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### 1) The Gauche Effect in XCH2CH2X Revisited

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* https://doi.org/10.1002/cphc.202100090
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* Published 7 Apr 2021 (early online 8 Feb 2021)
* Processed: 2021-4

We have quantum chemically investigated the rotational isomerism of 1,2-dihaloethanes XCH2CH2X (X = F, Cl, Br, I) at ZORA-BP86-D3(BJ)/QZ4P. Our Kohn-Sham molecular orbital (KS-MO) analyses reveal that hyperconjugative orbital interactions favor the gauche conformation in all cases (X = F−I), not only for X = F as in the current model of this so-called gauche effect. We show that, instead, it is the interplay of hyperconjugation with Pauli repulsion between lone-pair-type orbitals on the halogen substituents that constitutes the causal mechanism for the gauche effect. Thus, only in the case of the relatively small fluorine atoms, steric Pauli repulsion is too weak to overrule the gauche preference of the hyperconjugative orbital interactions. For the larger halogens, X⋅⋅⋅X steric Pauli repulsion becomes sufficiently destabilizing to shift the energetic preference from gauche to anti, despite the opposite preference of hyperconjugation.

### 2) Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study

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* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Universidade Federal de Lavras, University of Hradec Kralove, Radboud University
* Journal of Computational Chemistry
* https://doi.org/10.1002/jcc.26489
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* Published 15 Apr 2021 (early online 5 Feb 2021)
* Processed: 2021-4

We have performed a hierarchical ab initio benchmark and DFT performance study of D2Ch•••A− chalcogen bonds (Ch = S, Se; D, A = F, Cl). The ab initio benchmark study is based on a series of ZORA-relativistic quantum chemical methods [HF, MP2, CCSD, CCSD(T)], and all-electron relativistically contracted variants of Karlsruhe basis sets (ZORA-def2-SVP, ZORA-def2-TZVPP, ZORA-def2-QZVPP) with and without diffuse functions. The highest-level ZORA-CCSD(T)/ma-ZORA-def2-QZVPP counterpoise-corrected complexation energies (ΔECPC) are converged within 1.1–3.4 kcal mol−1 and 1.5–3.1 kcal mol−1 with respect to the method and basis set, respectively. Next, we used the ZORA-CCSD(T)/ma-ZORA-def2-QZVPP (ΔECPC) as reference data for analyzing the performance of 13 different ZORA-relativistic DFT approaches in combination with the Slater-type QZ4P basis set. We find that the three-best performing functionals are M06-2X, B3LYP, and M06, with mean absolute errors (MAE) of 4.1, 4.2, and 4.3 kcal mol−1, respectively. The MAE for BLYP-D3(BJ) and PBE amount to 8.5 and 9.3 kcal mol−1, respectively.

### 3) Viral G Protein-Coupled Receptors: Attractive Targets for Herpesvirus-Associated Diseases

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* Medicinal chemistry, AIMMS, Vrije Universiteit Brussel
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* https://doi.org/10.1124/pharmrev.120.000186
* Corresponding author: None
* Published 1 Apr 2021 (early online 10 Mar 2021)
* Processed: 2021-4

Herpesviruses are ubiquitous pathogens that establish lifelong, latent infections in their host. Spontaneous reactivation of herpesviruses is often asymptomatic or clinically manageable in healthy individuals, but reactivation events in immunocompromised or immunosuppressed individuals can lead to severe morbidity and mortality. Moreover, herpesvirus infections have been associated with multiple proliferative cardiovascular and post-transplant diseases. Herpesviruses encode viral G protein-coupled receptors (vGPCRs) that alter the host cell by hijacking cellular pathways and play important roles in the viral life cycle and these different disease settings. In this review, we discuss the pharmacological and signaling properties of these vGPCRs, their role in the viral life cycle, and their contribution in different diseases. Because of their prominent role, vGPCRs have emerged as promising drug targets, and the potential of vGPCR-targeting therapeutics is being explored. Overall, these vGPCRs can be considered as attractive targets moving forward in the development of antiviral, cancer, and/or cardiovascular disease treatments. SIGNIFICANCE STATEMENT: In the last decade, herpesvirus-encoded G protein-coupled receptors (GPCRs) have emerged as interesting drug targets with the growing understanding of their critical role in the viral life cycle and in different disease settings. This review presents the pharmacological properties of these viral receptors, their role in the viral life cycle and different diseases, and the emergence of therapeutics targeting viral GPCRs.

### 4) Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions

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* Synlett
* https://doi.org/10.1055/s-0040-1707284
* Corresponding author: Orian, L.
* Published Apr 2021 (early online 9 Oct 2020)
* Processed: 2021-4

Metal-mediated [2+2+2] cycloadditions of unsaturated molecules to cyclic and polycyclic organic compounds are a versatile synthetic route affording good yields and selectivity under mild conditions. In the last two decades, in silico investigations have unveiled important details about the mechanism and the energetics of the whole catalytic cycle. Particularly, a number of computational studies address the topic of half-sandwich catalysts which, due to their structural fluxionality, have been widely employed, since the 1980s. In these organometallic species, the metal is coordinated to an aromatic ring, typically the ubiquitous cyclopentadienyl anion, C 5H 5-(Cp) or to the Cp moiety of a larger polycyclic aromatic ligand (Cp′). During the catalytic process, the metal continuously 'slips' on the ring, changing its hapticity. This phenomenon of metal slippage and its implications for the catalyst's performance are discussed in this work, referring to the most important computational mechanistic studies reported in literature for Rh(I) half-metallocenes, with the purpose of providing hints for a rational design of this class of compounds. 1 Introduction 2 Mechanism of Metal-Catalyzed Acetylene [2+2+2] Cycloaddition to Benzene and the Problem of the Indenyl Effect 2.1 Acetylene-Acetonitrile [2+2+2] Co-cycloaddition to 2-Methylpyridine: Evidence of the Indenyl Effect 2.2 Heteroaromatic Catalysts and the Evidence of a Reverse Indenyl Effect 2.3 Booth's Mechanistic Hypothesis and the Evidence of the Indenyl Effect 3 Structure-Reactivity Correlation: The Slippage-Span Model 4 Conclusions and Perspectives.

### 5) Heterologous Expression of eth

* Ho, V. Q., Verboom, T., Rong, M. K., Habjan, E., Bitter, W., Speer, A.
* Organic Chemistry, AIMMS, Molecular Microbiology, Vrije Universiteit Amsterdam
* Antimicrobial agents and chemotherapy
* https://doi.org/10.1128/AAC.01445-20
* Corresponding author: Speer, A.
* Published Apr 2021 (early online None)
* Processed: 2021-4

A and katG in Mycobacterium marinum Enables the Rapid Identification of New Prodrugs Active against Mycobacterium tuberculosisScreening strategies for antituberculosis compounds using Mycobacterium tuberculosis are time consuming and require biosafety level 3 (BSL3) facilities, which makes the development of high-throughput assays difficult and expensive. Mycobacterium marinum, a close genetic relative of M. tuberculosis, possesses several advantages as a suitable model for tuberculosis drug screening. However, despite the high genetic similarity, there are some obvious differences in susceptibility to some tuberculosis drugs between these two species, especially for the prodrugs ethionamide and isoniazid. In this study, we aimed to improve M. marinum as a model for antituberculosis drug identification by heterologous expression of two common drug activators, EthA and KatG. These two activators were overexpressed in M. marinum, and the strains were tested against ethionamide, isoniazid, and a library of established antimycobacterial compounds from TB Alliance to compare drug susceptibility. Both in vitro and in vivo using zebrafish larvae, these genetically modified M. marinum strains showed significantly higher susceptibility against ethionamide and isoniazid, which require activation by EthA and KatG. More importantly, a strain overexpressing both ethA and katG was potentially more susceptible to approximately 20% of the antituberculosis hit compounds from the TB Alliance library. Most of these compounds were activated by EthA in M. marinum. Four of these compounds were selected for further analysis, and three of them showed obvious EthA-dependent activity against M. tuberculosis. Overall, our developed M. marinum strains are valuable tools for high-throughput discovery of potential novel antituberculosis prodrugs.

### 6) Analysis of missense variants in the human histamine receptor family reveals increased constitutive activity of e4106.30×30k variant in the histamine h1 receptor

* Ma, X., Segura, M. A., Zarzycka, B., Vischer, H. F., Leurs, R.
* Medicinal chemistry, AIMMS
* International Journal of Molecular Sciences
* https://doi.org/10.3390/ijms22073702
* Corresponding author: Leurs, R.
* Published 1 Apr 2021 (early online None)
* Processed: 2021-4

The Exome Aggregation Consortium has collected the protein-encoding DNA sequences of almost 61,000 unrelated humans. Analysis of this dataset for G protein-coupled receptor (GPCR) proteins (available at GPCRdb) revealed a total of 463 naturally occurring genetic missense variations in the histamine receptor family. In this research, we have analyzed the distribution of these missense variations in the four histamine receptor subtypes concerning structural segments and sites important for GPCR function. Four missense variants R1273.52×52H, R13934.57×57H, R4096.29×29H, and E4106.30×30 K, were selected for the histamine H1 receptor (H1R) that were hypothesized to affect receptor activity by interfering with the interaction pattern of the highly conserved D(E)RY motif, the so-called ionic lock. The E4106.30×30 K missense variant displays higher constitutive activity in G protein signaling as compared to wild-type H1R, whereas the opposite was observed for R1273.52×52H, R13934.57×57H, and R4096.29×29H. The E4106.30×30 K missense variant displays a higher affinity for the endogenous agonist histamine than wild-type H1R, whereas antagonist affinity was not affected. These data support the hypothesis that the E4106.30×30 K mutation shifts the equilibrium towards active conformations. The study of these selected missense variants gives additional insight into the structural basis of H1R activation and, moreover, highlights that missense variants can result in pharmacologically different behavior as compared to wild-type receptors and should consequently be considered in the drug discovery process.

### 7) A Quantitative Molecular Orbital Perspective of the Chalcogen Bond

* de Azevedo Santos, L., van der Lubbe, S. C., Hamlin, T. A., Ramalho, T. C., Matthias Bickelhaupt, F.
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* ChemistryOpen
* https://doi.org/10.1002/open.202100066
* Corresponding author: None
* Published 1 Apr 2021 (early online None)
* Processed: 2021-4

Invited for this month's cover are the groups of Prof. Dr. Teodorico C. Ramalho (Federal University of Lavras and University Hradec Kralove) and Prof. Dr. F. Matthias Bickelhaupt (Vrije Universiteit Amsterdam and Radboud University). The cover picture shows the key message of their work, that is, the covalency of the chalcogen bonds, in an elegantly simple and attractive manner. To that end, the chalcogen bonds are represented by schematic 3D structures of the bond donor D2 Ch and the bond acceptor A- , and their attractive interaction in green. Then, a colorful molecular orbital (MO) diagram where the HOMO-LUMO mixing is represented by the mixing of red (HOMO) and blue (LUMO) into purple (MO) is presented. Read the full text of their Full Paper at 10.1002/open.202000323.

### 8) Characterisation of (anti-)progestogenic and (anti-)androgenic activities in surface and wastewater using high resolution effectdirected analysis

* Houtman, C. J., Brewster, K., ten Broek, R., Duijve, B., van Oorschot, Y., Rosielle, M., Lamoree, M. H., Steen, R. J.
* E&H: Environmental Chemistry and Toxicology, AIMMS, The Water Laboratory
* Environment International
* https://doi.org/10.1016/j.envint.2021.106536
* Corresponding author: Lamoree, M. H.
* Published Aug 2021 (early online 1 Apr 2021)
* Processed: 2021-4

The quality of surface waters is threatened by pollution with low concentrations of bioactive chemicals, among which those interfering with steroid hormone systems. Induced by reports of anti-progestogenic activity in surface waters, a two-year four-weekly survey of (anti-)progestogenic activity was performed at three surface water locations in the Netherlands that serve as abstraction points for the production of drinking water. As certain endogenous and synthetic progestogenic compounds are also potent (anti-)androgens, these activities were also investigated. Anti-progestogenic and anti-androgenic activities were detected in the majority of the monitoring samples, sometimes in concentrations exceeding effect-based trigger values, indicating the need for further research. To characterize the compounds responsible for the activities, a high resolution Effect-Directed Analysis (hr-EDA) panel was combined with PR and AR CALUX bioassays, performed in agonistic and antagonistic modes. The influent and effluent of a domestic wastewater treatment plant (WWTP) were included as effluent is a possible emission source of active compounds. As drivers for androgenic and progestogenic activities several native and synthetic steroid hormones were identified in the WWTP samples, namely androstenedione, testosterone, DHT, levonorgestrel and cyproterone acetate. The pesticides metolachlor and cyazofamid were identified as contributors to both the anti-progestogenic and anti-androgenic activities in surface water. In addition, epiconazole contributed to the anti-progestogenic activities in the rivers Rhine and Enclosed Meuse. This study showed the strength of hr-EDA for the identification of bioactive compounds in environmental samples and shed light on the drivers of (anti-)progestogenic and (anti-)androgenic activities in the aquatic environment.

### 9) Proteome constraints reveal targets for improving microbial fitness in nutrient-rich environments

* Chen, Y., van Pelt-KleinJan, E., van Olst, B., Douwenga, S., Boeren, S., Bachmann, H., Molenaar, D., Nielsen, J., Teusink, B.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, Chalmers University of Technology, Wageningen University & Research, Vrije Universiteit Amsterdam, Technical University of Denmark, Copenhagen University
* Molecular Systems Biology
* https://doi.org/10.15252/msb.202010093
* Corresponding author: None
* Published 1 Apr 2021 (early online None)
* Processed: 2021-4

Cells adapt to different conditions via gene expression that tunes metabolism for maximal fitness. Constraints on cellular proteome may limit such expression strategies and introduce trade-offs. Resource allocation under proteome constraints has explained regulatory strategies in bacteria. It is unclear, however, to what extent these constraints can predict evolutionary changes, especially for microorganisms that evolved under nutrient-rich conditions, i.e., multiple available nitrogen sources, such as Lactococcus lactis. Here, we present a proteome-constrained genome-scale metabolic model of L.lactis (pcLactis) to interpret growth on multiple nutrients. Through integration of proteomics and flux data, in glucose-limited chemostats, the model predicted glucose and arginine uptake as dominant constraints at low growth rates. Indeed, glucose and arginine catabolism were found upregulated in evolved mutants. At high growth rates, pcLactis correctly predicted the observed shutdown of arginine catabolism because limited proteome availability favored lactate for ATP production. Thus, our model-based analysis is able to identify and explain the proteome constraints that limit growth rate in nutrient-rich environments and thus form targets of fitness improvement.

### 10) Short‐ and long‐term social recognition memory are differentially modulated by neuronal histamine

* Rani, B., Silva‐marques, B., Leurs, R., Passani, M. B., Blandina, P., Provensi, G.
* Medicinal chemistry, AIMMS, University of Florence, Universidade Federal de São Carlos
* Biomolecules
* https://doi.org/10.3390/biom11040555
* Corresponding author: Provensi, G.
* Published 9 Apr 2021 (early online None)
* Processed: 2021-4

The ability of recognizing familiar conspecifics is essential for many forms of social interaction including reproduction, establishment of dominance hierarchies, and pair bond formation in monogamous species. Many hormones and neurotransmitters have been suggested to play key roles in social discrimination. Here we demonstrate that disruption or potentiation of histaminergic neu-rotransmission differentially affects short (STM) and long‐term (LTM) social recognition memory. Impairments of LTM, but not STM, were observed in histamine‐deprived animals, either chronically (Hdc−/− mice lacking the histamine‐synthesizing enzyme histidine decarboxylase) or acutely (mice treated with the HDC irreversible inhibitor α‐fluoromethylhistidine). On the contrary, restriction of histamine release induced by stimulation of the H3R agonist (VUF16839) impaired both STM and LTM. H3R agonism‐induced amnesic effect was prevented by pre‐treatment with donepezil, an ac-etylcholinesterase inhibitor. The blockade of the H3R with ciproxifan, which in turn augmented histamine release, resulted in a procognitive effect. In keeping with this hypothesis, the procognitive effect of ciproxifan was absent in both Hdc−/− and αFMH‐treated mice. Our results suggest that brain histamine is essential for the consolidation of LTM but not STM in the social recognition test. STM impairments observed after H3R stimulation are probably related to their function as heterorecep-tors on cholinergic neurons.

### 11) Evaluation of chemicals of environmental concern in crumb rubber and water leachates from several types of synthetic turf football pitches

* Celeiro, M., Armada, D., Ratola, N., Dagnac, T., de Boer, J., Llompart, M.
* Environment and Health, AIMMS, University of Santiago de Compostela, University of Porto, Agronomic Research Centre (AGACAL-CIAM) – Unit of Organic Contaminants
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2020.128610
* Corresponding author: Llompart, M.
* Published May 2021 (early online 19 Oct 2020)
* Processed: 2021-5

Nowadays concern exists about the safety for both football players and the environment of recycled tire rubber used as infill in synthetic turf football pitches. In this study 40 target compounds, including polycyclic aromatic hydrocarbons (PAHs), plasticizers, antioxidants and vulcanization agents were determined in 50 synthetic football pitches of diverse characteristics to estimate environmental risks. This is the first study of crumb rubber sport facilities in Portugal. Analyses were performed by ultrasound-assisted extraction followed by gas chromatography-tandem mass spectrometry (UAE-GC-MS/MS). To evaluate the transfer of the target chemicals from the crumb rubber to the runoff water, water leachates collected from several football pitches were analyzed by solid-phase microextraction (SPME-GC-MS/MS). In addition, lab-scale runoff simulation experiments were performed to assess whether a persistent inflow of the target compounds from the football pitches into the runoff water wcould exist. Results revealed the presence of most of the target PAHs in crumb rubber at total concentrations up to 57 μg g−1, next to a high number of plasticizers and vulcanization agents. Runoff water collected from the football pitches contained up to 13 PAHs as well as other chemicals of environmental concern. In addition, continuous leaching of chemicals from the crumb rubber to the surrounding water was demonstrated. The transfer of target chemicals into the runoff water poses a potential risk for the aquatic environment.

### *12) Halide Perovskite-Lead Chalcohalide Nanocrystal Heterostructures*

* Imran, M., Peng, L., Pianetti, A., Pinchetti, V., Ramade, J., Zito, J., Di Stasio, F., Buha, J., Toso, S., Song, J., Infante, I., Bals, S., Brovelli, S., Manna, L.
* AIMMS, Theoretical Chemistry, Italian Institute of Technology, Shenzhen University, University of Milan - Bicocca, University of Antwerp, University of Genoa, Catholic University of the Sacred Heart
* Journal of the American Chemical Society
* https://doi.org/10.1021/jacs.0c10916
* Corresponding author: Song, J., Infante, I., Bals, S., Brovelli, S., Manna, L.
* Published 13 Jan 2021 (early online None)
* Processed: 2021-1

We report the synthesis of colloidal CsPbX3-Pb4S3Br2 (X = Cl, Br, I) nanocrystal heterostructures, providing an example of a sharp and atomically resolved epitaxial interface between a metal halide pe ...

### *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

...

### *14) An Environmental Dilemma for China During the COVID-19 Pandemic: The Explosion of Disposable Plastic Wastes*

* Liu, J., Vethaak, A. D., An, L., Liu, Q., Yang, Y., Ding, J.
* AIMMS, Environment and Health, Jiangnan University, Chinese Research Academy of Environmental Sciences, Nagoya University, Jiangsu Provincial Academy of Environmental Science, Deltares
* Bulletin of Environmental Contamination and Toxicology
* https://doi.org/10.1007/s00128-021-03121-x
* Corresponding author: Liu, J.
* Published Feb 2021 (early online 29 Jan 2021)
* Processed: 2021-2

Plastic pollution control has been on top of the political agenda in China. In January 2020, China announced a phased ban on the production and usage of various types of single-use plastics as a solut ...

### *15) How Lewis Acids Catalyze Ring-Openings of Cyclohexene Oxide*

* Hansen, T., Vermeeren, P., Yoshisada, R., Filippov, D. V., Van Der Marel, G. A., Codée, J. D., Hamlin, T. A.
* Chemistry and Pharmaceutical Sciences, Theoretical Chemistry, AIMMS, Leiden University
* Journal of Organic Chemistry
* https://doi.org/10.1021/acs.joc.0c02955
* Corresponding author: Hamlin, T. A.
* Published 4 Feb 2021 (early online None)
* Processed: 2021-2

We have quantum chemically studied the Lewis acid-catalyzed epoxide ring-opening reaction of cyclohexene epoxide by MeZH (Z = O, S, and NH) using relativistic dispersion-corrected density functional t ...

### *16) Analysis of recycled rubber: Development of an analytical method and determination of polycyclic aromatic hydrocarbons and heterocyclic aromatic compounds in rubber matrices*

* Skoczyńska, E., Leonards, P. E., Llompart, M., de Boer, J.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, Environment and Health, University of Santiago de Compostela
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2021.130076
* Corresponding author: Skoczyńska, E.
* Published Aug 2021 (early online 23 Feb 2021)
* Processed: 2021-2

Recycled crumb rubber (CR) is rich in compounds with unrecognized toxic potency; this study aims at the development of an analytical method that would allow identification and quantification of a very ...

### *17) Validating Differential Volatilome Profiles in Parkinson’s Disease*

* Sinclair, E., Walton-Doyle, C., Sarkar, D., Hollywood, K. A., Milne, J., Lim, S. H., Kunath, T., Rijs, A. M., Bie, R. M. A. D., Silverdale, M., Trivedi, D. K., Barran, P.
* BioAnalytical Chemistry, AIMMS
* ACS Central Science
* https://doi.org/10.1021/acscentsci.0c01028
* Corresponding author: None
* Published 24 Feb 2021 (early online None)
* Processed: 2021-2

...

### *18) 1,1,4,4-Tetracyanobutadiene-Functionalized Anthracenes: Regioselectivity of Cycloadditions in the Synthesis of Small Near-IR Dyes*

* Philippe, C., Bui, A. T., Batsongo-Boulingui, S., Pokladek, Z., Matczyszyn, K., Mongin, O., Lemiègre, L., Paul, F., Hamlin, T. A., Trolez, Y.
* Theoretical Chemistry, AIMMS, Université de Rennes 1, Wrocław University of Science and Technology
* Organic letters
* https://doi.org/10.1021/acs.orglett.1c00136
* Corresponding author: Trolez, Y.
* Published 19 Mar 2021 (early online 26 Feb 2021)
* Processed: 2021-3

Two small 1,1,4,4-tetracyanobutadiene-functionalized chromophores were obtained by careful leverage of the regioselectivity of the cycloaddition reaction of tetracyanoethylene with anthracene-ynamide ...

### *19) How metallylenes activate small molecules*

* Vermeeren, P., Doppert, M. T., Bickelhaupt, F. M., Hamlin, T. A.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Vrije Universiteit Amsterdam
* Chemical Science
* https://doi.org/10.1039/d0sc05987k
* Corresponding author: Hamlin, T. A.
* Published 28 Mar 2021 (early online 18 Feb 2021)
* Processed: 2021-3

We have studied the activation of dihydrogen by metallylenes using relativistic density functional theory (DFT). Our detailed activation strain and Kohn-Sham molecular orbital analyses have quantified ...

### *20) Combined cellomics and proteomics analysis reveals shared neuronal morphology and molecular pathway phenotypes for multiple schizophrenia risk genes*

* Rosato, M., Stringer, S., Gebuis, T., Paliukhovich, I., Li, K. W., Posthuma, D., Sullivan, P. F., Smit, A. B., van Kesteren, R. E.
* Molecular and Cellular Neurobiology, Complex Trait Genetics, AIMMS, Amsterdam Neuroscience - Cellular & Molecular Mechanisms, Amsterdam Neuroscience - Neurodegeneration, Amsterdam Neuroscience - Complex Trait Genetics, Center for Neurogenomics and Cognitive Research, University of North Carolina at Chapel Hill, Karolinska Institutet
* Molecular Psychiatry
* https://doi.org/10.1038/s41380-019-0436-y
* Corresponding author: van Kesteren, R. E.
* Published Mar 2021 (early online None)
* Processed: 2021-3

An enigma in studies of neuropsychiatric disorders is how to translate polygenic risk into disease biology. For schizophrenia, where > 145 significant GWAS loci have been identified and only a few gen ...

### *21) Effect of Extreme Weather Events on Contaminant Transport From Urban Run-Off to a Fjord System*

* Breedveld, G. D., Hansen, M. C., Hale, S. E., Allan, I. J., Hamers, T.
* E&H: Environmental Health and Toxicology, AIMMS, Norwegian Geotechnical Institute, University of Oslo, Norwegian Institute for Water Research
* Frontiers in Environmental Science
* https://doi.org/10.3389/fenvs.2021.601300
* Corresponding author: Breedveld, G. D.
* Published Mar 2021 (early online 4 Mar 2021)
* Processed: 2021-3

Urbanization has resulted in increased contaminant run-off in densely populated areas. Climate change is expected to result in a higher frequency of extreme weather events including torrential rainfal ...

### *22) Symposium on Lactic Acid Bacteria-reading while waiting for a meeting*

* Teusink, B., Kuipers, O. P., Moineau, S.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, University of Groningen, avenue de la MédecineUniversité Laval
* FEMS Microbiology Reviews
* https://doi.org/10.1093/femsre/fuaa049
* Corresponding author: None
* Published Mar 2021 (early online 16 Mar 2021)
* Processed: 2021-3

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### *23) The proteome of granulovacuolar degeneration and neurofibrillary tangles in Alzheimer’s disease*

* Hondius, D. C., Koopmans, F., Leistner, C., Pita-Illobre, D., Peferoen-Baert, R. M., Marbus, F., Paliukhovich, I., Li, K. W., Rozemuller, A. J., Hoozemans, J. J., Smit, A. B.
* Molecular and Cellular Neurobiology, Amsterdam Neuroscience - Cellular & Molecular Mechanisms, Amsterdam Neuroscience - Neurodegeneration, AIMMS, Center for Neurogenomics and Cognitive Research, Vrije Universiteit Amsterdam
* Acta Neuropathologica
* https://doi.org/10.1007/s00401-020-02261-4
* Corresponding author: Hondius, D. C.
* Published Mar 2021 (early online None)
* Processed: 2021-3

Granulovacuolar degeneration (GVD) is a common feature in Alzheimer’s disease (AD). The occurrence of GVD is closely associated with that of neurofibrillary tangles (NFTs) and GVD is even considered t ...

### *24) Not Carbon s–p Hybridization, but Coordination Number Determines C−H and C−C Bond Length*

* Vermeeren, P., Zeist, W., Hamlin, T. A., Guerra, C. F., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Chemistry: A European Journal
* https://doi.org/10.1002/chem.202004653
* Corresponding author: None
* Published 3 Mar 2021 (early online None)
* Processed: 2021-3

...

### *25) How the Lewis Base F– Catalyzes the 1,3-Dipolar Cycloaddition between Carbon Dioxide and Nitrilimines*

* Svatunek, D., Hansen, T., Houk, K. N., Hamlin, T. A.
* Theoretical Chemistry, Chemistry and Pharmaceutical Sciences, AIMMS
* The Journal of organic chemistry
* https://doi.org/10.1021/acs.joc.0c02963
* Corresponding author: None
* Published 5 Mar 2021 (early online None)
* Processed: 2021-3

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### *26) A flat embedding method for transmission electron microscopy reveals an unknown mechanism of tetracycline*

* Wenzel, M., Dekker, M. P., Wang, B., Burggraaf, M. J., Bitter, W., van Weering, J. R., Hamoen, L. W.
* Functional Genomics, Molecular Microbiology, AIMMS, Bioinformatics, University of Amsterdam, Chalmers University of Technology
* Communications biology
* https://doi.org/10.1038/s42003-021-01809-8
* Corresponding author: None
* Published 8 Mar 2021 (early online None)
* Processed: 2021-3

Transmission electron microscopy of cell sample sections is a popular technique in microbiology. Currently, ultrathin sectioning is done on resin-embedded cell pellets, which consumes milli- to decili ...

### *27) Differential Involvement of ACKR3 C-Tail in β-Arrestin Recruitment, Trafficking and Internalization*

* Zarca, A., Perez, C., van den Bor, J., Bebelman, J. P., Heuninck, J., de Jonker, R. J., Durroux, T., Vischer, H. F., Siderius, M., Smit, M. J.
* Medicinal chemistry, AIMMS, Vrije Universiteit Amsterdam, Université de Montpellier
* Cells
* https://doi.org/10.3390/cells10030618
* Corresponding author: None
* Published 11 Mar 2021 (early online None)
* Processed: 2021-3

Background: The atypical chemokine receptor 3 (ACKR3) belongs to the superfamily of G protein-coupled receptors (GPCRs). Unlike classical GPCRs, this receptor does not activate G proteins in most cell ...

### *28) Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radical-Coupling Reactions (Pn=N, P, As)The controlled release of well-defined radical species under mild conditions for subsequent use in selective reactions is an important and challenging task in synthetic chemistry. We show here that simple bismuth amide species [Bi(NAr2)3] readily release aminyl radicals [NAr2]. at ambient temperature in solution. These reactions yield the corresponding hydrazines, Ar2N−NAr2, as a result of highly selective N−N coupling. The exploitation of facile homolytic Bi−Pn bond cleavage for Pn−Pn bond formation was extended to higher homologues of the pnictogens (Pn=N–As): homoleptic bismuth amides mediate the highly selective dehydrocoupling of HPn*

* Oberdorf, K., Hanft, A., Ramler, J., Krummenacher, I., Bickelhaupt, F. M., Poater, J., Lichtenberg, C.
* Chemistry and Pharmaceutical Sciences, AIMMS, Theoretical Chemistry, University of Würzburg
* Angewandte Chemie - International Edition
* https://doi.org/10.1002/anie.202015514
* Corresponding author: Lichtenberg, C.
* Published 15 Mar 2021 (early online 14 Dec 2020)
* Processed: 2021-3

R2 to give R2Pn−PnR2. Analyses by NMR and EPR spectroscopy, single-crystal X-ray diffraction, and DFT calculations reveal low Bi−N homolytic bond-dissociation energies, suggest radical coupling in the ...

### *29) Bifunctional Hydrogen Bond Donor-Catalyzed Diels–Alder Reactions: Origin of Stereoselectivity and Rate Enhancement*

* Vermeeren, P., Hamlin, T. A., Bickelhaupt, F. M., Fernández, I.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Complutense University
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202004496
* Corresponding author: Hamlin, T. A.
* Published 17 Mar 2021 (early online 10 Nov 2020)
* Processed: 2021-3

The selectivity and rate enhancement of bifunctional hydrogen bond donor-catalyzed Diels–Alder reactions between cyclopentadiene and acrolein were quantum chemically studied using density functional t ...

### *30) Controlling the selectivity of aminergic GPCR ligands from the extracellular vestibule*

* Egyed, A., Kelemen, Á. A., Vass, M., Visegrády, A., Thee, S. A., Wang, Z., de Graaf, C., Brea, J., Loza, M. I., Leurs, R., Keserű, G. M.
* Medicinal chemistry, AIMMS, Eötvös Loránd Research Network, Gedeon, University of Santiago de Compostela
* Bioorganic Chemistry
* https://doi.org/10.1016/j.bioorg.2021.104832
* Corresponding author: Keserű, G. M.
* Published Jun 2021 (early online 19 Mar 2021)
* Processed: 2021-3

In addition to the orthosteric binding pocket (OBP) of GPCRs, recent structural studies have revealed that there are several allosteric sites available for pharmacological intervention. The secondary ...

### *31) An annotation database for chemicals of emerging concern in exposome research*

* Meijer, J., Lamoree, M., Hamers, T., Antignac, J. P., Hutinet, S., Debrauwer, L., Covaci, A., Huber, C., Krauss, M., Walker, D. I., Schymanski, E. L., Vermeulen, R., Vlaanderen, J.
* E&H: Environmental Chemistry and Toxicology, AIMMS, E&H: Environmental Health and Toxicology, École nationale vétérinaire, agroalimentaire et de l'alimentation, Nantes-Atlantique, INRAE, INRAE, University of Antwerp, Helmholtz Centre for Environmental Research, Icahn School of Medicine at Mount Sinai, University of Luxembourg, Utrecht University
* Environment International
* https://doi.org/10.1016/j.envint.2021.106511
* Corresponding author: Vlaanderen, J.
* Published Jul 2021 (early online 24 Mar 2021)
* Processed: 2021-3

Background: Chemicals of Emerging Concern (CECs) include a very wide group of chemicals that are suspected to be responsible for adverse effects on health, but for which very limited information is av ...

### *32) The Pauli Repulsion-Lowering Concept in Catalysis*

* Hamlin, T. A., Bickelhaupt, F. M., Fernández, I.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences
* Accounts of Chemical Research
* https://doi.org/10.1021/acs.accounts.1c00016
* Corresponding author: None
* Published 24 Mar 2021 (early online None)
* Processed: 2021-3

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### *33) Model selection reveals the butyrate-producing gut bacterium Coprococcus eutactus as predictor for language development in three-year-old rural Ugandan children*

* Kort, R., Schlösser, J., Vazquez, A. R., Atukunda, P., Muhoozi, G. K., Wacoo, A. P., Sybesma, W. F., Westerberg, A. C., Iversen, P. O., Schoen, E. D.
* Molecular Cell Physiology, AIMMS
* medRxiv
* https://doi.org/10.1101/2021.03.15.21253665
* Corresponding author: None
* Published 25 Mar 2021 (early online None)
* Processed: 2021-3

Introduction The metabolic activity of the gut microbiota plays a pivotal role in the gut-brain axis through the effects of bacterial metabolites on brain function and development. In this study we in ...

### *34) Do Sulfonamides Interact with Aromatic Rings?*

* Jian, J., Hammink, R., McKenzie, C. J., Bickelhaupt, F. M., Poater, J., Mecinović, J.
* Chemistry and Pharmaceutical Sciences, AIMMS, Theoretical Chemistry, University of Southern Denmark, Radboud University Nijmegen
* Chemistry - A European Journal
* https://doi.org/10.1002/chem.202004732
* Corresponding author: Mecinović, J.
* Published 26 Mar 2021 (early online 30 Dec 2020)
* Processed: 2021-3

Aromatic rings form energetically favorable interactions with many polar groups in chemical and biological systems. Recent molecular studies have shown that sulfonamides can chelate metal ions and for ...

### *35) How Oriented External Electric Fields Modulate Reactivity*

* Yu, S., 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.202004906
* Corresponding author: Hamlin, T. A.
* Published 26 Mar 2021 (early online 7 Dec 2020)
* Processed: 2021-3

A judiciously oriented external electric field (OEEF) can catalyze a wide range of reactions and can even induce endo/exo stereoselectivity of cycloaddition reactions. The Diels–Alder reaction between ...

### *36) Conventional and high resolution chemical characterization to assess refinery effluent treatment performance*

* Hjort, M., den Haan, K. H., Whale, G., Koekkoek, J., Leonards, P. E., Redman, A. D., Vaiopoulou, E.
* E&H: Environmental Chemistry and Toxicology, AIMMS, E&H: Environmental Bioanalytical Chemistry, Concawe, Klaas den Haan E&S Consulting, Shell Health Risk Science Team, ExxonMobil Petroleum and Chemical
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2021.130383
* Corresponding author: Hjort, M.
* Published Sep 2021 (early online 27 Mar 2021)
* Processed: 2021-3

Refinery effluents represent an emission source of hydrocarbons (HCs) and other constituents to the environment. Thus, characterisation of effluent quality in terms of concentrations of key parameters ...

### *37) Genome-wide data implicate terminal fusion automixis in king cobra facultative parthenogenesis*

* Card, D. C., Vonk, F. J., Smalbrugge, S., Casewell, N. R., Wüster, W., Castoe, T. A., Schuett, G. W., Booth, W.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of Texas at Arlington, Harvard University, Wageningen University & Research, Liverpool School of Tropical Medicine, Bangor University, Chiricahua Desert Museum, Georgia State University, University of Tulsa
* Scientific Reports
* https://doi.org/10.1038/s41598-021-86373-1
* Corresponding author: Booth, W.
* Published 31 Mar 2021 (early online None)
* Processed: 2021-3

Facultative parthenogenesis (FP) is widespread in the animal kingdom. In vertebrates it was first described in poultry nearly 70years ago, and since then reports involving other taxa have increased co ...