded by the sampling resolutions, instrumental sensitivities, and/or the scope of quantified MCs of past monitoring studies. Moreover, the ongoing deterioration of ammunition casings, which is closely tied to environmental conditions, might alter the likelihood of MC emissions and is understood only scarcely. This is especially the case for landlocked countries such as Switzerland, where freshwater lakes hold not less than 14 thousand tons of ammunition.



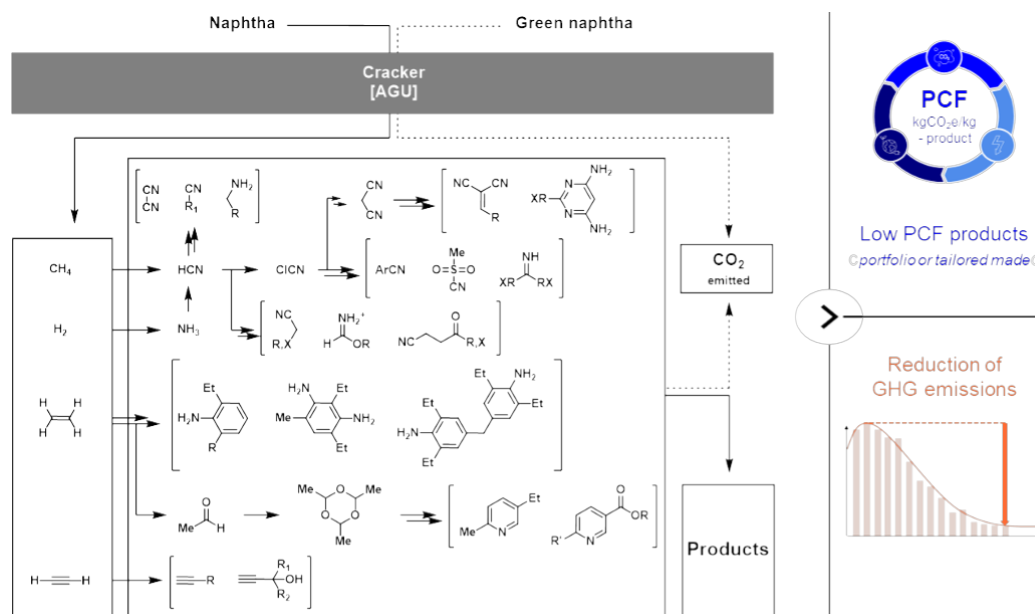
In our study, we are therefore designing sampling procedures and analytical methods to investigate the emission and fate processes of MCs from ammunition deposited in freshwater lakes. Specifically, we are developing methods for the quantification of 24 MCs and selected transformation products in water and sediments in the low to sub- ng/L and $\mu\text{g/kg}$ concentration range with liquid chromatography-high resolution tandem mass-spectrometry (LC-HRMS/MS). Limits of quantification for water analysis using evaporation for enrichment (0.01 to 1 $\mu\text{g/L}$) were significantly improved by implementing online solid-phase extraction (SPE) instead (0.1 to 10 ng/L). Using a solid-liquid extraction method for sediment analysis, very good absolute recoveries of 80-120% are obtained for 75% of our analytes. To support the evaluation of MCs distribution and ammunition casings deterioration, we are performing complementary analyses including (1) Pb-210 dating, (2) X-ray fluorescence (XRF) scanning with a focus on heavy metals, and (3) clay and total organic carbon (TOC) content estimation as indicators for MC sorption to sediment constituents. These analytical procedures are being applied to samples collected over selected open-water ammunition deposition sites in Switzerland. To increase sampling resolution, we successfully tested the deployment of a multicorer which allowed to simultaneously retrieve 6 cores of 60-80 cm at fixed relative horizontal distances at 215 m underwater in 20 min. This study will provide valuable information for the potential needs and risks of recovering ammunition lying at the bottom of Swiss lakes.

Turning Net-Zero Into Reality – Arxada's chemical network as key to unlock sustainable chemistry

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In today's world, the call for action to build a sustainable future resonates loudly, emphasizing the need for transformative solutions to reduce greenhouse gas (GHG) emissions. In this talk we discuss innovative approaches facilitated through Arxada's unique chemical network, to achieve net-zero products. Building on existing technologies we outline our strategy to transform a more than 100-year-old chemical network into a core asset for sustainable chemistry.



Two use-cases will be presented to explain how vertical integration can unlock high atom efficiencies[1] and net-zero production.

[1] Philipp Kohler, Eva Kirchner, Emilia Păunescu, Ulrich Mayerhöffer, *Helv. Chim. Acta*, 2024, 107, e202400048.

A Moment of Heat, a Lifetime Exposure? The Interplay of Temperature and Contaminants increases Pressure on Aquatic Invertebrates

J. Raths^{1,2}, M. Hermann¹, C. von Au^{1,2}, J. Hollender^{1,2}

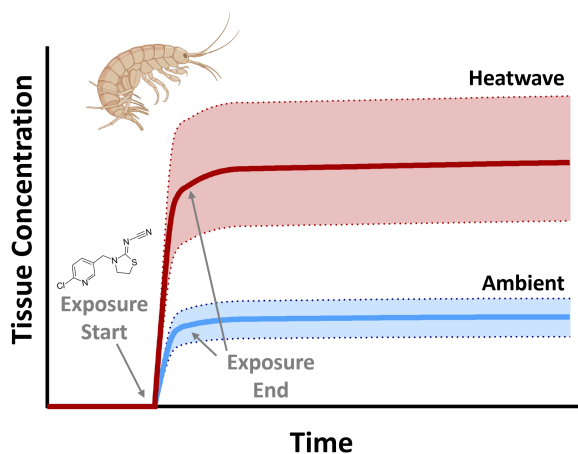
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Chemical pollution and climate change are major threats towards aquatic communities. Yet, the interactions of these stressors remain poorly understood. Especially the combination of chemical exposure and increasing heatwaves raises concern.¹ To understand the mechanisms of these stressor interactions, recent studies have explored the temperature-dependent toxicokinetics (uptake, elimination and transformation) of contaminants in aquatic invertebrates. These toxicokinetic processes define the internal concentrations in an organism and are a key connection between exposure and observed effects. However, such studies showed limitations for contaminants with strong receptor binding affinity (i.e. neonicotinoids) that were resistant towards elimination.²

In this talk, we will present a case study that examined temperature effects on the toxicokinetics of a neonicotinoid pesticide (thiacloprid) in aquatic invertebrates under laboratory and outdoor mesocosm conditions. For this purpose, a temperature dependent toxicokinetic model, including receptor-binding, was calibrated based on laboratory experiments with aquatic invertebrates exposed under static (fixed temperature and fixed exposure concentration) conditions. Additionally, experiments were performed using an outdoor mesocosm facility with a dynamic exposure (natural temperature fluctuations and exposure pulses) including a simulated heatwave (ambient temperature + 8°C).

Increasing temperature had an exponential effect on toxicokinetic rate constants. The temperature dependent toxicokinetic model showed a good fit for laboratory data ($R^2 = 0.78 - 0.98$) and allowed a correlation of temperature effects on toxicokinetics with other physiological parameters (i.e. respiration). Furthermore, the model accurately predicted tissue concentrations in the mesocosm experiment, thereby validating the model. The tissue concentrations were two times higher under heatwave conditions compared to ambient temperatures (46 vs. 25 $\mu\text{g kg}^{-1}$) and remained at this level even after the event of exposure due to insignificant elimination.

The presented study advanced the mechanistic understanding of the interaction of chemical exposure and changing climatic conditions. We highlight how extreme heat events can intensify risks caused by pesticides, especially when they show specific biological interactions such as strong receptor binding. These findings emphasize the need for regulatory strategies, such as dynamic models, to address the interactions of contaminants and a warming climate.



[1] Polazzo, F. et al. *Change Biol.* **2022**, 28 (4), 1248–1267.

[2] Raths et al., *Glob. Change Biol.* **2023**, 29 (5), 1390–1406.

Bioaccumulation of organic pesticides in fish cells for chemical risk assessment

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In vivo fish bioaccumulation testing is a costly, time-consuming, and ethically contentious requirement under pesticide regulatory frameworks. Fish cell lines offer validated *in vitro* alternatives that support the 3Rs principles of replacement, reduction, and refinement. In this study, we assessed the acute cytotoxicity and bioaccumulation of three organic pesticides (trifloxystrobin, tebuconazole, and tembotrione) using RTgill-W1 cells, derived from the gills of rainbow trout (*Oncorhynchus mykiss*), as an *in vitro* model. Non-toxic concentrations, derived from acute cytotoxicity testing per OECD TG 249, were used for bioaccumulation assessment.

Bioaccumulation factors were quantified using kinetic BCF (from uptake and elimination rate constants) and steady-state BCF approaches, and compared against *in vivo* measurements and QSAR estimates. Chemical analysis revealed compound-specific depletion in cell-containing exposures relative to cell-free controls, and biotransformation products were detected, confirming the biotransformation capacity of the cell line. Together, these findings demonstrate that RTgill-W1 cell assays can reliably capture bioaccumulation endpoints relevant to regulatory fish toxicity assessment, offering a practical and ethical alternative to animal testing.

A molecular mechanism for stress volatile perception in plants

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Wounded plants emit complex blends of volatile organic compounds that can alter the physiology of nearby plants, yet the identity of the active signals and the mechanisms by which they are perceived remain poorly understood. Here, we show that volatiles released from wounded maize plants induce defense responses in unwounded neighbors. To identify the active components, we used mutant emitter lines lacking specific volatile biosynthetic enzymes, resulting in the selective loss of individual compounds or compound classes. Using this approach, we show that green leaf volatiles (GLVs), a class of fatty acid-derived C6 aldehydes, alcohols, and esters that are rapidly induced by wounding, are both necessary and sufficient to induce defense responses in neighboring plants. Furthermore, we identify two homologous membrane-localized receptors that bind the GLVs *cis*-3-hexenol and *cis*-3-hexenyl acetate with high affinity and specificity. Loss of these receptors abolishes maize responsiveness to GLVs. Accordingly, receptor mutants are no longer able to detect and respond to herbivore-attacked neighbors. Forty years after the discovery of “talking trees,” these findings provide a molecular mechanism for plant volatile perception and demonstrate how plants can detect herbivory by sensing wound-induced volatiles through specific extracellular receptors.

Harnessing actinomycete-derived metabolites for late blight disease biocontrol

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Actinomycetes are well known for their capacity to produce a wide array of specialized metabolites with diverse biological activities, making them a valuable resource for the discovery of novel biocontrol agents. In previous work, we screened a collection of 175 actinomycete strains isolated from diverse Sudanese soils for inhibitory activity against *Phytophthora infestans*, the causal agent of late blight disease in potato and tomato. Using a comparative metabolomics and genomics approach, we identified approximately 75 potentially active metabolites and prioritized 15 candidate compounds for further investigation. Commercially available or synthesized standards of these compounds were subsequently evaluated against different developmental stages of *P. infestans*, including mycelial growth and spore germination, resulting in six active compounds, namely actinomycin D, antimycin A, borrelidin, ikarugamycin, macbecin I, and myriocin. In addition, their antimicrobial spectrum was assessed against a panel of plant pathogenic oomycetes and fungi to determine whether their activity is broad-spectrum or target-specific. Antimycin A and macbecin I exhibited strong antifungal activity against *Alternaria solani*, whereas actinomycin D and myriocin showed moderate inhibitory effects. In contrast, borrelidin displayed pronounced anti-oomycete activity against *Pythium ultimum*, while ikarugamycin specifically inhibited the zoospore germination of *P. infestans*. Notably, none of the tested compounds showed activity against *Rhizoctonia solani*. To facilitate translation toward practical application of promising biocontrol strains in Switzerland, a Swiss collection of actinomycetes (n = 238) was evaluated both *in vitro* and *in planta* against *P. infestans* and additional phytopathogens. Future analyses will determine whether active strains from both (Sudanese and Swiss) collections share biosynthetic gene clusters and metabolites responsible for their antagonistic effect against *P. infestans* or whether they act through different mechanisms. Overall, this project aims to exploit the metabolic diversity of actinomycetes to develop effective and sustainable biocontrol solutions against late blight disease, contributing to environmentally friendly plant protection strategies.

Cropping context and prior conspecific oviposition alter rape stem weevil behaviour: metabolomic insights into plant-insect interactions.

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Associative cropping, which consists of planting different crop species together, is increasingly promoted as a sustainable strategy to reduce pest pressure and enhance agroecosystem health and resilience. Planting oilseed rape (*Brassica napus*) alongside faba bean (*Vicia faba*) has proven to efficiently reduce oviposition punctures by the rape stem weevil (*Ceutorhynchus napi*), a major insect pest of oilseed rape. Using a combination of behavioural assays, volatile profiling and untargeted metabolomics, we investigated how cropping context influences plant-mediated interactions between host plants and ovipositing females. Results showed that previous oviposition by conspecifics induced contrasting behavioural responses depending on cropping system. While females preferentially oviposited on previously attacked plants grown in monoculture, oviposited plants grown in association with faba bean became less attractive than their non-attacked counterparts and no longer elicited oviposition preference. Volatile analyses revealed increased emissions in associated plants as compared to monocropped plants. In contrast, untargeted metabolomics identified oviposition as the primary driver of non-volatile metabolic variation, with comparatively limited effects of cropping context. Together, these results suggest that associative cropping modifies the chemical information available to host-seeking females. By potentially disrupting the positive feedback normally associated with conspecific oviposition, associative cropping may reduce aggregation behaviour and oviposition pressure. These findings provide new insights into the chemical ecology of diversified cropping systems and highlight how changes in plant diversity can alter chemical cues and reshape insect decision-making.

[1] Breitenmoser, S., Steinger, T., Baux, A., and Hiltbold, I. (2022). Intercropping winter oilseed rape (*Brassica napus* L.) has the potential to lessen the impact of the insect pest complex. *Agronomy*, 12, 723

[2] Magnin, L., Hiltbold, I., Jullien, A., and Baux, A. (2025). Intercropping mitigates incidence of the oilseed rape insect pest complex. *Pest Management Science*. Advance online publication.

Elucidating the Role of Floral and Herbivore-Induced Volatiles in *Maruca vitrata* Oviposition Behavior and Natural Enemy Attraction: Implications for Semiochemical-Based Pest Management

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Cowpea (*Vigna unguiculata*) suffers major yield losses from *Maruca vitrata*, whose ovipositing females rely on plant volatiles for host selection. Using GC–EAD and GC–MS, key floral compounds such as benzaldehyde and (*E*)-cinnamaldehyde were identified as oviposition cues, and a synthetic blend containing 3-vinylbenzaldehyde successfully mimicked flowering plants by inducing egg-laying. In contrast, herbivore-induced plant volatiles (HIPVs) emitted by infested plants including (*E*)-DMNT, indole, 1-octen-3-ol, and linalool—reduced oviposition and attracted parasitoids such as *Apanteles taragamae* and *Phanerotoma syleptae*. These results highlight the potential of semiochemicals for developing push–pull pest management strategies against *M. vitrata*.

Removal of Activated Corrosion Products in NPP Wastewater

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This work addresses the selective removal of cobalt from large-volume radioactive aqueous waste streams generated during nuclear power plant (NPP) operation. Efficient removal of ⁶⁰Co, a γ -emitting activation product, can reduce occupational exposure and complement conventional treatment routes such as evaporation.

Phosphate-based inorganic sorbents are attractive for radionuclide capture because of their structural stability, high density of sorption sites, and fast uptake kinetics [1]. In addition, the formation of sparingly soluble metal phosphate phases may enhance long-term immobilization under disposal-relevant conditions.

Here, we investigate the recently developed glaserite-type phosphate $\text{MgNaH}(\text{PO}_3)_2$ as a candidate material for cobalt immobilization. This material exhibits an open layered crystal structure, while the close match between the ionic radii of Mg^{2+} and Co^{2+} facilitates cation substitution within the phosphate framework. These features contribute to its high sorption capacity and selectivity [2,3].

The material shows rapid cobalt sorption kinetics, high uptake capacity, and strong selectivity in the presence of elevated Na, K, Mg and Ca concentrations representative of NPP wastewater. Rapid sorption of Zn, Cu, Ni, and Mn was also observed. These elements are relevant to NPP systems because their neutron activation can produce radiologically significant activation products, including ⁶⁵Zn, ⁶⁴Cu, ⁶³Ni, and ⁵⁴Mn.

To enable operation under flow-through conditions, $\text{MgNaH}(\text{PO}_3)_2$ was immobilized in a polyacrylonitrile (PAN) matrix, providing a practical route toward implementation in dynamic wastewater treatment systems.

[1] Y. Xie et al., J. Water Process Eng. 71, 107266 (2025)

[2] C. Yang et al., Chem. Eng. J. 486, 150362 (2024)

[3] L. Zeng et al., Resour. Conserv. Recycl. 212, 108005 (2025)

Development of a Near-Infrared Spectroscopy Workflow for Carbon and Nitrogen Prediction in Soil and Plant Samples

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Near-infrared (NIR) spectroscopy is a rapid and non-destructive analytical technique with strong potential for environmental and agricultural applications. In soil and plant systems, NIR spectroscopy can be used to estimate total carbon (C), total nitrogen (N), soil organic carbon (SOC), and C/N ratios, enabling fast screening of large sample sets with minimal sample preparation. Compared to conventional laboratory methods, NIR offers significant advantages in analysis speed, cost efficiency, and sustainability. However, reliable prediction models strongly depend on high-quality calibration datasets and standardized measurement conditions.

The objective of this work is to establish an NIR spectroscopy workflow for the prediction of C and N contents in heterogeneous soil and plant samples using elemental analysis as reference method. Soil and plant samples representing different soil textures, moisture conditions, and plant species are measured under standardized conditions. Combustion-based elemental analysis provides the reference values required for calibration and validation of spectroscopic models.

At the current stage of the project, the spectral database and calibration framework are still under development. Ring trial samples of leaves and soils as well as certified reference materials, including NIST standards, are used to establish robust calibration datasets. In addition, soil and plant samples from the WSL material database are integrated to cover a broad range of environmental conditions and sample compositions. This approach enables the development of both Switzerland-specific and internationally applicable calibration sets for future NIR-based prediction of C and N parameters. Address these challenges, preprocessing approaches and standardized workflows are systematically evaluated to improve robustness and reproducibility.

All spectral and elemental data are integrated into a structured database designed for future chemometric analysis and multivariate model development. This ongoing work provides the foundation for future high-throughput prediction of C and N in environmental samples and supports the development of scalable monitoring approaches for agricultural and ecological research.

Exposure to Plant Secondary Metabolites Through the European Diet

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Dietary exposure to plant bioactive compounds is difficult to quantify, as current food composition databases represent only a limited subset of the phytochemical diversity present in real diets. Here, we performed targeted and untargeted metabolomic profiling of more than 500 plant-based foods and beverages and integrated compound occurrence with EFSA food consumption data to estimate dietary exposure in a 70-kg European adult. Four bioactives representing distinct phytochemical classes and reported health-promoting activities were selected as case studies. First, the lignan secoisolariciresinol (SECO), a gut microbiota-derived precursor of the phytoestrogens enterodiol and enterolactone associated with cardiometabolic and anti-inflammatory benefits, was estimated at 703 µg/person/day, exceeding previous European estimates of approximately 170–230 µg/day. Second, coumarin, a benzopyrone with reported antioxidant and anti-inflammatory activities but whose intake is limited by hepatotoxicity at high doses, was estimated at 564 µg/person/day, below reported average dietary intakes (1–3 mg/day) and well below the EFSA tolerable daily intake. Third, the steroidal glycoalkaloid α -tomatine, investigated for cholesterol-lowering, anticancer and immunomodulatory properties, showed an estimated exposure of 45.5 µg/person/day, for which comparable population-level exposure data are currently lacking. Finally, the furocoumarin bergapten, a photoactive compound with reported anti-inflammatory and anticancer activities, was estimated at 345 µg/person/day, likewise representing one of the first population-level dietary exposure estimates. Despite their diverse chemical origins, estimated exposure to all four compounds was predominantly driven by the coffee, cocoa, tea, infusions food category, suggesting that beverage consumption is a major determinant of chronic phytochemical exposure. This food metabolome library provides a scalable framework for estimating population exposure to hundreds of plant bioactive compounds, facilitating compound prioritization for nutritional, toxicological, and One Health research.

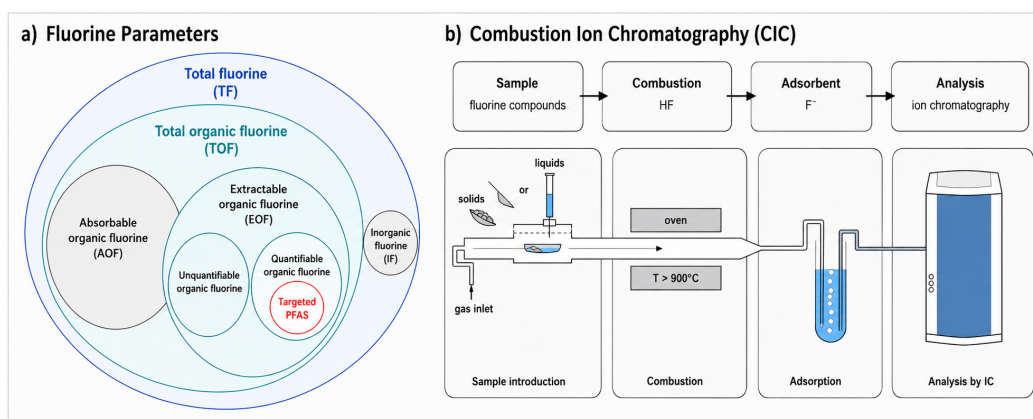
Opportunities and Limitations of Combustion Ion Chromatography (CIC) for PFAS Determination in Environmental Samples

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Per- and polyfluoroalkyl substances (PFAS) are persistent environmental contaminants that are frequently detected in water, soil, food, and consumer products. Targeted LC-MS/MS remains the gold standard for PFAS analysis but is limited to known analytes and may underestimate the total fluorinated compound burden.

Combustion ion chromatography (CIC) has recently gained attention as a complementary analytical approach for the determination of total fluorine (TF), total organic fluorine (TOF), extractable organic fluorine (EOF), and adsorbable organic fluorine (AOF). CIC enables the detection of both known and unknown fluorinated compounds, providing a more comprehensive assessment of fluorine contamination [1].



In this study, we evaluate the applicability of CIC as a cost-effective screening and mass-balance tool for PFAS investigations. Method performance was assessed using representative short- and long-chain perfluoroalkyl carboxylic acids (PFCAs) and perfluoroalkyl sulfonic acids (PFSAs). Typical LOQs were 1 µg F L⁻¹ for aqueous samples, while recoveries of individual PFAS standards ranged between 76 and 113 % depending on chain length and matrix composition. The method was applied to a variety of environmental matrices including surface water, groundwater, soil, food, and food-contact materials.

The results highlight both the strengths and limitations of CIC for environmental PFAS monitoring. While CIC provides valuable information on total fluorine content and can reveal the presence of unidentified fluorinated compounds, matrix effects and fluorine recovery remain critical factors influencing method performance. Ongoing work focuses on optimizing adsorbents and extraction procedures for AOF and EOF analysis. Overall, CIC represents a valuable complementary tool for PFAS screening and environmental monitoring.

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Plant Protection Products (PPPs) in Glacier Ice, Snow, and Meltwater Samples from Stein Glacier, Switzerland - Investigating the Occurrence and Spatial Distribution of Plant Protection Products in Remote Areas

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Abstract

Plant protection products (PPPs) are used in modern agriculture to protect crops from various pests and diseases. However, the distribution of these substances into non-target environmental compartments is problematic because of the potential risks they may pose to biotic and abiotic environments [1, 2, 3].

In this work, the presence of PPPs in glacier ice, snow, and meltwater samples collected from Stein Glacier in Switzerland was investigated. Chemical analysis was conducted by using solid phase extraction (SPE) and liquid chromatography tandem mass spectrometry (HPLC-ESI-MSMS). PPP occurrences and concentrations were compared to findings in the meltwater stream below the glacier. Moreover, the physicochemical properties of the compounds detected in the samples were investigated by considering different partitioning coefficients (K_{AW} , K_{OW} , K_{OA}), and half-lives ($DT_{50(air)}$) to assess the potential for environmental persistence and long-range atmospheric transport (LRAT). Our findings show a possible correlation between the amount of precipitation and $DT_{50(air)}$ with the number of compounds deposited on the glacier. Furthermore, PPP sales volumes in Switzerland were linked to the findings from the glacier ice, snow, and meltwater samples, as well as an ecological risk assessment was made to assess the water quality of the glacier samples. In general, many of the findings confirm the LRAT of these compounds.

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Biodegradation Testing of Constituents of Natural Complex Substances

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Because of the widespread use in consumer products, the question of the environmental impact of fragrances is central – namely the biodegradability of ingredients – and naturals used as fragrance ingredients are not an exemption here.

Some of these naturals are complex in chemical composition, consist of a high number of different chemical constituents, and are therefore commonly designated as Natural Complex Substances (NCS). Standard tests for ready biodegradability are not generally applicable for complex mixtures containing different types of chemicals [1]. A case-by-case evaluation has to take place on whether a biodegradability test on such a complex mixture would give conclusive information regarding the biodegradability of the mixture as such (i.e. regarding the biodegradability of all the constituents) or whether instead an investigation of the biodegradability of individual components of the mixture is required.

If sufficiently detailed composition information is not available on an NCS, gathering additional information on the composition of the NCS is the first step of the biodegradability assessment. Ideally all constituents $\geq 1\text{wt}\%$, and at least 80wt% of the NCS are identified. However, the minor constituents in the remaining unknowns of a given NCS are generally related to the identified constituents, as they are products of the same plant biochemistry pathways and hence expected to have similar biodegradation profiles.

The next step is gathering information on the biodegradability of the known individual constituents. While such information is typically available for constituents that are also used in their own right as fragrance substances, information on many other constituents was and in some cases is still missing. Thus, to complete the biodegradation assessment data needs to be generated for these “missing” constituents.

In this work, new biodegradation results for key constituents of fragrance NCSs will be presented. Case studies will also be used to show how this new data has allowed the completion of the biodegradation assessment of NCSs using the constituent approach where before crucial information was missing. Some NCSs were also tested as supplied for comparison of the constituent approach versus the whole substance approach.

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Investigating Regional Halocarbon Emissions: The Seoul Tracer Release Experiment

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Hydrofluorocarbons (HFCs) are potent greenhouse gases widely used as refrigerants, propellants, or in insulating foams. Their phasedown under the Kigali Amendment to the Montreal Protocol (2016) requires robust regional emission estimates to verify progress.¹ In 2020, East Asia accounted for 13.1% of global HFC emissions, and understanding its emission trends is crucial for evaluating compliance with international and global emissions.^{2,3}

In 2024/25, a large-scale controlled-release tracer experiment was conducted to estimate halocarbon emissions of the greater Seoul metropolitan area (SMA, South Korea). Ethyl fluoride (HFC-161)⁴ and hexafluorobutene (HFO-1336mzzE), both virtually absent from the background atmosphere, were released at a single location in Seoul as tracers with known emission strength. Release times were chosen based on FLEXPART⁵ transport model forecasts indicating when air masses would reach the AGAGE Gosan station (Jeju Island, 490 km south of the release location). This site is equipped with a Medusa GC-MS for in situ measurements of halogenated compounds. Additional flask samples were collected along the tracer trajectory at the Global Atmosphere Watch Observatory in Anmyeondo (138 km away) and at Mokpo National University (320 km away).

During two release experiments (Fall 2024 and Spring 2025), both tracers were detected at all sampling sites. The measurements show a strong correlation of the reference tracers with various HFCs. Preliminary emission estimates for the GSMA are presented, along with the experiment's challenges and limitations. Finally, a comparison to a full regional inversion, based on the continuous observations at Gosan, is conducted.

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Systemic defense induction by volatiles renders plants susceptible to manipulation by insect herbivores

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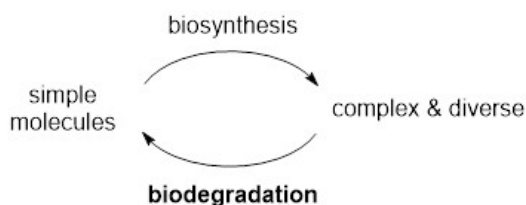
Upon herbivore attack, plants can induce systemic defenses through both vascular and volatile signals. So far, the relative contribution of the two pathways and the capacity of herbivores to interfere with them remains unclear. We quantified the contribution of herbivore-induced plant volatiles (HIPVs) to systemic defense induction in maize and tested to what extent herbivores can interfere with volatile mediated defense. We monitored real-time volatile emissions and measured phytohormone levels of systemic tissues following wounding. We assessed the role of volatile signals by mechanically blocking HIPV transmission. We then evaluated the contribution of Green Leaf Volatiles (GLVs) as systemic signals using a GLV biosynthesis mutant and synthetic complementation. Finally, we investigated how *Spodoptera* oral secretions (OS) influence systemic signaling during simulated herbivory. We found that systemic induction of plant volatiles can be fully explained by GLV signaling, without the need for vascular signals. Systemic responses were suppressed when volatiles were mechanically blocked and when GLV biosynthesis was impaired. *Spodoptera* OS reduced systemic induction of plant volatiles by reducing GLV emissions at the feeding site. Our results identify GLVs as primary systemic signals in maize and demonstrate that herbivores can attenuate systemic defense activation by interfering with GLV signaling during feeding.

***In vitro* reconstitution of bacterial degradation of plant toxins**

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Contemporary enzyme discovery focuses largely on elucidating the biosynthetic pathways that produce diverse and complex natural products. Yet understanding how natural and anthropogenic compounds affect living organisms and developing new processes for bioremediation, upcycling, and recycling may depend just as much on the enzymology of degradation. At first glance, the conversion of diverse, complex molecules into a small set of primary metabolites looks like the conceptual inverse of biosynthesis, which assembles simple building blocks into molecular diversity. The reality is likely more subtle: the types of transformation involved, their catalytic efficiencies, and the degree of catalytic promiscuity may differ between the logic of building and breaking complex compounds in ways that remain largely unexplored. Guided by these ideas, and in search of enzymes that catalyze useful bond-cleaving, isomerization, and oxidation reactions, we have begun to characterize naturally occurring pathways for alkaloid degradation. In this presentation, we discuss our results from this effort.

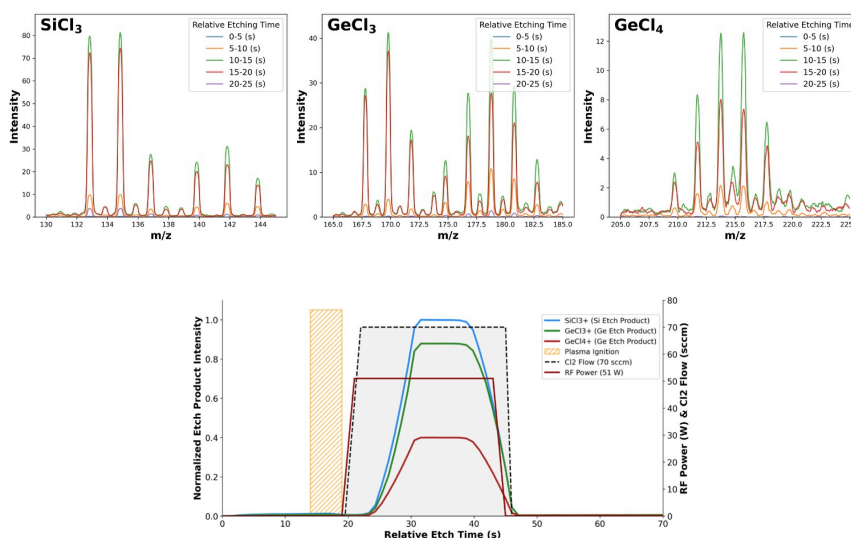


Real-Time EI-TOF-MS Monitoring of Byproducts during ICP Etching of GeSn- and Ge-on-Si

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GeSn is a promising group-IV material platform for photonic integration, but the gaseous byproducts formed during plasma etching remain poorly understood. In this work, Cl₂-based ICP etching of GeSn- and Ge-on-Si wafers was combined with online EI-TOF mass spectrometry to monitor exhaust gases in real time, while SEM was used to assess etch quality. The measurements revealed GeCl₃⁺- and GeCl₄⁺-related fragment families, lower-intensity GeN/GeO_x signals, and continuous SiCl₃⁺ signals from the simultaneously exposed Si substrate. Tin-chlorides were not clearly observed due to the low Sn concentration ($\leq 8\%$) and mass spectrometer sensitivity limits. The results show that byproduct formation depends on the applied plasma recipe and demonstrate a route to correlate plasma chemistry with etch performance by online EI-TOF-MS analysis. Crucially, the empirical detection of highly toxic GeCl₄ underscores the necessity for the right abatement system to identify environmental and health hazards.



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Identifying biocontrol traits and boosting them through amino acid adjuvants

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Chemical pesticides and copper-based products are widely used in agriculture but have a negative impact on the environment and on human health. Therefore, less harmful and more sustainable solutions are being explored. One of these is biocontrol, which relies on the use of living organisms to combat plant pathogens. However, while the efficacy of such biocontrol agents is well documented in vitro, their performance in the field remains limited.

This study aimed to evaluate whether specific amino acids could enhance the biocontrol activity of four bacterial strains (belonging to genera *Pseudomonas*, *Bacillus* and *Streptomyces*) against the oomycete *Phytophthora infestans*, the causal agent of late blight in *Solanaceae* plants. The focus was on the improvement of biocontrol-related traits and siderophore production, rather than solely on bacterial growth.

All twenty proteinogenic L-amino acids were tested in vitro by measuring the mycelial growth of *P. infestans* in the presence of biocontrol agents growing on media supplemented or not with individual amino acids. Some amino acids led to a significant reduction of mycelial growth of the pathogen and had different effects on siderophore production. Based on these results, four amino acids were selected to further investigate their influence on the emission of volatile compounds by the selected bacterial strains.

Certain amino acids, such as methionine, showed a significant effect on the ability of the bacteria to inhibit the oomycete. These results suggest that specific amino acids can act as adjuvants to enhance biocontrol performance of beneficial bacteria, offering a promising strategy to improve the effectiveness of biological control.

Effect of *Bacillus velezensis* K-165 volatiles on *Botrytis cinerea* and *Arabidopsis* protection

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The tomato root isolate *Bacillus velezensis* K-165 was shown to promote eggplant growth, but also to protect both eggplant and potato against the soilborne pathogen *Verticillium dahliae*. Moreover, strain K-165 was shown to induce systemic resistance against *V. dahliae* in *Arabidopsis thaliana*.

Our study's aim was to determine the role of volatile organic compounds (VOCs) released by K-165 in the direct inhibition of the pathogen *Botrytis cinerea* as well as in the induction of plant defenses. We show that the volatiles released by K-165 were dependent on its cultivation medium.

The VOCs released by K-165 when grown on PDA (but not on LB) inhibited the mycelium growth of *B. cinerea*, while *A. thaliana* plants exposed to VOCs released by K-165 grown on LB (but not on PDA) were more resistant to *B. cinerea*, suggesting that these VOCs induced plant defenses. Camalexin involvement in the VOCs-mediated plant defense stimulation was confirmed by an upregulation of genes involved in camalexin synthesis, an increase of the leaf camalexin concentration as well as by the loss of the VOCs' protective effects on pad3 mutant and cyp79B2/B3 double mutant plants infected with *B. cinerea*.

The VOCs released by K-165 cultivated on PDA and LB were identified by GC-MS. Five ketones were identified only when K-165 grew on PDA, while 2,5-dimethylpyrazine was released only when the strain grew on LB. The ketones were tested for effects on *B. cinerea* mycelial growth and shown to inhibit it when applied at high concentrations. 2,5-dimethylpyrazine was tested as plant defense inducer. Interestingly, exposure of *A. thaliana* wild-type (but not pad3 and cyp79B2/B3 double mutants) to 2,5-dimethylpyrazine showed a tendency for higher resistance against *B. cinerea*, suggesting that this VOC might be involved in K-165's induction of plant defenses.

Uptake via the leaf surface allows plants to perceive volatiles with closed stomata

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Plants can detect threats by perceiving airborne chemical signals [1, 2], but how these volatiles are taken up by the leaves is not well understood. Stomata are generally considered as the major uptake pathway. However, as stomata close at night or during drought, this may severely limit the capacity of plants to sense volatiles [3-5]. Using the crassulacean *Kalanchoë laxiflora*, which possesses CAM leaves that open their stomata at night, and C3 leaves that open their stomata during the day [6], we uncover that the leaf surface functions as an alternative volatile uptake pathway that unlocks volatile perception with closed stomata. We find that 80% of the wound-induced green leaf volatile (Z)-hexenyl acetate are taken up via the stomata, while 20% are taken up through an alternative pathway. Neither residual stomatal conductance nor hydathodes can account for the latter. Furthermore, the non-stomatal pathway shows a preference for lipophilic volatiles and is modulated by cuticular thickness and sub-epidermal airspaces. The leaf surface thus emerges as the most parsimonious non-stomatal volatile uptake pathway. Uptake via the leaf surface is highest when stomata are closed and can be enhanced through phytohormone application, demonstrating active regulation. Importantly, we show that volatile uptake via the leaf surface is sufficient to activate anti-herbivore defenses and resistance. Together, our findings reveal that plants can take up volatiles via the leaf surface when their stomata are closed, which allows them to perceive volatiles under variable environmental conditions.

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E-NICHE: A European Network In Chemical Ecology: Translating the language of life into sustainabilityC. Robert¹¹E-NICHE COST ACTION CA22102

The main aim and objective of this EU COST Action network is to unify European players in chemical ecology, enhancing cooperation, promoting visibility and sharing knowledge, tools, and platforms. It addresses major societal issues for environmental and sustainable development goals by describing chemodiversity, evolutionary forces, and global changes that will impact biodiversity and ecological interactions. E-NICHE is bringing together researchers and companies who study natural compounds that can act as semiochemicals (i.e., communication signals) across a diversity of organisms and ecological systems, including insects. This work will be nourished by a deeper understanding of the living world through the lens of chemical mediation, the main system of biological communication. It will also aim to prevent the loss of the chemical biodiversity found in nature, under threat because of global changes. Within this collaborative scientific effort, the participation of Young Researchers plays a key role in fostering innovation, ensuring continuity, and promoting inclusiveness within the European chemical ecology community.

Consequently, E-NICHE's overarching objective is to establish a strong, extended European CE network that catalyses international, interdisciplinary, and cross-sectoral exchanges with a view to building knowledge and intergenerational sustainable development solutions. Ultimately, the Action aims to build a European Association in Chemical Ecology as it exists already in Asia-Pacific (APACE) and the Latino Americas (ALAEQ) linked to the international one (ISCE).

¹⁸O-informed metabolomics reveals phosphorylation changes in microbial metabolic responses to environmental stressC. Shi¹, E. Evertz², F. Tamburini², T. Hofstetter^{1,3}

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Human activities induce stress to ecosystems, affecting the key functions provided by microorganisms. Under environmental perturbations and stress, microorganisms reconfigure their metabolism to adapt to the environmental changes. This offers the opportunity to develop chemical tracers that are indicative of microbial stress conditions and their potential to provide ecosystem functions. In this study, we aim to assess changes in ¹⁸O/¹⁶O ratios in cytosolic phosphate (cytosolic $\delta^{18}\text{O}(\text{PO}_4^{3-})$) as a proxy of microbial metabolic activity level. $\delta^{18}\text{O}(\text{PO}_4^{3-})$ has been used as an indicator of biological processes; however, which metabolic reactions drive $\delta^{18}\text{O}(\text{PO}_4^{3-})$ remains unknown. To address this challenge, we developed an ¹⁸O stable isotope labeling-based metabolomics workflow to track microbial phosphorylation and identify the key phosphoryl-transfer reactions regulating cytosolic $\delta^{18}\text{O}(\text{PO}_4^{3-})$. Specifically, we cultivated model microorganisms in batch cultures using H₂¹⁸O-labeled media under optimal and heat-stress conditions. By extracting metabolites at different time points and analyzing isotopic incorporation patterns via LC-HRMS, we mapped the differentiated metabolic pathways in the phosphorylation network. The results showed that the redox metabolism associated with oxidative phosphorylation was more responsive to heat stress, while metabolites tied to substrate-level phosphorylation in central carbon metabolism showed only minor or temporal variations. This research supports the use of $\delta^{18}\text{O}(\text{PO}_4^{3-})$ as an indicator of intracellular phosphorylation changes under stress, with broader implications for tracking microbial metabolic responses and phosphorus cycling in changing environmental conditions.