# AIMMS publication report for: 2022-09-07

### New papers: 2022-8/9

Wang, R., Hasanefendic, S., Von Hauff, E., Bossink, B. **The cost of photovoltaics: Re-evaluating grid parity for PV systems in China** (Renewable Energy, Jul 2022)[https://doi.org/10.1016/j.renene.2022.05.101]

Shaikh, B., Smith, L. P., Vasilescu, D., Marupilla, G., Wilson, M., Agmon, E., Agnew, H., Andrews, S. S., Anwar, A., Beber, M. E., Bergmann, F. T., Brooks, D., Brusch, L., Calzone, L., Choi, K., Cooper, J., Detloff, J., Drawert, B., Dumontier, M., Ermentrout, G. B., Faeder, J. R., Freiburger, A. P., Fröhlich, F., Funahashi, A., Garny, A., Gennari, J. H., Gleeson, P., Goelzer, A., Haiman, Z., Hasenauer, J., Hellerstein, J. L., Hermjakob, H., Hoops, S., Ison, J. C., Jahn, D., Jakubowski, H. V., Jordan, R., Kalaš, M., König, M., Liebermeister, W., Sheriff, R. S. M., Mandal, S., McDougal, R., Medley, J. K., Mendes, P., Müller, R., Myers, C. J., Naldi, A., Nguyen, T. V. N., Nickerson, D. P., Olivier, B. G., Patoliya, D., Paulevé, L., Petzold, L. R., Priya, A., Rampadarath, A. K., Rohwer, J. M., Saglam, A. S., Singh, D., Sinha, A., Snoep, J., Sorby, H., Spangler, R., Starruß, J., Thomas, P. J., Van Niekerk, D., Weindl, D., Zhang, F., Zhukova, A., Goldberg, A. P., Schaff, J. C., Blinov, M. L., Sauro, H. M., Moraru, I. I., Karr, J. R. **BioSimulators: a central registry of simulation engines and services for recommending specific tools** (Nucleic acids research, 5 Jul 2022)[https://doi.org/10.1093/nar/gkac331]

Deng, Y., Moo, E. V., Pérez Almería, C. V., Gentry, P. R., Vedel, L., Mathiesen, J. M., Bräuner-Osborne, H. **Delineation of the GPR15 receptor-mediated Gα protein signalling profile in recombinant mammalian cells** (Basic and Clinical Pharmacology and Toxicology, Aug 2022)[https://doi.org/10.1111/bcpt.13738]

Menzel, J. P., Boeije, Y., Bakker, T. M. A., Belić, J., Reek, J. N. H., de Groot, H. J. M., Visscher, L., Buda, F. **In Silico Optimization of Charge Separating Dyes for Solar Energy Conversion** (ChemSusChem, 5 Aug 2022)[https://doi.org/10.1002/cssc.202200594]

Ma, X., Gao, M., Vischer, H. F., Leurs, R. **A Nano BRET-Based H3R Conformational Biosensor to Study Real-Time H3 Receptor Pharmacology in Cell Membranes and Living Cells** (International Journal of Molecular Sciences, 1 Aug 2022)[https://doi.org/10.3390/ijms23158211]

Giarrusso, S., Neugarten, R., Baerends, E. J., Giesbertz, K. J. H. **Secondary Kinetic Peak in the Kohn-Sham Potential and Its Connection to the Response Step** (Journal of chemical theory and computation, 9 Aug 2022)[https://doi.org/10.1021/acs.jctc.2c00332]

Bosdriesz, E., Fernandes Neto, J. M., Sieber, A., Bernards, R., Blüthgen, N., Wessels, L. F. A. **Identifying mutant-specific multi-drug combinations using comparative network reconstruction** (iScience, 19 Aug 2022)[https://doi.org/10.1016/j.isci.2022.104760]

Blanas, A., Karsjens, H., de Ligt, A., Huijbers, E. J. M., van Loon, K., Denisov, S. S., Durukan, C., Engbersen, D. J. M., Groen, J., Hennig, S., Hackeng, T. M., van Beijnum, J. R., Griffioen, A. W. **Vaccination with a bacterial peptide conjugated to SARS-Co** (iScience, 19 Aug 2022)[https://doi.org/10.1016/j.isci.2022.104719]

Marvelous, C., de Azevedo Santos, L., Siegler, M. A., Fonseca Guerra, C., Bouwman, E. **Cleaner and stronger: how 8-quinolinolate facilitates formation of Co(iii)-thiolate from Co(ii)-disulfide complexes** (Dalton Transactions, 21 Aug 2022)[https://doi.org/10.1039/d2dt02106d]

Niezen, L. E., Staal, B. B. P., Lang, C., Philipsen, H. J. A., Pirok, B. W. J., Somsen, G. W., Schoenmakers, P. J. **Recycling gradient-elution liquid chromatography for the analysis of chemical-composition distributions of polymers** (Journal of Chromatography A, 30 Aug 2022)[https://doi.org/10.1016/j.chroma.2022.463386]

Blokker, E., van Zeist, W. J., Sun, X., Poater, J., van der Schuur, J. M., Hamlin, T. A., Bickelhaupt, F. M. **Methyl Substitution Destabilizes Alkyl Radicals** (Angewandte Chemie - International Edition, 5 Sep 2022)[https://doi.org/10.1002/anie.202207477]

Gstöttner, C., Haselberg, R., Wuhrer, M., Somsen, G. W., Domínguez-Vega, E. **Assessment of Macro- and Microheterogeneity of Monoclonal Antibodies Using Capillary Zone Electrophoresis Hyphenated with Mass Spectrometry** (None, 2022)[https://doi.org/10.1007/978-1-0716-2493-7\_9]

Haerkens, F., Kikken, C., Kirkels, L., van Amstel, M., Wouters, W., van Doornmalen, E., Francke, C., Hughes, S. **A new use for old drugs: identifying compounds with an anti-obesity effect using a high through-put semi-automated Caenorhabditis elegans screening platform** (Heliyon, Aug 2022)[https://doi.org/10.1016/j.heliyon.2022.e10108]

Pascha, M. N., Thijssen, V., Egido, J. E., Linthorst, M. W., Van Lanen, J. H., Van Dongen, D. A. A., Hopstaken, A. J. P., Van Kuppeveld, F. J. M., Snijder, J., De Haan, C. A. M., Jongkees, S. A. K. **Inhibition of H1 and H5 Influenza A Virus Entry by Diverse Macrocyclic Peptides Targeting the Hemagglutinin Stem Region** (Acs chemical biology, 4 Aug 2022)[https://doi.org/10.1021/acschembio.2c00040]

Nys, M., Zarkadas, E., Brams, M., Mehregan, A., Kambara, K., Kool, J., Casewell, N. R., Bertrand, D., Baenziger, J. E., Nury, H., Ulens, C. **The molecular mechanism of snake short-chain α-neurotoxin binding to muscle-type nicotinic acetylcholine receptors** (Nature Communications, 4 Aug 2022)[https://doi.org/10.1038/s41467-022-32174-7]

Perryman, R., Renziehausen, A., Shaye, H., Kostagianni, A. D., Tsiailanis, A. D., Thorne, T., Chatziathanasiadou, M. V., Sivolapenko, G. B., El Mubarak, M. A., Han, G. W., Zarzycka, B., Katritch, V., Lebon, G., Lo Nigro, C., Lattanzio, L., Morse, S. V., Choi, J. J., O'Neill, K., Kanaki, Z., Klinakis, A., Crook, T., Cherezov, V., Tzakos, A. G., Syed, N. **Inhibition of the angiotensin II type 2 receptor AT2R is a novel therapeutic strategy for glioblastoma** (Proceedings of the National Academy of Sciences of the United States of America, 9 Aug 2022)[https://doi.org/10.1073/pnas.2116289119]