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### 1) Switchable, Reagent-Controlled Diastereodivergent Photocatalytic Carbocyclisation of Imine-Derived α-Amino Radicals

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* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202107253
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* Published 2 Nov 2021 (early online 27 Feb 2021)
* Processed: 2021-11

A reagent-controlled stereodivergent carbocyclisation of aryl aldimine-derived, photocatalytically generated, α-amino radicals possessing adjacent conjugated alkenes, affording either bicyclic or tetracyclic products, is described. Under net reductive conditions using commercial Hantzsch ester, the α-amino radical species underwent a single stereoselective cyclisation to give trans-configured amino-indane structures in good yield, whereas using a substituted Hantzsch ester as a milder reductant afforded cis-fused tetracyclic tetrahydroquinoline frameworks, resulting from two consecutive radical cyclisations. Judicious choice of the reaction conditions allowed libraries of both single and dual cyclisation products to be synthesised with high selectivity, notable predictability, and good-to-excellent yields. Computational analysis employing DFT revealed the reaction pathway and mechanistic rationale behind this finely balanced yet readily controlled photocatalytic system.

### 2) Steering microbiomes by organic amendments towards climate-smart agricultural soils

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* Biology and Fertility of Soils
* https://doi.org/10.1007/s00374-021-01599-5
* Corresponding author: Brenzinger, K.
* Published Nov 2021 (early online 25 Sep 2021)
* Processed: 2021-11

We steered the soil microbiome via applications of organic residues (mix of cover crop residues, sewage sludge + compost, and digestate + compost) to enhance multiple ecosystem services in line with climate-smart agriculture. Our result highlights the potential to reduce greenhouse gases (GHG) emissions from agricultural soils by the application of specific organic amendments (especially digestate + compost). Unexpectedly, also the addition of mineral fertilizer in our mesocosms led to similar combined GHG emissions than one of the specific organic amendments. However, the application of organic amendments has the potential to increase soil C, which is not the case when using mineral fertilizer. While GHG emissions from cover crop residues were significantly higher compared to mineral fertilizer and the other organic amendments, crop growth was promoted. Furthermore, all organic amendments induced a shift in the diversity and abundances of key microbial groups. We show that organic amendments have the potential to not only lower GHG emissions by modifying the microbial community abundance and composition, but also favour crop growth-promoting microorganisms. This modulation of the microbial community by organic amendments bears the potential to turn soils into more climate-smart soils in comparison to the more conventional use of mineral fertilizers.

### 3) The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength

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* Processed: 2021-11

We have quantum chemically analyzed element−element bonds of archetypal HnX−YHn molecules (X, Y=C, N, O, F, Si, P, S, Cl, Br, I), using density functional theory. One purpose is to obtain a set of consistent homolytic bond dissociation energies (BDE) for establishing accurate trends across the periodic table. The main objective is to elucidate the underlying physical factors behind these chemical bonding trends. On one hand, we confirm that, along a period (e. g., from C−C to C−F), bonds strengthen because the electronegativity difference across the bond increases. But, down a period, our findings constitute a paradigm shift. From C−F to C−I, for example, bonds do become weaker, however, not because of the decreasing electronegativity difference. Instead, we show that the effective atom size (via steric Pauli repulsion) is the causal factor behind bond weakening in this series, and behind the weakening in orbital interactions at the equilibrium distance. We discuss the actual bonding mechanism and the importance of analyzing this mechanism as a function of the bond distance.

### 4) Intranasal vaccination with protein bodies elicit strong protection against Streptococcus pneumoniae colonization

* van Beek, L. F., Langereis, J. D., van den Berg van Saparoea, H. B., Gillard, J., Jong, W. S., van Opzeeland, F. J., Mesman, R., van Niftrik, L., Joosten, I., Diavatopoulos, D. A., Luirink, J., de Jonge, M. I.
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* Processed: 2021-11

Protein bodies (PBs) are particles consisting of insoluble, aggregated proteins with potential as a vaccine formulation. PBs can contain high concentrations of antigen, are stable and relatively resistant to proteases, release antigen slowly and are cost-effective to manufacture. Yet, the capacity of PBs to provoke immune responses and protection in the upper respiratory tract, a major entry route of respiratory pathogens, is largely unknown. In this study, we vaccinated mice intranasally with PBs comprising antigens from Streptococcus pneumoniae and evaluated the level of protection against nasopharyngeal colonization. PBs composed of the α-helical domain of pneumococcal surface protein A (PspAα) provided superior protection against colonization with S. pneumoniae compared to soluble PspAα. Immunization with soluble protein or PBs induced differences in antibody binding to pneumococci as well as a highly distinct antigen-specific nasal cytokine profile upon in vivo stimulation with inactivated S. pneumoniae. Moreover, immunization with PBs composed of conserved putative pneumococcal antigens reduced colonization by S. pneumoniae in mice, both as a single- and as a multi-antigen formulation. In conclusion, PBs represent a vaccine formulation that elicits strong mucosal immune responses and protection. The versatility of this platform offers opportunities for development of next-generation vaccine formulations.

### 5) Time-resolved relaxation and fragmentation of polycyclic aromatic hydrocarbons investigated in the ultrafast XUV-IR regime

* Lee, J. W., Tikhonov, D. S., Chopra, P., Maclot, S., Steber, A. L., Gruet, S., Allum, F., Boll, R., Cheng, X., Düsterer, S., Erk, B., Garg, D., He, L., Heathcote, D., Johny, M., Kazemi, M. M., Köckert, H., Lahl, J., Lemmens, A. K., Loru, D., Mason, R., Müller, E., Mullins, T., Olshin, P., Passow, C., Peschel, J., Ramm, D., Rompotis, D., Schirmel, N., Trippel, S., Wiese, J., Ziaee, F., Bari, S., Burt, M., Küpper, J., Rijs, A. M., Rolles, D., Techert, S., Eng-Johnsson, P., Brouard, M., Vallance, C., Manschwetus, B., Schnell, M.
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* Published Dec 2021 (early online 20 Oct 2021)
* Processed: 2021-12

Polycyclic aromatic hydrocarbons (PAHs) play an important role in interstellar chemistry and are subject to high energy photons that can induce excitation, ionization, and fragmentation. Previous studies have demonstrated electronic relaxation of parent PAH monocations over 10–100 femtoseconds as a result of beyond-Born-Oppenheimer coupling between the electronic and nuclear dynamics. Here, we investigate three PAH molecules: fluorene, phenanthrene, and pyrene, using ultrafast XUV and IR laser pulses. Simultaneous measurements of the ion yields, ion momenta, and electron momenta as a function of laser pulse delay allow a detailed insight into the various molecular processes. We report relaxation times for the electronically excited PAH\*, PAH+\* and PAH2+\* states, and show the time-dependent conversion between fragmentation pathways. Additionally, using recoil-frame covariance analysis between ion images, we demonstrate that the dissociation of the PAH2+ ions favors reaction pathways involving two-body breakup and/or loss of neutral fragments totaling an even number of carbon atoms.

### 6) The escherichia coli outer membrane β-barrel assembly machinery (Bam) crosstalks with the divisome

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* Molecular Microbiology, AIMMS, LaserLaB - Molecular Biophysics, University of Amsterdam
* International Journal of Molecular Sciences
* https://doi.org/10.3390/ijms222212101
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* Published 2 Nov 2021 (early online None)
* Processed: 2021-11

The BAM is a macromolecular machine responsible for the folding and the insertion of integral proteins into the outer membrane of diderm Gram-negative bacteria. In Escherichia coli, it consists of a transmembrane β-barrel subunit, BamA, and four outer membrane lipoproteins (BamB-E). Using BAM-specific antibodies, in E. coli cells, the complex is shown to localize in the lateral wall in foci. The machinery was shown to be enriched at midcell with specific cell cycle timing. The inhibition of septation by aztreonam did not alter the BAM midcell localization substantially. Furthermore, the absence of late cell division proteins at midcell did not impact BAM timing or localization. These results imply that the BAM enrichment at the site of constriction does not require an active cell division machinery. Expression of the Tre1 toxin, which impairs the FtsZ filamentation and therefore midcell localization, resulted in the complete loss of BAM midcell enrichment. A similar effect was observed for YidC, which is involved in the membrane insertion of cell division proteins in the inner membrane. The presence of the Z-ring is needed for preseptal peptidoglycan (PG) synthesis. As BAM was shown to be embedded in the PG layer, it is possible that BAM is inserted preferentially simultaneously with de novo PG synthesis to facilitate the insertion of OMPs in the newly synthesized outer membrane.

### 7) The two-way interaction between the molecules that cause vaginal malodour and lactobacilli: An opportunity for probiotics

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* Published 2 Nov 2021 (early online None)
* Processed: 2021-11

Vaginal malodour is a sign of dysbiosis. The biogenic amines (BAs) cadaverine, putrescine and tyramine are known to be causative compounds. Recent reports suggest these compounds produced by pathogens might have a role beyond causing malodour; namely inhibiting the growth of lactobacilli bacteria that are crucial in the maintenance of vaginal homeostasis. The aim of this study was to identify whether certain lactobacilli strains could reduce BAs and to evaluate how Lactobacillus species were affected by these compounds. Using LC–MS and HPLC-UV, five Lactobacillus crispatus strains were identified as being capable of significantly reducing BAs from the media under in vitro conditions. Through 16S rRNA gene sequencing of vaginal swabs exposed to Bas, cadaverine was found to reduce the relative abundance of lactobacilli. When L. crispatus was exposed to media supplemented with BAs with an HCl adjusted lower pH, its growth was enhanced, demonstrating the relevance of the maintenance of an acidic vaginal environment. If strains are to be developed for probiotic application to alleviate bacterial vaginosis and other conditions affecting large numbers of women worldwide, their ability to adapt to Bas and regulate pH should be part of the experimentation.

### 8) Age-related susceptibility to insulin resistance arises from a combination of CPT1B decline and lipid overload

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* https://doi.org/10.1186/s12915-021-01082-5
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* Published Dec 2021 (early online None)
* Processed: 2021-12

Background: The skeletal muscle plays a central role in glucose homeostasis through the uptake of glucose from the extracellular medium in response to insulin. A number of factors are known to disrupt the normal response to insulin leading to the emergence of insulin resistance (IR). Advanced age and a high-fat diet are factors that increase the susceptibility to IR, with lipid accumulation in the skeletal muscle being a key driver of this phenomenon. It is debated, however, whether lipid accumulation arises due to dietary lipid overload or from a decline of mitochondrial function. To gain insights into the interplay of diet and age in the flexibility of muscle lipid and glucose handling, we combined lipidomics, proteomics, mitochondrial function analysis and computational modelling to investigate young and aged mice on a low- or high-fat diet (HFD). Results: As expected, aged mice were more susceptible to IR when given a HFD than young mice. The HFD induced intramuscular lipid accumulation specifically in aged mice, including C18:0-containing ceramides and diacylglycerols. This was reflected by the mitochondrial β-oxidation capacity, which was upregulated by the HFD in young, but not in old mice. Conspicuously, most β-oxidation proteins were upregulated by the HFD in both groups, but carnitine palmitoyltransferase 1B (CPT1B) declined in aged animals. Computational modelling traced the flux control mostly to CPT1B, suggesting a CPT1B-driven loss of flexibility to the HFD with age. Finally, in old animals, glycolytic protein levels were reduced and less flexible to the diet. Conclusion: We conclude that intramuscular lipid accumulation and decreased insulin sensitivity are not due to age-related mitochondrial dysfunction or nutritional overload alone, but rather to their combined effects. Moreover, we identify CPT1B as a potential target to counteract age-dependent intramuscular lipid accumulation and thereby IR.

### 9) High biodiversity in a benzene-degrading nitrate-reducing culture is sustained by a few primary consumers

* Melkonian, C., Fillinger, L., Atashgahi, S., da Rocha, U. N., Kuiper, E., Olivier, B., Braster, M., Gottstein, W., Helmus, R., Parsons, J. R., Smidt, H., van der Waals, M., Gerritse, J., Brandt, B. W., Röling, W. F., Molenaar, D., van Spanning, R. J.
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* Communications biology
* https://doi.org/10.1038/s42003-021-01948-y
* Corresponding author: Melkonian, C.
* Published Dec 2021 (early online None)
* Processed: 2021-12

A key question in microbial ecology is what the driving forces behind the persistence of large biodiversity in natural environments are. We studied a microbial community with more than 100 different types of species which evolved in a 15-years old bioreactor with benzene as the main carbon and energy source and nitrate as the electron acceptor. Using genome-centric metagenomics plus metatranscriptomics, we demonstrate that most of the community members likely feed on metabolic left-overs or on necromass while only a few of them, from families Rhodocyclaceae and Peptococcaceae, are candidates to degrade benzene. We verify with an additional succession experiment using metabolomics and metabarcoding that these few community members are the actual drivers of benzene degradation. As such, we hypothesize that high species richness is maintained and the complexity of a natural community is stabilized in a controlled environment by the interdependencies between the few benzene degraders and the rest of the community members, ultimately resulting in a food web with different trophic levels.

### 10) High throughput screening of technological and biopreservation traits of a large set of wild lactic acid bacteria from Brazilian artisanal cheeses

* Margalho, L. P., Kamimura, B. A., Brexó, R. P., Alvarenga, V. O., Cebeci, A. S., Janssen, P. W., Dijkstra, A., Starrenburg, M. J., Sheombarsing, R. S., Cruz, A. G., Alkema, W., Bachmann, H., Sant'Ana, A. S.
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* Published Dec 2021 (early online None)
* Processed: 2021-12

This study aimed to evaluate technological (acidification, proteolysis, lipolysis, resistance to low pH, NaCl, and bile salts) and biopreservation (antimicrobial activity against foodborne pathogens) features of 1002 LAB by high throughput screening (HTS) methods. The LAB was isolated from 11 types of Brazilian artisanal cheeses (BAC) marketed in the main 5 producing regions. Remarkable intra-species variability in acidification rates have been found, which was most pronounced between isolates from Mina's artisanal cheeses, Caipira and Coalho cheeses. Lacticaseibacillus paracasei and Levilactobacillus brevis showed the fastest acidification rate; however, all isolates showed slower acidification rates than a lactococcal control strain (4.3 × lower). When testing inhibitory effects, > 75% of LAB isolates could inhibit the growth of Staphylococcus aureus ATCC 19095 and Listeria monocytogenes ATCC 7644. Two of these isolates, identified as Lactiplantibacillus plantarum and Lentilactobacillus buchneri, the sterile and neutral supernatants alone, were sufficient to inhibit L. monocytogenes growth. Principal component analysis (PCA) allowed the identification of functional groups based on proteolytic and lipolytic activity, osmotic stress resistance, and inhibition of L. monocytogenes. The type of cheese the isolates were recovered from influenced properties such as anti-listerial compounds and lipolytic enzyme production. The use of HTS and multivariate statistics allowed insights into a diverse set of LAB technological and biopreservation properties. These findings allow a profound knowledge of the heterogeneity of a large set of isolates, which can be further used to design starter cultures with varied and combined properties, such as biopreservation and technological features. Besides that, HTS makes it possible to analyze a vast panel of LAB strains, reducing costs and time within laboratory analysis, while avoiding the loss of information once all LAB are tested at the same time (differently from the traditional labor-intensive approach, in which a few numbers of strains is tested per time).

### 11) Metabolomics of sebum reveals lipid dysregulation in Parkinson’s disease

* Sinclair, E., Trivedi, D. K., Sarkar, D., Walton-Doyle, C., Milne, J., Kunath, T., Rijs, A. M., de Bie, R. M., Goodacre, R., Silverdale, M., Barran, P.
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* Nature Communications
* https://doi.org/10.1038/s41467-021-21669-4
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* Published Dec 2021 (early online None)
* Processed: 2021-12

Parkinson’s disease (PD) is a progressive neurodegenerative disorder, which is characterised by degeneration of distinct neuronal populations, including dopaminergic neurons of the substantia nigra. Here, we use a metabolomics profiling approach to identify changes to lipids in PD observed in sebum, a non-invasively available biofluid. We used liquid chromatography-mass spectrometry (LC-MS) to analyse 274 samples from participants (80 drug naïve PD, 138 medicated PD and 56 well matched control subjects) and detected metabolites that could predict PD phenotype. Pathway enrichment analysis shows alterations in lipid metabolism related to the carnitine shuttle, sphingolipid metabolism, arachidonic acid metabolism and fatty acid biosynthesis. This study shows sebum can be used to identify potential biomarkers for PD.

### 12) Overproducing the BAM complex improves secretion of difficult-to-secrete recombinant autotransporter chimeras

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* Microbial Cell Factories
* https://doi.org/10.1186/s12934-021-01668-2
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* Published Dec 2021 (early online None)
* Processed: 2021-12

Monomeric autotransporters have been used extensively to transport recombinant proteins or protein domains to the cell surface of Gram-negative bacteria amongst others for antigen display. Genetic fusion of such antigens into autotransporters has yielded chimeras that can be used for vaccination purposes. However, not every fusion construct is transported efficiently across the cell envelope. Problems occur in particular when the fused antigen attains a relatively complex structure in the periplasm, prior to its translocation across the outer membrane. The latter step requires the interaction with periplasmic chaperones and the BAM (β-barrel assembly machinery) complex in the outer membrane. This complex catalyzes insertion and folding of β-barrel outer membrane proteins, including the β-barrel domain of autotransporters. Here, we investigated whether the availability of periplasmic chaperones or the BAM complex is a limiting factor for the surface localization of difficult-to-secrete chimeric autotransporter constructs. Indeed, we found that overproduction of in particular the BAM complex, increases surface display of difficult-to-secrete chimeras. Importantly, this beneficial effect appeared to be generic not only for a number of monomeric autotransporter fusions but also for fusions to trimeric autotransporters. Therefore, overproduction of BAM might be an attractive strategy to improve the production of recombinant autotransporter constructs.

### *13) High-resolution infrared spectroscopy of naphthalene and acenaphthene dimers*

* Lemmens, A. K., Chopra, P., Garg, D., Steber, A. L., Schnell, M., Buma, W. J., Rijs, A. M.
* BioAnalytical Chemistry, AIMMS
* Molecular Physics
* https://doi.org/10.1080/00268976.2020.1811908
* Corresponding author: None
* Published 17 Jan 2021 (early online None)
* Processed: 2021-1

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### *14) Site-Specific N-Linked Glycosylation Analysis of Human Carcinoembryonic Antigen by Sheathless Capillary Electrophoresis-Tandem Mass Spectrometry*

* Pont, L., Kuzyk, V., Benavente, F., Sanz-Nebot, V., Mayboroda, O. A., Wuhrer, M., Lageveen-Kammeijer, G. S.
* BioAnalytical Chemistry, AIMMS, University of Barcelona, Leiden University
* Journal of Proteome Research
* https://doi.org/10.1021/acs.jproteome.0c00875
* Corresponding author: Benavente, F.
* Published 5 Mar 2021 (early online 9 Feb 2021)
* Processed: 2021-3

With 28 potential N-glycosylation sites, human carcinoembryonic antigen (CEA) bears an extreme amount of N-linked glycosylation, and approximately 60% of its molecular mass can be attributed to its ca ...

### *15) Combining High-Resolution Gas Chromatographic Continuous Fraction Collection with Nuclear Magnetic Resonance Spectroscopy: Possibilities of Analyzing a Whole GC Chromatogram*

* Van Mourik, L. M., Janssen, E., Breeuwer, R., Jonker, W., Koekkoek, J., Arrahman, A., Kool, J., Leonards, P. E.Pages:6158-6168
* E&H: Environmental Bioanalytical Chemistry, AIMMS, BioAnalytical Chemistry, E&H: Environmental Chemistry and Toxicology, Vrije Universiteit Amsterdam
* Analytical chemistry
* https://doi.org/10.1021/acs.analchem.1c00049
* Corresponding author: Van Mourik, L. M.
* Published 9 Apr 2021 (early online 9 Apr 2021)
* Processed: 2021-4

This study presents, for the first time, the successful application of analyzing a whole gas chromatography (GC) chromatogram by nuclear magnetic resonance (NMR) spectroscopy using a continuous repeat ...

### *16) FRET Analysis of RNA –Protein Interactions Using Spinach Aptamers*

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* Organic Chemistry, AIMMS, Vrije Universiteit Amsterdam
* None
* https://doi.org/10.1007/978-1-0716-1499-0\_13
* Corresponding author: Hennig, S.
* Published 2021 (early online None)
* Processed: 2021-6

The method development to analyze direct RNA–protein interaction is of high importance as not many homogeneous assay formats are available. The discovery of fluorescent light-up aptamers (FLAPs), shor ...

### *17) Internal shortest absent word queries*

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* Bioinformatics, AIMMS, Bio Informatics (IBIVU), Goldsmiths, University of London, Interdisciplinary Center Herzliya
* None
* https://doi.org/10.4230/LIPIcs.CPM.2021.6
* Corresponding author: Badkobeh, G.
* Published 2021 (early online None)
* Processed: 2021-6

Given a string T of length n over an alphabet Σ ⊂ {1, 2, . . ., nO(1)} of size s, we are to preprocess T so that given a range [i, j], we can return a representation of a shortest string over Σ that i ...

### *18) Metabolic modeling of fungi*

* Mendoza, S. N., Calhoun, S., Teusink, B., Aguilar-Pontes, M. V.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, United States Department of Energy, Utrecht University
* None
* https://doi.org/10.1016/B978-0-12-809633-8.21068-6
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* Published 2021 (early online None)
* Processed: 2021-6

Fungi have received special interest from the biotechnological sector focused on the production of active biomolecules and strain engineering. Genome-scale metabolic models (GEMs) are used to understa ...

### *19) Bicyclic β-Sheet Mimetics that Target the Transcriptional Coactivator β-Catenin and Inhibit Wnt Signaling*

* Wendt, M., Bellavita, R., Gerber, A., Efrém, N. L., van Ramshorst, T., Pearce, N. M., Davey, P. R., Everard, I., Vazquez-Chantada, M., Chiarparin, E., Grieco, P., Hennig, S., Grossmann, T. N.Pages:13937-13944
* Organic Chemistry, AIMMS, Vrije Universiteit Amsterdam, AstraZeneca, University of Naples Federico II
* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202102082
* Corresponding author: Grossmann, T. N.
* Published 14 Jun 2021 (early online None)
* Processed: 2021-6

Protein complexes are defined by the three-dimensional structure of participating binding partners. Knowledge about these structures can facilitate the design of peptidomimetics which have been applie ...

### *20) Managing service innovations at online travel agencies: evidence from China*

* Mu, Y., Bossink, B., Vinig, T., You, S.
* Science & Business Innovation, AIMMS, Sichuan Agricultural University, University of Amsterdam, Trip International
* Journal of Hospitality and Tourism Technology
* https://doi.org/10.1108/JHTT-08-2020-0190
* Corresponding author: Mu, Y.
* Published 5 Aug 2021 (early online 25 Jun 2021)
* Processed: 2021-8

PurposeResearch on service innovation management of online travel agencies (OTAs) remains relatively scarce. This study aims to illuminate the detailed components of managing service innovations at OT ...

### *21) Origin of the α-Effect in SN2 Reactions*

* Hansen, T., Vermeeren, P., Bickelhaupt, F. M., Hamlin, T. A.
* Chemistry and Pharmaceutical Sciences, Theoretical Chemistry, AIMMS
* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202106053
* Corresponding author: Hamlin, T. A.
* Published 13 Sep 2021 (early online 4 Jun 2021)
* Processed: 2021-9

The α-effect is a term used to explain the dramatically enhanced reactivity of α-nucleophiles (R−Y−X:−) compared to their parent normal nucleophile (R−X:−) by deviating from the classical Brønsted-typ ...

### *22) Association of exposure to organophosphate flame retardants and children's behavior at a median age of 18 months*

* Sugeng, E. J., de Cock, M., Leonards, P. E., van de Bor, M.
* E&H: Environmental Health and Toxicology, AIMMS, Environment and Health, E&H: Environmental Bioanalytical Chemistry
* Environmental Advances
* https://doi.org/10.1016/j.envadv.2021.100077
* Corresponding author: Sugeng, E. J.
* Published Oct 2021 (early online 12 Jun 2021)
* Processed: 2021-10

Exposure to polybrominated diphenyl ether (PBDE) flame retardants (FRs) could have adverse effects on neurodevelopment in children. Some organophosphate (OPFRs) are used as alternatives for the phased ...

### *23) SARS-Co*

* Djidrovski, I., Georgiou, M., Hughes, G. L., Patterson, E. I., Casas-Sanchez, A., Pennington, S. H., Biagini, G. A., Moya-Molina, M., van den Bor, J., Smit, M. J., Chung, G., Lako, M., Armstrong, L.
* Medicinal chemistry, AIMMS, Newcells Biotech, Newcastle University, Liverpool School of Tropical Medicine
* Stem Cells
* https://doi.org/10.1002/stem.3422
* Corresponding author: Armstrong, L.
* Published Oct 2021 (early online 21 Jun 2021)
* Processed: 2021-10

V-2 infects an upper airway model derived from induced pluripotent stem cellsAs one of the primary points of entry of xenobiotic substances and infectious agents into the body, the lungs are subject t ...

### *24) Seasonal Changes in Hemolymph Parameters of the Bivalve Modiolus kurilensis Bernard, 1983 from Vostok Bay, Sea of Japan*

* Grinchenko, A. V., Sokolnikova, Y. N., Ilyaskina, D. V., Kumeiko, V. V.
* AIMMS, E&H: Environmental Bioanalytical Chemistry, RAS - National Scientific Center of Marine Biology, Far Eastern Branch, Far Eastern Federal University
* Russian Journal of Marine Biology
* https://doi.org/10.1134/S1063074021040052
* Corresponding author: Grinchenko, A. V.
* Published Jul 2021 (early online None)
* Processed: 2021-7

Abstract: Hemolymph is one of the main tissues providing invertebrates’ immunity and homeostasis. Earlier, we showed that some of the hemolymph immune parameters of the common Far Eastern mollusk Modi ...

### *25) GW100: A Slater-Type Orbital Perspective*

* Förster, A., Visscher, L.
* AIMMS, Theoretical Chemistry
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.1c00308
* Corresponding author: Förster, A.
* Published 10 Aug 2021 (early online 8 Jul 2021)
* Processed: 2021-8

We calculate complete basis set (CBS) limit-extrapolated ionization potentials (IPs) and electron affinities (EA) with Slater-type basis sets for the molecules in the GW100 database. To this end, we p ...

### *26) Boron Tunneling in the “Weak” Bond-Stretch Isomerization of N−B Lewis Adducts*

* Nandi, A., Tarannam, N., Rodrigues Silva, D., Fonseca Guerra, C., Hamlin, T. A., Kozuch, S.
* Theoretical Chemistry, AIMMS, Ben-Gurion University of the Negev
* ChemPhysChem
* https://doi.org/10.1002/cphc.202100505
* Corresponding author: Kozuch, S.
* Published 15 Sep 2021 (early online 10 Jul 2021)
* Processed: 2021-9

Some nitrile-boron halide adducts exhibit a double-well potential energy surface with two distinct minima: a “long bond” geometry (LB, a van der Waals interaction mostly based on electrostatics, but i ...

### *27) Bioenergetics theory and components | Periplasmic electron-transport systems in bacteria*

* Richardson, D. J., Sawers, G., Van Spanning, R. J.
* Systems Bioinformatics, AIMMS, University of East Anglia, John Innes Centre
* None
* https://doi.org/10.1016/B978-0-12-819460-7.00601-0
* Corresponding author: Richardson, D. J.
* Published 2021 (early online None)
* Processed: 2021-8

The periplasmic compartment lies between the inner (cytoplasmic) and outer membranes of Gram-negative bacteria. It is frequently termed the ‘periplasmic space’, but this is a misnomer as the term ‘spa ...

### *28) Switch From Pauli-Lowering to LUMO-Lowering Catalysis in Brønsted Acid-Catalyzed Aza-Diels-Alder Reactions*

* Yu, S., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* ChemistryOpen
* https://doi.org/10.1002/open.202100172
* Corresponding author: Bickelhaupt, F. M.
* Published Aug 2021 (early online 5 Aug 2021)
* Processed: 2021-8

Brønsted acid-catalyzed inverse-electron demand (IED) aza-Diels-Alder reactions between 2-aza-dienes and ethylene were studied using quantum chemical calculations. The computed activation energy syste ...

### *29) Bidirectional string anchors: A new string sampling mechanism*

* Loukides, G., Pissis, S. P.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London
* None
* https://doi.org/10.4230/LIPIcs.ESA.2021.64
* Corresponding author: Loukides, G.
* Published 31 Aug 2021 (early online None)
* Processed: 2021-8

The minimizers sampling mechanism is a popular mechanism for string sampling introduced independently by Schleimer et al. [SIGMOD 2003] and by Roberts et al. [Bioinf. 2004]. Given two positive integer ...

### *30) Faster algorithms for longest common substring*

* Charalampopoulos, P., Kociumaka, T., Pissis, S. P., Radoszewski, J.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), Interdisciplinary Center Herzliya, University of California at Berkeley, University of Warsaw, Samsung R&D Institute Poland
* None
* https://doi.org/10.4230/LIPIcs.ESA.2021.30
* Corresponding author: Charalampopoulos, P.
* Published 31 Aug 2021 (early online None)
* Processed: 2021-8

In the classic longest common substring (LCS) problem, we are given two strings S and T, each of length at most n, over an alphabet of size σ, and we are asked to find a longest string occurring as a ...

### *31) Orbital transformations to reduce the 1-norm of the electronic structure Hamiltonian for quantum computing applications*

* Koridon, E., Yalouz, S., Senjean, B., Buda, F., Obrien, T. E., Visscher, L.
* Theoretical Chemistry, AIMMS, Leiden University, Alphabet Inc.
* Physical Review Research
* https://doi.org/10.1103/PhysRevResearch.3.033127
* Corresponding author: Senjean, B.
* Published Sep 2021 (early online 6 Aug 2021)
* Processed: 2021-9

Reducing the complexity of quantum algorithms to treat quantum chemistry problems is essential to demonstrate an eventual quantum advantage of noisy-intermediate scale quantum devices over their class ...

### *32) The EU chemicals strategy for sustainability: in support of the Bf*

* Barile, F. A., Berry, S. C., Blaauboer, B., Boobis, A., Bolt, H. M., Borgert, C., Dekant, W., Dietrich, D., Domingo, J. L., Galli, C. L., Gori, G. B., Greim, H., Hengstler, J. G., Heslop-Harrison, P., Kacew, S., Marquardt, H., Mally, A., Pelkonen, O., Savolainen, K., Testai, E., Tsatsakis, A., Vermeulen, N. P.
* Chemistry and Pharmaceutical Sciences, AIMMS, St. John's University, Queen Mary University of London, Utrecht University, Imperial College London, Dortmund University, Inc, University of Würzburg, University of Konstanz, Universidad Rovira i Virgili, University of Milan, The Health Policy Center, Technical University of Munich, University of Leicester, University of Ottawa, University of Hamburg, University of Oulu, Finnish Institute of Occupational Health, Istituto Superiore di Sanita, University of Crete
* Archives of Toxicology
* https://doi.org/10.1007/s00204-021-03125-w
* Corresponding author: Greim, H.
* Published Sep 2021 (early online 7 Aug 2021)
* Processed: 2021-9

R positionThe EU chemicals strategy for sustainability (CSS) asserts that both human health and the environment are presently threatened and that further regulation is necessary. In a recent Guest Edi ...

### *33) Effects of ligands on (de-)enhancement of plasmonic excitations of silver, gold and bimetallic nanoclusters: TD-DFT+TB calculations*

* Asadi-Aghbolaghi, N., Pototschnig, J., Jamshidi, Z., Visscher, L.
* Theoretical Chemistry, AIMMS
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp03220h
* Corresponding author: Visscher, L.
* Published 7 Sep 2021 (early online 11 Aug 2021)
* Processed: 2021-9

Metal nanoclusters can be synthesized in various sizes and shapes and are typically protected with ligands to stabilize them. These ligands can also be used to tune the plasmonic properties of the clu ...

### *34) Implementation of Relativistic Coupled Cluster Theory for Massively Parallel GPU-Accelerated Computing Architectures*

* Pototschnig, J. V., Papadopoulos, A., Lyakh, D. I., Repisky, M., Halbert, L., Severo Pereira Gomes, A., Jensen, H. J. A., Visscher, L.
* Theoretical Chemistry, AIMMS, Vrije Universiteit Amsterdam, Oak Ridge National Laboratory, UiT The Arctic University of Norway, Universite de Lille 2, University of Southern Denmark
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.1c00260
* Corresponding author: Pototschnig, J. V.
* Published 14 Sep 2021 (early online 9 Aug 2021)
* Processed: 2021-9

In this paper, we report reimplementation of the core algorithms of relativistic coupled cluster theory aimed at modern heterogeneous high-performance computational infrastructures. The code is design ...

### *35) SARS-CoV spike proteins can compete for electrolytes in physiological fluids according to structure-based quantum-chemical calculations*

* Margiotta, E., Fonseca Guerra, C.
* Theoretical Chemistry, AIMMS
* COMPUTATIONAL AND THEORETICAL CHEMISTRY
* https://doi.org/10.1016/j.comptc.2021.113392
* Corresponding author: Margiotta, E.
* Published Oct 2021 (early online 5 Aug 2021)
* Processed: 2021-10

The trimeric spike (S) glycoprotein is the trojan horse and the stronghold of the severe acute respiratory syndrome coronaviruses. Although several structures of the S-protein have been solved, a comp ...

### *36) Temporal transcriptomic alterations of cadmium exposed human i*

* Singh, P., Chandrasekaran, V., Hardy, B., Wilmes, A., Jennings, P., Exner, T. E.
* Molecular and Computational Toxicology, AIMMS, Edelweiss Connect GmbH, University of Basel, Seven Past Nine d.o.o.
* Toxicology in Vitro
* https://doi.org/10.1016/j.tiv.2021.105229
* Corresponding author: Jennings, P.
* Published Oct 2021 (early online 3 Aug 2021)
* Processed: 2021-10

PSC-derived renal proximal tubule-like cellsCadmium is a well-studied environmental pollutant where the kidney and particularly the proximal tubule cells are especially sensitive as they are exposed t ...

### *37) Macrocyclic peptides as allosteric inhibitors of nicotinamide: N-methyltransferase (NNMT)Nicotinamide N-methyltransferase (NNMT) methylates nicotinamide to form 1-methylnicotinamide (MNA) using S-Adenosyl-l-methionine (SAM) as the methyl donor. The complexity of the role of NNMT in healthy and disease states is slowly being elucidated and provides an indication that NNMT may be an interesting therapeutic target for a variety of diseases including cancer, diabetes, and obesity. Most inhibitors of NNMT described to date are structurally related to one or both of its substrates. In the search for structurally diverse NNMT inhibitors, an m*

* Van Haren, M. J., Zhang, Y., Thijssen, V., Buijs, N., Gao, Y., Mateuszuk, L., Fedak, F. A., Kij, A., Campagna, R., Sartini, D., Emanuelli, M., Chlopicki, S., Jongkees, S. A., Martin, N. I.
* Chemistry and Pharmaceutical Sciences, AIMMS, Leiden University, Utrecht University, Jagiellonian University in Kraków, Marche Polytechnic University
* RSC Chemical Biology
* https://doi.org/10.1039/d1cb00134e
* Corresponding author: Martin, N. I.
* Published 1 Oct 2021 (early online 19 Aug 2021)
* Processed: 2021-10

RNA display screening technique was used to identify macrocyclic peptides which bind to NNMT. Several of the cyclic peptides identified in this manner show potent inhibition of NNMT with IC50 values a ...

### *38) Atypical and Asymmetric 1,3-P,N Ligands: Synthesis, Coordination and Catalytic Performance of Cycloiminophosphanes*

* Rong, M. K., Holtrop, F., Bobylev, E. O., Nieger, M., Ehlers, A. W., Slootweg, J. C., Lammertsma, K.
* Organic Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Theoretical Chemistry, Vrije Universiteit Amsterdam, University of Helsinki
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202101921
* Corresponding author: Lammertsma, K.
* Published 7 Oct 2021 (early online 17 Aug 2021)
* Processed: 2021-10

Novel seven-membered cyclic imine-based 1,3-P,N ligands were obtained by capturing a Beckmann nitrilium ion intermediate generated in situ from cyclohexanone with benzotriazole, and then displacing it ...

### *39) Beyond the BEST Theorem: Fast Assessment of Eulerian Trails*

* Conte, A., Grossi, R., Loukides, G., Pisanti, N., Pissis, S. P., Punzi, G.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), University of Pisa, ERABLE Team, King's College London
* None
* https://doi.org/10.1007/978-3-030-86593-1\_11
* Corresponding author: Punzi, G.
* Published 2021 (early online None)
* Processed: 2021-9

Given a directed multigraph G= (V, E), with | V| = n nodes and | E| = m edges, and an integer z, we are asked to assess whether the number # ET(G) of node-distinct Eulerian trails of G is at least z; ...

### *40) Ion Homeostasis and Metabolome Analysis of Arabidopsis 14-3-3 Quadruple Mutants to Salt Stress*

* Gao, J., van Kleeff, P. J., de Boer, M. H., Erban, A., Kopka, J., Hincha, D. K., de Boer, A. H.
* Structural Biology, Medicinal chemistry, AIMMS, Vrije Universiteit Amsterdam, Max Planck Institute of Molecular Plant Physiology
* Frontiers in Plant Science
* https://doi.org/10.3389/fpls.2021.697324
* Corresponding author: de Boer, A. H.
* Published Sep 2021 (early online 13 Sep 2021)
* Processed: 2021-9

Salinity is one of the major abiotic stresses that limits agricultural productivity worldwide. Many proteins with defined functions in salt stress adaptation are controlled through interactions with m ...

### *41) Low-Order Scaling Quasiparticle Self-Consistent GW for Molecules*

* Förster, A., Visscher, L.
* Theoretical Chemistry, AIMMS
* Frontiers in Chemistry
* https://doi.org/10.3389/fchem.2021.736591
* Corresponding author: Förster, A.
* Published Sep 2021 (early online 3 Sep 2021)
* Processed: 2021-9

Low-order scaling GW implementations for molecules are usually restricted to approximations with diagonal self-energy. Here, we present an all-electron implementation of quasiparticle self-consistent ...

### *42) Noninterfering and simultaneous Stern-Gerlach and Heisenberg microscope experiments to measure the full electron coordinate in an entangled state*

* Gritsenko, O. V.
* Theoretical Chemistry, AIMMS
* Physical Review A
* https://doi.org/10.1103/PhysRevA.104.032210
* Corresponding author: Gritsenko, O. V.
* Published Sep 2021 (early online 10 Sep 2021)
* Processed: 2021-9

In two celebrated experiments of quantum mechanics, the Stern-Gerlach (SG) and Heisenberg microscope (HM) experiments, the electron spin sz and spatial r coordinates are measured separately. In this p ...

### *43) Origin of asynchronicity in Diels-Alder reactions*

* Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp02456f
* Corresponding author: Vermeeren, P.
* Published 28 Sep 2021 (early online 3 Sep 2021)
* Processed: 2021-9

Asynchronicity in Diels-Alder reactions plays a crucial role in determining the height of the reaction barrier. Currently, the origin of asynchronicity is ascribed to the stronger orbital interaction ...

### *44) A method to monitor the NAD+ metabolome—from mechanistic to clinical applications*

* Giner, M. P., Christen, S., Bartova, S., Makarov, M. V., Migaud, M. E., Canto, C., Moco, S.
* Molecular and Computational Toxicology, AIMMS, Nestle, University of South Alabama, Olon Ricerca Bioscience
* International Journal of Molecular Sciences
* https://doi.org/10.3390/ijms221910598
* Corresponding author: Moco, S.
* Published 1 Oct 2021 (early online 30 Sep 2021)
* Processed: 2021-10

Nicotinamide adenine dinucleotide (NAD+) and its reduced form (NADH) are coenzymes employed in hundreds of metabolic reactions. NAD+ also serves as a substrate for enzymes such as sirtuins, poly(ADP‐r ...

### *45) Synthesis of Carbazoles and Dihydrocarbazoles by a Divergent Cascade Reaction of Donor-Acceptor Cyclopropanes*

* Faltracco, M., Damian, M., Ruijter, E.
* Organic Chemistry, AIMMS, Vrije Universiteit Amsterdam, University of Genoa
* Organic letters
* https://doi.org/10.1021/acs.orglett.1c02795
* Corresponding author: Ruijter, E.
* Published 1 Oct 2021 (early online 20 Sep 2021)
* Processed: 2021-10

An alkylation/olefination cascade of indolecarboxaldehydes and phosphonate-functionalized donor-acceptor cyclopropanes affords functionalized dihydrocarbazoles and cyclohepta[cd]indoles in formal (3 + ...

### *46) Dipolar repulsion in α-halocarbonyl compounds revisited*

* Rodrigues Silva, D., De Azevedo Santos, L., Hamlin, T. A., Bickelhaupt, F. M., P. Freitas, M., Fonseca Guerra, C.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Universidade Federal de Lavras
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp02502c
* Corresponding author: Bickelhaupt, F. M.
* Published 7 Oct 2021 (early online 1 Sep 2021)
* Processed: 2021-10

The concept of dipolar repulsion has been widely used to explain several phenomena in organic chemistry, including the conformational preferences of carbonyl compounds. This model, in which atoms and ...

### *47) How Lewis Acids Catalyze Ene Reactions*

* Tiekink, E. H., Vermeeren, P., Bickelhaupt, F. M., Hamlin, T. A.
* AIMMS, Theoretical Chemistry, Chemistry and Pharmaceutical Sciences
* European Journal of Organic Chemistry
* https://doi.org/10.1002/ejoc.202101107
* Corresponding author: Vermeeren, P.
* Published 7 Oct 2021 (early online 12 Sep 2021)
* Processed: 2021-10

The catalytic effect of various Lewis acids (LAs) on the ene reaction between propene (ene) and but-3-en-2-one (enophile) was studied quantum chemically using density functional theory and with couple ...

### *48) Probing the formation of isolated cyclo-FF peptide clusters by far-infrared action spectroscopy*

* Bakels, S., Stroganova, I., Rijs, A. M.
* BioAnalytical Chemistry, AIMMS
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp03237b
* Corresponding author: Rijs, A. M.
* Published 7 Oct 2021 (early online 15 Sep 2021)
* Processed: 2021-10

Small cyclic peptides containing phenylalanine residues are prone to aggregate in the gas phase into highly hydrophobic chains. A combination of laser desorption, mass spectrometry and conformational ...

### *49) Project earthrise: Proceedings of the ninth annual conference of in*

* Prescott, S. L., Wegienka, G., Kort, R., Nelson, D. H., Gabrysch, S., Hancock, T., Kozyrskyj, A., Lowry, C. A., Redvers, N., Poland, B., Robinson, J., Moubarac, J. C., Warber, S., Jansson, J., Sinkkonen, A., Penders, J., Erdman, S., Nanan, R., Van Den Bosch, M., Schneider, K., Schroeck, N. J., Sobko, T., Harvie, J., Kaplan, G. A., Moodie, R., Lengnick, L., Prilleltensky, I., Celidwen, Y., Berman, S. H., Logan, A. C., Berman, B.
* Molecular Cell Physiology, AIMMS, Places and Planet, University of Western Australia, Telethon Kids Institute, University of Maryland, Baltimore, Henry Ford Health System, Independent Researcher, Heidelberg University, Member of the Leibniz Association, Charité – Universitätsmedizin Berlin, University of Victoria BC, Alberta Learning, University of Colorado Boulder, University of North Dakota, University of Toronto, University of Sheffield, University of Montréal, University of Michigan, Ann Arbor, Pacific Northwest National Laboratory, Luke Natural Resources Institute Finland, Maastricht University, Massachusetts Institute of Technology, University of Sydney, University of British Columbia, Existential-Humanistic Institute, Saybrook University, Columbia University, University of Detroit Mercy, The University of Hong Kong, Institute for a Sustainable Future, University of Melbourne, LLC, University of Miami, Independent Researcher
* International Journal of Environmental Research and Public Health
* https://doi.org/10.3390/ijerph182010654
* Corresponding author: Prescott, S. L.
* Published 2 Oct 2021 (early online None)
* Processed: 2021-10

VIVO planetary healthThe “Earthrise” photograph, taken on the 1968 Apollo 8 mission, became one of the most significant images of the 20th Century. It triggered a profound shift in environmental aware ...

### *50) Electronic spectra of ytterbium fluoride from relativistic electronic structure calculations*

* Pototschnig, J. V., Dyall, K. G., Visscher, L., Gomes, A. S. P.
* Theoretical Chemistry, AIMMS, Dirac Solutions, Universite de Lille 2
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp03701c
* Corresponding author: Pototschnig, J. V.
* Published 21 Oct 2021 (early online 1 Oct 2021)
* Processed: 2021-10

We report an investigation of the low-lying excited states of the YbF molecule-a candidate molecule for experimental measurements of the electron electric dipole moment-with 2-component based multi-re ...

### *51) Fast Intrinsic Emission Quenching in Cs4Pb*

* Petralanda, U., Biffi, G., Boehme, S. C., Baranov, D., Krahne, R., Manna, L., Infante, I.
* Photo Conversion Materials, Theoretical Chemistry, AIMMS, Italian Institute of Technology, University of Genoa
* Nano Letters
* https://doi.org/10.1021/acs.nanolett.1c02537
* Corresponding author: Manna, L.
* Published 27 Oct 2021 (early online 13 Oct 2021)
* Processed: 2021-10

Br6NanocrystalsCs4PbBr6 (0D) nanocrystals at room temperature have both been reported as nonemissive and green-emissive systems in conflicting reports, with no consensus regarding both the origin of t ...