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### 1) The cost of photovoltaics: Re-evaluating grid parity for PV systems in China

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* Processed: 2022-8

The price of photovoltaics (PV) has been steadily decreasing over the last decade, and many reports suggest that PV has become considerably cheaper than conventional electricity sources. In this paper, we critically evaluate the PV grid parity and use China as a case study. China is an interesting case study due to the wealth of data combined with the recent decrease in financial subsidies. Electricity costs are commonly compared in the literature using levelized costs of electricity (LCOE). However traditional LCOE analyses neglect important cost factors that are specific to PV, in particular the cost of grid integration. Here, we demonstrate that system LCOE calculation more accurately estimates the grid parity of PV. We find that the integration costs account for 15% of the total system costs, which cannot be neglected with the higher penetration of PV in the electricity system. Further, provincial grid parity indexes are greater than 1, indicating that the grid parity from a system LCOE perspective has not yet been achieved. The learning rate of Chinese PV is still relatively small, and we estimate that grid parity for PV in China will be achieved between 2020 and 2032, depending on the region. These findings shed new light on assessing grid parity of PV systems by considering relevant local parameters and thereby offer an assessment method framework and prediction modeling for assessing grid parity of PV installations.

### 2) BioSimulators: a central registry of simulation engines and services for recommending specific tools

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Computational models have great potential to accelerate bioscience, bioengineering, and medicine. However, it remains challenging to reproduce and reuse simulations, in part, because the numerous formats and methods for simulating various subsystems and scales remain siloed by different software tools. For example, each tool must be executed through a distinct interface. To help investigators find and use simulation tools, we developed BioSimulators (https://biosimulators.org), a central registry of the capabilities of simulation tools and consistent Python, command-line and containerized interfaces to each version of each tool. The foundation of BioSimulators is standards, such as CellML, SBML, SED-ML and the COMBINE archive format, and validation tools for simulation projects and simulation tools that ensure these standards are used consistently. To help modelers find tools for particular projects, we have also used the registry to develop recommendation services. We anticipate that BioSimulators will help modelers exchange, reproduce, and combine simulations.

### 3) Delineation of the GPR15 receptor-mediated Gα protein signalling profile in recombinant mammalian cells

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The GPR15 receptor is a G protein-coupled receptor (GPCR), which is activated by an endogenous peptide GPR15L(25–81) and a C-terminal peptide fragment GPR15L(71–81). GPR15 signals through the Gi/o pathway to decrease intracellular cyclic adenosine 3′,5′-monophosphate (cAMP). However, the activation profiles of the GPR15 receptor within Gi/o subtypes have not been examined. Moreover, whether the receptor can also couple to Gs, Gq/11 and G12/13 is unclear. Here, GPR15L(25–81) and GPR15L(71–81) are used as pharmacological tool compounds to delineate the GPR15 receptor-mediated Gα protein signalling using a G protein activation assay and second messenger assay conducted on living cells. The results show that the GPR15 receptor preferentially couples to Gi/o rather than other pathways in both assays. Within the Gi/o family, the GPR15 receptor activates all the subtypes (Gi1, Gi2, Gi3, GoA, GoB and Gz). The Emax and activation rates of Gi1, Gi2, Gi3, GoA and GoB are similar, whilst the Emax of Gz is smaller and the activation rate is significantly slower. The potencies of both peptides toward each Gi/o subtype have been determined. Furthermore, the GPR15 receptor signals through Gi/o to inhibit cAMP accumulation, which could be blocked by the application of the Gi/o inhibitor pertussis toxin.

### 4) In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion

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* Processed: 2022-8

Dye-sensitized photoelectrochemical cells are promising devices in solar energy conversion. However, several limitations still have to be addressed, such as the major loss pathway through charge recombination at the dye-semiconductor interface. Charge separating dyes constructed as push-pull systems can increase the spatial separation of electron and hole, decreasing the recombination rate. Here, a family of dyes, consisting of polyphenylamine donors, fluorene bridges, and perylene monoimide acceptors, was investigated in silico using a combination of semi-empirical nuclear dynamics and a quantum propagation of photoexcited electron and hole. To optimize the charge separation, several molecular design strategies were investigated, including modifying the donor molecule, increasing the π-bridge length, and decoupling the molecular components through steric effects. The combination of a triphenylamine donor, using an extended 2-fluorene π-bridge, and decoupling the different components by steric hindrance from side groups resulted in a dye with significantly improved charge separation properties in comparison to the original supramolecular complex.

### 5) A Nano BRET-Based H3R Conformational Biosensor to Study Real-Time H3 Receptor Pharmacology in Cell Membranes and Living Cells

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* Published 1 Aug 2022 (early online 26 Jul 2022)
* Processed: 2022-8

A NanoBRET-Based H3R Conformational Biosensor to Study Real-Time H3 Receptor Pharmacology in Cell Membranes and Living CellsConformational biosensors to monitor the activation state of G protein-coupled receptors are a useful addition to the molecular pharmacology assay toolbox to characterize ligand efficacy at the level of receptor proteins instead of downstream signaling. We recently reported the initial characterization of a NanoBRET-based conformational histamine H3 receptor (H3R) biosensor that allowed the detection of both (partial) agonism and inverse agonism on living cells in a microplate reader assay format upon stimulation with H3R ligands. In the current study, we have further characterized this H3R biosensor on intact cells by monitoring the effect of consecutive ligand injections in time and evaluating its compatibility with photopharmacological ligands that contain a light-sensitive azobenzene moiety for photo-switching. In addition, we have validated the H3R biosensor in membrane preparations and found that observed potency values better correlated with binding affinity values that were measured in radioligand competition binding assays on membranes. Hence, the H3R conformational biosensor in membranes might be a ready-to-use, high-throughput alternative for radioligand binding assays that in addition can also detect ligand efficacies with comparable values as the intact cell assay.

### 6) Secondary Kinetic Peak in the Kohn-Sham Potential and Its Connection to the Response Step

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* Processed: 2022-8

We consider a prototypical 1D model Hamiltonian for a stretched heteronuclear molecule and construct individual components of the corresponding KS potential, namely, the kinetic, the N - 1, and the conditional potentials. These components show very special features, such as peaks and steps, in regions where the density is drastically low. Some of these features are quite well-known, whereas others, such as a secondary peak in the kinetic potential or a second bump in the conditional potential, are less or not known at all. We discuss these features building on the analytical model treated in Giarrusso et al. J. Chem. Theory Comput. 2018, 14, 4151. In particular, we provide an explanation for the underlying mechanism which determines the appearance of both peaks in the kinetic potential and elucidate why these peaks delineate the region over which the plateau structure, due to the N - 1 potential, stretches. We assess the validity of the Heitler-London Ansatz at large but finite internuclear distance, showing that, if optimal orbitals are used, this model is an excellent approximation to the exact wave function. Notably, we find that the second natural orbital presents an extra node very far out on the side of the more electronegative atom.

### 7) Identifying mutant-specific multi-drug combinations using comparative network reconstruction

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* Processed: 2022-8

Targeted inhibition of aberrant signaling is an important treatment strategy in cancer, but responses are often short-lived. Multi-drug combinations have the potential to mitigate this, but to avoid toxicity such combinations must be selective and given at low dosages. Here, we present a pipeline to identify promising multi-drug combinations. We perturbed an isogenic PI3K mutant and wild-type cell line pair with a limited set of drugs and recorded their signaling state and cell viability. We then reconstructed their signaling networks and mapped the signaling response to changes in cell viability. The resulting models, which allowed us to predict the effect of unseen combinations, indicated that no combination selectively reduces the viability of the PI3K mutant cells. However, we were able to validate 25 of the 30 combinations that we predicted to be anti-selective. Our pipeline enables efficient prioritization of multi-drug combinations from the enormous search space of possible combinations.

### 8) Vaccination with a bacterial peptide conjugated to SARS-Co

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V-2 receptor-binding domain accelerates immunity and protects against COVID-19Poor immunogenicity of critical epitopes can hamper vaccine efficacy. To boost immune recognition of non- or low-immunogenic antigens, we developed a vaccine platform based on the conjugation of a target protein to a chimeric designer peptide (CDP) of bacterial origin. Here, we exploited this immune Boost (iBoost) technology to enhance the immune response against the receptor-binding domain (RBD) of the SARS-CoV-2 spike glycoprotein. Despite its fundamental role during viral infection, RBD is only moderately immunogenic. Immunization studies in mice showed that the conjugation of CDP to RBD induced superior immune responses compared to RBD alone. CDP-RBD elicited cross-reactive antibodies against the variants of concern Delta and Omicron. Furthermore, hamsters vaccinated with CDP-RBD developed potent neutralizing antibody responses and were fully protected from lung lesion formation upon challenge with SARS-CoV-2. In sum, we show that the iBoost conjugate vaccine technology provides a valuable tool for both quantitatively and qualitatively enhancing anti-viral immunity.

### 9) Cleaner and stronger: how 8-quinolinolate facilitates formation of Co(iii)-thiolate from Co(ii)-disulfide complexes

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* Processed: 2022-8

The formation of Co(iii)-thiolate complexes from Co(ii)-disulfide complexes using the anionic ligand 8-quinolinolate (quin−) has been studied experimentally and quantum chemically. Two Co(ii)-disulfide complexes [Co2(LxSSLx)(Cl)4] (x = 1 or 2; L1SSL1 = 2,2′-disulfanediylbis(N,N-bis(pyridin-2-ylmethyl)ethan-1-amine; L2SSL2 = 2,2′-disulfanedylbis (N-((6-methylpyridin-2-yl)methyl)-N-(pyridin-2-ylmethyl) ethan-1-amine) have been successfully converted with high yield to their corresponding Co(iii)-thiolate complexes upon addition of the ligand 8-quinolinolate. Using density functional theory (DFT) computations the d-orbital splitting energies of the cobalt-thiolate compounds [Co(L1S)(quin)]+ and [Co(L2S)(quin)]+ were estimated to be 3.10 eV and 3.07 eV, indicating a slightly smaller ligand-field strength of ligand L2SSL2 than of L1SSL1. Furthermore, the orientation of the quin− ligand in the thiolate compounds determines the stability of the thiolate complex. DFT computations show that the thiolate structure benefits from more electrostatic attraction when the oxygen atom of the quin− ligand is positioned trans to the sulfur atom of the [Co(L1S)]2+ fragment. Quin− is the first auxiliary ligand with which it appeared possible to induce the redox-conversion reaction in cobalt(ii) compounds of the relatively weak-field ligand L2SSL2

### 10) Recycling gradient-elution liquid chromatography for the analysis of chemical-composition distributions of polymers

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* Processed: 2022-8

Synthetic polymers typically show dispersity in molecular weight and potentially in chemical composition. For the analysis of the chemical-composition distribution (CCD) gradient liquid chromatography may be used. The CCD obtained using this method is often convoluted with an underlying molecular-weight distribution (MWD). In this paper we demonstrate that the influence of the MWD can be reduced using very steep gradients and that such gradients are best realized utilizing recycling gradient liquid chromatography (LC↻LC). This method allows for a more-accurate determination of the CCD and the assessment of (approximate) critical conditions (if these exist), even when high-molecular-weight standards of narrow dispersity are not readily available. The performance and usefulness of the approach is demonstrated for several polystyrene standards, and for the separation of statistical copolymers consisting of styrene/methyl methacrylate and methyl methacrylate/butyl methacrylate. For the latter case, approximate critical compositions of the copolymers were calculated from the critical compositions of two homopolymers and one copolymer of known chemical composition, allowing for a determination of the CCD of unknown samples. Using this approach it is shown that the copolymers elute significantly closer to the predicted critical compositions after recycling of the gradient. This is most clear for the lowest-molecular-weight copolymer (Mw = 4.2 kDa), for which the difference between measured and predicted elution composition decreases from 7.9% without recycling to 1.4% after recycling.

### 11) Methyl Substitution Destabilizes Alkyl Radicals

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* Processed: 2022-9

We have quantum chemically investigated how methyl substituents affect the stability of alkyl radicals MemH3−mC⋅ and the corresponding MemH3−mC−X bonds (X = H, CH3, OH; m = 0 – 3) using density functional theory at M06-2X/TZ2P. The state-of-the-art in physical organic chemistry is that alkyl radicals are stabilized upon an increase in their degree of substitution from methyl<primary<secondary<tertiary, and that this is the underlying cause for the decrease in C−H bond strength along this series. Here, we provide evidence that falsifies this model and show that, on the contrary, the MemH3−mC⋅ radical is destabilized with increasing substitution. The reason that the corresponding C−H bond nevertheless becomes weaker is that substitution destabilizes the sterically more congested MemH3−mC−H molecule even more.

### 12) Assessment of Macro- and Microheterogeneity of Monoclonal Antibodies Using Capillary Zone Electrophoresis Hyphenated with Mass Spectrometry

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This chapter focuses on the application of capillary zone electrophoresis hyphenated with mass spectrometry (CZE-MS) for the characterization of monoclonal antibodies (mAbs). mAbs are complex molecules comprising different glycoforms and many other posttranslational modifications. In addition to this inherent microheterogeneity, misassembling of antibodies can take place during production contributing to their macroheterogeneity. CZE-MS is a versatile and powerful technique which has demonstrated high potential for the assessment of both micro- and macroheterogeneity of mAbs. In this chapter, technical and practical considerations for the characterization of mAbs by CZE-MS are described. CE-MS interfacing, capillary coatings for the prevention of mAb adsorption, and sample preparation considerations are covered in detail. The assessment of the macro- and microheterogeneity is discussed and exemplified through three different approaches involving analysis of intact, enzymatically digested, and reduced antibodies. The examples also illustrate the use of two commercially available interfacing techniques (i.e., sheath liquid and sheathless) as well as different types of capillary coatings (positively charged and neutral coatings).

### 13) A new use for old drugs: identifying compounds with an anti-obesity effect using a high through-put semi-automated Caenorhabditis elegans screening platform

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* Processed: 2022-8

Obesity is one of the most common global health problems for all age groups with obese people at risk of a variety of associated health complications. Consequently, there is a need to develop new therapies that lower body fat without the side effects. However, obesity is a complex and systemic disease, so that in vitro results are not easily translatable to clinical situations. A promising way to circumnavigate these issues is to reposition already approved drugs for new treatments, enabling a more streamlined drug discovery process due to the availability of pre-existing pharmacological and toxicological datasets. Chemical libraries, such as the Prestwick Chemical Library of 1200 FDA approved drugs, are available for this purpose. We have developed a simple semi-automated whole-organism approach to screening the Prestwick Chemical Library for those compounds which reduce fat content using the model organism Caenorhabditis elegans. Our whole-organism approach to high-throughput screening identified 9 “lead” compounds that reduced fat within 2 weeks in the model. Further screening and analysis provided 4 “hit” compounds (Midodrine, Vinpocetine, Fenoprofen and Lamivudine) that showed significant promise as drugs to reduce fat levels. The effects of these candidates were found to further reduce fat content in nematodes where an nhr-49/PPAR mutation resulted in “overweight” worms. Upon unblinding the “hit” compounds, they were found to have recently been shown to have anti-obesity effects in mammalian models too. In developing a whole-animal chemical screen to identify pharmacological agents as potential anti-obesity compounds, we demonstrate how chemical libraries can be rapidly and relatively cheaply profiled for active hits. Using the nematode Caenorhabditis elegans thus enables drugs to be assessed for applicability in humans and provides a new incentive to explore drug repurposing as a feasible and efficient way to identify new anti-obesity compounds.

### 14) Inhibition of H1 and H5 Influenza A Virus Entry by Diverse Macrocyclic Peptides Targeting the Hemagglutinin Stem Region

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* Processed: 2022-8

Influenza A viruses pose a serious pandemic risk, while generation of efficient vaccines against seasonal variants remains challenging. There is thus a pressing need for new treatment options. We report here a set of macrocyclic peptides that inhibit influenza A virus infection at low nanomolar concentrations by binding to hemagglutinin, selected using ultrahigh-Throughput screening of a diverse peptide library. The peptides are active against both H1 and H5 variants, with no detectable cytotoxicity. Despite the high sequence diversity across hits, all tested peptides were found to bind to the same region in the hemagglutinin stem by HDX-MS epitope mapping. A mutation in this region identified in an escape variant confirmed the binding site. This stands in contrast to the immunodominance of the head region for antibody binding and suggests that macrocyclic peptides from in vitro display may be well suited for finding new druggable sites not revealed by antibodies. Functional analysis indicates that these peptides stabilize the prefusion conformation of the protein and thereby prevent virus-cell fusion. High-Throughput screening of macrocyclic peptides is thus shown here to be a powerful method for the discovery of novel broadly acting viral fusion inhibitors with therapeutic potential.

### 15) The molecular mechanism of snake short-chain α-neurotoxin binding to muscle-type nicotinic acetylcholine receptors

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* Published 4 Aug 2022 (early online None)
* Processed: 2022-8

Bites by elapid snakes (e.g. cobras) can result in life-threatening paralysis caused by venom neurotoxins blocking neuromuscular nicotinic acetylcholine receptors. Here, we determine the cryo-EM structure of the muscle-type Torpedo receptor in complex with ScNtx, a recombinant short-chain α-neurotoxin. ScNtx is pinched between loop C on the principal subunit and a unique hairpin in loop F on the complementary subunit, thereby blocking access to the neurotransmitter binding site. ScNtx adopts a binding mode that is tilted toward the complementary subunit, forming a wider network of interactions than those seen in the long-chain α-Bungarotoxin complex. Certain mutations in ScNtx at the toxin-receptor interface eliminate inhibition of neuronal α7 nAChRs, but not ofhuman muscle-type receptors. These observations explain why ScNtx binds more tightly to muscle-type receptors than neuronal receptors. Together, these data offer a framework for understanding subtype-specific actions of short-chain α-neurotoxins and inspire strategies for design of new snake antivenoms.

### 16) Inhibition of the angiotensin II type 2 receptor AT2R is a novel therapeutic strategy for glioblastoma

* Perryman, R., Renziehausen, A., Shaye, H., Kostagianni, A. D., Tsiailanis, A. D., Thorne, T., Chatziathanasiadou, M. V., Sivolapenko, G. B., El Mubarak, M. A., Han, G. W., Zarzycka, B., Katritch, V., Lebon, G., Lo Nigro, C., Lattanzio, L., Morse, S. V., Choi, J. J., O'Neill, K., Kanaki, Z., Klinakis, A., Crook, T., Cherezov, V., Tzakos, A. G., Syed, N.
* Medicinal chemistry, AIMMS, Imperial College London, University of Southern California, University of Ioannina, University of Surrey, University of Patras, Université de Montpellier, Ospedale San Croce e Carle, Academy of Athens
* Proceedings of the National Academy of Sciences of the United States of America
* https://doi.org/10.1073/pnas.2116289119
* Corresponding author: Syed, N.
* Published 9 Aug 2022 (early online 2 Aug 2022)
* Processed: 2022-8

Glioblastoma (GBM) is an aggressive malignant primary brain tumor with limited therapeutic options. We show that the angiotensin II (AngII) type 2 receptor (AT2R) is a therapeutic target for GBM and that AngII, endogenously produced in GBM cells, promotes proliferation through AT2R. We repurposed EMA401, an AT2R antagonist originally developed as a peripherally restricted analgesic, for GBM and showed that it inhibits the proliferation of AT2R-expressing GBM spheroids and blocks their invasiveness and angiogenic capacity. The crystal structure of AT2R bound to EMA401 was determined and revealed the receptor to be in an active-like conformation with helix- VIII blocking G-protein or β-arrestin recruitment. The architecture and interactions of EMA401 in AT2R differ drastically from complexes of AT2R with other relevant compounds. To enhance central nervous system (CNS) penetration of EMA401, we exploited the crystal structure to design an angiopep-2-tethered EMA401 derivative, A3E. A3E exhibited enhanced CNS penetration, leading to reduced tumor volume, inhibition of proliferation, and increased levels of apoptosis in an orthotopic xenograft model of GBM.

### *17) 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 ...

### *18) 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.
* AIMMS, Organic Chemistry, Molecular Microbiology, LaserLaB - Analytical Chemistry and Spectroscopy, Vrije Universiteit Amsterdam, University of Groningen
* Antibiotics
* https://doi.org/10.3390/antibiotics11020273
* Corresponding author: Grossmann, T. N.
* Published Feb 2022 (early online 19 Feb 2022)
* 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 ...

### *19) Effect of Different Exercise Training Modalities on Fasting Levels of Oxylipins and Endocannabinoids in Middle-Aged Sedentary Adults: A Randomized Controlled Trial*

* Jurado-Fasoli, L., Yang, W., Kohler, I., Dote-Montero, M., Osuna-Prieto, F. J., Di, X., Hankemeier, T., Krekels, E. H. J., Harms, A. C., Castillo, M. J., Amaro-Gahete, F. J., Martinez-Tellez, B.
* BioAnalytical Chemistry, AIMMS, University of Granada, Leiden University, Research and Development of Functional Food Centre (CIDAF), University of Almeria
* International journal of sport nutrition and exercise metabolism
* https://doi.org/10.1123/IJSNEM.2021-0332
* Corresponding author: Jurado-Fasoli, L.
* Published Jul 2022 (early online 26 Mar 2022)
* Processed: 2022-7

This study aimed to investigate the effects of different exercise training programs on fasting plasma levels of oxylipins, endocannabinoids (eCBs), and eCBs-like molecules in middle-aged sedentary adu ...

### *20) All-pairs suffix/prefix in optimal time using Aho-Corasick space*

* Loukides, G., Pissis, S. P.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London
* Information Processing Letters
* https://doi.org/10.1016/j.ipl.2022.106275
* Corresponding author: Pissis, S. P.
* Published Nov 2022 (early online 28 Apr 2022)
* Processed: 2022-4

The all-pairs suffix/prefix (APSP) problem is a classic problem in computer science with many applications in bioinformatics. Given a set {S1,…,Sk} of k strings of total length n, we are asked to find ...

### *21) Clustering Demographics and Sequences of Diagnosis Codes*

* Zhong, H., Loukides, G., Pissis, S. P.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London
* IEEE Journal of Biomedical and Health Informatics
* https://doi.org/10.1109/JBHI.2021.3129461
* Corresponding author: Loukides, G.
* Published May 2022 (early online 19 Nov 2021)
* Processed: 2022-5

A Relational-Sequential dataset (or RS-dataset for short) contains records comprised of a patient's values in demographic attributes and their sequence of diagnosis codes. The task of clustering an RS ...

### *22) Oil Absorbent Polypropylene Particles Stimulate Biodegradation of Crude Oil by Microbial Consortia*

* Vita, M. M., Iturbe-Espinoza, P., Bonte, M., Brandt, B. W., Braster, M., Brown, D. M., van Spanning, R. J. M.
* Systems Bioinformatics, Preventive Dentistry, Molecular Cell Physiology, AIMMS, Vrije Universiteit Amsterdam, Royal Dutch Shell PLC, Ministry of Infrastructure and Water Management, Ricardo
* Frontiers in Microbiology
* https://doi.org/10.3389/fmicb.2022.853285
* Corresponding author: Vita, M. M.
* Published May 2022 (early online 23 May 2022)
* Processed: 2022-5

Oil absorbent particles made from surface-modified polypropylene can be used to facilitate the removal of oil from the environment. In this study, we investigated to what extent absorbed oil was biode ...

### *23) Longest Palindromic Substring in Sublinear Time*

* Charalampopoulos, P., Pissis, S. P., Radoszewski, J.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), Reichman University, University of Warsaw
* None
* https://doi.org/10.4230/LIPIcs.CPM.2022.20
* Corresponding author: Charalampopoulos, P.
* Published 2022 (early online None)
* Processed: 2022-6

We revisit the classic algorithmic problem of computing a longest palidromic substring. This problem is solvable by a celebrated O(n)-time algorithm [Manacher, J. ACM 1975], where n is the length of t ...

### *24) Making de Bruijn Graphs Eulerian*

* Bernardini, G., Chen, H., Loukides, G., Pissis, S. P., Stougie, L., Sweering, M.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), Operations Analytics, Tinbergen Institute, Amsterdam Business Research Institute, University of Trieste, Centrum voor Wiskunde en Informatica, King's College London
* None
* https://doi.org/10.4230/LIPIcs.CPM.2022.12
* Corresponding author: Bernardini, G.
* Published 2022 (early online None)
* Processed: 2022-6

A directed multigraph is called Eulerian if it has a circuit which uses each edge exactly once. Euler's theorem tells us that a weakly connected directed multigraph is Eulerian if and only if every no ...

### *25) On Strings Having the Same Length-k Substrings*

* Bernardini, G., Conte, A., Gabory, E., Grossi, R., Loukides, G., Pissis, S. P., Punzi, G., Sweering, M.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), University of Trieste, Centrum voor Wiskunde en Informatica, University of Pisa, King's College London
* None
* https://doi.org/10.4230/LIPIcs.CPM.2022.16
* Corresponding author: Bernardini, G.
* Published 2022 (early online None)
* Processed: 2022-6

Let Substrk(X) denote the set of length-k substrings of a given string X for a given integer k > 0. We study the following basic string problem, called z-Shortest Sk-Equivalent Strings: Given a set Sk ...

### *26) Classical Force-Field Parameters for Cs*

* Pascazio, R., Zaccaria, F., Van Beek, B., Infante, I.
* Theoretical Chemistry, AIMMS, Italian Institute of Technology, University of Genoa, Vrije Universiteit Amsterdam
* Journal of Physical Chemistry C
* https://doi.org/10.1021/acs.jpcc.2c00600
* Corresponding author: Infante, I.
* Published 16 Jun 2022 (early online 1 Jun 2022)
* Processed: 2022-6

PbBr3Perovskite NanocrystalsUnderstanding the chemico-physical properties of colloidal semiconductor nanocrystals (NCs) requires exploration of the dynamic processes occurring at the NC surfaces, in p ...

### *27) Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings*

* Jian, J., Barkhatova, D., Hammink, R., Tinnemans, P., Bickelhaupt, F. M., Poater, J., Mecinović, J.
* Chemistry and Pharmaceutical Sciences, AIMMS, Theoretical Chemistry, University of Southern Denmark, Radboud University Nijmegen
* Journal of Organic Chemistry
* https://doi.org/10.1021/acs.joc.2c00533
* Corresponding author: Mecinović, J.
* Published 17 Jun 2022 (early online 2 Jun 2022)
* Processed: 2022-6

Imidazole-based compounds are widely found in natural products, synthetic molecules, and biomolecules. Noncovalent interactions between the imidazole ring and other functional groups play an important ...

### *28) Multi-task learning to leverage partially annotated data for PPI interface prediction*

* Capel, H., Feenstra, K. A., Abeln, S.
* Bioinformatics, AIMMS, Integrative Bioinformatics, Vrije Universiteit Amsterdam
* Scientific Reports
* https://doi.org/10.1038/s41598-022-13951-2
* Corresponding author: Abeln, S.
* Published 21 Jun 2022 (early online None)
* Processed: 2022-6

Protein protein interactions (PPI) are crucial for protein functioning, nevertheless predicting residues in PPI interfaces from the protein sequence remains a challenging problem. In addition, structu ...

### *29) Palladium-Catalyzed Activation of Carbon–Halogen Bonds: Electrostatics-Controlled Reactivity*

* Moloto, B. P., Vermeeren, P., Dalla Tiezza, M., Esterhuysen, C., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, University of Stellenbosch
* European Journal of Organic Chemistry
* https://doi.org/10.1002/ejoc.202200722
* Corresponding author: Bickelhaupt, F. M.
* Published 14 Jul 2022 (early online 22 Jun 2022)
* Processed: 2022-7

We have quantum chemically studied the palladium-mediated activation of C(spn)−X bonds (n=1–3; X=F, Cl, Br, I) in the archetypal model substrates H3C−CH2−X, H2C=CH−X, and HC≡C−X by a model bare pallad ...

### *30) " Commandeuring" Xenobiotic Metabolism: Advances in Understanding Xenobiotic Metabolism*

* Van Vugt-Lussenburg, B. M. A., Capinha, L., Reinen, J., Rooseboom, M., Kranendonk, M., Onderwater, R. C. A., Jennings, P.
* Molecular and Computational Toxicology, AIMMS, BioDetection Systems B.V., Charles River Den Bosch, Royal Dutch Shell PLC, NOVA University Lisbon, Materia Nova ASBL
* Chemical Research in Toxicology
* https://doi.org/10.1021/acs.chemrestox.2c00067
* Corresponding author: Van Vugt-Lussenburg, B. M. A.
* Published 18 Jul 2022 (early online 29 Jun 2022)
* Processed: 2022-7

The understanding of how exogenous chemicals (xenobiotics) are metabolized, distributed, and eliminated is critical to determine the impact of the chemical and its metabolites to the (human) organism. ...

### *31) GPCRs steer Gi and Gs selectivity via TM5-TM6 switches as revealed by structures of serotonin receptors*

* Huang, S., Xu, P., Shen, D. D., Simon, I. A., Mao, C., Tan, Y., Zhang, H., Harpsøe, K., Li, H., Zhang, Y., You, C., Yu, X., Jiang, Y., Zhang, Y., Gloriam, D. E., Xu, H. E.
* Medicinal chemistry, AIMMS, CAS - Shanghai Institute of Materia Medica, University of Chinese Academy of Sciences, ShanghaiTech University, Zhejiang University, University of Copenhagen, Key Laboratory of Immunity and Inflammatory Diseases of Zhejiang Province
* Molecular cell
* https://doi.org/10.1016/j.molcel.2022.05.031
* Corresponding author: Zhang, Y.
* Published 21 Jul 2022 (early online 16 Jun 2022)
* Processed: 2022-7

Serotonin (or 5-hydroxytryptamine, 5-HT) is an important neurotransmitter that activates 12 different G protein-coupled receptors (GPCRs) through selective coupling of Gs, Gi, or Gq proteins. The stru ...

### *32) Gastric Th17 Cells Specific for H+/K+-ATPase and Serum IL-17 Signature in Gastric Autoimmunity*

* Della Bella, C., Antico, A., Panozzo, M. P., Capitani, N., Petrone, L., Benagiano, M., D’Elios, S., Sparano, C., Azzurri, A., Pratesi, S., Cianchi, F., Ortiz-Princz, D., Bergman, M., Bizzaro, N., D’Elios, M. M.
* Molecular Microbiology, AIMMS, University of Florence, Hospital Alto Vicentino, University of Siena, Azienda Ospedaliera Careggi, University of Pisa, Toscana Centro Hospital, Universidad Central de Venezuela, San Antonio Hospital, Azienda Sanitaria Universitaria Integrata
* Frontiers in Immunology
* https://doi.org/10.3389/fimmu.2022.952674
* Corresponding author: D’Elios, M. M.
* Published Jul 2022 (early online 11 Jul 2022)
* Processed: 2022-7

Human gastric autoimmunity [autoimmune gastritis (AIG)] is characterized by inflammation of the gastric mucosa and parietal cell loss. The gastric parietal cell proton pump H+/K+-adenosine triphosphat ...

### *33) Phylogenetic Classification and Functional Review of Autotransporters*

* Clarke, K. R., Hor, L., Pilapitiya, A., Luirink, J., Paxman, J. J., Heras, B.
* Molecular Microbiology, AIMMS, LaserLaB - Molecular Biophysics, La Trobe University
* Frontiers in Immunology
* https://doi.org/10.3389/fimmu.2022.921272
* Corresponding author: Paxman, J. J.
* Published Jul 2022 (early online 1 Jul 2022)
* Processed: 2022-7

Autotransporters are the core component of a molecular nano-machine that delivers cargo proteins across the outer membrane of Gram-negative bacteria. Part of the type V secretion system, this large fa ...

### *34) Does parental exposure to nanoplastics modulate the response of Hediste diversicolor to other contaminants: A case study with arsenic*

* Silva, M. S. S., Oliveira, M., Almeida, H., Vethaak, A. D., Martínez-Gómez, C., Figueira, E., Pires, A.
* AIMMS, Environment and Health, University of Aveiro, Instituto Espanol de Oceanografia, Deltares
* Environmental Research
* https://doi.org/10.1016/j.envres.2022.113764
* Corresponding author: Pires, A.
* Published Nov 2022 (early online 5 Jul 2022)
* Processed: 2022-7

Plastic pollution is a serious problem in aquatic systems throughout the world. Despite the increasing number of studies addressing the impact of macro- and microplastics on biota, there is still a si ...

### *35) Distinct cell type-specific protein signatures in GRN and MAPT genetic subtypes of frontotemporal dementia*

* Miedema, S. S. M., Mol, M. O., Koopmans, F. T. W., Hondius, D. C., van Nierop, P., Menden, K., de Veij Mestdagh, C. F., van Rooij, J., Ganz, A. B., Paliukhovich, I., Melhem, S., Li, K. W., Holstege, H., Rizzu, P., van Kesteren, R. E., van Swieten, J. C., Heutink, P., Smit, A. B.
* Molecular and Cellular Neurobiology, Amsterdam Neuroscience - Neurodegeneration, Amsterdam Neuroscience - Cellular & Molecular Mechanisms, AIMMS, Center for Neurogenomics and Cognitive Research, Erasmus University Rotterdam, Vrije Universiteit Amsterdam, German Center for Neurodegenerative Diseases, Amsterdam UMC
* Acta Neuropathologica Communications
* https://doi.org/10.1186/s40478-022-01387-8
* Corresponding author: Miedema, S. S. M.
* Published 7 Jul 2022 (early online None)
* Processed: 2022-7

Frontotemporal dementia is characterized by progressive atrophy of frontal and/or temporal cortices at an early age of onset. The disorder shows considerable clinical, pathological, and genetic hetero ...

### *36) Conformational selection guides β-arrestin recruitment at a biased G protein–coupled receptor*

* Kleist, A. B., Jenjak, S., Sente, A., Laskowski, L. J., Szpakowska, M., Calkins, M. M., Anderson, E. I., McNally, L. M., Heukers, R., Bobkov, V., Peterson, F. C., Thomas, M. A., Chevigné, A., Smit, M. J., McCorvy, J. D., Babu, M. M., Volkman, B. F.
* Medicinal chemistry, AIMMS, Medical College of Wisconsin, Medical Research Council, Luxembourg Institute of Health, St. Jude Children Research Hospital
* Science
* https://doi.org/10.1126/science.abj4922
* Corresponding author: Volkman, B. F.
* Published 8 Jul 2022 (early online 7 Jul 2022)
* Processed: 2022-7

G protein–coupled receptors (GPCRs) recruit β-arrestins to coordinate diverse cellular processes, but the structural dynamics driving this process are poorly understood. Atypical chemokine receptors ( ...

### *37) Targeting the interaction of β-catenin and TCF/LEF transcription factors to inhibit oncogenic Wnt signaling*

* Koelman, E. M. R., Yeste-Vázquez, A., Grossmann, T. N.
* Organic Chemistry, AIMMS, Vrije Universiteit Amsterdam
* Bioorganic and Medicinal Chemistry
* https://doi.org/10.1016/j.bmc.2022.116920
* Corresponding author: Grossmann, T. N.
* Published 9 Jul 2022 (early online None)
* Processed: 2022-7

The Wnt/β-catenin signaling pathway is crucially involved in embryonic development, stem cell maintenance and tissue renewal. Hyperactivation of this pathway is associated with the development and pro ...

### *38) [Cover profile] How Ionization Catalyzes Diels-Alder Reactions*

* Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry (Weinheim an der Bergstrasse, Germany)
* https://doi.org/10.1002/chem.202201620
* Corresponding author: None
* Published 15 Jul 2022 (early online None)
* Processed: 2022-7

Invited for the cover of this issue are Pascal Vermeeren, Trevor A. Hamlin, and F. Matthias Bickelhaupt of the TheoCheM group at the Vrije Universiteit Amsterdam. The cover art depicts how ionizing th ...

### *39) 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) ...

### *40) Online Versus Offline Peer Feedback in Higher Education: A Meta-Analysis*

* Jongsma, M. V., Scholten, D. J., van Muijlwijk-Koezen, J. E., Meeter, M.
* LEARN! - Learning sciences, AIMMS, Innovations in Human Health & Life Sciences, Educational and Family Studies
* JOURNAL OF EDUCATIONAL COMPUTING RESEARCH
* https://doi.org/10.1177/07356331221114181
* Corresponding author: Scholten, D. J.
* Published 15 Jul 2022 (early online None)
* Processed: 2022-7

In recent years, the technical possibilities of educational technologies regarding online peer feedback have developed rapidly. However, the impact of online peer feedback activities compared to tradi ...

### *41) Physiologically Based Toxicokinetic Modeling of Bisphenols in Zebrafish (Danio rerio) Accounting for Variations in Metabolic Rates, Brain Distribution, and Liver Accumulation*

* Chelcea, I., Örn, S., Hamers, T., Koekkoek, J., Legradi, J., Vogs, C., Andersson, P. L.
* E&H: Environmental Health and Toxicology, AIMMS, E&H: Environmental Chemistry and Toxicology, Umeå University, Swedish University of Agricultural Sciences, Karolinska Institutet
* Environmental science & technology
* https://doi.org/10.1021/acs.est.2c01292
* Corresponding author: None
* Published 19 Jul 2022 (early online None)
* Processed: 2022-7

Bisphenol A (BPA) is an industrial chemical, which has raised human health and environmental concerns due to its endocrine-disrupting properties. BPA analogues are less well-studied despite their wide ...

### *42) The 1,3-Dipolar Cycloaddition: From Conception to Quantum Chemical Design*

* Beutick, S. E., Vermeeren, P., Hamlin, T. A.
* Theoretical Chemistry, AIMMS
* Chemistry - An Asian JournalArticle number:e202200553
* https://doi.org/10.1002/asia.202200553
* Corresponding author: Vermeeren, P.
* Published 28 Jul 2022 (early online 13 Jul 2022)
* Processed: 2022-7

The 1,3-dipolar cycloaddition (1,3-DCA) reaction, conceptualized by Rolf Huisgen in 1960, has proven immensely useful in organic, material, and biological chemistry. The uncatalyzed, thermal transform ...