# 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"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.General information** (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. 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.General information** (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)]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.General information** (Journal of Chemical Physics, 14 May 2021)[https://doi.org/10.1063/5.0053838]