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### 1) Influence of short- And long-term exposure on the biodegradation capacity of activated sludge microbial communities in ready biodegradability tests

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* Processed: 2021-1

Ready biodegradability tests (RBTs) are extensively used to screen the potential of chemicals to be biodegraded. The use of RBT protocols often results in large variations of test results that may lead to wrong interpretations. The present study aims to obtain a fundamental understanding of this variability. For this, we subjected the compounds 4-chloroaniline (4CA), carbamazepine (CBZ), metformin (MET), and N-methylpiperazine (NMP) to a variety of different test conditions. Inocula from five local wastewater treatment plants (WWTPs) were used in an attempt to enhance the Organisation for Economic Co-operation and Development (OECD) 310 biodegradability tests. The biodegradation capacity in RBTs, community composition and adaptation of the communities were compared after one week of pre-exposure in batch and four months exposure in chemostat. The results confirm that none of the test compounds is readily biodegradable in the standard OECD 310 RBT. However, when pre-exposure under either batch or chemostat conditions was included, 4CA was degraded in some cases and less variability among different inocula was observed for the transformation of MET. Bacterial communities from the five locations were found to be significantly different in composition from one another. In addition, pre-treatment performed before the RBT significantly changed the composition of each community. Results of this experiment show that short-term pre-exposure may increase the absolute number of degraders and deserves to be further investigated as a potential method to reduce the outcome variability of RBTs.

### 2) Critique of the “Comment” etitled “Pyrethroid exposure: Not so harmless after all” by Demeneix et al. (2020) published in the lancet diabetes endocrinology

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* Toxicology Letters
* https://doi.org/10.1016/j.toxlet.2020.12.020
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* Published 1 Apr 2021 (early online 4 Jan 2021)
* Processed: 2021-1

### 3) Serial propagation in water-in-oil emulsions selects for Saccharomyces cerevisiae strains with a reduced cell size or an increased biomass yield on glucose

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* Published Mar 2021 (early online 5 Jan 2021)
* Processed: 2021-1

In S. cerevisiae and many other micro-organisms an increase in metabolic efficiency (i.e. ATP yield on carbon) is accompanied by a decrease in growth rate. From a fundamental point of view, studying these yield-rate trade-offs provides insight in for example microbial evolution and cellular regulation. From a biotechnological point of view, increasing the ATP yield on carbon might increase the yield of anabolic products. We here aimed to select S. cerevisiae mutants with an increased biomass yield. Serial propagation of individual cells in water-in-oil emulsions previously enabled the selection of lactococci with increased biomass yields, and adapting this protocol for yeast allowed us to enrich an engineered Crabtree-negative S. cerevisiae strain with a high biomass yield on glucose. When we started the selection with an S. cerevisiae deletion collection, serial propagation in emulsion enriched hxk2Δ and reg1Δ strains with an increased biomass yield on glucose. Surprisingly, a tps1Δ strain was highly abundant in both emulsion- and suspension-propagated populations. In a separate experiment we propagated a chemically mutagenized S. cerevisiae population in emulsion, which resulted in mutants with a higher cell number yield on glucose, but no significantly changed biomass yield. Genome analyses indicate that genes involved in glucose repression and cell cycle processes play a role in the selected phenotypes. The repeated identification of mutations in genes involved in glucose-repression indicates that serial propagation in emulsion is a valuable tool to study metabolic efficiency in S. cerevisiae.

### 4) KLIFS: an overhaul after the first 5 years of supporting kinase research

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* Processed: 2021-1

Kinases are a prime target of drug development efforts with >60 drug approvals in the past two decades. Due to the research into this protein family, a wealth of data has been accumulated that keeps on growing. KLIFS-Kinase-Ligand Interaction Fingerprints and Structures-is a structural database focusing on how kinase inhibitors interact with their targets. The aim of KLIFS is to support (structure-based) kinase research through the systematic collection, annotation, and processing of kinase structures. Now,5years after releasing the initial KLIFS website, the database has undergone a complete overhaul with a new website, new logo, and new functionalities. In this article, we start by looking back at how KLIFS has been used by the research community, followed by a description of the renewed KLIFS, and conclude with showcasing the functionalities of KLIFS. Major changes include the integration of approved drugs and inhibitors in clinical trials, extension of the coverage to atypical kinases, and a RESTful API for programmatic access. KLIFS is available at the new domain https://klifs.net.

### 5) Unlocking Elementary Conversion Modes: ecmtool Unveils All Capabilities of Metabolic Networks

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* Published 8 Jan 2021 (early online None)
* Processed: 2021-1

The metabolic capabilities of cells determine their biotechnological potential, fitness in ecosystems, pathogenic threat levels, and function in multicellular organisms. Their comprehensive experimental characterization is generally not feasible, particularly for unculturable organisms. In principle, the full range of metabolic capabilities can be computed from an organism's annotated genome using metabolic network reconstruction. However, current computational methods cannot deal with genome-scale metabolic networks. Part of the problem is that these methods aim to enumerate all metabolic pathways, while computation of all (elementally balanced) conversions between nutrients and products would suffice. Indeed, the elementary conversion modes (ECMs, defined by Urbanczik and Wagner) capture the full metabolic capabilities of a network, but the use of ECMs has not been accessible until now. We explain and extend the theory of ECMs, implement their enumeration in ecmtool, and illustrate their applicability. This work contributes to the elucidation of the full metabolic footprint of any cell.

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

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* Science of the Total Environment
* https://doi.org/10.1016/j.scitotenv.2020.142566
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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 and the related adult and children exposure to these surfaces is growing. This study aims a thorough chemical characterization encompassing 42 hazardous compounds, including polycyclic aromatic hydrocarbons (PAHs), phthalates, adipates, antioxidants and vulcanization agents in a wide range of crumb rubber from different surfaces. For the extraction of the target compounds, a method based on ultrasound-assisted extraction followed by gas chromatography-tandem mass spectrometry (UAE-GC–MS/MS) has been validated. Forty crumb rubber samples coming from synthetic turf football pitches, outdoor and indoor playgrounds, urban pavements, commercial tiles and granulates, and scrap tires, were analyzed. In addition, green alternative materials, such as sand and artificial turf based on cork granulate infill were included to compare the levels of the target compounds with those of crumb rubber. Most of the analyzed recycled surfaces meet the recent limits proposed by the European Commission for rubber granulates and mulches, although they exceed in several cases the maximum levels allowed for rubber consumer products. Besides, most of the other target compounds, including several of them considered as endocrine disruptors, were detected in the analyzed samples, reaching parts per million concentrations.

### 7) Circular pattern matching with k mismatches

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* Journal of Computer and System Sciences
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* 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 this distance is no more than k. It is a variation of the well-studied k-mismatch problem. A multitude of papers has been devoted to solving the k-CPM problem, but only average-case upper bounds are known. In this paper, we present the first non-trivial worst-case upper bounds for this problem. Specifically, we show an O(nk)-time algorithm and an [Formula presented]-time algorithm. The latter algorithm applies in an extended way a technique that was very recently developed for the k-mismatch problem Bringmann et al. (2019) [10]. A preliminary version of this work appeared at FCT 2019 [35]. In this version we improve the time complexity of the second algorithm from [Formula presented] to [Formula presented].

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

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* AIMMS, Medicinal chemistry
* Current Opinion in Endocrine and Metabolic Research
* https://doi.org/10.1016/j.coemr.2020.10.005
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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 GPCRs with cancer has become apparent and offers new opportunities to target GPCRs in oncology. GPCR overexpression and mutations lead to aberrant activation of pro-oncogenic pathways inducing tumor progression. In this review, we describe how GPCRs activate some main signaling pathways that contribute to different cancer hallmarks, including cell transformation, proliferative signaling, immune evasion, angiogenesis, and metastasis. Thereafter, we highlight different approaches to target GPCRs, including small molecules and biologics (e.g. monoclonal antibodies and nanobodies) and combinatorial (immuno)therapies that are emerging with promising effects for cancer treatment.

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

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* NATURE MICROBIOLOGY
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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-wide studies have been largely limited to engineered communities, ex situ adapted cultures or synthetic assemblies. Here, we show how kefir, a natural milk-fermenting community of prokaryotes (predominantly lactic and acetic acid bacteria) and yeasts (family Saccharomycetaceae), realizes stable coexistence through spatiotemporal orchestration of species and metabolite dynamics. During milk fermentation, kefir grains (a polysaccharide matrix synthesized by kefir microorganisms) grow in mass but remain unchanged in composition. In contrast, the milk is colonized in a sequential manner in which early members open the niche for the followers by making available metabolites such as amino acids and lactate. Through metabolomics, transcriptomics and large-scale mapping of inter-species interactions, we show how microorganisms poorly suited for milk survive in—and even dominate—the community, through metabolic cooperation and uneven partitioning between grain and milk. Overall, our findings reveal how inter-species interactions partitioned in space and time lead to stable coexistence.

### *10) A schematic sampling protocol for contaminant monitoring in raptors*

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* Published Jan 2021 (early online 12 May 2020)
* Processed: 2021-1

Birds of prey, owls and falcons are widely used as sentinel species in raptor biomonitoring programmes. A major current challenge is to facilitate large-scale biomonitoring by coordinating contaminant ...

### *11) Receptor-based in vitro activities to assess human exposure to chemical mixtures and related health impacts*

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* Published Jan 2021 (early online 14 Oct 2020)
* Processed: 2021-1

Humans are exposed to a large number of chemicals from sources such as the environment, food, and consumer products. There is growing concern that human exposure to chemical mixtures, especially durin ...

### *12) Asymmetrical flow field-flow fractionation to probe the dynamic association equilibria of β-D-galactosidase*

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* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461719
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* Published 4 Jan 2021 (early online 13 Nov 2020)
* Processed: 2021-1

Protein dynamics play a significant role in many aspects of enzyme activity. Monitoring of structural changes and aggregation of biotechnological enzymes under native conditions is important to safegu ...

### *13) Rapid Screening α-Glucosidase Inhibitors from Natural Products by At-Line Nanofractionation with Parallel Mass Spectrometry and Bioactivity Assessment*

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* BioAnalytical Chemistry, AIMMS, Jinan University, SCIEX (China) Co., Ltd.
* Journal of Chromatography A
* https://doi.org/10.1016/j.chroma.2020.461740
* Corresponding author: Jiang, Z.
* Published 4 Jan 2021 (early online 23 Nov 2020)
* Processed: 2021-1

In this study, a novel at-line nanofractionation screening platform was successfully developed for the rapid screening and identification of α-glucosidase inhibitors from natural products. A time-cour ...

### *14) Reducing the influence of geometry-induced gradient deformation in liquid chromatographic retention modelling*

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* Journal of Chromatography A
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* Published 4 Jan 2021 (early online 13 Nov 2020)
* Processed: 2021-1

Rapid optimization of gradient liquid chromatographic (LC) separations often utilizes analyte retention modelling to predict retention times as function of eluent composition. However, due to the dwel ...

### *15) Influence maximization in the presence of vulnerable nodes: A ratio perspective*

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* Published 8 Jan 2021 (early online 20 Nov 2020)
* Processed: 2021-1

Influence maximization is a key problem seeking to identify users who will diffuse information to influence the largest number of other users in a social network. A drawback of the influence maximizat ...

### *16) Dynamic co-culture metabolic models reveal the fermentation dynamics, metabolic capacities and interplays of cheese starter cultures*

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* Published Jan 2021 (early online 14 Sep 2020)
* Processed: 2021-1

In this study, we have investigated the cheese starter culture as a microbial community through a question: can the metabolic behaviour of a co-culture be explained by the characterized individual org ...