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ABSTRACT BOOK

GLOBAL CHALLENGES. AN EMERGENCY FOR ENVIRONMENTAL SCIENCES.

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Institute
Chemicals have a fundamental role in our daily life. Over the last years, the worldwide consumption of chemicals has increased not only in volume but also in diversity. Due to their wide-spread use, chemicals are continuously released and can subsequently harm environmental health. Many well-known historical chemical pollution problems are the result of the release of highly persistent chemicals and hence persistency is seen as a major cause of concern [1]. The aim of this work was to explore opportunities to prevent environmental pollution early in the chemical life-cycle by redesigning structures for biodegradability whilst the initial function of the chemical is preserved. For our case-study, the NORMAN database was screened and triisobutyl phosphate (TiBP) was selected for redesign. TiBP is used as a flame-retardant on textiles and is persistent in sediments [2]. Alternatives for TiBP were generated with an *in silico* approach, creating a large virtual library with circa 8.2 million chemical structures. Relevant properties for these structures (including LogKow) were predicted with QSAR models. A multi-criteria selection process was developed by assigning a 'desirability score' to the generated structures. The scoring system revealed chemical alternatives with an improved profile of predicted environmental properties. From the top 500, one alternative structure was selected and synthesized based on expert judgement. Properties of the new chemical are currently tested. The developed approach can identify chemical structures with improved (environmental) properties, and is in line with current policy goals as defined under e.g. the EU Green Deal. Safe and sustainable-by-design chemicals can play a pivotal role in enabling a circular economy by 2050 when aligned with concepts of circular chemistry [3]. [1] Cousins, I. T., Ng, C. A., Wang, Z., & Scheringer, M. (2019). Why is high persistence alone a major cause of concern?. Environmental Science: Processes & Impacts, 21(5), 781-792. [2] Alygizakis, N. A., Oswald, P., Thomaidis, N. S., Schymanski, E. L., Aalizadeh, R., Schulze, T., ... & Slobodnik, J. (2019). NORMAN digital sample freezing platform: A European virtual platform to exchange liquid chromatography high resolution-mass spectrometry data and screen suspects in "digitally frozen" environmental samples. TrAC Trends in Analytical Chemistry, 115, 129-137. [3] Keijer, T., Bakker, V., & Slootweg, J. C. (2019). Circular chemistry to enable a circular economy. Nature chemistry, 11(3), 190-195.

Marine and Freshwater Pelagic and Benthic Harmful Algal Blooms: Toxins Production, Detection, Fate, Effects, Monitoring and Management.

4.11.04
Development and Evaluation of a Sensitive, Diffusive Gradients in Thin-Films (DGT) Method for Determining microcystin-LR Concentrations in Freshwater and Seawater
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A Diffusive Gradients in Thin-Films (DGT) passive sampling technique was developed for microcystin-LR (MCLR), one of the most common and toxic microcystins. Three types of resins (HP20, SP700, and XAD18) were evaluated for MC-LR uptake kinetics, capacities, and extraction efficiencies and simple procedures were developed for determining MC-LR concentration in binding disc extracts by Adda-ELISA (U.S. EPA Method 546). The XAD18-DGT/Adda-ELISA method had a 7-d deployment time detection limit of ≈0.05 µg/L and capacity of > 250 µg/L of MC-LR in water samples which encompass U.S. EPA and WHO advisory concentrations for drinking and recreational waters. The XAD18-DGT/Adda-ELISA method determined time-averaged MC-LR concentrations in waters with wide ranging pH (4.9–8.3) and ionic strength (0.04–0.8 M) under well-stirred and quiescent conditions with 90–101% accuracy. In addition to high sensitivity and accuracy, the method is simple, inexpensive, and applicable for determining MC-LR and related MCs concentrations in waterbodies with wide ranging chemical characteristics and hydrodynamic conditions.

4.11.07
Cylindrospermopsin and Glyphosate Accumulation in Lettuce (Lactuca sativa) Simultaneously Exposed to Both Toxicants in Hydroponic and Soil Systems
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In nature, the simultaneous occurrence of multiple emergent contaminants such as cyanotoxins (e.g., cylindrospermopsin (CYN)) and herbicides (e.g., glyphosate (GLY)), is highly expectable and it can be anticipated, mainly in the aquatic and terrestrial environments. The use of contaminated water for irrigation can be hazardous to the agricultural sector and some studies have reported that, individually, these contaminants can be accumulated in the edible tissues exerting a negative influence on crop plants safety and ultimately in human health. Furthermore, recent studies have suggested that some cyanotoxins (e.g., microcystins) can change the membrane permeability of roots, resulting in changes in the accumulation rates of other contaminants in plants. Since edible plants are exposed to a wide variety of substances through irrigation water, there is increasing concern in the potential adverse effects of the interactions between those substances when present simultaneously, especially when this can have potential public health consequences. The aim of this study was to determine the accumulation of CYN in *Lactuca sativa* simultaneously exposed to GLY at environmentally relevant concentrations. Lettuce plants were exposed for 15 days to 50 µg/L or kg of CYN-containing crude extract (*Chrysosporum ovalisporum* culture - LEGE X-001) and 750 µg/L or kg of GLY, in hydroponic and soil systems, respectively. The concentration of CYN and GLY in lettuce plants (roots and leaves) was determined by LC/MS-MS. The results show that, at the described conditions, CYN was accumulated in roots (0.06-7.62 µg CYN/g Dw) and leaves (0.13-1.1 µg CYN/g Dw) of lettuce, especially when plants were exposed in hydroponic system. However, interestingly, when lettuce plants were exposed simultaneously to both toxicants the concentration of CYN assimilated by lettuce plants (roots and leaves) was respectively, 1.5-fold and 1-3-2.2-fold lower than in the exposure to isolated CYN. Conversely, the plants exposed to the mixture in soil system, showed that the concentration of GLY incorporated by lettuce (roots and leaves) was higher than in the exposure to the isolated compound (0.04 - 0.21 µg GLY/g and < LOQ - 0.84 µg GLY/g, respectively). This finding highlights the potential for the enhancement of GLY accumulation in lettuce plants due to their co-occurrence with CYN, and it underlines the importance of further research regarding the mechanism involved. **Keywords:** Bioaccumulation, cylindrospermopsin, *Lactuca sativa*, glyphosate. **Acknowledgements:** This work has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 823860.

4.11.08
Effects of Cylindrospermopsin and Glyphosate at Environmentally Relevant Concentrations on Growth and Mineral Content of Beetroot PLANTS (Beta vulgaris)
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Natural toxins produced by freshwater cyanobacteria, such as cylindrospermopsin (CYN), have been regarded as an emergent environmental threat. Cyanotoxins can be applied directly to soil by using contaminated water for agricultural irrigation. Despite the risks for food safety, the impact of cyanotoxins in agriculture is not yet fully understood. Furthermore, in soil-plant system the