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Looking for Ways out of the PFAS Mess

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Per- and polyfluoroalkyl substances (PFASs) have been used for decades in a wide variety of consumer products and in numerous industrial processes and in components of a broad range of devices and machinery. Many of these uses were in open applications leading to direct releases of PFASs to the environment; in addition, large amounts of PFASs have been released with waste streams to water, air and soil. All of this has led to a widespread contamination of the environment and human food and drinking water by a set of approximately 50 to 100 PFASs, mostly perfluoroalkyl carboxylic acids (PFCAs), perfluoroalkyl sulfonic acids (PFSAAs), and perfluoroalkyl ether carboxylic acids (PFECAs), and precursors of these substances. In response to this concerning situation, regulatory action has been taken or initiated in many countries or regions, ranging from bans of individual PFASs to bans of PFASs in all consumer products and to the EU's proposal of a restriction of PFASs as a class, and also including setting (or adjusting) limit values for PFASs in food, drinking water, surface water, and soil. Also in Switzerland, there is currently a lot of regulatory and political activity around PFASs, including the development of new limit values and several parliamentary motions submitted recently. PFAS manufacturers are facing numerous lawsuits in several countries, mostly by water providers and affected communities, and may have to pay billions of USD for compensation or settlement.

The fluorochemical industry and many industry branches using PFASs currently seem to be in a process of abandoning PFAS uses in consumer products [1], which is an important, but long overdue development. The main group of PFASs that will continue to be used, at least in certain, highly demanding applications, is fluoropolymers (FPs). PFAS emissions from FP production processes have been reduced, but are still substantial [2], which constitutes an important environmental footprint of FPs. FP manufacturers and users claim that emissions from FP production can and will be further reduced, whereas government authorities in many European countries support the EU's restriction proposal, which includes FPs. For FP uses without sufficient alternatives, the proposal foresees transition times of more than 12 years. Importantly, innovation processes leading to alternatives to PFASs, also FPs, are underway [3].

In this situation, many societal actors (regulators, industry, policy makers, scientists, civil society groups, the media, public health institutions, and more) have to find responses to a range of challenging questions, including: what are preferable regulatory approaches to the PFAS problem, and what are their pros and cons? How was it possible that the PFAS problem has escalated into such a serious situation? What are the alternatives to PFASs in all the many PFAS uses that need to be ceased now? To what extent is remediation and clean-up possible, and what does it cost? Who will be responsible in the long-term for national action on PFASs? How can all societal actors contribute to an open process that facilitates the transition to alternatives wherever possible?

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Overview on PFASs Contamination in Swiss Soils

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Due to their persistence, widespread use, and toxicity per- and polyfluoroalkyl substances (PFASs) are a reason of concern for the environment and human health. They are a major challenge for chemical soil protection. To set soil threshold values and prioritize measures, knowledge on PFAS concentrations in soil is crucial.

For Switzerland, only information on background concentrations of PFASs in soil has been available so far^[1]. To have a better understanding of the PFAS distribution in Swiss soils, a data collection of measurements of PFASs in Swiss soils has been initiated.

Measurement results of over 1000 samples were gathered with most of the data originating from cantonal measurement campaigns. The objectives of the campaigns were varied, some assessing PFAS background concentrations in soil, while others screened for potentially contaminated sites or further assessed known contaminated sites.

This study summarizes the current knowledge on PFAS soil levels in Switzerland. In addition, it sheds light on the PFAS distribution within soil, on most relevant PFAS sources, and on patterns associated with different PFAS uses. These results are very useful for improving our understanding of the concentration of PFASs in soil and will be a relevant contribution to the derivation of soil threshold values in Switzerland.

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The Food Contact Chemicals Priority List (FCCprio List)

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Food packaging is essential for preserving food quality and extending shelf life, but it also poses environmental and health risks due to resource use, pollution, and chemical exposure. While many tools help assess environmental impacts, chemical safety has so far lacked a solid evidence-based approach. To address this gap, we created the FCCprio List - a list of priority Food Contact Chemicals (FCCs) [1] - and integrated it into the Understanding Packaging (UP) Scorecard to support more holistic, sustainable packaging decisions. The FCCprio List was created by applying the evidence-based PlastChem methodology [2] to the more than 15'000 known FCCs [3,4]. Using officially recognized (harmonized) hazard data, chemicals were prioritized if they met any of the following criteria: PBT (persistent, bioaccumulative & toxic), vPvB (very persistent & very bioaccumulative), PMT (persistent, mobile & toxic), vPvM (very persistent & very mobile), carcinogenic, mutagenic, toxic for reproduction, toxic for specific target organs upon repeated exposure, or endocrine disrupting. Prioritized FCCs were subsequently ranked into four tiers based on their evidence for human exposure from food contact materials (FCMs) [3,4,5]. To enhance usability, FCCs were also grouped by chemical structure. In total, 1'222 FCCs are hazardous based on harmonized hazard data sources. Of these, 94 FCCs migrate from FCMs and have been detected in human biomonitoring programs (Tier 1). The remaining 1'128 FCCs have not been detected in human biomonitoring programs, of these, 264 chemicals migrate from FCMs (Tier 2), 224 have been detected in FCMs (Tier 3), and 640 FCCs have not been detected experimentally but are potentially used in the production of in FCMs (Tier 4). Of all known FCCs, 12'317 (81%) currently lack harmonized hazard data and cannot be considered for prioritization. The FCCprio List helps to identify, screen, and avoid the most hazardous chemicals in FCMs and supports the development of safe and sustainable food packaging. Integrating it into the UP Scorecard empowers decision-makers to navigate the complex trade-offs inherent in food packaging choices and facilitates the transition toward products that minimize impacts on both environmental and human health.

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Halogenated nitramines: a novel class of disinfection byproducts

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Potentially harmful disinfection byproducts, formed through the reaction of disinfectants with natural water constituents, are a long-standing challenge of water disinfection. Recently, chloronitramide was revealed as the long-standing unidentified product of chloramine decay [1]. Chloronitramide as a disinfection byproduct, is unique, in that it is formed in the decomposition of chloramines and does not, to our knowledge, require additional precursors, unlike regulated disinfection byproduct classes, including trihalomethanes, haloacetic acids, and nitrosamines. Although the structure of chloronitramide was finally elucidated last year, it remains unknown if brominated and iodated analogues form in drinking water systems. To this end, work is underway to synthesize pure standards of chloronitramide, bromonitramide, and idonitramide. We have developed successful synthetic routes albeit with modest yields to produce chloronitramide and bromonitramide. Optimized synthetic pathways will be discussed along with challenges in the analytical methodologies needed for these disinfection byproducts. Drinking water samples from chloraminated water systems that have source water with elevated bromide and iodide levels will be obtained to determine whether these bromonitramide and idonitramide are formed in real systems. Overall, these results will inform risk assessment by providing occurrence data for halogenated nitramines, a novel class of disinfection byproducts.

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Investigating Urban Halocarbon Emissions: A Seoul Tracer Release Experiment

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Hydrofluorocarbons (HFCs), the replacement substances of (hydro)chlorofluorocarbons ((H)CFCs), are regulated under the Kyoto Protocol (1997) and, more recently, also under the Kigali amendment (2016) to the Montreal Protocol, which targets a reduction of HFC production and consumption over the following decades.^{1,2} To achieve this, HFCs are being replaced by hydrofluoroolefins (HFOs) and other low-global-warming-potential substitutes.³ Monitoring compliance with these treaties by observing halogenated substances in the atmosphere is crucial. This can be achieved by atmospheric measurements using gas chromatography-mass spectrometry (GC-MS), combined with modeling, to yield regional and global emission estimates.^{4,5}

In this project, we have conducted a deliberate-release tracer experiment to estimate halocarbon emissions of the Seoul metropolitan area. Ethyl fluoride (HFC-161)⁶ and hexafluorobutane (HFO-1336mzzE), which are practically absent in the atmosphere, were released in the City of Seoul. Release times were carefully selected when favorable meteorological conditions allowed air masses to reach the in-situ measurement site at Gosan (Jeju Island), 485 km away, and further remote sites, Anmyeondo (138 km) and Mokpo (320 km), for flask sampling in between. FLEXPART⁷ was used to forecast the trajectory and dispersion of the plume, and the release and sampling timing were adjusted accordingly. During the first release in November 2024, both tracers were detected at the flask sampling sites Anmyeondo and Mokpo, as well as at Gosan station. First results show a stable correlation with various urban-used HFCs. First emission estimations from Seoul will be shown, using the November 2024 release. A second release is planned for Spring 2025, and the data will be included for more detailed estimates.

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Plant amino acid metabolism is central in response to pathogenic and beneficial bacteria

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Plants interact with organisms in their environment via metabolites. Primary compounds such as sugars and amino acids serve as nutrients for heterotrophic organisms, and secondary compounds often act as signals, attracting or deterring specific organisms [1]. Our team found that root exudates, compounds released by roots into the rhizosphere, are dynamic, responding to various environmental and experimental stimuli [2]. However, how plants respond on a general metabolic level to presence of microbes remained unclear. Here, we investigated changes in plant metabolic profiles to pathogenic or beneficial bacteria with an untargeted, direct injection mass spectrometry method. With this, we identify multiple chemical classes changing with different temporal dynamics in response to pathogens. Coupled with an RNAseq experiment and integrated analysis of the multi-omic dataset, we reveal the central importance of amino acid metabolism in pathogen responses.

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A polymer-based quantification of Tire wear particles (TWP) in atmospheric deposition samples using pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS)

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Tire wear particles (TWPs) constitute a significant source of environmental microplastics and airborne particulate matter (PM_{2.5} and PM₁₀). Global per capita emissions range from 0.23 to 4.7 kg per year, with an average of 0.81 kg per year.¹ TWPs contribute 5–10% of oceanic plastic pollution and 3–7% of ambient PM_{2.5}, exacerbating the global health burden of air pollution.¹ In addition to representing the primary anthropogenic source of zinc (Zn), TWPs contain over 200 toxic organic compounds in the environment.² Given their pervasive distribution, accurate quantification of TWPs across diverse geographical regions and understanding their transport pathways through air and water are critical for assessing environmental and public health risks. However, estimating TWP emissions remains analytically challenging due to variations in tire composition across different manufacturers, varying usage conditions, and varying tire ages.

Traditional analytical methods, including Fourier-transform infrared (FTIR) spectroscopy, elemental analysis, and single-marker detection through gas chromatography-mass spectrometry (GC-MS) or high-performance liquid chromatography (HPLC), encounter limitations in consistently quantifying tire wear particles (TWPs) due to matrix interferences. In response to these challenges, we have developed an integrated pyrolysis gas chromatography-mass spectrometry (Py-GC-MS) method that quantifies the total polymer content of TWPs, rather than depending on individual markers. This innovative approach incorporates optimized sample preparation techniques to minimize interference from co-occurring environmental contaminants. By thoroughly analyzing both primary and secondary pyrolysis products of tire rubber, our method facilitates a more precise and comprehensive quantification of TWPs.

Furthermore, we applied this methodology to atmospheric deposition samples collected from different locations in Switzerland. The data, combined with land use statistics, will estimate the annual atmospheric input of TWP into these areas. These findings will provide a basis for assessing the environmental risks associated with TWPs and their derived chemicals.

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Passive Air Sampling and Bee Pollen Analysis Reveals Distribution of Current-Use Pesticides in Agricultural Landscapes

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Current-use pesticides (CUPs) are crucial to modern agricultural practices, yet their off-target transport poses environmental and human health risks. Passive air sampling using polyurethane foam (PUF) is a practical method for monitoring CUPs occurrence, transport, and temporal patterns [1]. In parallel, biomonitoring using pollinators has emerged as a valuable approach to investigate CUPs distribution and persistence in the environment [2].

This study evaluates the persistence and distribution of CUPs using an integrated approach that combines passive air sampling with PUF disks and biomonitoring through bee pollen analysis. Five beehives and thirteen PUF samplers were strategically installed around a controlled area covering 39 agricultural fields (~600,000 m²). Detailed pesticide application records, including the specific compounds used, quantities, and locations, were compiled, along with continuous meteorological data. Weekly bee pollen and biweekly PUF samples were collected from late April to late October 2023.

Airborne pesticide concentrations were estimated using a previously published model for effective sampling volumes [3], adapted to CUPs physicochemical properties and local meteorological conditions. The results revealed short-term changes in pesticide levels and dispersion over distances greater than two kilometres from their application sites. Additionally, bee pollen analysis confirmed that pesticides persisted on crops beyond their intended periods, contaminating untreated and off-crop areas more than 800 meters from application sites. Fractionation of pollen samples by plant species further confirmed multiple contamination sources, including directly treated crops and untreated off-crop plants.

Overall, this study provides a comprehensive view of how CUPs are distributed and persist in the environment. The presented approach improves the spatial and temporal resolution of CUPs contamination by revealing new perspectives on pesticide presence, transport, and longevity. These findings highlight significant exposure risks for non-target organisms, particularly pollinators, and emphasise the need for complementary sampling techniques to guide effective mitigation and environmental protection policies.

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Decoding pest dynamics in associated oilseed rape: insights from chemical and behavioral mechanisms

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Winter oilseed rape (WOR, *Brassica napus*) is an economically important crop which faces increasing threats from multiple herbivorous insects. The emergence of insecticide resistance coupled with neonicotinoid bans in certain regions of the world drives the need for efficient alternative control measures. Recent studies have highlighted the potential of multi-cropping practices on lowering pest pressure in WOR fields. However, underlying mechanisms shaping multi-trophic interactions in diversified WOR landscapes are largely unknown. Here we present how service planting with faba bean (*Vicia faba*) can impact glucosinolate production in oilseed rape, with associated plants displaying altered defense responses to herbivory by an important coleopteran pest, the cabbage stem flea beetle (CSFB). Behavioral assays with adult beetles revealed that such shifts in secondary metabolite production could further explain part of protective mechanisms service planting can offer. Moreover, olfactometer assays suggest that service cropping influences the emission of volatile organic compounds, which may affect pest behavior and movement at larger spatial scales. Results obtained from laboratory and field experiments help shed light on complex chemical and behavioral interactions driving pest dynamics in diversified agroecosystems.

Proteolytic Activity and Substrate Specificity of Lake Geneva

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Heterotrophic microorganisms in lakewater secrete proteases which contribute to the turnover of dissolved organic matter and the degradation of peptidic contaminants. However, little is known about the identities and substrate specificities of these proteases. Using Multiplex Substrate Profiling by Mass Spectrometry (MSP-MS)¹, we sought to characterize the global proteolytic fingerprint of the extracellular proteases present in Lake Geneva. We identified preferred enzymatic cleavage next to positively charged and certain non-polar amino acids, while cleavage next to negatively charged residues was disfavored. Specifically, many of the detected cleavage sites were predominantly surrounded by arginine and lysine, consistent with a trypsin-like substrate specificity. This pattern was conserved across seasons and water depths and was shared with two other Swiss lakes. In contrast, we observed variability in the number and types of cleavage sites across samples, suggesting spatial and temporal differences in overall extracellular protease diversity. Our findings expand our understanding of protein stability in lake ecosystems and may be used to predict the fate of peptidic contaminants in the environment.

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Water-based amide coupling with sustainable xylose acetals as co-solvents: A novel organic base-free strategy

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Amide bond formation is one of the most fundamental and widely used chemical transformations, playing a crucial role in the synthesis of pharmaceuticals, agrochemicals, and bulk chemicals. Despite its industrial significance, traditional amide coupling methodologies often require highly polar, petroleum-derived solvents such as N,N-dimethylformamide (DMF), acetonitrile, or N-methyl-2-pyrrolidone (NMP) to efficiently solubilize polar coupling reagents,¹ which are essential for activating carboxylic acids toward nucleophilic attack by amines. These solvents are not only derived from non-renewable resources but are also associated with significant environmental and human health concerns, including reprotoxicity.

To address these issues, aqueous reaction media supplemented with surfactants have been explored as a more sustainable alternative. However, these methodologies still rely on toxic and hazardous non-renewable organic bases such as pyridine, 2,6-lutidine, or triethylamine, which are often used in excess and, in turn, act as co-solvents.^{2,3} A major challenge in developing greener alternatives lies in maintaining efficient solubilization of all reagents in a strictly aqueous medium while ensuring high reactivity and selectivity. Inorganic bases offer a more sustainable alternative, yet they often lead to lower reactivity and reduced selectivity in amide bond formation due to their weaker solubilization and buffering capabilities.

This work presents a novel organic base-free amide coupling strategy that leverages biomass-derived xylose acetals as key additives.⁴ By utilizing these renewable sugar-based compounds, we aim to improve the solubility and reactivity of coupling agents in aqueous media, thereby reducing reliance on hazardous polar aprotic solvents and organic bases. Additionally, xylose acetals play a crucial role in counterbalancing the intrinsic lower reactivity and selectivity induced by inorganic bases, offering an efficient and more sustainable approach to amide bond formation.

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Environmental implications of soluble versus immobilized *Candida glabrata* ketoreductase for the production of chiral alcohols

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Chiral alcohols are versatile and essential building blocks in pharmaceutical, food and fragrance industries. And with the application of biocatalysis, their synthesis can be achieved in milder conditions of temperature, pressure and with less organic solvents needed, and thus, is an environmentally friendlier process at a financially competitive cost [1]. To ease the integration of this transformations of industry, their immobilization allows them to be recycled and removed from the reaction, simplifying the work-up and enhancing the cost-effectiveness of this strategy.[2] In this project, we study the immobilization and implication of using a mutant of *Candida glabrata* ketoreductase (CgKR1 F92C/F94W),[1] quantifying the environmental impact of producing chiral alcohols with this immobilized enzyme versus the soluble enzyme through a life cycle assessment (LCA).

The immobilization screening of CgKR1-F92C/F94W was performed with various supports (methacrylate, silica, agarose, cellulose) and binding chemistries. From those, the best immobilization was achieved with a silica containing primary amines and cross-linking with glutaraldehyde post-immobilization, with a recovered activity of 100% to 50% over five cycles and a final immobilized activity of 1.1 U/g to 0.5 U/g. This biocatalyst was applied successfully to the synthesis of various chiral alcohols (see figure). Using these results, we performed the LCA analysis and the results were evaluated and used to make an extrapolation of the environmental impact of producing chiral alcohols with immobilized enzymes at industrial scale.

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Cobalt Depletion by Inorganic Sorbents

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This project focuses on the selective sorption of cobalt from large volumes of aqueous waste generated during the operation of nuclear power plants, particularly at the Gösgen plant (KKG). The removal of ⁶⁰Co, a long-lived radionuclide with high-energy γ -radiation, using a selective inorganic sorbent, integrated into the purification system, could provide a sustainable alternative to the current practice of evaporating tens of tons of such waste daily, thus lowering doses to personnel.

Activated corrosion products of structural materials of pressurized water reactors are a primary source of radioactivity in wastewater. The treatment of such waste, characterized by its complex composition and varying levels of radioactivity, is critical for nuclear power plant operation. Among traditional and advanced decontamination technologies, adsorption stands out due to its cost-effectiveness, operational simplicity, and high efficiency [1].

Cobalt extraction from various waste streams is particularly challenging due to its typically low concentration relative to a broad spectrum of competing ions present in higher quantities. Furthermore, cobalt often exists in complexed forms and colloidal particles, requiring additional processing steps to ensure its efficient removal [2]. Inorganic sorbents play a key role in sorption due to their safety in long-term management and the final solid inorganic waste to be disposed of.

Metal phosphates have demonstrated high efficiency in radionuclide removal due to their structural stability, abundance of adsorption sites, and fast adsorption kinetics [3]. A deeper understanding of the involved adsorption mechanisms is essential for the development of more effective and stable sorbents. To contribute to this field, we synthesized $\text{MgNa}_2\text{H}(\text{PO}_3)_2$, a promising sorbent for cobalt removal, and confirmed its structure and purity using PXRD, FT-IR, and SEM/EDX analyses. Our ongoing research within a project under the auspices of *swissnuclear* aims to evaluate the behavior of this sorption compound under the complex multi-component wastewater conditions occurring at KKG.

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[2] International Atomic Energy Agency, IAEA-TECDOC-1336, 2003.

[3] Y. Xie, et al, Journal of Water Process Engineering, 2025, 71.

Accelerating Environmental Fate Assessments: A Novel Read-Across Approach Using Activated Sludge to Predict Degradation Half-Lives in Soil

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Agrochemicals and active pharmaceutical ingredients play a vital role in modern society, yet their environmental persistence poses significant risks to ecosystems and public health. Current regulatory frameworks for assessing chemical degradation in environmental systems, particularly OECD guidelines 307 and 308, require substantial time and resources, limiting their application during early chemical design phases. This study presents an innovative time-efficient alternative using activated sludge experiments to predict environmental degradation rates. Through a 'read-across' approach, we demonstrated accurate predictions of chemical half-lives in soil ($DT50_{OECD307}$) and water-sediment systems ($DT50_{OECD308}$) based on two key parameters: activated sludge degradation half-life and organic carbon-water partition coefficient (KOC). Our calibrated regression models surpassed the accuracy of existing *in silico* prediction tools, offering a robust framework for rapid environmental fate assessment. This methodology holds the potential to accelerate the development of environmentally sustainable chemicals while maintaining regulatory compliance, potentially transforming early-phase chemical design processes.

Iron-induced Reduction of Iodate in Secondary Organic Aerosol

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Secondary organic aerosol (SOA) is formed by the oxidation of volatile organic compounds and is one of the main contributors to the global atmospheric aerosol mass. Transition metal ions (TMI), like Iron (Fe), occur in aerosol particles due to, e.g., mineral dust or other iron containing particles. They can undergo metal dissolution processes and be complexed by organic compounds from SOA. Furthermore, oceans and volcanic activity emit iodine into the atmosphere, in the form of gas phase I₂, iodinated organics or iodate (IO₃⁻). TMI can influence redox processes of secondary organics and iodate in aerosol particles. The reduction of iodate through the Briggs-Rauscher / Bray-Liebhafsky mechanism leads to the release of reactive iodine species to the gas phase, which contributes to the degradation of atmospheric ozone.

To investigate possible reduction pathways and product yields of iron (III) citrate (FeCit) and iodate containing SOA, coated wall flow tube (CWFT) experiments were performed [1,2]. Citric acid (CA) served as a proxy for SOA. The reaction products were measured under irradiation and in the dark with a CO₂ analyzer, cavity enhanced absorption spectroscopy (CE-DOAS), and chemical ionization mass spectrometry (CIMS).

We are currently modelling these CWFT experiments with the kinetic multilayer model KM-MEMO. Comparing the experimental results to the simulations will allow us to assess the importance of different chemical mechanisms and to determine relevant rate parameters. KM-MEMO was previously used successfully to model iron carboxylate photochemistry in the FeCit system without iodate [3].

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[2] M. Reza, L. Iezzi, H. Finkenzeller, A. Roose, M. Ammann, R. Volkamer, *Iodine Activation from Iodate Reduction in Aqueous Films via Photocatalyzed and Dark Reactions*. ACS Earth and Space Chemistry, 2024, 8(12), 2495-2508.
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Insights into the Biosynthetic Pathway of Multihexose Benzoxazinoids in Maize (*Zea mays*)

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Benzoxazinoids (BXDs) are plant specialized metabolites exerting a pivotal role in plant nutrition, allelopathy, and defenses. Multihexose BXDs were previously observed in cereal-based food products, such as whole-grain bread, but their synthesis *in planta* remained unclear. Our data show that drought, but not elevated CO₂ nor temperature, induced the production of di-, tri-, and even tetrahexose BXDs in maize. The drought-mediated induction of multihexose BXDs was common among several maize lines. Bioinformatic analyses identified two UDP-glycosyltransferase candidates that, when heterologously expressed in *E. coli*, catalyzed the glucosylation of BXD glucosides, producing multihexose derivatives. We report here on our recent efforts to further characterize the BXD synthetic pathway and its relevance in maize-environment interactions.

The heterogeneous reaction of HNO₃ and HCl with CaCO₃ in the context of stratospheric aerosol injection and its impact on stratospheric ozone

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Lack of action in climate change mitigation is driving research on solar radiation modification via stratospheric aerosol injection (SAI), i.e., the injection of aerosols or their precursors into the stratosphere to increase Earth's albedo, inducing global cooling. The idea evolved from observations of the cooling effect of large volcanic eruptions, which emitted SO₂ into the stratosphere. Therefore, SAI research mainly focused on sulfur dioxide (SO₂) injection, the main precursor of H₂SO₄ aerosols. However, SO₂ injection could lead to adverse side effects such as stratospheric ozone depletion, stratospheric heating, and sizable effects on the large-scale atmospheric circulation. Recent studies suggested that injection of solid particles such as calcite (CaCO₃), alumina (Al₂O₃) and diamond (C) instead of SO₂ could reduce some of these adverse side effects. However, the expected improvements are subject to large uncertainties. Like H₂SO₄, heterogeneous chemistry on solid particles in the stratosphere can increase ozone depletion by moving passive chlorine reservoir species such as HCl or ClONO₂ into their active, ozone depleting form (e.g., ClO). The degree to which the extent is smaller than for the same reactions with liquid H₂SO₄ particles remains poorly constrained. Furthermore, alkaline materials such as CaCO₃ are subject to acid-base reactions resulting in an uptake of acidic gases which could have beneficial or adverse effects on stratospheric ozone. We constrain some of these uncertainties by experimental work on heterogeneous chemistry of CaCO₃ in presence of gaseous HCl, HNO₃, and H₂SO₄ under near-stratospheric conditions. CaCO₃ powder was exposed to controlled gas mixtures closely above either a binary HNO₃/H₂SO₄ or HCl/H₂SO₄ solution for several days. Relative Humidity (RH) was set at a stratospheric value of 5% and temperature ranged between -20°C and -40°C. The surface passivation effect induced by reaction with H₂SO₄ was as well investigated. X-Ray Photoelectron Spectroscopy (XPS), an X-ray analysis technique to obtain elemental composition of the first surface nm was used to probe surface reactions.

Evaluation of scalability parameters in synthesis using agitator bead mills for mechanochemistry

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¹WAB-GROUP®

Mechanochemistry, the study of chemical reactions driven by mechanical force, has emerged as a promising approach for more sustainable chemical processes. Unlike conventional methods that rely on heat, solvents, or other energy-intensive techniques, mechanochemistry utilizes mechanical energy to initiate or accelerate reactions, often under milder conditions. This offers significant advantages, including reduced energy consumption, minimized waste, and the replacement of hazardous solvents with greener alternatives.

The goal of WAB-GROUP® is to develop cutting-edge technologies to provide customers with state-of-the-art solutions (the picture shows the principles of a continuous flow reactor). To assess the potential of the existing equipment for mechanochemical processes, a thorough evaluation of key process parameters was conducted, including heat transfer coefficients for various product flows, cooling media, and process settings, as well as residence time distributions under multiple operating conditions, and micro mixing efficiency. These studies aimed to fully characterize WAB mills and identify their properties towards mechanochemical applications.

A particular focus was placed on the **WAB IMPA°CT REACTOR**®, which integrates both conventional flow chemistry and bead milling technology.

Heat transfer was found to be highly dependent on cooling flow characteristics, and optimization strategies were analytically defined to address these challenges. The residence time is influenced by geometry, flow characteristics, tip speed, and bead filling degree. By optimizing these parameters, the internal recirculation flow can be controlled, achieving an ideal residence time distribution for specific reactions. Our findings show that the mills operate within a range similar to traditional reactors, from near-ideal CSTR behavior to plug-flow characteristics, depending on the chosen process settings.

This presentation will provide an overview of characterization results and proposed optimization strategies, highlighting the benefits of bead mills for synthetic applications. Applications [1] and the overall benefits of the technology for chemistry and the environment will also be discussed.

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The three Is of sustainable agricultureC. Screpanti¹

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The soil is a key component of future sustainable agroecosystems and food production. We are witnessing a recent resurgence in interest in the soil health concept to face the increasing threats. As result, the responsible management of agriculture soils is a priority. This triggers new efforts for the development and adoption of new technological solutions. Several calls for actions are in place to quest for a multistakeholder dialogue. More public-private partnership or any other form of collaborations are becoming imperative. Notably, there is an urgency to accelerate the translational Science. In this respect, the private sector will have a fundamental role to play. To effectively reap the benefits from the deployment of the science and technology, the private sector can explore new model for innovation. To this end, here a framework is proposed hinging on the three: ideation, integration, and information. A few examples will be illustrated. A roadmap will be presented with the goal to stimulate the debate on how fundamental and applied research, can merge with new entrepreneurial initiatives to full reap the benefits for farmers and society.

Using ^{18}O -assisted phosphometabolomics to elucidate key enzymatic pathways regulating microbial phosphorus metabolism under stress

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Climate change, biodiversity loss, chemical pollution, and other environmental changes driven by anthropogenic perturbations are disrupting microbial ecosystem functions and threatening food security and clean water supply. However, there is limited understanding on how microorganisms regulate their metabolism to adapt to these perturbations. We hypothesize that the holistic metabolic activity is shifted under stress, and thus limiting the ability of microorganisms to provide essential ecosystem services.

In this study, we aim to assess the metabolic activity through quantifying changes in phosphorus metabolism using ^{18}O -assisted phosphometabolomics. We chose phosphorus metabolism to estimate the holistic metabolic activity due to the essential role of phosphoryl-transfer reactions in cellular metabolism, such as intracellular energy transfer and storage, signal transduction, and post-translational modification. We posit that the enzymatic dynamics of phosphoryl-transfer reactions can be estimated by the isotope ratio of $^{18}\text{O}/^{16}\text{O}$ in cytosolic phosphate (cytosolic $\delta^{18}\text{O}(\text{PO}_4^{3-})$) as a proxy.

To test this hypothesis, we developed a method to track microbial phosphorus fluxes through different phosphoryl-transfer reactions under stress conditions, such as heat shock and nutrient limitation. Specifically, we used cell media with ^{18}O labeled water to trace ^{18}O incorporation into phosphometabolites in model organisms, such as *Escherichia coli* and *Bacillus subtilis*. By quantifying the enrichment of ^{18}O in both targeted and untargeted phosphometabolites with LC-HRMS, we elucidated the changes in the phosphoryl-transfer network under stress (Figure attached). Combining the measurements of cytosolic $\delta^{18}\text{O}(\text{PO}_4^{3-})$, we expect to evaluate how oxygen isotope fractionation expressed in cytosolic phosphate reflects the phosphometabolites turnover, and their dynamics induced by stress. Preliminary results suggested shifts in the turnover of phosphoenolpyruvate (PEP), sugar phosphates, and nucleoside phosphates under stress, which is also reflected in cytosolic $\delta^{18}\text{O}(\text{PO}_4^{3-})$. Phosphometabolomics, moreover, support further development of ^{18}O metabolic modeling. The outcomes of this study will contribute to a framework aiming to characterize holistic metabolic activities influenced by environmental perturbations.

Assessing the Environmental Hazard of Synthetic Phenolic Antioxidants

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Synthetic phenolic antioxidants (SPAs) are contaminants of emerging concern due to their extensive use in a wide range of applications, e.g., as preserving agents in plastics, fire retardants, synthetic fibers, fuels, and even foods. As a result, SPAs are now frequently detected in various environmental matrices, including natural water bodies, sediments, air or biota. Although prior studies have shown that certain SPAs and their transformation products can exhibit toxic effects in living organisms, data on their environmental fate and (eco-)toxicity remains sparse for a majority of compounds in this diverse and large class of substances.

This project aims to address this knowledge gap by investigating key environmental hazards of SPAs, namely persistence and (eco-)toxicity. As a first step, we assess the persistence of a broad range of SPAs as well as the formation of transformation products (i.e., ~80 substances), using activated sludge biotransformation assays. In this context, our goal is to streamline biodegradation experiments so that they are rapid yet robustly predictive of the compounds' tendency to be biotransformed by complex environmental microbial communities, allowing for more efficient data collection for persistence assessment. Besides screening a large number of substances and developing a targeted LCMS analytical method, we will use these experimental systems to further explore a recently proposed alternative hazard assessment concept i.e., the cumulative and persistent toxicity equivalents (CTE/PTE) concept. The CTE/PTE concept couples biotransformation experiments with animal-free *in vitro* bioassays to test different cellular toxicity pathways so that key hazards of parent compounds and transformation products can be detected and quantified.

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

High throughput mass spectrometry method development for dissolved organic matter characterisation

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Dissolved organic matter (DOM) plays a major role in global carbon cycling and contributes to natural carbon dioxide (CO₂) emissions. DOM is a complex mixture, containing mainly carbon, nitrogen, oxygen, and hydrogen, and is found in all aquatic systems, including lakes and rivers. High resolution mass spectrometry is one of the most convenient tools to study transformations of DOM. Furthermore, high resolution mass spectrometry can be enhanced by pairing with ultra high performance liquid chromatography. Specifically, we were interested in increasing the resolution in the analysis of DOM and its transformation products by the development of a chromatographic and mass spectrometric method. Herein, we developed a mixture of compounds known to be present in DOM that covered a range of classes (e.g., lipids, lignin, tannins, etc.) with similar features to DOM. This defined mixture was used to test a number of different columns (including C4 chemistries, C8 chemistries, C18 chemistries, among others), gradients and mass spectrometric methods. The data was processed and peak evaluated automatically, using peak symmetry, retention time and peak resolution, providing us with a score for the most suitable methods. The results of this work will improve our understanding of DOM and its transformation products.

Hazard Assessment of Synthetic Antioxidants for Safe-by-Design Development

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Antioxidants are commonly found additives in a variety of industrial products, ranging from food to fuels, with the purpose of slowing their degradation caused by oxidation[1, 2]. Especially for synthetic antioxidants their widespread use and lack of data on potential hazards for ecosystems and human health contribute to them being recognized as contaminants of emerging concern [3]. In this study, experimental and regulatory data on a broad range of chemicals used as antioxidants was collected in order to gain a clearer picture of the issue and its scope. The data was examined with respect to the environmental hazard characteristics defined under REACH regulation of the European Union: ready biodegradability, bioaccumulation, toxicity and mobility [4]. Established in-silico tools were used to fill the gaps in the data and predict potential transformation products as well as their toxicity. Analysis of the data shows that only a small percentage of the investigated compounds can be considered benign and that the relationship between molecular structure and hazard profile of a compound is complex. This work is part of a larger, interdisciplinary project aiming to develop a framework for the design of novel, environmentally safe antioxidants based on high-throughput persistence and (eco-)toxicity screening and machine-learning techniques for generative modeling of molecules. The findings presented here highlight the necessity for new approaches in the assessment of chemical risk in general and the relevance of the 2022 "safe and sustainable by design chemicals and materials" framework [5] in particular and establish a baseline for the development of new safe and sustainable by design antioxidants that will follow.

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^{35}Cl NQR as a Site-Specific Characterization Technique for Chlorinated CompoundsA. G. Nobile¹, C. Copéret^{1*}¹Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir Prelog Weg 1-5 CH-8093 Zürich, Switzerland

Chlorinated molecules are widely used in making plastics, solvents, pesticides, and medicines.[1] However, they can also be harmful pollutants that pose risks to health and the environment.[2] Despite their relevance, understanding the structure of these chlorine-containing compounds is challenging, especially because chlorine atoms (which have a nuclear spin of 3/2) produce weak and broad signals in standard solid-state NMR, making them hard to detect. To overcome this, we use a method called ^{35}Cl Nuclear Quadrupole Resonance (NQR), which is highly sensitive to chlorine's local chemical environment.[3] In this study, we use DFT (Density Functional Theory) to model a variety of chlorine-containing organic compounds and predict their NQR signatures, defined by two key parameters: C_Q (quadrupolar coupling constant) and η_Q (asymmetry parameter). Our goal is to see how these parameters can help identify chlorine in different chemical environments. This information can then be used to better detect and understand chlorine pollution in the environment.

The predicted ν_Q frequencies of 80 chlorine-containing organic compounds (Fig. 1A) representing a large range of possible chlorine-carbon environments. We noticed that acyl chlorides, sp^2 , sp^3 and sp -bound chlorine can indeed be distinguished from either their ν_Q or from the quadrupolar parameters. We then used the predicted values to measure NQR signals for 16 signals of reference molecules (Fig. 1B) and found a clear link between the amount of chlorine and the observed frequency. Finally, we tested this approach on a prototypical example, namely PVC (polyvinyl chloride, Fig. 1C). We could distinguish terminal from central chlorine atoms. We also saw that isomers, defects, and intermolecular interactions affected the signal's position.

In this work, we have explored the potential application of ^{35}Cl NQR for characterizing chlorinated compounds, common environmental pollutants with significant health and ecological risks. We first established a protocol for predicting and measuring the quadrupolar constants of different organic chlorides. These parameters allow for differentiation of Cl functionalities based on their hybridization, functional group, and neighboring Cl. These findings are then applied to PVC to differentiate isomers, defects, and intermolecular interactions. These results represent a step toward the detection of chlorine pollutants and the understanding of PVC depolymerization processes.

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