# AIMMS publication report for: 2020-08-31

### New papers: 2020-08

Luo, L., Straatsma, T. P., Suarez, L. E., Broer, R., Bykov, D., D'Azevedo, E. F., Faraji, S. S., Gottiparthi, K. C., De Graaf, C., Harris, J. A., Havenith, R. W., Jensen, H. J., Joubert, W., Kathir, R. K., Larkin, J., Li, Y. W., Lyakh, D. I., Messer, O. E., Norman, M. R., Oefelein, J. C., Sankaran, R., Tillack, A. F., Barnes, A. L., Visscher, L., Wells, J. C., Wibowo, M. **Pre-exascale accelerated application development: The ORNL Summit experience** (IBM Journal of Research and Development, 1 May 2020)[https://doi.org/10.1147/JRD.2020.2965881]

Verweij, E. W., Al Araaj, B., Prabhata, W. R., Prihandoko, R., Nijmeijer, S., Tobin, A. B., Leurs, R., Vischer, H. F. **Differential Role of Serines and Threonines in Intracellular Loop 3 and C-Terminal Tail of the Histamine H4 Receptor in β-Arrestin and G Protein-Coupled Receptor Kinase Interaction, Internalization, and Signaling** (ACS Pharmacology and Translational Science, 10 Apr 2020)[https://doi.org/10.1021/acsptsci.0c00008]

Hintzen, J. C., Poater, J., Kumar, K., Al Temimi, A. H., Pieters, B. J., Paton, R. S., Bickelhaupt, F. M., Mecinović, J. **Comparison of molecular recognition of trimethyllysine and trimethylthialysine by epigenetic reader proteins** (Molecules, Apr 2020)[https://doi.org/10.3390/molecules25081918]

Kool, J. **Picofractionation & MS imaging: Analytics for pathology profiling of venoms** (Toxicon : official journal of the International Society on Toxinology, 20 Apr 2020)[https://doi.org/10.1016/j.toxicon.2019.10.024]

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?** (Toxicology Letters, 1 Oct 2020)[https://doi.org/10.1016/j.toxlet.2020.04.008]

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?** (Toxicology in Vitro, Sep 2020)[https://doi.org/10.1016/j.tiv.2020.104861]

Joost, M., Nieger, M., Lutz, M., Ehlers, A. W., Slootweg, J. C., Lammertsma, K. **Synthesis, Structures, and Electronic Properties of O- And S-Heterocyclic Carbene Complexes of Iridium, Copper, Silver, and Gold** (Organometallics, 26 May 2020)[https://doi.org/10.1021/acs.organomet.0c00066]

Koenderink, J. B., van den Heuvel, J. J., Bilos, A., Vredenburg, G., Vermeulen, N. P., Russel, F. G. **Human multidrug resistance protein 4 (MRP4) is a cellular efflux transporter for paracetamol glutathione and cysteine conjugates** (Archives of Toxicology, 1 Sep 2020)[https://doi.org/10.1007/s00204-020-02793-4]

Zhu, D., Zito, J., Pinchetti, V., Dang, Z., Olivati, A., Pasquale, L., Tang, A., Zaffalon, M. L., Meinardi, F., Infante, I., De Trizio, L., Manna, L., Brovelli, S. **Compositional Tuning of Carrier Dynamics in Cs2Na1- x** (ACS Energy Letters, 12 Jun 2020)[https://doi.org/10.1021/acsenergylett.0c00914]

Nordholt, N., van Heerden, J. H., Bruggeman, F. J. **Biphasic Cell-Size and Growth-Rate Homeostasis by Single Bacillus subtilis Cells** (Current Biology, 22 Jun 2020)[https://doi.org/10.1016/j.cub.2020.04.030]

Aerts, J. W., Riedo, A., Melton, D. J., Martini, S., Flahaut, J., Meierhenrich, U. J., Meinert, C., Myrgorodska, I., Lindner, R., Ehrenfreund, P. **Biosignature Analysis of Mars Soil Analogs from the Atacama Desert: Challenges and Implications for Future Missions to Mars** (Astrobiology, Jun 2020)[https://doi.org/10.1089/ast.2019.2063]

Reid, G., Sybesma, W., Matovu, W., Onyango, A., Westerik, N., Kort, R. **Empowering women through probiotic fermented food in East Africa** (Journal of global health, Jun 2020)[https://doi.org/10.7189/jogh.10.010330]

Charalampopoulos, P., Pissis, S. P., Radoszewski, J., Walen, T., Zuba, W. **Unary Words Have the Smallest Levenshtein k-Neighbourhoods** (None, 9 Jun 2020)[https://doi.org/10.4230/LIPIcs.CPM.2020.10]

Zhang, L., Yamazaki, K., Leitch, J. A., Manzano, R., Atkinson, V. A., Hamlin, T. A., Dixon, D. J. **Dual catalytic enantioselective desymmetrization of allene-tethered cyclohexanones** (Chemical Science, 28 Jun 2020)[https://doi.org/10.1039/d0sc02878a]

Soave, M., Heukers, R., Kellam, B., Woolard, J., Smit, M. J., Briddon, S. J., Hill, S. J. **Monitoring Allosteric Interactions with CXCR4 Using Nano** (None, 30 Jun 2020)[https://doi.org/10.1016/j.chembiol.2020.06.006]

Di Zazzo, A., Yang, W., Coassin, M., Micera, A., Antonini, M., Piccinni, F., De Piano, M., Kohler, I., Harms, A. C., Hankemeier, T., Bonini, S., Mashaghi, A. **Correction to: Signaling lipids as diagnostic biomarkers for ocular surface cicatrizing conjunctivitis** (Journal of Molecular Medicine, Jul 2020)[https://doi.org/10.1007/s00109-020-01938-3]

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?** (Archives of Toxicology, Jul 2020)[https://doi.org/10.1007/s00204-020-02800-8]

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]

Pichon, X., Robert, M. C., Bertrand, E., Singer, R. H., Tutucci, E. **New Generations of MS2 Variants and MCP Fusions to Detect Single m** (None, 2020)[https://doi.org/10.1007/978-1-0716-0712-1\_7]

Tutucci, E., Singer, R. H. **Simultaneous Detection of m** (None, 2020)[https://doi.org/10.1007/978-1-0716-0712-1\_4]

Gerber, A., Roeder, R. G. **The CTD Is Not Essential for the Post-Initiation Control of RNA Polymerase II Activity** (None, 21 Jul 2020)[https://doi.org/10.1016/j.jmb.2020.07.010]

Houtman, C. J., ten Broek, R., van Oorschot, Y., Kloes, D., van der Oost, R., Rosielle, M., Lamoree, M. H. **High resolution effect-directed analysis of steroid hormone (ant)agonists in surface and wastewater quality monitoring** (Environmental Toxicology and Pharmacology, Nov 2020)[https://doi.org/10.1016/j.etap.2020.103460]

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]

### New papers: 2020

Dalla Tiezza, M., Bickelhaupt, F. M., Flohé, L., Maiorino, M., Ursini, F., Orian, L. **A dual attack on the peroxide bond. The common principle of peroxidatic cysteine or selenocysteine residues** (Redox Biology, Jul 2020)[https://doi.org/10.1016/j.redox.2020.101540]

Förster, A., Visscher, L. **Double hybrid DFT calculations with Slater type orbitals** (Journal of Computational Chemistry, 5 Jul 2020)[https://doi.org/10.1002/jcc.26209]

Hansen, T., Vermeeren, P., Haim, A., van Dorp, M. J., Codée, J. D., Bickelhaupt, F. M., Hamlin, T. A. **Regioselectivity of Epoxide Ring-Openings via SN2 Reactions Under Basic and Acidic Conditions** (European Journal of Organic Chemistry, 7 Jul 2020)[https://doi.org/10.1002/ejoc.202000590]

Kooijman, S. A., Lika, K., Augustine, S., Marn, N., Kooi, B. W. **The energetic basis of population growth in animal kingdom** (Ecological Modelling, 15 Jul 2020)[https://doi.org/10.1016/j.ecolmodel.2020.109055]

Ortega Ugalde, S., Wallraven, K., Speer, A., Bitter, W., Grossmann, T. N., Commandeur, J. N. **Acetylene containing cyclo(L-Tyr-L-Tyr)-analogs as mechanism-based inhibitors of CYP121A1 from Mycobacterium tuberculosis** (Biochemical Pharmacology, Jul 2020)[https://doi.org/10.1016/j.bcp.2020.113938]

Gerritse, J., Leslie, H. A., de Tender, C. A., Devriese, L. I., Vethaak, A. D. **Fragmentation of plastic objects in a laboratory seawater microcosm** (Scientific Reports, 1 Dec 2020)[https://doi.org/10.1038/s41598-020-67927-1]

Bossink, B. **Learning strategies in sustainable energy demonstration projects: What organizations learn from sustainable energy demonstrations** (Renewable and Sustainable Energy Reviews, Oct 2020)[https://doi.org/10.1016/j.rser.2020.110025]

Krebs, A., van Vugt-Lussenburg, B. M. A., Waldmann, T., Albrecht, W., Boei, J., Ter Braak, B., Brajnik, M., Braunbeck, T., Brecklinghaus, T., Busquet, F., Dinnyes, A., Dokler, J., Dolde, X., Exner, T. E., Fisher, C., Fluri, D., Forsby, A., Hengstler, J. G., Holzer, A., Janstova, Z., Jennings, P., Kisitu, J., Kobolak, J., Kumar, M., Limonciel, A., Lundqvist, J., Mihalik, B., Moritz, W., Pallocca, G., Ulloa, A. P. C., Pastor, M., Rovida, C., Sarkans, U., Schimming, J. P., Schmidt, B. Z., Stöber, R., Strassfeld, T., van de Water, B., Wilmes, A., van der Burg, B., Verfaillie, C. M., von Hellfeld, R., Vrieling, H., Vrijenhoek, N. G., Leist, M.Pages:2435-2461 **The EU-Tox** (Archives of Toxicology, 6 Jul 2020)[https://doi.org/10.1007/s00204-020-02802-6]

Johansson, H. K., Damdimopoulou, P., van Duursen, M. B., Boberg, J., Franssen, D., de Cock, M., Jääger, K., Wagner, M., Velthut-Meikas, A., Xie, Y., Connolly, L., Lelandais, P., Mazaud-Guittot, S., Salumets, A., Draskau, M. K., Filis, P., Fowler, P. A., Christiansen, S., Parent, A. S., Svingen, T. **Putative adverse outcome pathways for female reproductive disorders to improve testing and regulation of chemicals** (None, 7 Jul 2020)[https://doi.org/10.1007/s00204-020-02834-y]

van den Brand, A. D., Rubinstein, E., de Jong, P. C., van den Berg, M., van Duursen, M. B. **Assessing anti-estrogenic effects of AHR ligands in primary human and rat endometrial epithelial cells** (Reproductive Toxicology, Sep 2020)[https://doi.org/10.1016/j.reprotox.2020.07.00310.1016/j.reprotox.2020.07.003]

Dulio, V., Koschorreck, J., van Bavel, B., van den Brink, P., Hollender, J., Munthe, J., Schlabach, M., Aalizadeh, R., Agerstrand, M., Ahrens, L., Allan, I., Alygizakis, N., Barcelo’, D., Bohlin-Nizzetto, P., Boutroup, S., Brack, W., Bressy, A., Christensen, J. H., Cirka, L., Covaci, A., Derksen, A., Deviller, G., Dingemans, M. M., Engwall, M., Fatta-Kassinos, D., Gago-Ferrero, P., Hernández, F., Herzke, D., Hilscherová, K., Hollert, H., Junghans, M., Kasprzyk-Hordern, B., Keiter, S., Kools, S. A., Kruve, A., Lambropoulou, D., Lamoree, M., Leonards, P., Lopez, B., López de Alda, M., Lundy, L., Makovinská, J., Marigómez, I., Martin, J. W., McHugh, B., Miège, C., O’Toole, S., Perkola, N., Polesello, S., Posthuma, L., Rodriguez-Mozaz, S., Roessink, I., Rostkowski, P., Ruedel, H., Samanipour, S., Schulze, T., Schymanski, E. L., Sengl, M., Tarábek, P., Ten Hulscher, D., Thomaidis, N., Togola, A., Valsecchi, S., van Leeuwen, S., von der Ohe, P., Vorkamp, K., Vrana, B., Slobodnik, J. **The NORMAN Association and the European Partnership for Chemicals Risk Assessment (PARC): let’s cooperate!The Partnership for Chemicals Risk Assessment (PARC) is currently under development as a joint research and innovation programme to strengthen the scientific basis for chemical risk assessment in the EU. The plan is to bring chemical risk assessors and managers together with scientists to accelerate method development and the production of necessary data and knowledge, and to facilitate the transition to next-generation evidence-based risk assessment, a non-toxic environment and the European Green Deal. The NORMAN Network is an independent, well-established and competent network of more than 80 organisations in the field of emerging substances and has enormous potential to contribute to the implementation of the PARC partnership. NORMAN stands ready to provide expert advice to PARC, drawing on its long experience in the development, harmonisation and testing of advanced tools in relation to chemicals of emerging concern and in support of a European Early Warning System to unravel the risks of contaminants of emerging concern (CECs) and close the gap between research and innovation and regulatory processes. In this commentary we highlight the tools developed by NORMAN that we consider most relevant to supporting the PARC initiative: (i) joint data space and cutting-edge research tools for risk assessment of contaminants of emerging concern; (ii) collaborative European framework to improve data quality and comparability; (iii) advanced data analysis tools for a European early warning system and (iv) support to national and European chemical risk assessment thanks to harnessing, combining and sharing evidence and expertise on CECs. By combining the extensive knowledge and experience of the NORMAN network with the financial and policy-related strengths of the PARC initiative, a large step towards the goal of a non-toxic environment can be taken.General information** (Environmental Sciences Europe, 1 Dec 2020)[https://doi.org/10.1186/s12302-020-00375-w]

Loha, K. M., Lamoree, M., De Boer, J. **Pesticide residue levels in vegetables and surface waters at the Central Rift Valley (CRV) of Ethiopia** (Environmental Monitoring and Assessment, 27 Jul 2020)[https://doi.org/10.1007/s10661-020-08452-6]

de Weert, J., Smedes, F., Beeltje, H., de Zwart, D., Hamers, T. **Time integrative sampling properties of Speedisk and silicone rubber passive samplers determined by chemical analysis and in vitro bioassay testing** (Chemosphere, Nov 2020)[https://doi.org/10.1016/j.chemosphere.2020.127498]

Geurink, L., van Tricht, E., Dudink, J., Pajic, B., van de Griend, C. E. S. **Four-step approach to efficiently develop capillary gel electrophoresis methods for viral vaccine protein analysis** (None, 8 Jul 2020)[https://doi.org/10.1002/elps.202000107]

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]

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