# AIMMS publication report for: 2021-05-31

### New papers: 2021-4/5

de Azevedo Santos, L., van der Lubbe, S. C., Hamlin, T. A., Ramalho, T. C., Bickelhaupt, F. M. **A Quantitative Molecular Orbital Perspective of the Chalcogen Bond** (ChemistryOpen, Apr 2021)[https://doi.org/10.1002/open.202000323]

Kooi, D. P., Weckman, T., Gori-Giorgi, P. **Dispersion without Many-Body Density Distortion: Assessment on Atoms and Small Molecules** (Journal of chemical theory and computation, 13 Apr 2021)[https://doi.org/10.1021/acs.jctc.1c00102]

Su, G., Thomson, C. J., Yamazaki, K., Rozsar, D., Christensen, K. E., Hamlin, T. A., Dixon, D. J. **A bifunctional iminophosphorane squaramide catalyzed enantioselective synthesis of hydroquinazolines: Via intramolecular aza-Michael reaction to α,β-unsaturated esters** (Chemical Science, 7 May 2021)[https://doi.org/10.1039/d1sc00856k]

Dalla Tiezza, M., Bickelhaupt, F. M., Flohé, L., Orian, L. **Proton Transfer and SN2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx** (ChemPlusChem, Apr 2021)[https://doi.org/10.1002/cplu.202000660]

Sijm, M., Maes, L., de Esch, I. J., Caljon, G., Sterk, G. J., Leurs, R. **Structure Activity Relationship of N-Substituted Phenyldihydropyrazolones Against Trypanosoma cruzi Amastigotes** (Frontiers in Chemistry, Apr 2021)[https://doi.org/10.3389/fchem.2021.608438]

Asseri, A. H., Godoy-Hernandez, A., Goojani, H. G., Lill, H., Sakamoto, J., McMillan, D. G., Bald, D. **Cardiolipin enhances the enzymatic activity of cytochrome bd and cytochrome bo 3 solubilized in dodecyl-maltoside** (Scientific Reports, Dec 2021)[https://doi.org/10.1038/s41598-021-87354-0]

Kagami, L., Roca-Martínez, J., Gavaldá-García, J., Ramasamy, P., Feenstra, K. A., Vranken, W. F. **Online biophysical predictions for SARS-Co** (BMC Molecular and Cell Biology, 23 Apr 2021)[https://doi.org/10.1186/s12860-021-00362-w]

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. **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"** (Toxicology Letters, 1 Aug 2021)[https://doi.org/10.1016/j.toxlet.2021.03.008]

Loru, D., Steber, A. L., Pinacho, P., Gruet, S., Temelso, B., Rijs, A. M., Pérez, C., Schnell, M. **How does the composition of a PAH influence its microsolvation? A rotational spectroscopy study of the phenanthrene-water and phenanthridine-water clusters** (Physical Chemistry Chemical Physics, 28 Apr 2021)[https://doi.org/10.1039/D1CP00898F]

Koenis, M. A., Nicu, V. P., Visscher, L., Kuehn, C., Bremer, M., Krier, M., Untenecker, H., Zhumaev, U., Küstner, B., Buma, W. J. **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.** (Physical Chemistry Chemical Physics, 28 Apr 2021)[https://doi.org/10.1039/d1cp00854d]

Kazandjian, T. D., Arrahman, A., Still, K. B., Somsen, G. W., Vonk, F. J., Casewell, N. R., Wilkinson, M. C., Kool, J. **Anticoagulant Activity of Naja nigricollis Venom Is Mediated by Phospholipase A2 Toxins and Inhibited by Varespladib** (Toxins, May 2021)[https://doi.org/10.3390/toxins13050302]

van Pelt-KleinJan, E., de Groot, D. H., Teusink, B. **Understanding FBA solutions under multiple nutrient limitations** (Metabolites, May 2021)[https://doi.org/10.3390/metabo11050257]

Hou, Q., Stringer, B., Waury, K., Capel, H., Haydarlou, R., Xue, F., Abeln, S., Heringa, J., Feenstra, K. A. **SeRenDIP-CE: Sequence-based Interface Prediction for Conformational Epitopes** (Bioinformatics (Oxford, England), 11 May 2021)[https://doi.org/10.1101/2020.11.19.390500]

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. **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** (Reproductive Toxicology, Jun 2021)[https://doi.org/10.1016/j.reprotox.2021.04.004]

Daas, T. J., Grossi, J., Vuckovic, S., Musslimani, Z. H., Kooi, D. P., Seidl, M., Giesbertz, K. J., Gori-Giorgi, P. **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)]** (Journal of Chemical Physics, 14 May 2021)[https://doi.org/10.1063/5.0053838]