# AIMMS publication report for: 2020-09-14

### New papers: 2020-09

Iversen, P. O., Atukunda, P., Kort, R., Ueland, P. M., Westerberg, A. C., Muhoozi, G. K. M. **No associations between microbiota signaling substances and cognitive, language and motor development among three-year-old rural Ugandan children** (Acta Paediatrica, 29 Apr 2020)[https://doi.org/10.1111/apa.15330]

Vuckovic, S., Fabiano, E., Gori-Giorgi, P., Burke, K. **MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory** (Journal of chemical theory and computation, 14 Jul 2020)[https://doi.org/10.1021/acs.jctc.0c00049]

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]

Munday, J. C., Kunz, S., Kalejaiye, T. D., Siderius, M., Schroeder, S., Paape, D., Alghamdi, A. H., Abbasi, Z., Huang, S. X., Donachie, A. M., William, S., Sabra, A. N., Sterk, G. J., Botros, S. S., Brown, D. G., Hoffman, C. S., Leurs, R., de Koning, H. P. **Cloning and functional complementation of ten Schistosoma mansoni phosphodiesterases expressed in the mammalian host stages** (PLoS Neglected Tropical Diseases, 30 Jul 2020)[https://doi.org/10.1371/journal.pntd.0008447]

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]

### 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]