# AIMMS publication report for: 2020-10-12

### New papers: 2020-9/10

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]