# AIMMS publication report for: 2020-10-12

### New papers: 2020-9/10

Landa, I., Westbroek, H., Janssen, F., van Muijlwijk-Koezen, J. E., Meeter, M. **Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking** (Science & Education, 7 Aug 2020)[https://doi.org/https://doi.org/10.1007/s11191-020-00145-3]

Narsaria, A. K., Ruijter, J. D., Hamlin, T. A., Ehlers, A. W., Guerra, C. F., Lammertsma, K., Bickelhaupt, F. M. **Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimides** (Journal of Computational Chemistry, 5 Jun 2020)[https://doi.org/10.1002/jcc.26188]

van de Ven, H. C., Purmova, J., Groeneveld, G., Bos, T. S., Gargano, A. F., van der Wal, S., Mengerink, Y., Schoenmakers, P. J. **Living with breakthrough: Two-dimensional liquid-chromatography separations of a water-soluble synthetically grafted bio-polymer** (Separations, Sep 2020)[https://doi.org/10.3390/separations7030041]

Stasyuk, O. A., Solà, M., Swart, M., Fonseca Guerra, C., Krygowski, T. M., Szatylowicz, H. **Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs** (ChemPhysChem, 15 Sep 2020)[https://doi.org/10.1002/cphc.202000434]

Perpiñá-Viciano, C., Işbilir, A., Zarca, A., Caspar, B., Kilpatrick, L. E., Hill, S. J., Smit, M. J., Lohse, M. J., Hoffmann, C. **Kinetic analysis of the early signaling steps of the human chemokine receptor CXCR4G protein–coupled receptors (GPCRs) are biologic switches that transduce extracellular stimuli into intracellular responses in the cell. Temporally resolving GPCR transduction pathways is key to understanding how cell signaling occurs. Here, we investigate the kinetics and dynamics of the activation and early signaling steps of the CXC chemokine receptor (CXCR) 4 in response to its natural ligands CXC chemokine ligand (CXCL) 12 and macrophage migration inhibitory factor (MIF), using Förster resonance energy transfer–based approaches. We show that CXCR4 presents a multifaceted response to CXCL12, with receptor activation (=0.6 seconds) followed by a rearrangement in the receptor/G protein complex (=1 seconds), a slower dimer rearrangement (=1.7 seconds), and prolonged G protein activation (=4 seconds). In comparison, MIF distinctly modulates every step of the transduction pathway, indicating distinct activation mechanisms and reflecting the different pharmacological properties of these two ligands. Our study also indicates that CXCR4 exhibits some degree of ligand-independent activity, a relevant feature for drug development.General information** (Molecular Pharmacology, 1 Aug 2020)[https://doi.org/10.1124/MOL.119.118448]

Landa, I., Westbroek, H., Janssen, F., van Muijlwijk, J., Meeter, M. **Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking** (Science and Education, 1 Oct 2020)[https://doi.org/10.1007/s11191-020-00145-3]

Pípal, M., Legradi, J., Smutná, M., Kočí, T., Priebojová, J., Bláhová, L., Krauss, M., Hilscherová, K. **Neurobehavioral effects of cyanobacterial biomass field extracts on zebrafish embryos and potential role of retinoids** (Aquatic Toxicology, Nov 2020)[https://doi.org/10.1016/j.aquatox.2020.105613]

Fumagalli, A., Heuninck, J., Pizzoccaro, A., Moutin, E., Koenen, J., Séveno, M., Durroux, T., Junier, M. P., Schlecht-Louf, G., Bachelerie, F., Schütz, D., Stumm, R., Smit, M. J., Guérineau, N. C., Chaumont-Dubel, S., Marin, P. **The atypical chemokine receptor 3 interacts with Connexin 43 inhibiting astrocytic gap junctional intercellular communication** (Nature Communications, 1 Dec 2020)[https://doi.org/10.1038/s41467-020-18634-y]

### New papers: 2020

Krahfuß, M. J., Nitsch, J., Bickelhaupt, F. M., Marder, T. B., Radius, U. **N-Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence** (Chemistry - A European Journal, 1 Sep 2020)[https://doi.org/10.1002/chem.202001062]

Yu, S., Vermeeren, P., van Dommelen, K., Bickelhaupt, F. M., Hamlin, T. A. **Understanding the 1,3-Dipolar Cycloadditions of Allenes** (Chemistry - A European Journal, 4 Sep 2020)[https://doi.org/10.1002/chem.202000857]

De Santis, M., Belpassi, L., Jacob, C. R., Severo Pereira Gomes, A., Tarantelli, F., Visscher, L., Storchi, L. **Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions** (Journal of chemical theory and computation, 8 Sep 2020)[https://doi.org/10.1021/acs.jctc.0c00603]

Buchholz, F., Theophilou, I., Giesbertz, K. J., Ruggenthaler, M., Rubio, A. **Light-Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics** (Journal of chemical theory and computation, 8 Sep 2020)[https://doi.org/10.1021/acs.jctc.0c00469]

Xie, C., Albulescu, L. O., Bittenbinder, M. A., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J. **Neutralizing effects of small molecule inhibitors and metal chelators on coagulopathic Viperinae snake venom toxins** (Biomedicines, Sep 2020)[https://doi.org/10.3390/BIOMEDICINES8090297]