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### 1) Bioactivation of trichloroethylene to three regioisomeric glutathione conjugates by liver fractions and recombinant human glutathione transferases: species differences and implications for human risk assessment

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* Toxicology Letters
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* Published 1 Feb 2021 (early online None)
* Processed: 2021-2

Enzymatic conjugation of glutathione (GSH) to trichloroethylene (TCE) followed by catabolism to the corresponding cysteine-conjugate, S-(dichlorovinyl)-L-cysteine (DCVC), and subsequent bioactivation by renal cysteine conjugate beta-lyases is considered to play an important role in the nephrotoxic effects observed in TCE-exposed rat and human. In this study, it is shown for the first time that three regioisomers of GSH-conjugates of TCE are formed by rat and human liver fractions, namely S-(1,2-trans-dichlorovinyl)-glutathione (1,2-trans-DCVG), S-(1,2-cis-dichlorovinyl)-glutathione (1,2-cis-DCVG) and S-2,2-dichlorovinyl-glutathione (2,2-DCVG). In incubations of TCE with rat liver fractions their amounts decreased in order of 1,2-cis-DCVG > 1,2-trans-DCVG > 2,2-DCVG. Human liver cytosol showed a more than 10-fold lower activity of GSH-conjugation, with amounts of regioisomers decreasing in order 2,2-DCVG > 1,2-trans-DCVG > 1,2-cis-DCVG. Incubations with recombinant human GSTs suggest that GSTA1-1 and GSTA2-2 play the most important role in human liver cytosol. GSTP1-1, which produces regioisomers in order 1,2-trans-DCVG > 2,2-cis-DCVG > 1,2-cis-DCVG, is likely to contribute to extrahepatic GSH-conjugation of TCE. Analysis of the products formed by a beta-lyase mimetic model showed that both 1,2-trans-DCVC and 1,2-cis-DCVC are converted to reactive products that form cross-links between the model nucleophile 4-(4-nitrobenzyl)-pyridine (NBP) and thiol-species. No NBP-alkylation was observed with 2,2-DCVC corresponding to its low cytotoxicity and mutagenicity. The lower activity of GSH-conjugation of TCE by human liver fractions, in combination with the lower fraction of potential nephrotoxic and mutagenic 1,2-DCVG-isomers, suggest that humans are at much lower risk for TCE-associated nephrotoxic effects than rats.

### 2) Temporal tracking of quantum-dot apatite across in vitro mycorrhizal networks shows how host demand can influence fungal nutrient transfer strategies

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* Published Feb 2021 (early online 28 Sep 2020)
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Arbuscular mycorrhizal fungi function as conduits for underground nutrient transport. While the fungal partner is dependent on the plant host for its carbon (C) needs, the amount of nutrients that the fungus allocates to hosts can vary with context. Because fungal allocation patterns to hosts can change over time, they have historically been difficult to quantify accurately. We developed a technique to tag rock phosphorus (P) apatite with fluorescent quantum-dot (QD) nanoparticles of three different colors, allowing us to study nutrient transfer in an in vitro fungal network formed between two host roots of different ages and different P demands over a 3-week period. Using confocal microscopy and raster image correlation spectroscopy, we could distinguish between P transfer from the hyphae to the roots and P retention in the hyphae. By tracking QD-apatite from its point of origin, we found that the P demands of the younger root influenced both: (1) how the fungus distributed nutrients among different root hosts and (2) the storage patterns in the fungus itself. Our work highlights that fungal trade strategies are highly dynamic over time to local conditions, and stresses the need for precise measurements of symbiotic nutrient transfer across both space and time.

### 3) Results of WEPAL-QUASIMEME/NORMANs first global interlaboratory study on microplastics reveal urgent need for harmonization

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* Published 10 Jun 2021 (early online 4 Feb 2021)
* Processed: 2021-2

To survey the conformity and quality of results among laboratories for microplastics determination worldwide, an international laboratory intercomparison and development exercise was organized. The 34 participants were requested to determine the polymer type and number or mass of polymer particles in 12 samples, i.e. six samples containing of pre-production pellets, five dissolvable soda tablets containing different (smaller) polymer particles and one blank soda tablet. A novel method for providing the test materials in aluminium strips was used. Thirty laboratories (88%) submitted data using their own method of choice, resulting in a variety of identification and quantification methods (n = 7). The majority of the labs (53–100%) correctly identified the type of polymer in all samples but one. The performance of the laboratories in quantifying and weighing the pellets was very good. The analysis of the number of the particles in the soda tablets varied considerably between laboratories (29–91%). The results of this study highlight the complexity of microplastics analysis and the need for harmonization of both reporting format and methods. Continued development and assessment of the comparability among analytical methods and laboratories are urgently needed to support monitoring programmes, research and decision-making.

### 4) IUPACpal: efficient identification of inverted repeats in IUPAC-encoded DNA sequences

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* Published Dec 2021 (early online 6 Feb 2021)
* Processed: 2021-2

Background: An inverted repeat is a DNA sequence followed downstream by its reverse complement, potentially with a gap in the centre. Inverted repeats are found in both prokaryotic and eukaryotic genomes and they have been linked with countless possible functions. Many international consortia provide a comprehensive description of common genetic variation making alternative sequence representations, such as IUPAC encoding, necessary for leveraging the full potential of such broad variation datasets. Results: We present IUPACpal, an exact tool for efficient identification of inverted repeats in IUPAC-encoded DNA sequences allowing also for potential mismatches and gaps in the inverted repeats. Conclusion: Within the parameters that were tested, our experimental results show that IUPACpal compares favourably to a similar application packaged with EMBOSS. We show that IUPACpal identifies many previously unidentified inverted repeats when compared with EMBOSS, and thatthis is also performed with orders of magnitude improved speed.

### 5) Intercellular communication induces glycolytic synchronization waves between individually oscillating cells

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* Published 9 Feb 2021 (early online None)
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Many organs have internal structures with spatially differentiated and sometimes temporally synchronized groups of cells. The mechanisms leading to such differentiation and coordination are not well understood. Here we design a diffusion-limited microfluidic system to mimic a multicellular organ structure with peripheral blood flow and test whether a group of individually oscillating yeast cells could form subpopulations of spatially differentiated and temporally synchronized cells. Upon substrate addition, the dynamic response at single-cell level shows glycolytic oscillations, leading to wave fronts traveling through the monolayered population and to synchronized communities at well-defined positions in the cell chamber. A detailed mechanistic model with the architectural structure of the flow chamber incorporated successfully predicts the spatial-temporal experimental data, and allows for a molecular understanding of the observed phenomena. The intricate interplay of intracellular biochemical reaction networks leading to the oscillations, combined with intercellular communication via metabolic intermediates and fluid dynamics of the reaction chamber, is responsible for the generation of the subpopulations of synchronized cells. This mechanism, as analyzed from the model simulations, is experimentally tested using different concentrations of cyanide stress solutions. The results are reproducible and stable, despite cellular heterogeneity, and the spontaneous community development is reminiscent of a zoned cell differentiation often observed in multicellular organs.

### 6) In vitro biotransformation and evaluation of potential transformation products of chlorinated paraffins by high resolution accurate mass spectrometry

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* Journal of Hazardous Materials
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* Published 5 Mar 2021 (early online 10 Oct 2020)
* Processed: 2021-3

Chlorinated paraffins (CPs) are high production chemicals, which leads to their ubiquitous presence in the environment. To date, few studies have measured CPs in humans and typically at relatively low concentrations, despite indications that exposure may be high compared to various persistent organic pollutants. The aim of this study is to investigate the in vitro biotransformation of CPs by human liver fractions. We determined the changes of the CP concentrations after the enzymatic transformation with human liver microsomes using a two-tiered in vitro approach. CP concentrations decreased with human liver microsomes, with the decreases of 33–94% after incubating with different groups of enzymes for 2 h. The profiles of CP rapidly shifted after the incubation with human liver microsomes. In addition, the concentrations of CPs and the biotransformation products were tentatively measured using high-resolution mass spectrometric analysis, including very short CP (carbon chain length <10), alcohols, ketones, and carboxylic acids. C‒C bond cleavage is a potential transformation pathway for CPs, and ketones are potential products of CP biotransformation, especially for long-chain CPs (C>17). The ketone products may be investigated as CP exposure biomarker in biomonitoring studies.

### *7) Hazardous compounds in recreational and urban recycled surfaces made from crumb rubber. Compliance with current regulation and future perspectives*

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* Published 10 Feb 2021 (early online 29 Sep 2020)
* Processed: 2021-2

Crumb rubber obtained from scrap tires is greatly employed for the construction of different facilities for sport, recreational and other uses. However, in recent years the concern about their safety ...

### *8) Circular pattern matching with k mismatches*

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* Published Feb 2021 (early online 29 Jul 2020)
* Processed: 2021-2

We consider the circular pattern matching with k mismatches (k-CPM) problem in which one is to compute the minimal Hamming distance of every length-m substring of T and any cyclic rotation of P, if th ...

### *9) G protein-coupled receptors as promising targets in cancer*

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* AIMMS, Medicinal chemistry
* Current Opinion in Endocrine and Metabolic Research
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* Published Feb 2021 (early online 26 Oct 2020)
* Processed: 2021-2

G protein-coupled receptors (GPCRs) control diverse cellular functions, and their dysregulation is involved in a plethora of diseases including tumorigenesis. In the last decade, the association of GP ...

### *10) Metabolic cooperation and spatiotemporal niche partitioning in a kefir microbial community*

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* Published Feb 2021 (early online None)
* Processed: 2021-2

Microbial communities often undergo intricate compositional changes yet also maintain stable coexistence of diverse species. The mechanisms underlying long-term coexistence remain unclear as system-wi ...

### *11) Neurotoxicity and underlying cellular changes of 21 mitochondrial respiratory chain inhibitors*

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* Published Feb 2021 (early online 29 Jan 2021)
* Processed: 2021-2

Inhibition of complex I of the mitochondrial respiratory chain (cI) by rotenone and methyl-phenylpyridinium (MPP +) leads to the degeneration of dopaminergic neurons in man and rodents. To formally de ...

### *12) A state-averaged orbital-optimized hybrid quantum–classical algorithm for a democratic description of ground and excited states*

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* Processed: 2021-1

In the noisy intermediate-scale quantum (NISQ) era, solving the electronic structure problem from chemistry is considered as the ‘killer application’ for near-term quantum devices. In spite of the suc ...