# AIMMS publication report for: 2021-03-22

1. Bioactivation of trichloroethylene to three regioisomeric gl (2021-2)
2. *Hazardous compounds in recreational and urban recycled surfa (2021-2)*
3. *Circular pattern matching with k mismatches (2021-2)*
4. *G protein-coupled receptors as promising targets in cancer (2021-2)*
5. *Metabolic cooperation and spatiotemporal niche partitioning (2021-2)*
6. *Neurotoxicity and underlying cellular changes of 21 mitochon (2021-2)*
7. *Temporal tracking of quantum-dot apatite across in vitro myc (2021-2)*
8. *Results of WEPAL-QUASIMEME/NORMANs first global interlaborat (2021-2)*
9. *IUPACpal: efficient identification of inverted repeats in IU (2021-2)*
10. *Intercellular communication induces glycolytic synchronizati (2021-2)*
11. *In vitro biotransformation and evaluation of potential trans (2021-3)*
12. *Decabromodiphenylether trends in the European environment: B (2021-2)*
13. *Microplastics and human health: Knowledge gaps should be add (2021-2)*
14. *Computational modelling of the Δ4 and Δ5 adrenal steroidogen (2021-2)*
15. *Nature of Alkali- and Coinage-Metal Bonds versus Hydrogen Bo (2021-2)*
16. *Discovery of fragments inducing conformational effects in dy (2021-2)*
17. *Tetrahydrophthalazinone inhibitor of phosphodiesterase with (2021-2)*
18. *Optimization of a low flow sampler for improved assessment o (2021-2)*

### 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) 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.
* Environment and Health, AIMMS, University of Santiago de Compostela, Agronomic Research Centre (AGACAL-CIAM) – Unit of Organic Contaminants
* 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 ...

### *3) 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 ...

### *4) 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 ...

### *5) 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 ...

### *6) 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 ...

### *7) 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 ...

### *8) 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 ...

### *9) 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 ...

### *10) 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 ...

### *11) 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 ...

### *12) 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.
* E&H: Environmental Chemistry and Toxicology, AIMMS, E&H: Environmental Bioanalytical Chemistry, Environment and Health, Centre for the Environment Fisheries and Aquaculture Science, Norwegian Polar Institute, Lancaster University
* Science of the Total Environment
* https://doi.org/10.1016/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, sewa ...

### *13) 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

...

### *14) 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. T ...

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

* Larrañaga, O., Arrieta, A., Fonseca Guerra, C., Bickelhaupt, F. M., de Cózar, A.
* 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 ...

### *16) 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 functi ...

### *17) 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 disp ...

### *18) 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 b ...