# AIMMS publication report for: 2022-02-23

### New papers: 2022-1/2

Fernandes, A. R., Vetter, W., Dirks, C., van Mourik, L., Cariou, R., Sprengel, J., Heeb, N., Lentjes, A., Krätschmer, K. **Determination of chlorinated paraffins (CPs): Analytical conundrums and the pressing need for reliable and relevant standards** (Chemosphere, Jan 2022)[https://doi.org/10.1016/j.chemosphere.2021.131878]

Wang, J., Baerends, E. J. **Self-Consistent-Field Method for Correlated Many-Electron Systems with an Entropic Cumulant Energy** (Physical review letters, 3 Jan 2022)[https://doi.org/10.1103/PhysRevLett.128.013001]

Loghmani, S. B., Veith, N., Sahle, S., Bergmann, F. T., Olivier, B. G., Kummer, U. **Inspecting the Solution Space of Genome-Scale Metabolic Models** (Metabolites, 5 Jan 2022)[https://doi.org/10.3390/metabo12010043]

Rozsar, D., Formica, M., Yamazaki, K., Hamlin, T. A., Dixon, D. J. **Bifunctional Iminophosphorane-Catalyzed Enantioselective Sulfa-Michael Addition to Unactivated α,β-Unsaturated Amides** (Journal of the American Chemical Society, 6 Jan 2022)[https://doi.org/10.1021/jacs.1c11898]

Rabbers, I., Gottstein, W., Feist, A. M., Teusink, B., Bruggeman, F. J., Bachmann, H. **Selection for Cell Yield Does Not Reduce Overflow Metabolism in Escherichia coli** (Molecular biology and evolution, 7 Jan 2022)[https://doi.org/10.1093/molbev/msab345]

Zaccaria, F., Zhang, B., Goldoni, L., Imran, M., Zito, J., Van Beek, B., Lauciello, S., De Trizio, L., Manna, L., Infante, I. **The Reactivity of CsPbBr3Nanocrystals toward Acid/Base Ligands** (ACS Nano, 10 Jan 2022)[https://doi.org/10.1021/acsnano.1c09603]

Hughes, S., Kolsters, N., van de Klashorst, D., Kreuter, E., Berger Büter, K. **An extract of Rosaceae,Solanaceae and Zingiberaceae increases health span and mobility in Caenorhabditis elegans** (BMC Nutrition, Dec 2022)[https://doi.org/10.1186/s40795-022-00498-8]

De Esch, I. J., Erlanson, D. A., Jahnke, W., Johnson, C. N., Walsh, L. **Fragment-to-Lead Medicinal Chemistry Publications in 2020** (Journal of medicinal chemistry, 13 Jan 2022)[https://doi.org/10.1021/acs.jmedchem.1c01803]

Slagboom, J., Kaal, C., Arrahman, A., Vonk, F. J., Somsen, G. W., Calvete, J. J., Wüster, W., Kool, J. **Analytical strategies in venomics** (Microchemical Journal, Apr 2022)[https://doi.org/10.1016/j.microc.2022.107187]

van Mourik, L. M., Crum, S., Martinez-Frances, E., van Bavel, B., Leslie, H. A., de Boer, J., Cofino, W. P. **Corrigendum to “Results of WEPAL-QUASIMEME/NORMANs first global interlaboratory study on microplastics reveal urgent need for harmonization”: [Sci. Total Environ. 772 (2021) 145071 10.1016/j.scitotenv.2021.145071 (ISSN 0048-9697)]** (Science of the Total Environment, 10 May 2022)[https://doi.org/10.1016/j.scitotenv.2022.153237]

Shiomi, S., Shennan, B. D., Yamazaki, K., Fuentes De Arriba, Á. L., Vasu, D., Hamlin, T. A., Dixon, D. J. **A New Organocatalytic Desymmetrization Reaction Enables the Enantioselective Total Synthesis of Madangamine e** (Journal of the American Chemical Society, 26 Jan 2022)[https://doi.org/10.1021/jacs.1c12040]

Brandsma, S. H., Leonards, P. E., Koekkoek, J. C., Samsonek, J., Puype, F. **Migration of hazardous contaminants from WEEE contaminated polymeric toy material by mouthing** (Chemosphere, May 2022)[https://doi.org/10.1016/j.chemosphere.2022.133774]

Jonkers, T. J., Meijer, J., Vlaanderen, J. J., Vermeulen, R. C., Houtman, C. J., Hamers, T., Lamoree, M. H. **High-Performance Data Processing Workflow Incorporating Effect-Directed Analysis for Feature Prioritization in Suspect and Nontarget Screening** (Environmental Science and Technology, 1 Feb 2022)[https://doi.org/10.1021/acs.est.1c04168]

Fiedler, H., van der Veen, I., de Boer, J. **Assessment of four rounds of interlaboratory tests within the UNEP-coordinated POPs projects** (Chemosphere, Feb 2022)[https://doi.org/10.1016/j.chemosphere.2021.132441]

Fiedler, H., van der Veen, I., de Boer, J. **Interlaboratory assessments for dioxin-like POPs (2016/2017 and 2018/2019)** (Chemosphere, Feb 2022)[https://doi.org/10.1016/j.chemosphere.2021.132449]

Somerville, V., Grigaitis, P., Battjes, J., Moro, F., Teusink, B. **Use and limitations of genome-scale metabolic models in food microbiology** (Current Opinion in Food Science, Feb 2022)[https://doi.org/10.1016/j.cofs.2021.12.010]

Nieuwland, C., Hamlin, T. A., Fonseca Guerra, C., Barone, G., Bickelhaupt, F. M. **B-DNA Structure and Stability: The Role of Nucleotide Composition and Order** (ChemistryOpen, 1 Feb 2022)[https://doi.org/10.1002/open.202200013]

Haigis, A., Ottermanns, R., Schiwy, A., Hollert, H., Legradi, J.Pages:133863 **Getting more out of the zebrafish light dark transition test** (Chemosphere, May 2022)[https://doi.org/10.1016/j.chemosphere.2022.133863]

Hansen, T., Roozee, J. C., Bickelhaupt, F. M., Hamlin, T. A. **How Solvation Influences the SN2 versus E2 Competition** (Journal of Organic Chemistry, 4 Feb 2022)[https://doi.org/10.1021/acs.joc.1c02354]

Ventouri, I. K., Loeber, S., Somsen, G. W., Schoenmakers, P. J., Astefanei, A. **Field-flow fractionation for molecular-interaction studies of labile and complex systems: A critical review** (Analytica Chimica Acta, 8 Feb 2022)[https://doi.org/10.1016/j.aca.2021.339396]

Tian, L., Skoczynska, E., Siddhanti, D., van Putten, R. J., Leslie, H. A., Gruter, G. J. M. **Quantification of polyethylene terephthalate microplastics and nanoplastics in sands, indoor dust and sludge using a simplified in-matrix depolymerization method** (Marine Pollution Bulletin, 9 Feb 2022)[https://doi.org/10.1016/j.marpolbul.2022.113403]

Elsemman, I. E., Rodriguez Prado, A., Grigaitis, P., Garcia Albornoz, M., Harman, V., Holman, S. W., van Heerden, J., Bruggeman, F. J., Bisschops, M. M., Sonnenschein, N., Hubbard, S., Beynon, R., Daran-Lapujade, P., Nielsen, J., Teusink, B. **Whole-cell modeling in yeast predicts compartment-specific proteome constraints that drive metabolic strategies** (Nature Communications, 10 Feb 2022)[https://doi.org/10.1038/s41467-022-28467-6]

Stringer, B., de Ferrante, H., Abeln, S., Heringa, J., Feenstra, K. A., Haydarlou, R. **PIPENN: Protein Interface Prediction from sequence with an Ensemble of Neural Nets** (Bioinformatics (Oxford, England), 12 Feb 2022)[https://doi.org/10.1101/2021.09.03.45883210.1093/bioinformatics/btac071]

Xu, M., Legradi, J., Leonards, P. **Using comprehensive lipid profiling to study effects of PFHx** (Science of the Total Environment, 20 Feb 2022)[https://doi.org/10.1016/j.scitotenv.2021.151739]