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### 1) pH dependencies of glycolytic enzymes of yeast under in vivo-like assay conditions

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Under carbon source transitions, the intracellular pH of Saccharomyces cerevisiae is subject to change. Dynamics in pH modulate the activity of the glycolytic enzymes, resulting in a change in glycolytic flux and ultimately cell growth. To understand how pH affects the global behavior of glycolysis and ethanol fermentation, we measured the activity of the glycolytic and fermentative enzymes in S. cerevisiae under in vivo-like conditions at different pH. We demonstrate that glycolytic enzymes exhibit differential pH dependencies, and optima, in the pH range observed during carbon source transitions. The forward reaction of GAPDH shows the highest decrease in activity, 83%, during a simulated feast/famine regime upon glucose removal (cytosolic pH drop from 7.1 to 6.4). We complement our biochemical characterization of the glycolytic enzymes by fitting the Vmax to the progression curves of product formation or decay over time. The fitting analysis shows that the observed changes in enzyme activities require changes in Vmax, but changes in Km cannot be excluded. Our study highlights the relevance of pH as a key player in metabolic regulation and provides a large set of quantitative data that can be explored to improve our understanding of metabolism in dynamic environments.

### 2) Assessment of the Second-Order Statically Screened Exchange Correction to the Random Phase Approximation for Correlation Energies

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With increasing interelectronic distance, the screening of the electron-electron interaction by the presence of other electrons becomes the dominant source of electron correlation. This effect is described by the random phase approximation (RPA) which is therefore a promising method for the calculation of weak interactions. The success of the RPA relies on the cancellation of errors, which can be traced back to the violation of the crossing symmetry of the 4-point vertex, leading to strongly overestimated total correlation energies. By the addition of second-order screened exchange (SOSEX) to the correlation energy, this issue is substantially reduced. In the adiabatic connection (AC) SOSEX formalism, one of the two electron-electron interaction lines in the second-order exchange term is dynamically screened (SOSEX(W, vc)). A related SOSEX expression in which both electron-electron interaction lines are statically screened (SOSEX(W(0), W(0))) is obtained from the G3W2 contribution to the electronic self-energy. In contrast to SOSEX(W, vc), the evaluation of this correlation energy expression does not require an expensive numerical frequency integration and is therefore advantageous from a computational perspective. We compare the accuracy of the statically screened variant to RPA and RPA+SOSEX(W, vc) for a wide range of chemical reactions. While both methods fail for barrier heights, SOSEX(W(0), W(0)) agrees very well with SOSEX(W, vc) for charged excitations and noncovalent interactions where they lead to major improvements over RPA.

### 3) Particle on a Ring Model for Teaching the Origin of the Aromatic Stabilization Energy and the Hückel and Baird Rules

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Simple mathematical models can serve to reveal the essence of experimental phenomena and scientific concepts. The particle in a box (PIB), for example, is widely used in undergraduate programs to teach the quantum mechanical principles behind the UV-vis spectra of conjugated polyenes and polyynes. In this work, the particle on a ring (POR) and the PIB models are used to elucidate the concept of aromaticity in Introductory Chemistry courses. Thus, we explain the origin of the aromatic stabilization energy, Hückel's rule, and Baird's rule. Besides applications, the limitations of the POR and PIB models are also discussed.

### 4) Self-Consistent Implementation of Kohn-Sham Adiabatic Connection Models with Improved Treatment of the Strong-Interaction Limit

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Adiabatic connection models (ACMs), which interpolate between the limits of weak and strong interaction, are powerful tools to build accurate exchange-correlation functionals. If the exact weak-interaction expansion from the second-order perturbation theory is included, a self-consistent implementation of these functionals is challenging and still absent in the literature. In this work, we fill this gap by presenting a fully self-consistent-field (SCF) implementation of some popular ACM functionals. While using second-order perturbation theory at weak interactions, we have also introduced new generalized gradient approximations (GGAs), beyond the usual point-charge-plus-continuum model, for the first two leading terms at strong interactions, which are crucial to ensure robustness and reliability. We then assess the SCF-ACM functionals for molecular systems and for prototypical strong-correlation problems. We find that they perform well for both the total energy and the electronic density and that the impact of SCF orbitals is directly connected to the accuracy of the ACM functional form. For the H2 dissociation, the SCF-ACM functionals yield significant improvements with respect to standard functionals also thanks to the use of the new GGAs for the strong-coupling functionals.

### 5) Linoleic acid-derived oxylipins and isoprostanes plasma levels are influenced by 1,25-Dihydroxyvitamin D levels in middle-aged sedentary adults: The FIT-AGEING study

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Introduction: Vitamin D – concretely its active form 1,25-dihydroxyvitamin D (1,25(OH)2D) – maintains several physiological processes. Oxylipins are oxidized lipids derived from ω-6 and ω-3 polyunsaturated fatty acids involved in inflammation. Little is known about the association of 1,25(OH)2D with inflammatory parameters in middle-aged populations – who could be at risk of vitamin D deficiency –. The aim of this study was to investigate the relationship between 1,25(OH)2D plasma levels with circulating white blood cells, platelets counts and oxylipins levels. Materials and methods: A total of 74 (53 % women) middle-aged (40–65 years old) adults were recruited for this cross-sectional study. 1,25(OH)2D plasma levels were measured using an immunochemiluminometric assay. White blood cells and platelets were analyzed by hemocytometry. ω-6 and ω-3 oxylipins plasma levels were measured using liquid chromatography - tandem mass spectrometry. Simple and multiple linear regression models, and Pearson correlation analyses, were performed to study the association of 1,25(OH)2D levels with WBC and platelets counts, and oxylipins, respectively. Results: 1,25(OH)2D plasma levels were positively related with linoleic acid-derived oxylipins and isoprostanes plasma levels, whereas an inverse relationship with dihomo-γ-linolenic acid/linoleic acid and arachidonic acid/linoleic acid ratios was unveiled. No significant associations were observed for circulating ω-3 oxylipins, white blood cells levels or platelets count. Conclusions: Linoleic acid-derived oxylipins and isoprostanes plasma levels may be influenced by 1,25(OH)2D plasma levels. Further investigations are needed to elucidate the impact of other vitamin D forms upon circulating oxylipins levels.

### 6) High-Resolution Bioassay Profiling with Complemented Sensitivity and Resolution for Pancreatic Lipase Inhibitor Screening

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* Processed: 2022-10

How to rapidly and accurately screen bioactive components from complex natural products remains a major challenge. In this study, a screening platform for pancreatic lipase (PL) inhibitors was established by combining magnetic beads-based ligand fishing and high-resolution bioassay profiling. This platform was well validated using a mixture of standard compounds, i.e., (-)- epigallocatechin gallate (EGCG), luteolin and schisandrin. The dose–effect relationship of high-resolution bioassay profiling was demonstrated by the standard mixture with different concentrations for each compound. The screening of PL inhibitors from green tea extract at the concentrations of 0.2, 0.5 and 1.0 mg/mL by independent high-resolution bioassay profiling was performed. After sample pre-treatment by ligand fishing, green tea extract at the concentration of 0.2 mg/mL was specifically enriched and simplified, and consequently screened through the high-resolution bioassay profiling. As a result, three PL inhibitors, i.e., EGCG, (-)-Gallocatechin gallate (GCG) and (-)-Epicatechin gallate (ECG), were rapidly identified from the complex matrix. The established platform proved to be capable of enriching affinity binders and eliminating nonbinders in sample pre-treatment by ligand fishing, which overcame the technical challenges of high-resolution bioassay profiling in the aspects of sensitivity and resolution. Meanwhile, the high-resolution bioassay profiling possesses the ability of direct bioactive assessment, parallel structural analysis and identification after separation. The established platform allowed more accurate and rapid screening of PL inhibitors, which greatly facilitated natural product-based drug screening.

### 7) Mixture Risk Assessment of Complex Real-Life Mixtures—The PANORAMIX Project

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Humans are involuntarily exposed to hundreds of chemicals that either contaminate our environment and food or are added intentionally to our daily products. These complex mixtures of chemicals may pose a risk to human health. One of the goals of the European Union’s Green Deal and zero-pollution ambition for a toxic-free environment is to tackle the existent gaps in chemical mixture risk assessment by providing scientific grounds that support the implementation of adequate regulatory measures within the EU. We suggest dealing with this challenge by: (1) characterising ‘real-life’ chemical mixtures and determining to what extent they are transferred from the environment to humans via food and water, and from the mother to the foetus; (2) establishing a high-throughput whole-mixture-based in vitro strategy for screening of real-life complex mixtures of organic chemicals extracted from humans using integrated chemical profiling (suspect screening) together with effect-directed analysis; (3) evaluating which human blood levels of chemical mixtures might be of concern for children’s development; and (4) developing a web-based, ready-to-use interface that integrates hazard and exposure data to enable component-based mixture risk estimation. These concepts form the basis of the Green Deal project PANORAMIX, whose ultimate goal is to progress mixture risk assessment of chemicals.

### 8) Peptide-based covalent inhibitors of protein–protein interactions

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Protein–protein interactions (PPI) are involved in all cellular processes and many represent attractive therapeutic targets. However, the frequently rather flat and large interaction areas render the identification of small molecular PPI inhibitors very challenging. As an alternative, peptide interaction motifs derived from a PPI interface can serve as starting points for the development of inhibitors. However, certain proteins remain challenging targets when applying inhibitors with a competitive mode of action. For that reason, peptide-based ligands with an irreversible binding mode have gained attention in recent years. This review summarizes examples of covalent inhibitors that employ peptidic binders and have been tested in a biological context.

### 9) Grape polyphenols decrease circulating branched chain amino acids in overfed adults

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* Processed: 2022-10

Introduction and aims: Dietary polyphenols have long been associated with health benefits, including the prevention of obesity and related chronic diseases. Overfeeding was shown to rapidly induce weight gain and fat mass, associated with mild insulin resistance in humans, and thus represents a suitable model of the metabolic complications resulting from obesity. We studied the effects of a polyphenol-rich grape extract supplementation on the plasma metabolome during an overfeeding intervention in adults, in two randomized parallel controlled clinical trials. Methods: Blood plasma samples from 40 normal weight to overweight male adults, submitted to a 31-day overfeeding (additional 50% of energy requirement by a high calorie-high fructose diet), given either 2 g/day grape polyphenol extract or a placebo at 0, 15, 21, and 31 days were analyzed (Lyon study). Samples from a similarly designed trial on females (20 subjects) were collected in parallel (Lausanne study). Nuclear magnetic resonance (NMR)-based metabolomics was conducted to characterize metabolome changes induced by overfeeding and associated effects from polyphenol supplementation. The clinical trials are registered under the numbers NCT02145780 and NCT02225457 at ClinicalTrials.gov. Results: Changes in plasma levels of many metabolic markers, including branched chain amino acids (BCAA), ketone bodies and glucose in both placebo as well as upon polyphenol intervention were identified in the Lyon study. Polyphenol supplementation counterbalanced levels of BCAA found to be induced by overfeeding. These results were further corroborated in the Lausanne female study. Conclusion: Administration of grape polyphenol-rich extract over 1 month period was associated with a protective metabolic effect against overfeeding in adults.

### 10) SAR exploration of the non-imidazole histamine H3 receptor ligand ZEL-H16 reveals potent inverse agonism

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Histamine H3 receptor (H3R) agonists without an imidazole moiety remain very scarce. Of these, ZEL-H16 (1) has been reported previously as a high-affinity non-imidazole H3R (partial) agonist. Our structure-activity relationship analysis using derivatives of 1 identified both basic moieties as key interaction motifs and the distance of these from the central core as a determinant for H3R affinity. However, in spite of the reported H3R (partial) agonism, in our hands, 1 acts as an inverse agonist for Gαi signaling in a CRE-luciferase reporter gene assay and using an H3R conformational sensor. Inverse agonism was also observed for all of the synthesized derivatives of 1. Docking studies and molecular dynamics simulations suggest ionic interactions/hydrogen bonds to H3R residues D1143.32 and E2065.46 as essential interaction points.

### 11) A Combined Bioassay and Nanofractionation Approach to Investigate the Anticoagulant Toxins of Mamba and Cobra Venoms and Their Inhibition by Varespladib

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Envenomation by elapid snakes primarily results in neurotoxic symptoms and, consequently, are the primary focus of therapeutic research concerning such venoms. However, mounting evidence suggests these venoms can additionally cause coagulopathic symptoms, as demonstrated by some Asian elapids and African spitting cobras. This study sought to investigate the coagulopathic potential of venoms from medically important elapids of the genera Naja (true cobras), Hemachatus (rinkhals), and Dendroaspis (mambas). Crude venoms were bioassayed for coagulant effects using a plasma coagulation assay before RPLC/MS was used to separate and identify venom toxins in parallel with a nanofractionation module. Subsequently, coagulation bioassays were performed on the nanofractionated toxins, along with in-solution tryptic digestion and proteomics analysis. These experiments were then repeated on both crude venoms and on the nanofractionated venom toxins with the addition of either the phospholipase A2 (PLA2) inhibitor varespladib or the snake venom metalloproteinase (SVMP) inhibitor marimastat. Our results demonstrate that various African elapid venoms have an anticoagulant effect, and that this activity is significantly reduced for cobra venoms by the addition of varespladib, though this inhibitor had no effect against anticoagulation caused by mamba venoms. Marimastat showed limited capacity to reduce anticoagulation in elapids, affecting only N. haje and H. haemachatus venom at higher doses. Proteomic analysis of nanofractionated toxins revealed that the anticoagulant toxins in cobra venoms were both acidic and basic PLA2s, while the causative toxins in mamba venoms remain uncertain. This implies that while PLA2 inhibitors such as varespladib and metalloproteinase inhibitors such as marimastat are viable candidates for novel snakebite treatments, they are not likely to be effective against mamba envenomings.

### 12) Acute and long-term exercise differently modulate plasma levels of oxylipins, endocannabinoids, and their analogues in young sedentary adults: A sub-study and secondary analyses from the ACTIBATE randomized controlled-trial

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Background: Fatty acid-derived lipid mediators including oxylipins, endocannabinoids (eCBs), and their analogues, have emerged as key metabolites in the inflammatory and immune response to physiological stressors. Methods: This report was based on a sub-study and secondary analyses the ACTIBATE single-center unblinded randomized controlled trial (ClinicalTrials.gov ID: NCT02365129). The study was performed in the Sport and Health University Research Institute and the Virgen de las Nieves University Hospital of the University of Granada. Eligible participants were young, sedentary adults with no chronic diseases. Here, we performed both an acute endurance and resistance exercise sub-studies (n = 14 and 17 respectively), and a 24-week supervised exercise intervention, combining endurance and resistance exercise training at moderate-intensity (MOD-EX) or vigorous-intensity (VIG-EX) exercise groups, in young sedentary adults. Randomization was performed by unrestricted randomization. Plasma levels of oxylipins, eCBs, and their analogues were measured using liquid chromatography-tandem mass spectrometry. Findings: Both endurance and resistance exercise increased by +50% the plasma levels of dihomo-γ-linolenic acid and arachidonic acid (AA) omega-6 derived oxylipins, as well as eicosapentaenoic acid and docosahexaenoic acid omega-3 derived after 3 and 120 min of the bout of exercise (all η2 ≥ 0.219 and P ≤ 0.039). These exercise modalities also increased the levels of anandamide and eCBs analogues (+25%). 145 young sedentary adults were assigned to a control (CON, n = 54), a MOD-EX (n = 48) or a VIG-EX (n = 43). 102 participants were included in the final long-term analyses (CON, n = 36; MOD-EX, n = 33; and VIG-EX, n = 33) of the trial. After 24-week of supervised exercise, MOD-EX decreased plasma levels of omega-6 oxylipins, concretely linoleic acid (LA) and adrenic acid derived oxylipins, and the eCBs analogues OEA and LEA in comparison to the CON (all P ≤ 0.021). VIG-EX decreased LA-derived oxylipins and LEA compared to CON. No relevant adverse events were recorded. Interpretation: Endurance and resistance exercises acutely increased plasma levels of oxylipins, eCBs, and their analogues, whereas 24 weeks of exercise training decreased fasting plasma levels of omega-6 oxylipins, and eCBs analogues in young, sedentary adults. Funding: See Acknowledgments section.

### 13) Stability of alkyl carbocations

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The traditional and widespread rationale behind the stability trend of alkyl-substituted carbocations is incomplete. Through state-of-the-art quantum chemical analyses, we quantitatively established a generally overlooked driving force behind the stability of carbocations, namely, that the parent substrates are substantially destabilized by the introduction of substituents, often playing a dominant role in solution. This stems from the repulsion between the substituents and the C-X bond.

### 14) Methanotrophy by a Mycobacterium species that dominates a cave microbial ecosystem

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So far, only members of the bacterial phyla Proteobacteria and Verrucomicrobia are known to grow methanotrophically under aerobic conditions. Here we report that this metabolic trait is also observed within the Actinobacteria. We enriched and cultivated a methanotrophic Mycobacterium from an extremely acidic biofilm growing on a cave wall at a gaseous chemocline interface between volcanic gases and the Earth’s atmosphere. This Mycobacterium, for which we propose the name Candidatus Mycobacterium methanotrophicum, is closely related to well-known obligate pathogens such as M. tuberculosis and M. leprae. Genomic and proteomic analyses revealed that Candidatus M. methanotrophicum expresses a full suite of enzymes required for aerobic growth on methane, including a soluble methane monooxygenase that catalyses the hydroxylation of methane to methanol and enzymes involved in formaldehyde fixation via the ribulose monophosphate pathway. Growth experiments combined with stable isotope probing using 13C-labelled methane confirmed that Candidatus M. methanotrophicum can grow on methane as a sole carbon and energy source. A broader survey based on 16S metabarcoding suggests that species closely related to Candidatus M. methanotrophicum may be abundant in low-pH, high-methane environments.

### 15) Computationally designed GPCR quaternary structures bias signaling pathway activation

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Communication across membranes controls critical cellular processes and is achieved by receptors translating extracellular signals into selective cytoplasmic responses. While receptor tertiary structures can be readily characterized, receptor associations into quaternary structures are challenging to study and their implications in signal transduction remain poorly understood. Here, we report a computational approach for predicting receptor self-associations, and designing receptor oligomers with various quaternary structures and signaling properties. Using this approach, we designed chemokine receptor CXCR4 dimers with reprogrammed binding interactions, conformations, and abilities to activate distinct intracellular signaling proteins. In agreement with our predictions, the designed CXCR4s dimerized through distinct conformations and displayed different quaternary structural changes upon activation. Consistent with the active state models, all engineered CXCR4 oligomers activated the G protein Gi, but only specific dimer structures also recruited β-arrestins. Overall, we demonstrate that quaternary structures represent an important unforeseen mechanism of receptor biased signaling and reveal the existence of a bias switch at the dimer interface of several G protein-coupled receptors including CXCR4, mu-Opioid and type-2 Vasopressin receptors that selectively control the activation of G proteins vs β-arrestin-mediated pathways. The approach should prove useful for predicting and designing receptor associations to uncover and reprogram selective cellular signaling functions.

### 16) Synthesis and Structure-Activity Studies of β-Barrel Assembly Machine Complex Inhibitor MRL-494

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In the hunt for new antibiotics with activity against Gram-negative pathogens, the outer membrane β-barrel assembly machine (BAM) complex has become an increasingly interesting target. The recently reported BAM complex inhibitor, MRL-494, was discovered via a screening campaign for molecules that target the outer membrane. Notably, MRL-494 was reported to be an unintended byproduct generated during the synthesis of an unrelated compound, and as such no synthesis of the compound was disclosed. We here present a convenient and reliable route for the synthesis of MRL-494 that scales well. The antibacterial activity measured for synthesized MRL-494 matches that reported in the literature. Furthermore, MRL-494 was found to exhibit potent synergistic activity with rifampicin against Gram-negative bacteria, including E. coli, K. pneumoniae, A. baumannii, and P. aeruginosa. MRL-494 was also found to cause outer membrane disruption and induction of the Rcs stress response pathway. In addition, we undertook a focused structure-activity study specifically aimed at elucidating the roles played by the two guanidine moieties contained within the structure of MRL-494.

### 17) Chemometric Strategies for Fully Automated Interpretive Method Development in Liquid Chromatography

* Bos, T. S., Boelrijk, J., Molenaar, S. R. A., Van 'T Veer, B., Niezen, L. E., Van Herwerden, D., Samanipour, S., Stoll, D. R., Forré, P., Ensing, B., Somsen, G. W., Pirok, B. W. J.
* BioAnalytical Chemistry, AIMMS, University of Amsterdam, Center for Analytical Sciences Amsterdam, Gustavus Adolphus College
* Analytical chemistry
* https://doi.org/10.1021/acs.analchem.2c03160
* Corresponding author: Pirok, B. W. J.
* Published 22 Nov 2022 (early online 1 Nov 2022)
* Processed: 2022-11

The majority of liquid chromatography (LC) methods are still developed in a conventional manner, that is, by analysts who rely on their knowledge and experience to make method development decisions. In this work, a novel, open-source algorithm was developed for automated and interpretive method development of LC(-mass spectrometry) separations ("AutoLC"). A closed-loop workflow was constructed that interacted directly with the LC system and ran unsupervised in an automated fashion. To achieve this, several challenges related to peak tracking, retention modeling, the automated design of candidate gradient profiles, and the simulation of chromatograms were investigated. The algorithm was tested using two newly designed method development strategies. The first utilized retention modeling, whereas the second used a Bayesian-optimization machine learning approach. In both cases, the algorithm could arrive within 4-10 iterations (i.e., sets of method parameters) at an optimum of the objective function, which included resolution and analysis time as measures of performance. Retention modeling was found to be more efficient while depending on peak tracking, whereas Bayesian optimization was more flexible but limited in scalability. We have deliberately designed the algorithm to be modular to facilitate compatibility with previous and future work (e.g., previously published data handling algorithms).

### *18) Full humanization of the glycolytic pathway in Saccharomyces cerevisiae*

* Boonekamp, F. J., Knibbe, E., Vieira-Lara, M. A., Wijsman, M., Luttik, M. A., van Eunen, K., Ridder, M. D., Bron, R., Almonacid Suarez, A. M., van Rijn, P., Wolters, J. C., Pabst, M., Daran, J. M., Bakker, B. M., Daran-Lapujade, P.
* Molecular Cell Physiology, AIMMS, Delft University of Technology, University of Groningen
* Cell Reports
* https://doi.org/10.1016/j.celrep.2022.111010
* Corresponding author: None
* Published 28 Jun 2022 (early online None)
* Processed: 2022-6

Although transplantation of single genes in yeast plays a key role in elucidating gene functionality in metazoans, technical challenges hamper humanization of full pathways and processes. Empowered by ...

### *19) Front Cover: How Ionization Catalyzes Diels‐Alder Reactions (Chem. Eur. J. 40/2022)General information*

* Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry – A European Journal
* https://doi.org/10.1002/chem.202201619
* Corresponding author: None
* Published 15 Jul 2022 (early online None)
* Processed: 2022-7

Front Cover: How Ionization Catalyzes Diels‐Alder Reactions (Chem. Eur. J. 40/2022) ...

### *20) Endurance in the face of environmental transformations: a practice-oriented perspective on organizational identity*

* Hasanefendic, S., Donina, D.
* Science & Business Innovation, AIMMS, Nicolaus Copernicus University in Toruń
* Studies in Higher Education
* https://doi.org/10.1080/03075079.2022.2061448
* Corresponding author: Donina, D.
* Published 2022 (early online 11 Apr 2022)
* Processed: 2022-4

The effect of environmental transformations on organizational identity in universities has been addressed from different perspectives, yet considering micro-dynamics and impact on actual practices of ...

### *21) Fragment Screening Yields a Small-Molecule Stabilizer of 14-3-3 Dimers That Modulates Client Protein Interactions*

* Brink, H. J., Riemens, R., Thee, S., Beishuizen, B., da Costa Pereira, D., Wijtmans, M., de Esch, I., Smit, M. J., de Boer, A. H.
* Medicinal chemistry, Chemistry and Pharmaceutical Sciences, AIMMS, Molecular and Computational Toxicology, Amsterdam Institute for Molecular and Life Sciences (AIMMS)
* ChemBioChem
* https://doi.org/10.1002/cbic.202200178
* Corresponding author: Smit, M. J.
* Published 5 Sep 2022 (early online 29 Jun 2022)
* Processed: 2022-9

The development of protein-protein interaction (PPI) inhibitors has been a successful strategy in drug development. However, the identification of PPI stabilizers has proven much more challenging. Her ...

### *22) Of problems and opportunities—How to treat and how to not treat crystallographic fragment screening data*

* Weiss, M. S., Wollenhaupt, J., Correy, G. J., Fraser, J. S., Heine, A., Klebe, G., Krojer, T., Thunissen, M., Pearce, N. M.
* Organic Chemistry, AIMMS, Helmholtz Centre Berlin for Materials and Energy, University of California at San Francisco, University of Marburg, Lund University
* Protein Science
* https://doi.org/10.1002/pro.4391
* Corresponding author: Weiss, M. S.
* Published Sep 2022 (early online 29 Aug 2022)
* Processed: 2022-9

In their recent commentary in Protein Science, Jaskolski et al. analyzed three randomly picked diffraction data sets from fragment-screening group depositions from the PDB and, based on that, they cla ...

### *23) Correction to: Colloidal Bi-Doped Cs2Ag1- xNaxInCl6Nanocrystals: Undercoordinated Surface Cl Ions Limit Their Light Emission Efficiency*

* Zhang, B., Wang, M., Ghini, M., Melcherts, A. E. M., Zito, J., Goldoni, L., Infante, I., Guizzardi, M., Scotognella, F., Kriegel, I., De Trizio, L., Manna, L.
* Theoretical Chemistry, AIMMS, University of Genoa, Italian Institute of Technology, Utrecht University, Polytechnic University of Milan
* ACS Materials Letters
* https://doi.org/10.1021/acsmaterialslett.2c00568
* Corresponding author: Wang, M.
* Published 5 Sep 2022 (early online 9 Aug 2022)
* Processed: 2022-9

Understanding and tuning the ligand shell composition in colloidal halide perovskite nanocrystals (NCs) has been done systematically only for Pb-based perovskites, while much less is known on the surf ...

### *24) Semiquantitative Characterization of Bromo-chloro Paraffins and Olefins in the Australian Environment*

* He, C., Van Mourik, L., Brandsma, S., Thai, P., Wang, X., Chen, S., Thomas, K. V., Mueller, J. F.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, University of Queensland
* Environmental Science and Technology
* https://doi.org/10.1021/acs.est.2c03576
* Corresponding author: He, C.
* Published 6 Sep 2022 (early online 17 Aug 2022)
* Processed: 2022-9

A semiquantitative high-resolution mass spectrometry method was developed and applied to assess the occurrence of bromo-/chloro paraffins (BCPs) and olefins (BCOs) in the environment. More than 400 po ...

### *25) Racemization Pathway for MoO2(acac)2*

* Dhimba, G., Muller, A., Lammertsma, K.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of Johannesburg
* Inorganic Chemistry
* https://doi.org/10.1021/acs.inorgchem.2c00824
* Corresponding author: Lammertsma, K.
* Published 26 Sep 2022 (early online 18 Aug 2022)
* Processed: 2022-9

Favored over Ray-Dutt, Bailar, and Conte-Hippler TwistsChiral cis-MoO2(acac)2racemizes via four pathways that agree with and extend upon Muetterties' topological analysis for dynamic MX2(chel)2complex ...

### *26) Integrative biology of persister cell formation: molecular circuitry, phenotypic diversification and fitness effects*

* Berkvens, A., Chauhan, P., Bruggeman, F. J.
* AIMMS, Systems Bioinformatics, Structural Biology
* Journal of the Royal Society Interface
* https://doi.org/10.1098/rsif.2022.0129
* Corresponding author: Bruggeman, F. J.
* Published Sep 2022 (early online 14 Sep 2022)
* Processed: 2022-9

Microbial populations often contain persister cells, which reduce the extinction risk upon sudden stresses. Persister cell formation is deeply intertwined with physiology. Due to this complexity, it c ...

### *27) Uptake, Transport, and Toxicity of Pristine and Weathered Micro- and Nanoplastics in Human Placenta Cells*

* Dusza, H. M., Katrukha, E. A., Nijmeijer, S. M., Akhmanova, A., Vethaak, A. D., Walker, D. I., Legler, J.
* Environment and Health, AIMMS, Institute for Environmental Studies, Utrecht University, Icahn School of Medicine at Mount Sinai
* Environmental Health Perspectives
* https://doi.org/10.1289/EHP10873
* Corresponding author: None
* Published Sep 2022 (early online 21 Sep 2022)
* Processed: 2022-9

BACKGROUND: The first evidence of micro- and nanoplastic (MNP) exposure in the human placenta is emerging. However, the toxicokinetics and toxicity of MNPs in the placenta, specifically environmentall ...

### *28) Response of Mycobacterium smegmatis to the Cytochrome bcc Inhibitor Q203*

* Chauhan, P., van der Meulen, S. A., Simões Caetano, J. M., Goojani, H. G., Botman, D., van Spanning, R., Lill, H., Bald, D.
* Structural Biology, AIMMS, Systems Bioinformatics, LaserLaB - Analytical Chemistry and Spectroscopy, LaserLaB - Molecular Biophysics, Vrije Universiteit Amsterdam
* International Journal of Molecular Sciences
* https://doi.org/10.3390/ijms231810331
* Corresponding author: Chauhan, P.
* Published 2 Sep 2022 (early online None)
* Processed: 2022-9

For the design of next-generation tuberculosis chemotherapy, insight into bacterial defence against drugs is required. Currently, targeting respiration has attracted strong attention for combatting dr ...

### *29) ProteinGLUE multi-task benchmark suite for self-supervised protein modeling*

* Capel, H., Weiler, R., Dijkstra, M., Vleugels, R., Bloem, P., Feenstra, K. A.
* Computer Science, Integrative Bioinformatics, Artificial intelligence, Network Institute, Knowledge Representation and Reasoning, Bioinformatics, AIMMS, Vrije Universiteit Amsterdam
* Scientific Reports
* https://doi.org/10.1038/s41598-022-19608-4
* Corresponding author: Feenstra, K. A.
* Published 26 Sep 2022 (early online None)
* Processed: 2022-9

Self-supervised language modeling is a rapidly developing approach for the analysis of protein sequence data. However, work in this area is heterogeneous and diverse, making comparison of models and m ...