# 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]

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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]

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