# AIMMS publication report for: 2020-09-28

### New papers: 2020-8/09

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]

Faltracco, M., Sukowski, V., Van Druenen, M., Hamlin, T. A., Bickelhaupt, F. M., Ruijter, E. **Diastereoselective Synthesis of β-Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsuji-Trost Allylation** (Journal of Organic Chemistry, 7 Aug 2020)[https://doi.org/10.1021/acs.joc.0c00575]

Bunduc, C. M., Bitter, W., Houben, E. N. G.Pages:315-335 **Structure and Function of the Mycobacterial Type VII Secretion Systems** (Annual Review of Microbiology, 13 Jul 2020)[https://doi.org/10.1146/annurev-micro-012420-081657]

Koenis, M. A., Chibueze, C. S., Jinks, M. A., Nicu, V. P., Visscher, L., Goldup, S. M., Buma, W. J. **Vibrational circular dichroism spectroscopy for probing the expression of chirality in mechanically planar chiral rotaxanes** (Chemical Science, 28 Aug 2020)[https://doi.org/10.1039/d0sc02485f]

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]

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]

Sénard, T., Gargano, A. F., Falck, D., de Taeye, S. W., Rispens, T., Vidarsson, G., Wuhrer, M., Somsen, G. W., Domínguez-Vega, E. **MS-Based Allotype-Specific Analysis of Polyclonal Ig** (Frontiers in Immunology, 21 Aug 2020)[https://doi.org/10.3389/fimmu.2020.02049]

Daly, C. A., Smit, M. J., Plouffe, B. **The constitutive activity of the viral-encoded G protein-coupled receptor US28 supports a complex signalling network contributing to cancer development** (Biochemical Society transactions, 28 Aug 2020)[https://doi.org/10.1042/BST20190988]

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]

### New papers: 2020

Sugeng, E. J., de Cock, M., Leonards, P. E., van de Bor, M. **Toddler behavior, the home environment, and flame retardant exposure** (Chemosphere, Aug 2020)[https://doi.org/10.1016/j.chemosphere.2020.126588]

Jonkers, T. J., Steenhuis, M., Schalkwijk, L., Luirink, J., Bald, D., Houtman, C. J., Kool, J., Lamoree, M. H., Hamers, T. **Development of a high-throughput bioassay for screening of antibiotics in aquatic environmental samples** (Science of the Total Environment, 10 Aug 2020)[https://doi.org/10.1016/j.scitotenv.2020.139028]

Autrup, H., Barile, F. A., Berry, S. C., Blaauboer, B. J., 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., Vermeulen, N. P. **Human exposure to synthetic endocrine disrupting chemicals (S-EDCs) is generally negligible as compared to natural compounds with higher or comparable endocrine activity. How to evaluate the risk of the S-EDCs?** (Environmental Toxicology and Pharmacology, Aug 2020)[https://doi.org/10.1016/j.etap.2020.103396]

Autrup, H., Barile, F. A., Berry, S. C., Blaauboer, B. J., 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., Vermeulen, N. P. **Human exposure to synthetic endocrine disrupting chemicals (S-EDCs) is generally negligible as compared to natural compounds with higher or comparable endocrine activity. How to evaluate the risk of the S-EDCs?** (Chemico-Biological Interactions, 1 Aug 2020)[https://doi.org/10.1016/j.cbi.2020.109099]

Narsaria, A. K., Rauch, F., Krebs, J., Endres, P., Friedrich, A., Krummenacher, I., Braunschweig, H., Finze, M., Nitsch, J., Bickelhaupt, F. M., Marder, T. B. **Computationally Guided Molecular Design to Minimize the LE/CT Gap in D-π-A Fluorinated Triarylboranes for Efficient TADF via D and π-Bridge Tuning** (Advanced Functional Materials, 1 Aug 2020)[https://doi.org/10.1002/adfm.202002064]

Wang, J., Guo, J., Chen, H., Huang, X., Somsen, G. W., Song, F., Jiang, Z. **A single-step preparation of carbohydrate functionalized monoliths for separation and trapping of polar compounds** (Journal of Chromatography A, 27 Sep 2020)[https://doi.org/10.1016/j.chroma.2020.461481]

Hapka, M., Pernal, K., Gritsenko, O. V. **Local Enhancement of Dynamic Correlation in Excited States: Fresh Perspective on Ionicity and Development of Correlation Density Functional Approximation Based on the On-Top Pair Density** (The journal of physical chemistry letters, 6 Aug 2020)[https://doi.org/10.1021/acs.jpclett.0c01616]

van der Stel, W., Carta, G., Eakins, J., Darici, S., Delp, J., Forsby, A., Bennekou, S. H., Gardner, I., Leist, M., Danen, E. H., Walker, P., van de Water, B., Jennings, P. **Correction to: Multiparametric assessment of mitochondrial respiratory inhibition in Hep** (Archives of Toxicology, Aug 2020)[https://doi.org/10.1007/s00204-020-02849-5]

Keating, S. M., Waltemath, D., König, M., Zhang, F., Dräger, A., Chaouiya, C., Bergmann, F. T., Finney, A., Gillespie, C. S., Helikar, T., Hoops, S., Malik-Sheriff, R. S., Moodie, S. L., Moraru, I. I., Myers, C. J., Naldi, A., Olivier, B. G., Sahle, S., Schaff, J. C., Smith, L. P., Swat, M. J., Thieffry, D., Watanabe, L., Wilkinson, D. J., Blinov, M. L., Begley, K., Faeder, J. R., Gómez, H. F., Hamm, T. M., Inagaki, Y., Liebermeister, W., Lister, A. L., Lucio, D., Mjolsness, E., Proctor, C. J., Raman, K., Rodriguez, N., Shaffer, C. A., Shapiro, B. E., Stelling, J., Swainston, N., Tanimura, N., Wagner, J., Meier-Schellersheim, M., Sauro, H. M., Palsson, B., Bolouri, H., Kitano, H., Funahashi, A., Hermjakob, H., Doyle, J. C., Hucka, M., Adams, R. R., Allen, N. A., Angermann, B. R., Antoniotti, M., Bader, G. D., Červený, J., Courtot, M., Cox, C. D., Dalle Pezze, P., Demir, E., Denney, W. S., Dharuri, H., Dorier, J., Drasdo, D., Ebrahim, A., Eichner, J., Elf, J., Endler, L., Evelo, C. T., Flamm, C., Fleming, R. M., Fröhlich, M., Glont, M., Gonçalves, E., Golebiewski, M., Grabski, H., Gutteridge, A., Hachmeister, D., Harris, L. A., Heavner, B. D., Henkel, R., Hlavacek, W. S., Hu, B., Hyduke, D. R., de Jong, H., Juty, N., Karp, P. D., Karr, J. R., Kell, D. B., Keller, R., Kiselev, I., Klamt, S., Klipp, E., Knüpfer, C., Kolpakov, F., Krause, F., Kutmon, M., Laibe, C., Lawless, C., Li, L., Loew, L. M., Machne, R., Matsuoka, Y., Mendes, P., Mi, H., Mittag, F., Monteiro, P. T., Natarajan, K. N., Nielsen, P. M., Nguyen, T., Palmisano, A., Pettit, J. B., Pfau, T., Phair, R. D., Radivoyevitch, T., Rohwer, J. M., Ruebenacker, O. A., Saez-Rodriguez, J., Scharm, M., Schmidt, H., Schreiber, F., Schubert, M., Schulte, R., Sealfon, S. C., Smallbone, K., Soliman, S., Stefan, M. I., Sullivan, D. P., Takahashi, K., Teusink, B., Tolnay, D., Vazirabad, I., von Kamp, A., Wittig, U., Wrzodek, C., Wrzodek, F., Xenarios, I., Zhukova, A., Zucker, J. **SBML Level 3: an extensible format for the exchange and reuse of biological models** (Molecular Systems Biology, 1 Aug 2020)[https://doi.org/10.15252/msb.20199110]

de Araújo, J. S., França da Silva, C., Batista, D. D. G. J., Nefertiti, A., Fiuza, L. F. D. A., Fonseca-Berzal, C. R., Bernardino da Silva, P., Batista, M. M., Sijm, M., Kalejaiye, T. D., de Koning, H. P., Maes, L., Sterk, G. J., Leurs, R., Soeiro, M. D. N. C. **Efficacy of Novel Pyrazolone Phosphodiesterase Inhibitors in Experimental Mouse Models of Trypanosoma cruzi** (Antimicrobial agents and chemotherapy, 20 Aug 2020)[https://doi.org/10.1128/AAC.00414-20]