SETAC EUROPE 2021

SETAC EUROPE 31ST ANNUAL MEETING

ABSTRACT BOOK

GLOBAL CHALLENGES. AN EMERGENCY FOR ENVIRONMENTAL SCIENCES.

3–6 MAY 2021 | VIRTUAL

PRINT ISSN 2309-8031 - ONLINE ISSN 2310-3043 © 2021
Society of Environmental Toxicology and Chemistry Europe (SETAC Europe)

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

simultaneous occurrence of cyanotoxins and pesticides can be highly expectable. Pesticides, especially residues of glyphosate (GLY), have been frequently detected in soils and have been recognized to contribute to soil toxicity. Beetroot (*Beta vulgaris*) are root vegetables, extensively consumed worldwide with great importance for human nourishment and economy. It is, therefore, important to evaluate the effects of using water contaminated with CYN and GLY on beetroot cultivation. This study aimed to assess the effects of environmentally relevant concentrations of CYN, GLY and a mixture of both on growth and mineral content of beetroot (roots and leaves) cultivated in soil system. Plants were exposed in controlled conditions to CYN-crude extracts (50µg/kg) (*Chrysosporum ovalisporum* culture - LEGE X-001), isolated and in mixture with GLY (750 µg/kg) for 4 months. Beetroot growth was assessed by determining its fresh (Fw) and dry weight (Dw). The determination of mineral content was made by inductively coupled plasma-mass spectrometry (ICP-MS), after sample mineralization by microwave-assisted acid digestion. The results denote that Fw and Dw of beetroot (leaves and roots, respectively) were significantly changed (<i>P

4.11.09

Risk Assessment of Cyanotoxins in Agriculture - an Overview of the Effects in Plant Performance, Yield and Contamination

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Fresh water resources in many countries are vulnerable due to their biogeographical and climatic characteristics. Moreover higher water consumption and higher human impacts in the downstream water bodies is leading to a higher eutrophication with increased incidence and intensity of cyanobacteria blooms and their toxins. The scarcity of clean water resources leads to the compulsory use of water containing cyanobacteria and their toxins in agriculture. Research carried out in particular in the last decade, has showed that Microcystins (MCs), the most prevalent group of cyanotoxins in freshwaters in the world, can induce several adverse effects in plants (terrestrial and aquatic) including agricultural species. Among the effects reported are the inhibition in germination and growth, morphological alterations in roots and aerial organs, impairment of photosynthesis, and reduced yield. Nevertheless, the impacts in crops depend on many factors, including genetic. Other plant stress factors can also enhance the toxicity of cyanotoxins. In this work, a review is carried on the toxic effects of cyanotoxins in agricultural plants, focusing in particular those linked to environmental realistic scenarios. This analysis highlights that MCs at 1 µg/l, are not harmful to plants thereby, can be acceptable in irrigation waters. Moreover, most crops may tolerate MCs to a concentration up to 10 µg/l. Few morphological and physiological impairments were linked to exposure to this range of concentrations. Moreover, the toxicity of the water with 10 µg/l MCs, can be ameliorated for instance by promoting the growth of crop species that are more tolerant to MCs or, by withholding the use of contaminated water during germination and seedling development, since the sensitivity of crops increase considerably in these stages of development. These procedures will also help avoid the accumulation of MCs in plants and edible tissues and avoid food safety issues.In conclusion, this range of concentrations can be considered in the domains of water management and water treatment for agricultural purposes; and also in terms of future regulation development, concerning the maximum levels of cyanotoxins (MCs) admitted in irrigation waters. **Keywords:** Cyanotoxins, Microcystins, Crops, Phytotoxicty, Food safety.
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.

4.11.10

Generating Ecotoxicity Information on Cyanotoxins and Prymnesins Using Extracts of Cultures and Surface Water Samples

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There is a lack of information to estimate safe levels for aquatic life concerning the toxicity of natural toxins produced by cyanobacteria and the freshwater invasive microalgae *Prymnesium parvum*. Given the uncertainty of standards for toxins, the cost of using them to conduct acute and chronic toxicity tests and their potential impurities, a new approach is proposed using cultures and ambient samples. In this study we have used laboratory cultures of a toxin producing unicellular *Microcystis aeruginosa* and *P. parvum* and non-toxin producing filamentous *Anabaena flos-aquae.* Each culture was centrifuged to remove each species from its culture media, then resuspended in moderately hard water. The *M. aeruginosa* culture was then frozen/thawed three times at -20 °C following procedures used for ELISA analyses. A similar lysing procedure was also used on lake water samples. Acute 48-hr tests and 7-day short term chronic tests were conducted with a cell density of 3.73×10^6 (2017), 4.42×10^6 (2018), 4.16×10^6 (2019) and 1.75×10^6 (2020) cell/ml (average microcystin concentrations 73, 52, 37, and 855 ug/L) with *Ceriodaphnia dubia*, *Neocloeon triangulifer*, *Hyalella azteca* and larval *Pimephales promelas*. A stock concentration of 1746 ug/L was prepared for 100% exposure. For all studies, exposures were conducted at 0, 6.25, 12.5, 25, 50 and 100% of the stock concentration. Microcystin concentrations in the lysed samples as high as 74 ug/L did not cause any acute toxicity greater than the lab water controls to any of the 4-test species. *A. flos-aquae* caused mortality greater than the controls to *N. triangulifer.* For chronic tests, 80 L of the culture *M. aeruginosa* were used. No treatment levels exhibited any adverse survival effects in *C. dubia*, *P. promelas* or *H. azteca* tests. The only adverse effects noted in these tests were the sub-lethal point estimate endpoints for reproduction inhibition (IC_{25}=30.96% [1.37×10^6 cells/ml]) in the *C. dubia* bioassay. August 2017 Lake Harsha sample (total # of cells 300,000 cells/ml) was not acutely toxic to any of the 4-test species. For chronic toxicity lake water sample, the long term lethal concentration (LC_{50})% was 7.81, 15.33, and 7.59 in *C. dubia*, *P. promelas* and *N. triangulifer* tests, and IC_{25} were 1.03, 8.36, and 1.14 %, respectively. For *P. parvum* LC_{50}s were 493,850 cells/ml for *C. dubia* and 121,761 cells/ml *N. triangulifer*. One observation that was made is that cultures of similar cells/ml did not produce the same concentration of intracellular toxin.

4.11.11

Toxicity of microalgae to non-target organisms is related to species, fraction and culturing

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Exopolymers (EPS) of microalgae are promising candidates as additives for lubricants. The EPS producing red algae *Dixoniella grisea* is not described as toxin producing species in the literature while some strains of the also EPS producing cyanobacterium *Cyanothece* sp. are. In addition, culture conditions may affect quality and quantity of both EPS and toxins. For using microalgae as sustainable suppliers of raw materials, negative effects to different non-target organisms need to be excluded under a broad set of algal culture conditions. For this purpose, a rapid screening using a set of non-target organisms representing three different exposure pathways, namely *Daphnia magna*, *Folsomia candida* and *Enchytraeus crypticus*, was developed. It was used to test the culture, parts of the culture, the algal material and EPS for their potential to induce acute toxicity in any of these species. Each culture was tested singly to take into account the culture conditions in the evaluation. Overall, EPS most frequently caused toxic effects to any of the non-target organisms. Of all test species, *E. crypticus* was most often affected. The culture conditions had different impact for the different algae strains tested, so that analytical results of the test substance composition were compared to identify possible drivers of ecotoxicity. All kinds of samples were analysed for their monosaccharide, fatty acid, and amino acid composition, and