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### 1) Bioactivation of trichloroethylene to three regioisomeric glutathione conjugates by liver fractions and recombinant human glutathione transferases: species differences and implications for human risk assessment

* Capinha, L., Jennings, P., Commandeur, J. N.
* Molecular and Computational Toxicology, AIMMS
* Toxicology Letters
* https://doi.org/10.1016/j.toxlet.2021.01.021
* Corresponding author: None
* Published 1 Feb 2021 (early online None)
* Processed: 2021-2

Enzymatic conjugation of glutathione (GSH) to trichloroethylene (TCE) followed by catabolism to the corresponding cysteine-conjugate, S-(dichlorovinyl)-L-cysteine (DCVC), and subsequent bioactivation by renal cysteine conjugate beta-lyases is considered to play an important role in the nephrotoxic effects observed in TCE-exposed rat and human. In this study, it is shown for the first time that three regioisomers of GSH-conjugates of TCE are formed by rat and human liver fractions, namely S-(1,2-trans-dichlorovinyl)-glutathione (1,2-trans-DCVG), S-(1,2-cis-dichlorovinyl)-glutathione (1,2-cis-DCVG) and S-2,2-dichlorovinyl-glutathione (2,2-DCVG). In incubations of TCE with rat liver fractions their amounts decreased in order of 1,2-cis-DCVG > 1,2-trans-DCVG > 2,2-DCVG. Human liver cytosol showed a more than 10-fold lower activity of GSH-conjugation, with amounts of regioisomers decreasing in order 2,2-DCVG > 1,2-trans-DCVG > 1,2-cis-DCVG. Incubations with recombinant human GSTs suggest that GSTA1-1 and GSTA2-2 play the most important role in human liver cytosol. GSTP1-1, which produces regioisomers in order 1,2-trans-DCVG > 2,2-cis-DCVG > 1,2-cis-DCVG, is likely to contribute to extrahepatic GSH-conjugation of TCE. Analysis of the products formed by a beta-lyase mimetic model showed that both 1,2-trans-DCVC and 1,2-cis-DCVC are converted to reactive products that form cross-links between the model nucleophile 4-(4-nitrobenzyl)-pyridine (NBP) and thiol-species. No NBP-alkylation was observed with 2,2-DCVC corresponding to its low cytotoxicity and mutagenicity. The lower activity of GSH-conjugation of TCE by human liver fractions, in combination with the lower fraction of potential nephrotoxic and mutagenic 1,2-DCVG-isomers, suggest that humans are at much lower risk for TCE-associated nephrotoxic effects than rats.

### 2) Results of WEPAL-QUASIMEME/NORMANs first global interlaboratory study on microplastics reveal urgent need for harmonization

* van Mourik, L. M., Crum, S., Martinez-Frances, E., van Bavel, B., Leslie, H. A., de Boer, J., Cofino, W. P.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, E&H: Environmental Chemistry and Toxicology, Environment and Health, Wageningen University & Research, Norwegian Institute for Water Research
* Science of the Total Environment
* https://doi.org/10.1016/j.scitotenv.2021.145071
* Corresponding author: van Mourik, L. M.
* Published 10 Jun 2021 (early online 4 Feb 2021)
* Processed: 2021-2

To survey the conformity and quality of results among laboratories for microplastics determination worldwide, an international laboratory intercomparison and development exercise was organized. The 34 participants were requested to determine the polymer type and number or mass of polymer particles in 12 samples, i.e. six samples containing of pre-production pellets, five dissolvable soda tablets containing different (smaller) polymer particles and one blank soda tablet. A novel method for providing the test materials in aluminium strips was used. Thirty laboratories (88%) submitted data using their own method of choice, resulting in a variety of identification and quantification methods (n = 7). The majority of the labs (53–100%) correctly identified the type of polymer in all samples but one. The performance of the laboratories in quantifying and weighing the pellets was very good. The analysis of the number of the particles in the soda tablets varied considerably between laboratories (29–91%). The results of this study highlight the complexity of microplastics analysis and the need for harmonization of both reporting format and methods. Continued development and assessment of the comparability among analytical methods and laboratories are urgently needed to support monitoring programmes, research and decision-making.

### 3) Results of WEPAL-QUASIMEME/NORMANs first global interlaboratory study on microplastics reveal urgent need for harmonization

* van Mourik, L. M., Crum, S., Martinez-Frances, E., van Bavel, B., Leslie, H. A., de Boer, J., Cofino, W. P.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, E&H: Environmental Chemistry and Toxicology, Environment and Health, Wageningen University & Research, Norwegian Institute for Water Research
* Science of the Total Environment
* https://doi.org/https://doi.org/10.1016/j.scitotenv.2021.14507110.1016/j.scitotenv.2021.145071
* Corresponding author: van Mourik, L. M.
* Published 10 Jun 2021 (early online 4 Feb 2021)
* Processed: 2021-2

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### 4) Decabromodiphenylether trends in the European environment: Bird eggs, sewage sludge and surficial sediments

* Leslie, H. A., Brandsma, S. H., Barber, J. L., Gabrielsen, G. W., Bersuder, P., Barry, J., Shore, R. F., Walker, L. A., de Boer, J.
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* Science of the Total Environment
* https://doi.org/https://doi.org/10.1016/j.scitotenv.2021.14517410.1016/j.scitotenv.2021.145174
* Corresponding author: de Boer, J.
* Published 20 Jun 2021 (early online 11 Feb 2021)
* Processed: 2021-2

Concern on relatively high levels and the potential bioaccumulation of decabromodiphenylether (BDE209) has led to a European 8-year monitoring program on trends in BDE209 concentrations in birds, sewage sludge and sediments from seven countries. BDE209 was analysed in four environmental matrices: sparrowhawk eggs (UK), glaucous gull eggs (Bear Island, Norway), sewage sludge (UK, Ireland and the Netherlands) and sediment (France, Germany, the Netherlands, UK and Ireland). BDE209 was detected in most of the glaucous gull and sparrow hawk eggs but neither increasing nor decreasing trends in these BDE209 levels were observed. An indication for debromination of BDE209 in sparrowhawk eggs was found. BDE209 concentrations in sediments ranged from very low ng/g (88 ng/g on an organic carbon (OC) basis) concentrations, in the rivers Elbe, Ems, Seine and the Outer Humber, to high μg/g (120 μg/g OC), in the Western Scheldt, Liverpool Bay and River Mersey. Apart from decreasing values in the Western Scheldt sediment no further decreases in BDE209 concentrations were observed over time, neither in sediment nor in sewage sludge showing that the voluntary emissions control program of the bromine industry only had a local effect. In contrast to the sewage sludge samples from the Netherlands (mean 355 ng/g dry weight (dw) or 1026 ng/g OC), the BDE209 concentrations in the UK increased at all sites from 2006 to 2011 (8092 ng/g dw or 22,367 ng/g OC). The BDE209 levels in several UK sediments and sewage sludge were still very high at the end of the program in 2012, most likely caused by frequent use of BDE209 in the textile industry. This may be indicative of the persistence of BDE209 and the limited degradation into lower brominated congeners in sediment, although it cannot be excluded that ongoing BDE209 emissions have played a role as well.

### 5) Microplastics and human health: Knowledge gaps should be addressed to ascertain the health risks of microplastics

* Vethaak, A. D., Legler, J.
* AIMMS, Environment and Health
* Science
* https://doi.org/10.1126/science.abe5041
* Corresponding author: Vethaak, A. D.
* Published 12 Feb 2021 (early online None)
* Processed: 2021-2

### 6) Computational modelling of the Δ4 and Δ5 adrenal steroidogenic pathways provides insight into hypocortisolism

* Louw, C., van Schalkwyk, E. J., Conradie, R., Louw, R., Engelbrecht, Y., Storbeck, K. H., Swart, A. C., van Niekerk, D. D., Snoep, J. L., Swart, P.
* AIMMS, Molecular Cell Physiology, University of Stellenbosch, Stellenbosch University
* Molecular and cellular endocrinology
* https://doi.org/10.1016/j.mce.2021.111194
* Corresponding author: Swart, P.
* Published 15 Apr 2021 (early online 13 Feb 2021)
* Processed: 2021-2

This study demonstrates the application of a mathematical steroidogenic model, constructed with individual in vitro enzyme characterisations, to simulate in vivo steroidogenesis in a diseased state. This modelling approach was applied to the South African Angora goat, that suffers from hypocortisolism caused by altered adrenal function. These animals are extremely vulnerable to cold stress, leading to substantial monetary loss in the mohair industry. The Angora goat has increased CYP17A1 17,20-lyase enzyme activity in comparison with hardy livestock species. Determining the effect of this altered adrenal function on adrenal steroidogenesis during a cold stress response is difficult. We developed a model describing adrenal steroidogenesis under control conditions, and under altered steroidogenic conditions where the animal suffers from hypocortisolism. The model is parameterised with experimental data from in vitro enzyme characterisations of a hardy control species. The increased 17,20-lyase activity of the Angora goat CYP17A1 enzyme was subsequently incorporated into the model and the response to physiological stress is simulated under both control and altered adrenal steroidogenic conditions.

### 7) Nature of Alkali- and Coinage-Metal Bonds versus Hydrogen Bonds

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* Theoretical Chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, University of the Basque Country, Ikerbasque Basque Foundation for Science
* Chemistry - An Asian Journal
* https://doi.org/10.1002/asia.202001201
* Corresponding author: Bickelhaupt, F. M., de Cózar, A.
* Published 15 Feb 2021 (early online 29 Dec 2020)
* Processed: 2021-2

We have quantum chemically studied the structure and nature of alkali- and coinage-metal bonds (M-bonds) versus that of hydrogen bonds between A−M and B− in archetypal [A−M⋅⋅⋅B]− model systems (A, B=F, Cl and M=H, Li, Na, Cu, Ag, Au), using relativistic density functional theory at ZORA-BP86-D3/TZ2P. We find that coinage-metal bonds are stronger than alkali-metal bonds which are stronger than the corresponding hydrogen bonds. Our main purpose is to understand how and why the structure, stability and nature of such bonds are affected if the monovalent central atom H of hydrogen bonds is replaced by an isoelectronic alkali- or coinage-metal atom. To this end, we have analyzed the bonds between A−M and B− using the activation strain model, quantitative Kohn-Sham molecular orbital (MO) theory, energy decomposition analysis (EDA), and Voronoi deformation density (VDD) analysis of the charge distribution.

### 8) Discovery of fragments inducing conformational effects in dynamic proteins using a second-harmonic generation biosensor

* FitzGerald, E. A., Butko, M. T., Boronat, P., Cederfelt, D., Abramsson, M., Ludviksdottir, H., van Muijlwijk-Koezen, J. E., de Esch, I. J., Dobritzsch, D., Young, T., Danielson, U. H.
* Innovations in Human Health & Life Sciences, AIMMS, Chemistry and Pharmaceutical Sciences, Uppsala University, Beactica, Biodesy, Inc., VU University
* RSC Advances
* https://doi.org/10.1039/d0ra09844b
* Corresponding author: Danielson, U. H.
* Published 17 Feb 2021 (early online None)
* Processed: 2021-2

Biophysical screening of compound libraries for the identification of ligands that interact with a protein is efficient, but does typically not reveal if (or how) ligands may interfere with its functional properties. For this a biochemical/functional assay is required. But for proteins whose function is dependent on a conformational change, such assays are typically complex or have low throughput. Here we have explored a high-throughput second-harmonic generation (SHG) biosensor to detect fragments that induce conformational changes upon binding to a protein in real time and identify dynamic regions. Multiwell plate format SHG assays were developed for wild-type and six engineered single-cysteine mutants of acetyl choline binding protein (AChBP), a homologue to ligand gated ion channels (LGICs). They were conjugated with second harmonic-active labelsviaamine or maleimide coupling. To validate the assay, it was confirmed that the conformational changes induced in AChBP by nicotinic acetyl choline receptor (nAChR) agonists and antagonists were qualitatively different. A 1056 fragment library was subsequently screened against all variants and conformational modulators of AChBP were successfully identified, with hit rates from 9-22%, depending on the AChBP variant. A subset of four hits was selected for orthogonal validation and structural analysis. A time-resolved grating-coupled interferometry-based biosensor assay confirmed the interaction to be a reversible 1-step 1 : 1 interaction, and provided estimates of affinities and interaction kinetic rate constants (KD= 0.28-63 μM,ka= 0.1-6 μM−1s−1,kd=1 s−1). X-ray crystallography of two of the fragments confirmed their binding at a previously described conformationally dynamic site, corresponding to the regulatory site of LGICs. These results reveal that SHG has the sensitivity to identify fragments that induce conformational changes in a protein. A selection of fragment hits with a response profile different to known LGIC regulators was characterized and confirmed to bind to dynamic regions of the protein.

### 9) Tetrahydrophthalazinone inhibitor of phosphodiesterase with in vitro activity against intracellular trypanosomatids

* De Araújo, J. S., Peres, R. B., Da Silva, P. B., Batista, M. M., Sterk, G. J., Maes, L., Caljon, G., Leurs, R., De Koning, H. P., Kalejaiye, T. D., De Nazaré Correia Soeiro, M.
* Medicinal chemistry, AIMMS, Fundação Oswaldo Cruz, University of Antwerp, University of Glasgow
* Antimicrobial agents and chemotherapy
* https://doi.org/10.1128/AAC.00960-20
* Corresponding author: De Nazaré Correia Soeiro, M.
* Published 17 Feb 2021 (early online None)
* Processed: 2021-2

The phosphodiesterase inhibitor tetrahydrophthalazinone NPD-008 was explored by phenotypic in vitro screening, target validation, and ultrastructural approaches against Trypanosoma cruzi. NPD-008 displayed activity against different forms and strains of T. cruzi (50% effective concentration [EC50], 6.6 to 39.5mM). NPD-008 increased cAMP levels of T. cruzi and its combination with benznidazole gave synergistic interaction. It was also moderately active against intracellular amastigotes of Leishmania amazonensis and Leishmania infantum, confirming a potential activity profile as an antitrypanosomatid drug candidate.

### 10) Optimization of a low flow sampler for improved assessment of gas and particle bound exposure to chlorinated paraffins

* Al Saify, I., Cioni, L., van Mourik, L. M., Brandsma, S. H., Warner, N. A.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, Norwegian Institute for Air Research, Vrije Universiteit Amsterdam, UiT The Arctic University of Norway
* Chemosphere
* https://doi.org/10.1016/j.chemosphere.2021.130066
* Corresponding author: Warner, N. A.
* Published Jul 2021 (early online 23 Feb 2021)
* Processed: 2021-2

An optimized low volume sampler was developed to determine both gas- and particle bound concentrations of short and medium-chain chlorinated paraffins (S/MCCPs). Background contamination was limited by the sampler design, providing method quantification limits (MQLs) at least two orders of magnitude lower than other studies within the gas (MQL: 500 pg (ΣSCCPs), 1.86 ng (ΣMCCPs)) and particle (MQL: 500 pg (ΣSCCPs), 1.72 ng (ΣMCCPs) phases. Good repeatability was observed between parallel indoor measurements (RSD ≤ 9.3% (gas), RSD ≤ 14% (particle)) with no breakthrough/saturation observed after a week of continuous sampling. For indoor air sampling, SCCPs were dominant within the gas phase (17 ± 4.9 ng/m3) compared to MCCPs (2.7 ± 0.8 ng/m3) while the opposite was observed in the particle bound fraction (0.28 ± 0.11 ng/m3 (ΣSCCPs) vs. 2.7 ± 1.0 ng/m3 (ΣMCCPs)). Only SCCPs in the gas phase could be detected reliably during outdoor sampling and were considerably lower compared to indoor concentrations (0.27 ± 0.10 ng/m3). Separation of the gas and particle bound phase was found to be crucial in applying the appropriate response factors for quantification based on the deconvoluted S/MCCP sample profile, thus avoiding over- (gas phase) or underestimation (particle phase) of reported concentrations. Very short chain chlorinated paraffins (vSCCPs, C5-C9) were also detected at equal or higher abundance compared to SCCP congener groups (C10-C13) congener groups, indicating an additional human indoor inhalation risk.

### *11) Hazardous compounds in recreational and urban recycled surfaces made from crumb rubber. Compliance with current regulation and future perspectives*

* Celeiro, M., Armada, D., Dagnac, T., de Boer, J., Llompart, M.
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* Science of the Total Environment
* https://doi.org/10.1016/j.scitotenv.2020.142566
* Corresponding author: Llompart, M.
* Published 10 Feb 2021 (early online 29 Sep 2020)
* Processed: 2021-2

Crumb rubber obtained from scrap tires is greatly employed for the construction of different facilities for sport, recreational and other uses. However, in recent years the concern about their safety ...

### *12) Circular pattern matching with k mismatches*

* Charalampopoulos, P., Kociumaka, T., Pissis, S. P., Radoszewski, J., Rytter, W., Straszyński, J., Waleń, T., Zuba, W.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London, University of Warsaw, Bar-Ilan University
* Journal of Computer and System Sciences
* https://doi.org/10.1016/j.jcss.2020.07.003
* Corresponding author: Pissis, S. P.
* Published Feb 2021 (early online 29 Jul 2020)
* Processed: 2021-2

We consider the circular pattern matching with k mismatches (k-CPM) problem in which one is to compute the minimal Hamming distance of every length-m substring of T and any cyclic rotation of P, if th ...

### *13) G protein-coupled receptors as promising targets in cancer*

* Perez Almeria, C. V., Setiawan, I. M., Siderius, M., Smit, M. J.
* AIMMS, Medicinal chemistry
* Current Opinion in Endocrine and Metabolic Research
* https://doi.org/10.1016/j.coemr.2020.10.005
* Corresponding author: Smit, M. J.
* Published Feb 2021 (early online 26 Oct 2020)
* Processed: 2021-2

G protein-coupled receptors (GPCRs) control diverse cellular functions, and their dysregulation is involved in a plethora of diseases including tumorigenesis. In the last decade, the association of GP ...

### *14) Metabolic cooperation and spatiotemporal niche partitioning in a kefir microbial community*

* Blasche, S., Kim, Y., Mars, R. A., Machado, D., Maansson, M., Kafkia, E., Milanese, A., Zeller, G., Teusink, B., Nielsen, J., Benes, V., Neves, R., Sauer, U., Patil, K. R.
* Systems Bioinformatics, AIMMS, Systems Bioinformatics, European Molecular Biology Laboratory, Swiss Federal Institute of Technology Zurich, Chr. Hansen AS, University of Cambridge, Chalmers University of Technology
* NATURE MICROBIOLOGY
* https://doi.org/10.1038/s41564-020-00816-5
* Corresponding author: Patil, K. R.
* Published Feb 2021 (early online None)
* Processed: 2021-2

Microbial communities often undergo intricate compositional changes yet also maintain stable coexistence of diverse species. The mechanisms underlying long-term coexistence remain unclear as system-wi ...

### *15) Neurotoxicity and underlying cellular changes of 21 mitochondrial respiratory chain inhibitors*

* Delp, J., Cediel-Ulloa, A., Suciu, I., Kranaster, P., van Vugt-Lussenburg, B. M., Munic Kos, V., van der Stel, W., Carta, G., Bennekou, S. H., Jennings, P., van de Water, B., Forsby, A., Leist, M.
* Molecular and Computational Toxicology, AIMMS, University of Konstanz, Karolinska Institutet, Uppsala University, BioDetection Systems B.V., Leiden University, Technical University of Denmark, Stockholm University
* Archives of Toxicology
* https://doi.org/10.1007/s00204-020-02970-5
* Corresponding author: Leist, M.
* Published Feb 2021 (early online 29 Jan 2021)
* Processed: 2021-2

Inhibition of complex I of the mitochondrial respiratory chain (cI) by rotenone and methyl-phenylpyridinium (MPP +) leads to the degeneration of dopaminergic neurons in man and rodents. To formally de ...

### *16) Temporal tracking of quantum-dot apatite across in vitro mycorrhizal networks shows how host demand can influence fungal nutrient transfer strategies*

* van’t Padje, A., Oyarte Galvez, L., Klein, M., Hink, M. A., Postma, M., Shimizu, T., Kiers, E. T.
* Animal Ecology, Bioinformatics, AIMMS, Bio Informatics (IBIVU), Wageningen University & Research, Vrije Universiteit Amsterdam, University of Amsterdam, AMOLF
* ISME Journal
* https://doi.org/10.1038/s41396-020-00786-w
* Corresponding author: van’t Padje, A.
* Published Feb 2021 (early online 28 Sep 2020)
* Processed: 2021-2

Arbuscular mycorrhizal fungi function as conduits for underground nutrient transport. While the fungal partner is dependent on the plant host for its carbon (C) needs, the amount of nutrients that the ...

### *17) IUPACpal: efficient identification of inverted repeats in IUPAC-encoded DNA sequences*

* Alamro, H., Alzamel, M., Iliopoulos, C. S., Pissis, S. P., Watts, S.
* Bioinformatics, AIMMS, Bio Informatics (IBIVU), King's College London, Princess Nourah Bint Abdulrahman University, King Saud University
* BMC Bioinformatics
* https://doi.org/10.1186/s12859-021-03983-2
* Corresponding author: Pissis, S. P.
* Published Dec 2021 (early online 6 Feb 2021)
* Processed: 2021-2

Background: An inverted repeat is a DNA sequence followed downstream by its reverse complement, potentially with a gap in the centre. Inverted repeats are found in both prokaryotic and eukaryotic geno ...

### *18) Intercellular communication induces glycolytic synchronization waves between individually oscillating cells*

* Mojica-Benavides, M., van Niekerk, D. D., Mijalkov, M., Snoep, J. L., Mehlig, B., Volpe, G., Goksör, M., Adiels, C. B.
* Molecular Cell Physiology, AIMMS, University of Gothenburg, University of Stellenbosch, Karolinska Institutet
* Proceedings of the National Academy of Sciences of the United States of America
* https://doi.org/10.1073/pnas.2010075118
* Corresponding author: Adiels, C. B.
* Published 9 Feb 2021 (early online None)
* Processed: 2021-2

Many organs have internal structures with spatially differentiated and sometimes temporally synchronized groups of cells. The mechanisms leading to such differentiation and coordination are not well u ...

### *19) In vitro biotransformation and evaluation of potential transformation products of chlorinated paraffins by high resolution accurate mass spectrometry*

* He, C., van Mourik, L., Tang, S., Thai, P., Wang, X., Brandsma, S. H., Leonards, P. E., Thomas, K. V., Mueller, J. F.
* E&H: Environmental Bioanalytical Chemistry, AIMMS, University of Queensland, Dongguan University of Technology
* Journal of Hazardous Materials
* https://doi.org/10.1016/j.jhazmat.2020.124245
* Corresponding author: He, C.
* Published 5 Mar 2021 (early online 10 Oct 2020)
* Processed: 2021-3

Chlorinated paraffins (CPs) are high production chemicals, which leads to their ubiquitous presence in the environment. To date, few studies have measured CPs in humans and typically at relatively low ...

### *20) Discovery of Diaryl Ether Substituted Tetrahydrophthalazinones as Tbr*

* de Heuvel, E., Kooistra, A. J., Edink, E., van Klaveren, S., Stuijt, J., van der Meer, T., Sadek, P., Mabille, D., Caljon, G., Maes, L., Siderius, M., de Esch, I. J., Sterk, G. J., Leurs, R.
* Medicinal chemistry, AIMMS, Chemistry and Pharmaceutical Sciences, University of Antwerp, VU University
* Frontiers in Chemistry
* https://doi.org/10.3389/fchem.2020.608030
* Corresponding author: Leurs, R.
* Published 21 Jan 2021 (early online None)
* Processed: 2021-1

PDEB1 Inhibitors Following Structure-Based Virtual ScreeningSeveral members of the 3′,5′-cyclic nucleotide phosphodiesterase (PDE) family play an essential role in cellular processes, which has labele ...

### *21) On the Origin of Regioselectivity in Palladium-Catalyzed Oxidation of Glucosides*

* Wan, I. C., Hamlin, T. A., Eisink, N. N., Marinus, N., de Boer, C., Vis, C. A., Codée, J. D., Witte, M. D., Minnaard, A. J., Bickelhaupt, F. M.
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* European Journal of Organic Chemistry
* https://doi.org/10.1002/ejoc.202001453
* Corresponding author: Witte, M. D., Minnaard, A. J., Bickelhaupt, F. M.
* Published 26 Jan 2021 (early online 18 Dec 2020)
* Processed: 2021-1

The palladium-catalyzed oxidation of glucopyranosides has been investigated using relativistic density functional theory (DFT) at ZORA-BLYP−D3(BJ)/TZ2P. The complete Gibbs free energy profiles for the ...