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### 1) Studying protein structure and function by native separation–mass spectrometry

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Alterations in protein structure may have profound effects on biological function. Analytical techniques that permit characterization of proteins while maintaining their conformational and functional state are crucial for studying changes in the higher order structure of proteins and for establishing structure–function relationships. Coupling of native protein separations with mass spectrometry is emerging rapidly as a powerful approach to study these aspects in a reliable, fast and straightforward way. This Review presents the available native separation modes for proteins, covers practical considerations on the hyphenation of these separations with mass spectrometry and highlights the involvement of affinity-based separations to simultaneously obtain structural and functional information of proteins. The impact of these approaches is emphasized by selected applications addressing biomedical and biopharmaceutical research questions.

### 2) Adaptive changes of sediment microbial communities associated with cleanup of oil spills in Nigerian mangrove forests

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The objectives of this study were to assess the influence on microbial communities resulting from i) the physical removal of free oil (pre-treatment or post-treatment), and ii) the level of oiling within a contaminated former mangrove forest. Sediment samples were collected before and after the removal of free oil. Before the process of remediation, a highly biodiverse mangrove microbiome which had adapted to history of recurring oil spills was observed. After removing the surface oil, the microbial diversity of the sediments reduced, with members of the phyla Firmicutes and Proteobacteria becoming dominant. This indicates that while water flushing reduced overall microbial diversity, it stimulated the growth of a more specialized bacterial community reported to be involved in hydrocarbon biodegradation. These results provide new insights on microbial communities and their succession in mangrove forest sediments, that will be useful for monitoring oil cleaning programs using water flushing to remove free oil.

### 3) Gradient Expansions for the Large-Coupling Strength Limit of the Møller-Plesset Adiabatic Connection

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The adiabatic connection that has, as weak-interaction expansion, the Møller-Plesset perturbation series has been recently shown to have a large coupling-strength expansion, in terms of functionals of the Hartree-Fock density with a clear physical meaning. In this work, we accurately evaluate these density functionals and we extract second-order gradient coefficients from the data for neutral atoms, following ideas similar to the ones used in the literature for exchange, with some modifications. These new gradient expansions will be the key ingredient for performing interpolations that have already been shown to reduce dramatically MP2 errors for large noncovalent complexes. As a byproduct, our investigation of neutral atoms with large number of electrons N indicates that the second-order gradient expansion for exchange grows as N log(N) rather than as N, as often reported in the literature.

### 4) Integrate mechanistic evidence from new approach methodologies (NAMs) into a read-across assessment to characterise trends in shared mode of action

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Read-across approaches often remain inconclusive as they do not provide sufficient evidence on a common mode of action across the category members. This read-across case study on thirteen, structurally similar, branched aliphatic carboxylic acids investigates the concept of using human-based new approach methods, such as in vitro and in silico models, to demonstrate biological similarity. Five out of the thirteen analogues have preclinical in vivo studies. Three out of them induced lipid accumulation or hypertrophy in preclinical studies with repeated exposure, which leads to the read-across hypothesis that the analogues can potentially induce hepatic steatosis. To confirm the selection of analogues, the expression patterns of the induced differentially expressed genes (DEGs) were analysed in a human liver model. With increasing dose, the expression pattern within the tested analogues got more similar, which serves as a first indication of a common mode of action and suggests differences in the potency of the analogues. Hepatic steatosis is a well-known adverse outcome, for which over 55 adverse outcome pathways have been identified. The resulting adverse outcome pathway (AOP) network, comprised a total 43 MIEs/KEs and enabled the design of an in vitro testing battery. From the AOP network, ten MIEs, early and late KEs were tested to systematically investigate a common mode of action among the grouped compounds. The targeted testing of AOP specific MIE/KEs shows that biological activity in the category decreases with side chain length. A similar trend was evident in measuring liver alterations in zebra fish embryos. However, activation of single MIEs or early KEs at in vivo relevant doses did not necessarily progress to the late KE “lipid accumulation”. KEs not related to the read-across hypothesis, testing for example general mitochondrial stress responses in liver cells, showed no trend or biological similarity. Testing scope is a key issue in the design of in vitro test batteries. The Dempster-Shafer decision theory predicted those analogues with in vivo reference data correctly using one human liver model or the CALUX reporter assays. The case study shows that the read-across hypothesis is the key element to designing the testing strategy. In the case of a good mechanistic understanding, an AOP facilitates the selection of reliable human in vitro models to demonstrate a common mode of action. Testing DEGs, MIEs and early KEs served to show biological similarity, whereas the late KEs become important for confirmation, as progression from MIEs to AO is not always guaranteed.

### 5) BRET-Based Biosensors to Measure Agonist Efficacies in Histamine H1 Receptor-Mediated G Protein Activation, Signaling and Interactions with GRKs and β-Arrestins

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The histamine H1 receptor (H1R) is a G protein-coupled receptor (GPCR) and plays a key role in allergic reactions upon activation by histamine which is locally released from mast cells and basophils. Consequently, H1R is a well-established therapeutic target for antihistamines that relieve allergy symptoms. H1R signals via heterotrimeric Gq proteins and is phosphorylated by GPCR kinase (GRK) subtypes 2, 5, and 6, consequently facilitating the subsequent recruitment of β-arrestin1 and/or 2. Stimulation of a GPCR with structurally different agonists can result in preferential engagement of one or more of these intracellular signaling molecules. To evaluate this so-called biased agonism for H1R, bioluminescence resonance energy transfer (BRET)-based biosensors were applied to measure H1R signaling through heterotrimeric Gq proteins, second messengers (inositol 1,4,5-triphosphate and Ca2+), and receptor-protein interactions (GRKs and β-arrestins) in response to histamine, 2-phenylhistamines, and histaprodifens in a similar cellular background. Although differences in efficacy were observed for these agonists between some functional readouts as compared to reference agonist histamine, subsequent data analysis using an operational model of agonism revealed only signaling bias of the agonist Br-phHA-HA in recruiting β-arrestin2 to H1R over Gq biosensor activation.

### 6) In vitro and in vivo preclinical venom inhibition assays identify metalloproteinase inhibiting drugs as potential future treatments for snakebite envenoming by Dispholidus typus

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* Processed: 2022-3

Snakebite envenoming affects more than 250,000 people annually in sub-Saharan Africa. Envenoming by Dispholidus typus (boomslang) results in venom-induced consumption coagulopathy (VICC), whereby highly abundant prothrombin-activating snake venom metalloproteinases (SVMPs) consume clotting factors and deplete fibrinogen. The only available treatment for D. typus envenoming is the monovalent SAIMR Boomslang antivenom. Treatment options are urgently required because this antivenom is often difficult to source and, at US$6000/vial, typically unaffordable for most snakebite patients. We therefore investigated the in vitro and in vivo preclinical efficacy of four SVMP inhibitors to neutralise the effects of D. typus venom; the matrix metalloproteinase inhibitors marimastat and prinomastat, and the metal chelators dimercaprol and DMPS. The venom of D. typus exhibited an SVMP-driven procoagulant phenotype in vitro. Marimastat and prinomastat demonstrated equipotent inhibition of the SVMP-mediated procoagulant activity of the venom in vitro, whereas dimercaprol and DMPS showed considerably lower potency. However, when tested in preclinical murine models of envenoming using mixed sex CD1 mice, DMPS and marimastat demonstrated partial protection against venom lethality, demonstrated by prolonged survival times of experimental animals, whereas dimercaprol and prinomastat failed to confer any protection at the doses tested. The preclinical results presented here demonstrate that DMPS and marimastat show potential as novel small molecule-based therapeutics for D. typus snakebite envenoming. These two drugs have been previously shown to be effective against Echis ocellatus VICC in preclinical models, and thus we conclude that marimastat and DMPS should be further explored as potentially valuable early intervention therapeutics to broadly treat VICC following snakebite envenoming in sub-Saharan Africa.

### 7) Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins

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Nε-Methylation of lysine residues in histones plays an essential role in the regulation of eukaryotic transcription. The ‘highest’ methylation mark, Nε-trimethyllysine, is specifically recognised by Nε-trimethyllysine binding ‘reader’ domains, and undergoes demethylation, as catalysed by 2-oxoglutarate dependent JmjC oxygenases. We report studies on the recognition of the closest positively charged Nε-trimethyllysine analogue, i.e. its trimethylphosphonium derivative (KPme3), by Nε-trimethyllysine histone binding proteins and Nε-trimethyllysine demethylases. Calorimetric and computational studies with histone binding proteins reveal that H3KP4me3 binds more tightly than the natural H3K4me3 substrate, though the relative differences in binding affinity vary. Studies with JmjC demethylases show that some, but not all, of themcan accept the phosphonium analogue of their natural substrates and that the methylation state selectivity can be changed by substitution of nitrogen for phosphorus. The combined results reveal that very subtle changes, e.g. substitution of nitrogen for phosphorus, can substantially affect interactions between ligand and reader domains / demethylases, knowledge that we hope will inspire the development of highly selective small molecules modulating their activity.

### 8) One planet: one health. A call to support the initiative on a global science–policy body on chemicals and waste

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The chemical pollution crisis severely threatens human and environmental health globally. To tackle this challenge the establishment of an overarching international science–policy body has recently been suggested. We strongly support this initiative based on the awareness that humanity has already likely left the safe operating space within planetary boundaries for novel entities including chemical pollution. Immediate action is essential and needs to be informed by sound scientific knowledge and data compiled and critically evaluated by an overarching science–policy interface body. Major challenges for such a body are (i) to foster global knowledge production on exposure, impacts and governance going beyond data-rich regions (e.g., Europe and North America), (ii) to cover the entirety of hazardous chemicals, mixtures and wastes, (iii) to follow a one-health perspective considering the risks posed by chemicals and waste on ecosystem and human health, and (iv) to strive for solution-oriented assessments based on systems thinking. Based on multiple evidence on urgent action on a global scale, we call scientists and practitioners to mobilize their scientific networks and to intensify science–policy interaction with national governments to support the negotiations on the establishment of an intergovernmental body based on scientific knowledge explaining the anticipated benefit for human and environmental health.

### 9) A quantitative AOP of mitochondrial toxicity based on data from three cell lines

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Adverse Outcome Pathways (AOPs) are increasingly used to support the integration of in vitro data in hazard assessment for chemicals. Quantitative AOPs (qAOPs) use mathematical models to describe the relationship between key events (KEs). In this paper, data obtained in three cell lines, LHUMES, HepG2 and RPTEC/TERT1, using similar experimental protocols, was used to calibrate a qAOP of mitochondrial toxicity for two chemicals, rotenone and deguelin. The objectives were to determine whether the same qAOP could be used for the three cell types, and to test chemical-independence by cross-validation with a dataset obtained on eight other chemicals in LHUMES cells. Repeating the calibration approach for both chemicals in three cell lines highlighted various practical difficulties. Even when the same readouts of KEs are measured, the mathematical functions used to describe the key event relationships may not be the same. Cross-validation in LHUMES cells was attempted by estimating chemical-specific potency at the molecular initiating events and using the rest of the calibrated qAOP to predict downstream KEs: toxicity of azoxystrobin, carboxine, mepronil and thifluzamide was underestimated. Selection of most relevant readouts and accurate characterization of the molecular initiating event for cross-validation are critical when designing in vitro experiments targeted at calibrating qAOPs.

### 10) A bacterial extracellular vesicle-based intranasal vaccine against SARS-Co

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* Published 14 Mar 2022 (early online None)
* Processed: 2022-3

V-2 protects against disease and elicits neutralizing antibodies to wild-type and Delta variantsSeveral vaccines have been introduced to combat the coronavirus infectious disease-2019 (COVID-19) pandemic, caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Current SARS-CoV-2 vaccines include mRNA-containing lipid nanoparticles or adenoviral vectors that encode the SARS-CoV-2 Spike (S) protein of SARS-CoV-2, inactivated virus, or protein subunits. Despite growing success in worldwide vaccination efforts, additional capabilities may be needed in the future to address issues such as stability and storage requirements, need for vaccine boosters, desirability of different routes of administration, and emergence of SARS-CoV-2 variants such as the Delta variant. Here, we present a novel, well-characterized SARS-CoV-2 vaccine candidate based on extracellular vesicles (EVs) of Salmonella typhimurium that are decorated with the mammalian cell culture-derived Spike receptor-binding domain (RBD). RBD-conjugated outer membrane vesicles (RBD-OMVs) were used to immunize the golden Syrian hamster (Mesocricetus auratus) model of COVID-19. Intranasal immunization resulted in high titres of blood anti-RBD IgG as well as detectable mucosal responses. Neutralizing antibody activity against wild-type and Delta variants was evident in all vaccinated subjects. Upon challenge with live virus, hamsters immunized with RBD-OMV, but not animals immunized with unconjugated OMVs or a vehicle control, avoided body mass loss, had lower virus titres in bronchoalveolar lavage fluid, and experienced less severe lung pathology. Our results emphasize the value and versatility of OMV-based vaccine approaches.

### 11) Global evaluation of the chemical hazard of recycled tire crumb rubber employed on worldwide synthetic turf football pitches

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* Processed: 2022-3

Social and environmental concern about the use of crumb rubber from end-of-life car tires in the construction of different sport and recreational facilities is increasing due to the presence of hazardous compounds. The aim of this research was the assessment of 42 organic chemicals, including polycyclic aromatic hydrocarbons (PAHs), phthalates, adipates, antioxidants and vulcanisation agents in a large number of infill samples (91) from synthetic turf football pitches of diverse characteristics and geographical origin. Samples were taken worldwide, in 17 countries on 4 continents, to show the global dimension of this problem. Ultrasound assisted extraction was employed to extract the target compounds, followed by gas chromatography coupled to tandem-mass spectrometry (UAE-GC–MS/MS). Seventy-eight crumb rubber samples as well as thirteen samples of alternatives materials, such as cork granulates, thermoplastic elastomers and coconut fibre, were analyzed. The results highlight the presence of all target PAH in most rubber samples at concentrations up to μg g−1, including the eight ECHA (European Chemicals Agency) PAHs considered as carcinogenic, and anthracene (ANC), pyrene (PYR) and benzo[ghi]perylene (B[ghi]P), catalogued as substances of very high concern (SVHC). Endocrine disruptors such as some plasticizers (mainly phthalates), and other compounds like benzothiazole (BTZ) and 2-mercaptobenzothiazole (MBTZ) were found reaching the mg g−1 level. This confirms the presence of the hazardous substances in the recycled crumb rubber samples collected all around the world. Three crumb rubber samples exceeded the limit of 20 μg g−1 for the sum of the eight ECHA PAHs. Regarding the chemical composition of other infill alternatives, cork appears to be adequate, while the thermoplastic elastomers contained high levels of some plasticizers. In addition, the plastic infill as well as the crumb rubber both are microplastics. Microplastics are considered contaminants of emerging concern since they do not biodegrade and remain in the environment for a long time.

### 12) Discovery and quantification of plastic particle pollution in human blood

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* Environment International
* https://doi.org/10.1016/j.envint.2022.107199
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* Published 24 Mar 2022 (early online None)
* Processed: 2022-3

### 13) Hydrophilic interaction chromatography – mass spectrometry for metabolomics and proteomics: state-of-the-art and current trends

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* Microchemical Journal
* https://doi.org/10.1016/j.microc.2021.106986
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* Published Apr 2022 (early online 15 Nov 2021)
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Among all the –omics approaches, proteomics and metabolomics have received increased attention over the last decade. Both approaches have reached a certain level of maturity, showing their relevance in numerous clinical applications, including biomarkers discovery, improved diagnosis, staging, and prognosis of diseases, as well as a better knowledge on various (patho-)physiological processes. Analytically, reversed-phase liquid chromatography – mass spectrometry (RPLC-MS) is considered the golden standard in proteomics and metabolomics, due to its ease of use and reproducilibity. However, RPLC-MS alone is not sufficient to resolve the complexity of the proteome, while very polar metabolites are typically poorly retained. In this context, hydrophilic interaction chromatography (HILIC) represents an attractive complementary approach, due to its orthogonal separation mechanism. This review presents an overview of the literature reporting the application of HILIC-MS in metabolomics and proteomics. For metabolomics the focus is on the analysis of bioactive lipids, amino acids, organic acids, and nucleotides/nucleosides, whereas for proteomics the analysis of complex samples and protein post-translational modifications therein using bottom-up, middle up/down proteomics and intact protein analysis is discussed. The review handles the technological aspects related to the use of HILIC-MS in both proteomics and metabolomics, paying attention to stationary phases, mobile phase conditions, injection volume and column temperature. Recent trends and developments in the application of HILIC-MS in proteomics and metabolomics are also presented and discussed, highlighting the advantages the technique can provide in addition or complementary to RPLC-MS, as well as the current limitations and possible solutions.

### 14) Optical control of Class A G protein-coupled receptors with photoswitchable ligands

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* Published Apr 2022 (early online None)
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The field of photopharmacology of Class A GPCR ligands has recently attracted attention. In this review we analyze 31 papers on currently available photoswitchable ligands for Class A GPCRs. Using the six most recurring terms of all combined paper abstracts, one can extract the overarching goal of this area of research: “Photoswitchable ligands control receptor activity with light” (represented in the TOC graphic). We analyze the design, photochemistry and pharmacology of the photoswitchable ligands. Trends, challenges and limitations will be discussed. A number of efficient photoswitchable ligands that allow optical modulation of GPCR function in various in vitro assays are presented. Moreover, optical modulation of in vivo GPCR function is within reach and the first reports to this end are highlighted.

### 15) Workflows for optimization of enzyme cascades and whole cell catalysis based on enzyme kinetic characterization and pathway modelling

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* Published Apr 2022 (early online 15 Nov 2021)
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To move towards a circular bioeconomy, sustainable strategies for the utilization of renewable, non-food biomass wastes such as lignocellulose, are needed. To this end, an efficient bioconversion of D-xylose – after D-glucose the most abundant sugar in lignocellulose – is highly desirable. Most standard organisms used in biotechnology are limited in metabolising D-xylose, and also in vitro enzymatic strategies for its conversion have not been very successful. We herein discuss that bioconversion of D-xylose is mostly hampered by missing knowledge on the kinetic properties of the enzymes involved in its metabolism. We propose a combination of classical enzyme characterizations and mathematical modelling approaches as a workflow for rational, model-based design to optimize enzyme cascades and/or whole cell biocatalysts for efficient D-xylose metabolism.

### *16) Kinetic Modeling of Saccharomyces cerevisiae Central Carbon Metabolism: Achievements, Limitations, and Opportunities*

* Lao-Martil, D., Verhagen, K. J., Schmitz, J. P., Teusink, B., Wahl, S. A., van Riel, N. A.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Eindhoven University of Technology, Friedrich-Alexander University Erlangen-Nürnberg, DSM Food Specialties, University of Amsterdam
* Metabolites
* https://doi.org/10.3390/metabo12010074
* Corresponding author: Lao-Martil, D.
* Published Jan 2022 (early online None)
* Processed: 2022-1

Central carbon metabolism comprises the metabolic pathways in the cell that process nutrients into energy, building blocks and byproducts. To unravel the regulation of this network upon glucose pertur ...

### *17) Mapping the cellular response to electron transport chain inhibitors reveals selective signaling networks triggered by mitochondrial perturbation*

* van der Stel, W., Yang, H., Vrijenhoek, N. G., Schimming, J. P., Callegaro, G., Carta, G., Darici, S., Delp, J., Forsby, A., White, A., le Dévédec, S., Leist, M., Jennings, P., Beltman, J. B., van de Water, B., Danen, E. H.
* Molecular and Computational Toxicology, AIMMS, Leiden University, University of Konstanz, Stockholm University, Unilever
* Archives of Toxicology
* https://doi.org/10.1007/s00204-021-03160-7
* Corresponding author: van de Water, B.
* Published Jan 2022 (early online 21 Oct 2021)
* Processed: 2022-1

Mitochondrial perturbation is a key event in chemical-induced organ toxicities that is incompletely understood. Here, we studied how electron transport chain (ETC) complex I, II, or III (CI, CII and C ...

### *18) Analytical Nonadiabatic Couplings and Gradients within the State-Averaged Orbital-Optimized Variational Quantum Eigensolver*

* Yalouz, S., Koridon, E., Senjean, B., Lasorne, B., Buda, F., Visscher, L.
* Theoretical Chemistry, AIMMS, Université de Montpellier, Leiden University
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.1c00995
* Corresponding author: Yalouz, S.
* Published 8 Feb 2022 (early online 14 Jan 2022)
* Processed: 2022-2

We introduce several technical and analytical extensions to our recent state-averaged orbital-optimized variational quantum eigensolver (SA-OO-VQE) algorithm (see Yalouz et al. Quantum Sci. Technol. 2 ...

### *19) Density-Corrected DFT Explained: Questions and Answers*

* Song, S., Vuckovic, S., Sim, E., Burke, K.
* Theoretical Chemistry, AIMMS, Yonsei University, University of California at Irvine
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.1c01045
* Corresponding author: Sim, E.
* Published 8 Feb 2022 (early online 28 Jan 2022)
* Processed: 2022-2

HF-DFT, the practice of evaluating approximate density functionals on Hartree-Fock densities, has long been used in testing density functional approximations. Density-corrected DFT (DC-DFT) is a gener ...

### *20) Absorbing knowledge from an emerging field: The role of interfacing by proponents in big pharma*

* Romasanta, A. K., van der Sijde, P., de Esch, I. J.
* Medicinal chemistry, Organization Sciences, Network Institute, Organization & Processes of Organizing in Society (OPOS), Chemistry and Pharmaceutical Sciences, AIMMS
* Technovation
* https://doi.org/10.1016/j.technovation.2021.102363
* Corresponding author: Romasanta, A. K.
* Published Feb 2022 (early online None)
* Processed: 2022-2

Engaging with knowledge from an emerging field, with its promises and limitations still uncertain, can be challenging for incumbent firms. Proponents of novel technologies within these firms then play ...

### *21) Stapling of Peptides Potentiates: The Antibiotic Treatment of Acinetobacter baumannii In Vivo*

* Schouten, G. K., Paulussen, F. M., Kuipers, O. P., Bitter, W., Grossmann, T. N., van Ulsen, P.Pages:273
* Molecular Microbiology, AIMMS, Organic Chemistry, LaserLaB - Analytical Chemistry and Spectroscopy, Vrije Universiteit Amsterdam, University of Groningen
* Antibiotics
* https://doi.org/10.3390/antibiotics1102027310.3390/antibiotics11020273
* Corresponding author: Grossmann, T. N.
* Published Feb 2022 (early online None)
* Processed: 2022-2

The rising incidence of multidrug resistance in Gram-negative bacteria underlines the urgency for novel treatment options. One promising new approach is the synergistic combination of antibiotics with ...

### *22) Targeting the ATP synthase in bacterial and fungal pathogens: beyond Mycobacterium tuberculosis*

* Vestergaard, M., Bald, D., Ingmer, H.
* AIMMS, Structural Biology, University of Copenhagen
* Journal of Global Antimicrobial Resistance
* https://doi.org/10.1016/j.jgar.2022.01.026
* Corresponding author: Ingmer, H.
* Published Jun 2022 (early online 4 Feb 2022)
* Processed: 2022-2

The ATP synthase is a multicomponent enzyme that is largely conserved across the kingdoms of life. In many species the ATP synthase is central in the synthesis of ATP by using the electrochemical prot ...

### *23) Global interlaboratory assessments on PCBs, organochlorine pesticides and brominated flame retardants in various environmental matrices 2017/2019*

* de Boer, J., van der Veen, I., Fiedler, H.
* Environment and Health, AIMMS, E&H: Environmental Bioanalytical Chemistry, Örebro University
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2022.133991
* Corresponding author: de Boer, J.
* Published May 2022 (early online 12 Feb 2022)
* Processed: 2022-2

In support of the United Nations Environment Programme (UNEP) global monitoring plan under the Stockholm Convention contributing laboratories were offered to take part in a series of interlaboratory a ...

### *24) Probing the Lewis Acidity of Boronic Acids through Interactions with Arene Substituents*

* Jian, J., Hammink, R., McKenzie, C. J., Bickelhaupt, F. M., Poater, J., Mecinović, J.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of Southern Denmark, Radboud University Nijmegen
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202104044
* Corresponding author: Mecinović, J.
* Published 16 Feb 2022 (early online 27 Dec 2021)
* Processed: 2022-2

Boronic acids are Lewis acids that exist in equilibrium with boronate forms in aqueous solution. Here we experimentally and computationally investigated the Lewis acidity of 2,6-diarylphenylboronic ac ...

### *25) Innovations in analytical methods to assess the occurrence of microplastics in soil*

* Perez, C. N., Carré, F., Hoarau-Belkhiri, A., Joris, A., Leonards, P. E., Lamoree, M. H.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, E&H: Environmental Chemistry and Toxicology, Vrije Universiteit Amsterdam, Institut national de l'environnement industriel et des risques, Institut Scientifique de Service Public
* Journal of Environmental Chemical Engineering
* https://doi.org/10.1016/j.jece.2022.107421
* Corresponding author: Lamoree, M. H.
* Published Jun 2022 (early online 17 Feb 2022)
* Processed: 2022-2

The occurrence of microplastics (MPs, particles <5 mm) in the environment has raised concerns globally due to their extensive use, slow degradation, low recycling rates, and potential risks to the eco ...

### *26) Plasma Levels of Bile Acids Are Related to Cardiometabolic Risk Factors in Young Adults*

* Osuna-Prieto, F. J., Rubio-Lopez, J., Di, X., Yang, W., Kohler, I., Rensen, P. C., Ruiz, J. R., Martinez-Tellez, B.
* BioAnalytical Chemistry, AIMMS, University of Granada, Research and Development of Functional Food Centre (CIDAF), Complejo Hospitalario de Jaen, Leiden University
* The Journal of clinical endocrinology and metabolism
* https://doi.org/10.1210/clinem/dgab773
* Corresponding author: None
* Published 17 Feb 2022 (early online 26 Oct 2021)
* Processed: 2022-2

CONTEXT: Bile acids (BA) are known for their role in intestinal lipid absorption and can also play a role as signaling molecules to control energy metabolism. Prior evidence suggests that alterations ...

### *27) Comparing the nature of quantum plasmonic excitations for closely spaced silver and gold dimers*

* Jamshidi, Z., Asadi-Aghbolaghi, N., Morad, R., Mahmoudi, E., Sen, S., Maaza, M., Visscher, L.
* Theoretical Chemistry, AIMMS, University of South Africa, Sharif University of Technology
* The Journal of chemical physics
* https://doi.org/10.1063/5.0079258
* Corresponding author: None
* Published 21 Feb 2022 (early online 15 Feb 2022)
* Processed: 2022-2

In the new field of quantum plasmonics, plasmonic excitations of silver and gold nanoparticles are utilized to manipulate and control light-matter interactions at the nanoscale. While quantum plasmons ...

### *28) Quantification of Geometric Errors Made Simple: Application to Main-Group Molecular Structures*

* Vuckovic, S.
* Theoretical Chemistry, AIMMS
* Journal of Physical Chemistry A
* https://doi.org/10.1021/acs.jpca.1c10688
* Corresponding author: Vuckovic, S.
* Published 24 Feb 2022 (early online 10 Feb 2022)
* Processed: 2022-2

Nearly all electronic structure simulations begin with obtaining approximate geometries, making a systematic quantification of errors in approximate molecular structures of key importance. Recently, t ...