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

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* https://doi.org/10.1002/open.202000323
* Corresponding author: Bickelhaupt, F. M.
* Published Apr 2021 (early online 17 Feb 2021)
* Processed: 2021-4

We have quantum chemically analyzed the structure and stability of archetypal chalcogen-bonded model complexes D2Ch⋅⋅⋅A− (Ch = O, S, Se, Te; D, A = F, Cl, Br) using relativistic density functional theory at ZORA-M06/QZ4P. Our purpose is twofold: (i) to compute accurate trends in chalcogen-bond strength based on a set of consistent data; and (ii) to rationalize these trends in terms of detailed analyses of the bonding mechanism based on quantitative Kohn-Sham molecular orbital (KS-MO) theory in combination with a canonical energy decomposition analysis (EDA). At odds with the commonly accepted view of chalcogen bonding as a predominantly electrostatic phenomenon, we find that chalcogen bonds, just as hydrogen and halogen bonds, have a significant covalent character stemming from strong HOMO−LUMO interactions. Besides providing significantly to the bond strength, these orbital interactions are also manifested by the structural distortions they induce as well as the associated charge transfer from A− to D2Ch.

### 2) Dispersion without Many-Body Density Distortion: Assessment on Atoms and Small Molecules

* Kooi, D. P., Weckman, T., Gori-Giorgi, P.
* Theoretical Chemistry, AIMMS
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.1c00102
* Corresponding author: Kooi, D. P.
* Published 13 Apr 2021 (early online 10 Mar 2021)
* Processed: 2021-4

The "fixed diagonal matrices"(FDM) dispersion formalism [ Kooi, D. P.; et al. J. Phys. Chem. Lett. 2019, 10, 1537 ] is based on a supramolecular wave function constrained to leave the diagonal of the many-body density matrix of each monomer unchanged, reducing dispersion to a balance between kinetic energy and monomer-monomer interaction. The corresponding variational optimization leads to expressions for the dispersion energy in terms of the ground-state pair densities of the isolated monomers only, providing a framework to build new approximations without the need for polarizabilities or virtual orbitals. Despite the underlying microscopic real space mechanism being incorrect, as in the exact case there is density relaxation, the formalism has been shown to give extremely accurate (or even exact) dispersion coefficients for H and He. The question we answer in this work is how accurate the FDM expressions can be for isotropic and anisotropic C6 dispersion coefficients when monomer pair densities are used from different levels of theory, namely Hartree-Fock, MP2, and CCSD. For closed-shell systems, FDM with CCSD monomer pair densities yield a mean average percent error for isotropic C6 dispersion coefficients of about 7% and a maximum absolute error within 18%, with a similar accuracy for anisotropies. The performance for open-shell systems is less satisfactory, with CCSD pair densities performing sometimes worse than Hartree-Fock or MP2. In the present implementation, the computational cost on top of the monomer's ground-state calculations is O(N4). The results show little sensitivity to the basis set used in the monomer's calculations.

### 3) A bifunctional iminophosphorane squaramide catalyzed enantioselective synthesis of hydroquinazolines: Via intramolecular aza-Michael reaction to α,β-unsaturated esters

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* https://doi.org/10.1039/d1sc00856k
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* Published 7 May 2021 (early online 18 Mar 2021)
* Processed: 2021-5

An efficient synthesis of enantioenriched hydroquinazoline cores via a novel bifunctional iminophosphorane squaramide catalyzed intramolecular aza-Michael reaction of urea-linked α,β-unsaturated esters is described. The methodology exhibits a high degree of functional group tolerance around the forming hydroquinazoline aryl core and wide structural variance on the nucleophilic N atom of the urea moiety. Excellent yields (up to 99%) and high enantioselectivities (up to 97 : 3 er) using both aromatic and less acidic aliphatic ureas were realized. The potential industrial applicability of the transformation was demonstrated in a 20 mmol scale-up experiment using an adjusted catalyst loading of 2 mol%. The origin of enantioselectivity and reactivity enhancement provided by the squaramide motif has been uncovered computationally using density functional theory (DFT) calculations, combined with the activation strain model (ASM) and energy decomposition analysis (EDA).

### 4) Proton Transfer and SN2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx

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* ChemPlusChem
* https://doi.org/10.1002/cplu.202000660
* Corresponding author: Orian, L.
* Published Apr 2021 (early online 9 Nov 2020)
* Processed: 2021-4

The so-called peroxidatic cysteines and selenocysteines in proteins reduce hydroperoxides through a dual attack to the peroxide bond in a two-step mechanism. First, a proton dislocation from the thiol/selenol to a close residue of the enzymatic pocket occurs. Then, a nucleophilic attack of the anionic cysteine/selenocysteine to one O atom takes place, while the proton is shuttled back to the second O atom, promoting the formation of a water molecule. In this computational study, we use a molecular model of GPx to demonstrate that the enzymatic environment significantly lowers the barrier of the latter SN2 step. Particularly, in our Se-based model the energy barriers for the two steps are 29.82 and 2.83 kcal mol−1, both higher than the corresponding barriers computed in the enzymatic cluster, i. e., 21.60 and null, respectively. Our results, obtained at SMD-B3LYP-D3(BJ)/6-311+G(d,p), cc-pVTZ//B3LYP-D3(BJ)/6-311G(d,p), cc-pVTZ level of theory, show that the mechanistic details can be well reproduced using an oversimplified model, but the energetics is definitively more favorable in the GPx active site. In addition, we pinpoint the role of the chalcogen in the peroxide reduction process, rooting the advantages of the presence of selenium in its acidic and nucleophilic properties.

### 5) Structure Activity Relationship of N-Substituted Phenyldihydropyrazolones Against Trypanosoma cruzi Amastigotes

* Sijm, M., Maes, L., de Esch, I. J., Caljon, G., Sterk, G. J., Leurs, R.
* Medicinal chemistry, Chemistry and Pharmaceutical Sciences, AIMMS, University of Antwerp
* Frontiers in Chemistry
* https://doi.org/10.3389/fchem.2021.608438
* Corresponding author: Leurs, R.
* Published Apr 2021 (early online 30 Apr 2021)
* Processed: 2021-4

Current drugs for Chagas disease have long treatment regimens with occurrence of adverse drug effects leading to poor treatment compliance. Novel and efficacious medications are therefore highly needed. We previously reported on the discovery of NPD-0227 (2-isopropyl-5-(4-methoxy-3-(pyridin-3-yl)phenyl)-4,4-dimethyl-2,4-dihydro-3H-pyrazol-3-one) as a potent in vitro inhibitor of Trypanosoma cruzi (pIC50 = 6.4) with 100-fold selectivity over human MRC-5 cells. The present work describes a SAR study on the exploration of substituents on the phenylpyrazolone nitrogen. Modifications were either done directly onto this pyrazolone nitrogen or alternatively by introducing a piperidine linker. Attention was pointed toward the selection of substituents with a cLogP preferably below NPD-0227s cLogP of 3.5. Generally the more apolar compounds showed better activities then molecules with cLogPs <2.0. Several new compounds were identified with potencies that are in the same range as NPD-0227 (pIC50 = 6.4) and promising selectivities. While the potency could not be improved, valuable SAR was obtained. Furthermore the introduction of a piperidine linker offers new opportunities for derivatization as valuable novel starting points for future T. cruzi drug discovery.

### 6) Cardiolipin enhances the enzymatic activity of cytochrome bd and cytochrome bo 3 solubilized in dodecyl-maltoside

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* Structural Biology, AIMMS, Delft University of Technology, Kyushu Institute of Technology
* Scientific Reports
* https://doi.org/10.1038/s41598-021-87354-0
* Corresponding author: Bald, D.
* Published Dec 2021 (early online 13 Apr 2021)
* Processed: 2021-4

Cardiolipin (CL) is a lipid that is found in the membranes of bacteria and the inner membranes of mitochondria. CL can increase the activity of integral membrane proteins, in particular components of respiratory pathways. We here report that CL activated detergent-solubilized cytochrome bd, a terminal oxidase from Escherichia coli. CL enhanced the oxygen consumption activity ~ twofold and decreased the apparent KM value for ubiquinol-1 as substrate from 95µM to 35µM. Activation by CL was also observed for cytochrome bd from two Gram-positive species, Geobacillus thermodenitrificans and Corynebacterium glutamicum, and for cytochrome bo3 from E. coli. Taken together, CL can enhance the activity of detergent-solubilized cytochrome bd and cytochrome bo3.

### 7) Online biophysical predictions for SARS-Co

* Kagami, L., Roca-Martínez, J., Gavaldá-García, J., Ramasamy, P., Feenstra, K. A., Vranken, W. F.
* Bioinformatics, AIMMS, Integrative Bioinformatics, Free Universities of Brussels, Vrije Universiteit Brussel, Flanders Institute for Biotechnology, Ghent University
* BMC Molecular and Cell Biology
* https://doi.org/10.1186/s12860-021-00362-w
* Corresponding author: Vranken, W. F.
* Published 23 Apr 2021 (early online None)
* Processed: 2021-4

V-2 proteinsBACKGROUND: The SARS-CoV-2 virus, the causative agent of COVID-19, consists of an assembly of proteins that determine its infectious and immunological behavior, as well as its response to therapeutics. Major structural biology efforts on these proteins have already provided essential insights into the mode of action of the virus, as well as avenues for structure-based drug design. However, not all of the SARS-CoV-2 proteins, or regions thereof, have a well-defined three-dimensional structure, and as such might exhibit ambiguous, dynamic behaviour that is not evident from static structure representations, nor from molecular dynamics simulations using these structures. MAIN: We present a website ( https://bio2byte.be/sars2/ ) that provides protein sequence-based predictions of the backbone and side-chain dynamics and conformational propensities of these proteins, as well as derived early folding, disorder, β-sheet aggregation, protein-protein interaction and epitope propensities. These predictions attempt to capture the inherent biophysical propensities encoded in the sequence, rather than context-dependent behaviour such as the final folded state. In addition, we provide the biophysical variation that is observed in homologous proteins, which gives an indication of the limits of their functionally relevant biophysical behaviour.CONCLUSION: The https://bio2byte.be/sars2/ website provides a range of protein sequence-based predictions for 27 SARS-CoV-2 proteins, enabling researchers to form hypotheses about their possible functional modes of action.

### 8) Corrigendum to “Critique of the “Comment” etitled “Pyrethroid exposure: not so harmless after all” by Demeniex et al. (2020) published in the lancet diabetes endocrinology"

* Barile, F. A., Berry, S. C., Blaauboer, B., Boobis, A., Bolt, H., Borgert, C. J., Dekant, W., Dietrich, D., Domingo, J. L., Gori, G. B., Greim, H., Hengstler, J., Kacew, S., Marquardt, H., Pelkonen, O., Savolainen, K., Heslop-Harrison, P., 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, Pere Virgili Health Research Institute, The Health Policy Center, Technical University of Munich, University of Ottawa, Toxicology, University of Oulu, Finnish Institute of Occupational Health, University of Leicester, University of Crete
* Toxicology Letters
* https://doi.org/10.1016/j.toxlet.2021.03.008
* Corresponding author: Greim, H.
* Published 1 Aug 2021 (early online 24 Apr 2021)
* Processed: 2021-4

The authors regret that the letter inaccurately refers to “the lancet diabetes endocrinology” and “The Lancet” while it should read: “The Lancet Diabetes & Endocrinology”. The correct title of the letter should read: “Critique of the “Comment” entitled: “Pyrethroid exposure: Not so harmless after all” by Demeneix et al. (2020) published in The Lancet Diabetes & Endocrinology”. The authors wish to clarify that the comment was published in The Lancet Diabetes & Endocrinology and not The Lancet. The authors also wish to clarify that The Lancet Diabetes & Endocrinology chose not to publish their criticism of the article because the correspondence content published in The Lancet Diabetes & Endocrinology is only accepted within 8 weeks of publication of the original item.

### 9) How does the composition of a PAH influence its microsolvation? A rotational spectroscopy study of the phenanthrene-water and phenanthridine-water clusters

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* BioAnalytical Chemistry, AIMMS, German Electron Synchrotron, College of Charleston, Kiel University
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/D1CP00898F
* Corresponding author: Loru, D.
* Published 28 Apr 2021 (early online 6 Apr 2021)
* Processed: 2021-4

We report on the noncovalent intermolecular interactions established between the polycyclic aromatic hydrocarbons phenanthrene and phenanthridine with water. Such noncovalent interactions involving extended aromatic systems and water molecules are ubiquitous in a variety of chemical and biological systems. Our study provides spectroscopic results on simple model systems to understand the impact that an extended aromatic surface and the presence of a heteroatom have on the nature of the noncovalent interactions established with the solvent. Microhydrated phenanthrene and phenanthridine clusters with up to three water molecules have been observed and unambiguously characterised by means of broadband rotational spectroscopy and quantum chemical calculations. The presence of a nitrogen atom in the backbone of phenanthridine remarkably affects the geometries of the water clusters and the interaction networks at play, with O-H⋯N and C-H⋯O interactions becoming preferred in the phenanthridine-water clusters over the O-H⋯π interactions seen in the phenanthrene-water clusters. The presence of this heteroatom induces nuclear quadrupole coupling, which was used to understand the cooperativity effects found with increasing cluster size. Our results provide important insight to draw a more complete picture of the noncovalent interactions involving solvent molecules and aromatic systems larger than benzene, and they can be significant to enhance our understanding of the aromatic-polar interactions at play in a myriad of chemical and biological contexts.

### 10) Vibrational circular dichroism studies of exceptionally strong chirality inducers in liquid crystals7,7′-Disubstituted 2,2′-methylenedioxy-1,1′-binaphthyls are highly efficient chirality inducers in nematic liquid crystals.

* Koenis, M. A., Nicu, V. P., Visscher, L., Kuehn, C., Bremer, M., Krier, M., Untenecker, H., Zhumaev, U., Küstner, B., Buma, W. J.
* Theoretical Chemistry, AIMMS, University of Amsterdam, Lucian Blaga University of Sibiu, Merck KGaA, Radboud University Nijmegen
* Physical Chemistry Chemical Physics
* https://doi.org/10.1039/d1cp00854d
* Corresponding author: Buma, W. J.
* Published 28 Apr 2021 (early online 9 Apr 2021)
* Processed: 2021-4

The absolute configuration of these compounds is, however, hard to determine as they only crystallize as racemic mixtures. In this work a Vibrational Circular Dichroism (VCD) study is reported that provides an unambiguous determination of the absolute configuration of these compounds. An in-depth General Coupled Oscillator (GCO) analysis of the source of the VCD signal reveals that the unusual structure of these binaphthyl compounds inherently leads to strong and robust VCD bands. Combined with linear transit calculations, our VCD studies allow for the determination of key structural parameters.

### 11) Anticoagulant Activity of Naja nigricollis Venom Is Mediated by Phospholipase A2 Toxins and Inhibited by Varespladib

* Kazandjian, T. D., Arrahman, A., Still, K. B., Somsen, G. W., Vonk, F. J., Casewell, N. R., Wilkinson, M. C., Kool, J.
* BioAnalytical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Liverpool School of Tropical Medicine
* Toxins
* https://doi.org/10.3390/toxins13050302
* Corresponding author: None
* Published May 2021 (early online 23 Apr 2021)
* Processed: 2021-5

Bites from elapid snakes typically result in neurotoxic symptoms in snakebite victims. Neurotoxins are, therefore, often the focus of research relating to understanding the pathogenesis of elapid bites. However, recent evidence suggests that some elapid snake venoms contain anticoagulant toxins which may help neurotoxic components spread more rapidly. This study examines the effects of venom from the West African black-necked spitting cobra (Naja nigricollis) on blood coagulation and identifies potential coagulopathic toxins. An integrated RPLC-MS methodology, coupled with nanofractionation, was first used to separate venom components, followed by MS, proteomics and coagulopathic bioassays. Coagulation assays were performed on both crude and nanofractionated N. nigricollis venom toxins as well as PLA2s and 3FTx purified from the venom. Assays were then repeated with the addition of either the phospholipase A2 inhibitor varespladib or the snake venom metalloproteinase inhibitor marimastat to assess whether either toxin inhibitor is capable of neutralizing coagulopathic venom activity. Subsequent proteomic analysis was performed on nanofractionated bioactive venom toxins using tryptic digestion followed by nanoLC-MS/MS measurements, which were then identified using Swiss-Prot and species-specific database searches. Varespladib, but not marimastat, was found to significantly reduce the anticoagulant activity of N. nigricollis venom and MS and proteomics analyses confirmed that the anticoagulant venom components mostly consisted of PLA2 proteins. We, therefore, conclude that PLA2s are the most likely candidates responsible for anticoagulant effects stimulated by N. nigricollis venom.

### 12) Understanding FBA solutions under multiple nutrient limitations

* van Pelt-KleinJan, E., de Groot, D. H., Teusink, B.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics
* Metabolites
* https://doi.org/10.3390/metabo11050257
* Corresponding author: Teusink, B.
* Published May 2021 (early online 21 Apr 2021)
* Processed: 2021-5

Genome-scale stoichiometric modeling methods, in particular Flux Balance Analysis (FBA) and variations thereof, are widely used to investigate cell metabolism and to optimize biotechno-logical processes. Given (1) a metabolic network, which can be reconstructed from an organism’s genome sequence, and (2) constraints on reaction rates, which may be based on measured nutrient uptake rates, FBA predicts which reactions maximize an objective flux, usually the production of cell components. Although FBA solutions may accurately predict the metabolic behavior of a cell, the actual flux predictions are often hard to interpret. This is especially the case for conditions with many constraints, such as for organisms growing in rich nutrient environments: it remains unclear why a certain solution was optimal. Here, we rationalize FBA solutions by explaining for which properties the optimal combination of metabolic strategies is selected. We provide a graphical formalism in which the selection of solutions can be visualized; we illustrate how this perspective provides a glimpse of the logic that underlies genome-scale modeling by applying our formalism to models of various sizes.

### 13) SeRenDIP-CE: Sequence-based Interface Prediction for Conformational Epitopes

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* Computer Science, Bioinformatics, AIMMS, Integrative Bioinformatics, Bio Informatics (IBIVU), IBIVU - Center for Integrative Bioinformatics, Shandong University
* Bioinformatics (Oxford, England)
* https://doi.org/10.1101/2020.11.19.390500
* Corresponding author: None
* Published 11 May 2021 (early online 11 May 2021)
* Processed: 2021-5

MOTIVATION: Antibodies play an important role in clinical research and biotechnology, with their specificity determined by the interaction with the antigen's epitope region, as a special type of protein-protein interaction (PPI) interface. The ubiquitous availability of sequence data, allows us to predict epitopes from sequence in order to focus time-consuming wet-lab experiments towards the most promising epitope regions. Here, we extend our previously developed sequence-based predictors for homodimer and heterodimer PPI interfaces to predict epitope residues that have the potential to bind an antibody.RESULTS: We collected and curated a high quality epitope dataset from the SAbDab database. Our generic PPI heterodimer predictor obtained an AUC-ROC of 0.666 when evaluated on the epitope test set. We then trained a random forest model specifically on the epitope dataset, reaching AUC 0.694. Further training on the combined heterodimer and epitope datasets, improves our final predictor to AUC 0.703 on the epitope test set. This is better than the best state-of-the-art sequence-based epitope predictor BepiPred-2.0. On one solved antibody-antigen structure of the COVID19 virus spike RNA binding domain, our predictor reaches AUC 0.778. We added the SeRenDIP-CE Conformational Epitope predictors to our webserver, which is simple to use and only requires a single antigen sequence as input, which will help make the method immediately applicable in a wide range of biomedical and biomolecular research.AVAILABILITY: Webserver, source code and datasets at www.ibi.vu.nl/programs/serendipwww/.

### 14) Endocrine, metabolic and apical effects of in utero and lactational exposure to non-dioxin-like 2,2´,3,4,4´,5,5´-heptachlorobiphenyl (PCB 180): A postnatal follow-up study in rats

* Alarcón, S., Esteban, J., Roos, R., Heikkinen, P., Sánchez-Pérez, I., Adamsson, A., Toppari, J., Koskela, A., Finnilä, M. A., Tuukkanen, J., Herlin, M., Hamscher, G., Leslie, H. A., Korkalainen, M., Halldin, K., Schrenk, D., Håkansson, H., Viluksela, M.
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* Reproductive Toxicology
* https://doi.org/10.1016/j.reprotox.2021.04.004
* Corresponding author: Esteban, J.
* Published Jun 2021 (early online 13 May 2021)
* Processed: 2021-5

PCB 180 is a persistent and abundant non-dioxin-like PCB (NDL-PCB). We determined the developmental toxicity profile of ultrapure PCB 180 in developing offspring following in utero and lactational exposure with the focus on endocrine, metabolic and retinoid system alterations. Pregnant rats were given total doses of 0, 10, 30, 100, 300 or 1000 mg PCB 180/kg bw on gestational days 7-10 by oral gavage, and the offspring were sampled on postnatal days (PND) 7, 35 and 84. Decreased serum testosterone and triiodothyronine concentrations on PND 84, altered liver retinoid levels, increased liver weights and induced 7-pentoxyresorufin O-dealkylase (PROD) activity were the sensitive effects used for margin of exposure (MoE) calculations. Liver weights were increased together with induction of the metabolizing enzymes cytochrome P450 (CYP) 2B1, CYP3A1, and CYP1A1. Less sensitive effects included decreased serum estradiol and increased luteinizing hormone levels in females, decreased prostate and seminal vesicle weight and increased pituitary weight in males, increased cortical bone area and thickness of tibial diaphysis in females and decreased cortical bone mineral density in males. Developmental toxicity profiles were partly different in male and female offspring, males being more sensitive to increased liver weight, PROD induction and decreased thyroxine concentrations. MoE assessment indicated that the 95th percentile of current maternal PCB 180 concentrations do not exceed the estimated tolerable human lipid-based PCB 180 concentration. Although PCB 180 is much less potent than dioxin-like compounds, it shares several toxicological targets suggesting a potential for interactions.

### 15) Erratum: "Large coupling-strength expansion of the Møller-Plesset adiabatic connection: From paradigmatic cases to variational expressions for the leading terms" [J. Chem. Phys., 153, 214112 (2020)]

* Daas, T. J., Grossi, J., Vuckovic, S., Musslimani, Z. H., Kooi, D. P., Seidl, M., Giesbertz, K. J., Gori-Giorgi, P.
* Theoretical Chemistry, AIMMS, Vrije Universiteit Amsterdam
* Journal of Chemical Physics
* https://doi.org/10.1063/5.0053838
* Corresponding author: Gori-Giorgi, P.
* Published 14 May 2021 (early online 10 May 2021)
* Processed: 2021-5

We correct an error in Eq. (19) of the article, namely, a missing factor 1/2. The correct equation reads (Farmula Presenred) This is only a misprint in the article and does not affect any of the results, which were obtained from the correct equations.

### *16) The Gauche Effect in XCH2CH2X Revisited*

* Rodrigues Silva, D., de Azevedo Santos, L., Hamlin, T. A., Fonseca Guerra, C., Freitas, M. P., Bickelhaupt, F. M.
* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, Universidade Federal de Lavras
* ChemPhysChem
* https://doi.org/10.1002/cphc.202100090
* Corresponding author: Fonseca Guerra, C.
* 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 ...

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

* de Azevedo Santos, L., Ramalho, T. C., Hamlin, T. A., Bickelhaupt, F. M.
* 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
* Corresponding author: de Azevedo Santos, L., Ramalho, T. C., Hamlin, T. A., Bickelhaupt, F. M.
* 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-relat ...

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

* De Groof, T. W., Elder, E. G., Siderius, M., Heukers, R., Sinclair, J. H., Smit, M. J.
* Medicinal chemistry, AIMMS, Vrije Universiteit Brussel
* Pharmacological reviews
* 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 ind ...

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

* Orian, L., Bickelhaupt, F. M.
* Chemistry and Pharmaceutical Sciences, AIMMS, University of Padova
* 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. I ...

### *20) 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 tu ...

### *21) 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 ...

### *22) 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.
* Theoretical Chemistry, AIMMS, Universidade Federal de Lavras, University of Hradec Kralove, Vrije Universiteit Amsterdam, Radboud University Nijmegen
* 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 A ...

### *23) 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-progesto ...

### *24) 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. Resou ...

### *25) 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 ...

### *26) 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, inc ...

### *27) 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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### *28) Generalization of Intrinsic Orbitals to Kramers-Paired Quaternion Spinors, Molecular Fragments, and Valence Virtual Spinors*

* Senjean, B., Sen, S., Repisky, M., Knizia, G., Visscher, L.
* Theoretical Chemistry, AIMMS, UiT The Arctic University of Norway, Pennsylvania State University
* Journal of chemical theory and computation
* https://doi.org/10.1021/acs.jctc.0c00964
* Corresponding author: Senjean, B.
* Published 9 Mar 2021 (early online 8 Feb 2021)
* Processed: 2021-3

Localization of molecular orbitals finds its importance in the representation of chemical bonding (and antibonding) and in the local correlation treatments beyond mean-field approximation. In this pap ...