# AIMMS publication report for: 2022-11-23

### New papers: 2022-10/11

Luzia, L., Lao-Martil, D., Savakis, P., van Heerden, J., van Riel, N., Teusink, B. **pH dependencies of glycolytic enzymes of yeast under in vivo-like assay conditions** (FEBS Journal, Oct 2022)[https://doi.org/10.1111/febs.16459]

Förster, A. **Assessment of the Second-Order Statically Screened Exchange Correction to the Random Phase Approximation for Correlation Energies** (Journal of chemical theory and computation, 11 Oct 2022)[https://doi.org/10.1021/acs.jctc.2c00366]

Solà, M., Bickelhaupt, F. M. **Particle on a Ring Model for Teaching the Origin of the Aromatic Stabilization Energy and the Hückel and Baird Rules** (Journal of Chemical Education, 11 Oct 2022)[https://doi.org/10.1021/acs.jchemed.2c00523]

Śmiga, S., Della Sala, F., Gori-Giorgi, P., Fabiano, E. **Self-Consistent Implementation of Kohn-Sham Adiabatic Connection Models with Improved Treatment of the Strong-Interaction Limit** (Journal of chemical theory and computation, 11 Oct 2022)[https://doi.org/10.1021/acs.jctc.2c00352]

Vázquez-Lorente, H., Jurado-Fasoli, L., Kohler, I., Di, X., Yang, W., Osuna-Prieto, F. J., Asadov, S., Frias-Rodríguez, J. F., Castillo-Garzón, M. J., Amaro-Gahete, F. J. **Linoleic acid-derived oxylipins and isoprostanes plasma levels are influenced by 1,25-Dihydroxyvitamin D levels in middle-aged sedentary adults: The FIT-AGEING study** (Experimental Gerontology, Nov 2022)[https://doi.org/10.1016/j.exger.2022.111954]

Jian, J., Yuan, J., Fan, Y., Wang, J., Zhang, T., Kool, J., Jiang, Z. **High-Resolution Bioassay Profiling with Complemented Sensitivity and Resolution for Pancreatic Lipase Inhibitor Screening** (Molecules, 2 Oct 2022)[https://doi.org/10.3390/molecules27206923]

Escher, B. I., Lamoree, M., Antignac, J. P., Scholze, M., Herzler, M., Hamers, T., Jensen, T. K., Audebert, M., Busquet, F., Maier, D., Oelgeschläger, M., Valente, M. J., Boye, H., Schmeisser, S., Dervilly, G., Piumatti, M., Motteau, S., König, M., Renko, K., Margalef, M., Cariou, R., Ma, Y., Treschow, A. F., Kortenkamp, A., Vinggaard, A. M. **Mixture Risk Assessment of Complex Real-Life Mixtures—The PANORAMIX Project** (International Journal of Environmental Research and Public Health, 2 Oct 2022)[https://doi.org/10.3390/ijerph192012990]

Paulussen, F. M., Grossmann, T. N. **Peptide-based covalent inhibitors of protein–protein interactions** (Journal of Peptide Science, 14 Oct 2022)[https://doi.org/10.1002/psc.3457]

Bartova, S., Madrid-Gambin, F., Fernández, L., Carayol, J., Meugnier, E., Segrestin, B., Delage, P., Vionnet, N., Boizot, A., Laville, M., Vidal, H., Marco, S., Hager, J., Moco, S. **Grape polyphenols decrease circulating branched chain amino acids in overfed adults** (Frontiers in nutrition, 26 Oct 2022)[https://doi.org/10.3389/fnut.2022.998044]

Wágner, G., Mocking, T. A. M., Ma, X., Slynko, I., Da Costa Pereira, D., Breeuwer, R., Rood, N. J. N., van der Horst, C., Vischer, H. F., de Graaf, C., de Esch, I. J. P., Wijtmans, M., Leurs, R. **SAR exploration of the non-imidazole histamine H3 receptor ligand ZEL-H16 reveals potent inverse agonism** (Archiv der Pharmazie, 30 Oct 2022)[https://doi.org/10.1002/ardp.202200451]

Arrahman, A., Kazandjian, T. D., Still, K. B. M., Slagboom, J., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J. **A Combined Bioassay and Nanofractionation Approach to Investigate the Anticoagulant Toxins of Mamba and Cobra Venoms and Their Inhibition by Varespladib** (Toxins, Nov 2022)[https://doi.org/10.3390/toxins14110736]

Jurado-Fasoli, L., Di, X., Sanchez-Delgado, G., Yang, W., Osuna-Prieto, F. J., Ortiz-Alvarez, L., Krekels, E., Harms, A. C., Hankemeier, T., Schönke, M., Aguilera, C. M., Llamas-Elvira, J. M., Kohler, I., Rensen, P. C. N., Ruiz, J. R., Martinez-Tellez, B. **Acute and long-term exercise differently modulate plasma levels of oxylipins, endocannabinoids, and their analogues in young sedentary adults: A sub-study and secondary analyses from the ACTIBATE randomized controlled-trial** (Ebiomedicine, Nov 2022)[https://doi.org/10.1016/j.ebiom.2022.104313]

Hansen, T., Vermeeren, P., Bickelhaupt, F. M., Hamlin, T. A. **Stability of alkyl carbocations** (Chemical communications (Cambridge, England), 7 Nov 2022)[https://doi.org/10.1039/d2cc04034d]

van Spanning, R. J. M., Guan, Q., Melkonian, C., Gallant, J., Polerecky, L., Flot, J. F., Brandt, B. W., Braster, M., Iturbe Espinoza, P., Aerts, J. W., Meima-Franke, M. M., Piersma, S. R., Bunduc, C. M., Ummels, R., Pain, A., Fleming, E. J., van der Wel, N. N., Gherman, V. D., Sarbu, S. M., Bodelier, P. L. E., Bitter, W. **Methanotrophy by a Mycobacterium species that dominates a cave microbial ecosystem** (NATURE MICROBIOLOGY, 3 Nov 2022)[https://doi.org/10.1038/s41564-022-01252-3]

Paradis, J. S., Feng, X., Murat, B., Jefferson, R. E., Sokrat, B., Szpakowska, M., Hogue, M., Bergkamp, N. D., Heydenreich, F. M., Smit, M. J., Chevigné, A., Bouvier, M., Barth, P. **Computationally designed GPCR quaternary structures bias signaling pathway activation** (Nature Communications, 11 Nov 2022)[https://doi.org/10.1038/s41467-022-34382-7]

Wade, N., Wesseling, C. M. J., Innocenti, P., Slingerland, C. J., Koningstein, G. M., Luirink, J., Martin, N. I. **Synthesis and Structure-Activity Studies of β-Barrel Assembly Machine Complex Inhibitor MRL-494** (ACS Infectious Diseases, 11 Nov 2022)[https://doi.org/10.1021/acsinfecdis.2c00459]

Bos, T. S., Boelrijk, J., Molenaar, S. R. A., Van 'T Veer, B., Niezen, L. E., Van Herwerden, D., Samanipour, S., Stoll, D. R., Forré, P., Ensing, B., Somsen, G. W., Pirok, B. W. J. **Chemometric Strategies for Fully Automated Interpretive Method Development in Liquid Chromatography** (Analytical chemistry, 22 Nov 2022)[https://doi.org/10.1021/acs.analchem.2c03160]