# AIMMS publication report for: 2021-05-03

### New papers: 2021-4/5

Rodrigues Silva, D., de Azevedo Santos, L., Hamlin, T. A., Fonseca Guerra, C., Freitas, M. P., Bickelhaupt, F. M. **The Gauche Effect in XCH2CH2X Revisited** (ChemPhysChem, 7 Apr 2021)[https://doi.org/10.1002/cphc.202100090]

de Azevedo Santos, L., Ramalho, T. C., Hamlin, T. A., Bickelhaupt, F. M. **Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study** (Journal of Computational Chemistry, 15 Apr 2021)[https://doi.org/10.1002/jcc.26489]

De Groof, T. W., Elder, E. G., Siderius, M., Heukers, R., Sinclair, J. H., Smit, M. J. **Viral G Protein-Coupled Receptors: Attractive Targets for Herpesvirus-Associated Diseases** (Pharmacological reviews, 1 Apr 2021)[https://doi.org/10.1124/pharmrev.120.000186]

Orian, L., Bickelhaupt, F. M. **Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions** (Synlett, Apr 2021)[https://doi.org/10.1055/s-0040-1707284]

Ho, V. Q., Verboom, T., Rong, M. K., Habjan, E., Bitter, W., Speer, A. **Heterologous Expression of eth** (Antimicrobial agents and chemotherapy, Apr 2021)[https://doi.org/10.1128/AAC.01445-20]

Ma, X., Segura, M. A., Zarzycka, B., Vischer, H. F., Leurs, R. **Analysis of missense variants in the human histamine receptor family reveals increased constitutive activity of e4106.30×30k variant in the histamine h1 receptor** (International Journal of Molecular Sciences, 1 Apr 2021)[https://doi.org/10.3390/ijms22073702]

de Azevedo Santos, L., van der Lubbe, S. C., Hamlin, T. A., Ramalho, T. C., Matthias Bickelhaupt, F. **A Quantitative Molecular Orbital Perspective of the Chalcogen Bond** (ChemistryOpen, 1 Apr 2021)[https://doi.org/10.1002/open.202100066]

Houtman, C. J., Brewster, K., ten Broek, R., Duijve, B., van Oorschot, Y., Rosielle, M., Lamoree, M. H., Steen, R. J. **Characterisation of (anti-)progestogenic and (anti-)androgenic activities in surface and wastewater using high resolution effectdirected analysis** (Environment International, Aug 2021)[https://doi.org/10.1016/j.envint.2021.106536]

Chen, Y., van Pelt-KleinJan, E., van Olst, B., Douwenga, S., Boeren, S., Bachmann, H., Molenaar, D., Nielsen, J., Teusink, B. **Proteome constraints reveal targets for improving microbial fitness in nutrient-rich environments** (Molecular Systems Biology, 1 Apr 2021)[https://doi.org/10.15252/msb.202010093]

Rani, B., Silva‐marques, B., Leurs, R., Passani, M. B., Blandina, P., Provensi, G. **Short‐ and long‐term social recognition memory are differentially modulated by neuronal histamine** (Biomolecules, 9 Apr 2021)[https://doi.org/10.3390/biom11040555]

Celeiro, M., Armada, D., Ratola, N., Dagnac, T., de Boer, J., Llompart, M. **Evaluation of chemicals of environmental concern in crumb rubber and water leachates from several types of synthetic turf football pitches** (Chemosphere, May 2021)[https://doi.org/10.1016/j.chemosphere.2020.128610]