# AIMMS publication report for: 2021-12-31

### New papers: 2020-11/12

de Jong, G. B., Ortega, N., Lutz, M., Lammertsma, K., Slootweg, J. C. **Easy Access to Phosphine-Borane Building Blocks** (Chemistry - A European Journal, 4 Dec 2020)[https://doi.org/10.1002/chem.202002367]

Vermeeren, P., Hansen, T., Jansen, P., Swart, M., Hamlin, T. A., Bickelhaupt, F. M. **A Unified Framework for Understanding Nucleophilicity and Protophilicity in the SN2/E2 Competition** (Chemistry - A European Journal, 1 Dec 2020)[https://doi.org/10.1002/chem.202003831]

Keiffer, S., Carneiro, M. G., Hollander, J., Kobayashi, M., Pogoryelev, D., Ab, E., Theisgen, S., Müller, G., Siegal, G. **NMR in target driven drug discovery: why not?** (Journal of Biomolecular NMR, Nov 2020)[https://doi.org/10.1007/s10858-020-00343-9]

Kleerebezem, M., Bachmann, H., van Pelt-KleinJan, E., Douwenga, S., Smid, E. J., Teusink, B., van Mastrigt, O. **Lifestyle, metabolism and environmental adaptation in Lactococcus lactis** (FEMS Microbiology Reviews, 24 Nov 2020)[https://doi.org/10.1093/femsre/fuaa033]

Bruggeman, F. J., Planqué, R., Molenaar, D., Teusink, B. **Searching for principles of microbial physiology** (FEMS Microbiology Reviews, 24 Nov 2020)[https://doi.org/10.1093/femsre/fuaa034]

Rodrigues Silva, D., de Azevedo Santos, L., P. Freitas, M., Fonseca Guerra, C., Hamlin, T. A. **Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides** (Chemistry - An Asian Journal, 1 Dec 2020)[https://doi.org/10.1002/asia.202001127]

van der Lubbe, S. C., Vermeeren, P., Fonseca Guerra, C., Bickelhaupt, F. M. **The Nature of Nonclassical Carbonyl Ligands Explained by Kohn–Sham Molecular Orbital Theory** (Chemistry - A European Journal, 1 Dec 2020)[https://doi.org/10.1002/chem.202003768]

Giesbertz, K. J. **Implications of the unitary invariance and symmetry restrictions on the development of proper approximate one-body reduced-density-matrix functionals** (Physical Review A, 16 Nov 2020)[https://doi.org/10.1103/PhysRevA.102.052814]

Işbilir, A., Möller, J., Arimont, M., Bobkov, V., Perpiñá-Viciano, C., Hoffmann, C., Inoue, A., Heukers, R., de Graaf, C., Smit, M. J., Annibale, P., Lohse, M. J. **Advanced fluorescence microscopy reveals disruption of dynamic CXCR4 dimerization by subpocket-specific inverse agonists** (Proceedings of the National Academy of Sciences of the United States of America, 17 Nov 2020)[https://doi.org/10.1073/pnas.2013319117]

Jangrouei, M. R., Pernal, K., Gritsenko, O. V. **Universal on-top description of electron correlation in the ground and excited many-electron states with correlon quasiparticles** (Physical Review A, 25 Nov 2020)[https://doi.org/10.1103/PhysRevA.102.052829]

Makraki, E., Darby, J. F., Carneiro, M. G., Firth, J. D., Heyam, A., Ab, E., O'Brien, P., Siegal, G., Hubbard, R. E. **Fragment-derived modulators of an industrial β-glucosidase** (The Biochemical journal, 27 Nov 2020)[https://doi.org/10.1042/BCJ20200507]

van de Velde, B., Guillarme, D., Kohler, I. **Supercritical fluid chromatography – Mass spectrometry in metabolomics: Past, present, and future perspectives** (Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 15 Dec 2020)[https://doi.org/10.1016/j.jchromb.2020.122444]

Hernandez-Valdes, J. A., aan de Stegge, M., Hermans, J., Teunis, J., van Tatenhove-Pel, R. J., Teusink, B., Bachmann, H., Kuipers, O. P. **Enhancement of amino acid production and secretion by Lactococcus lactis using a droplet-based biosensing and selection system** (Metabolic Engineering Communications, Dec 2020)[https://doi.org/10.1016/j.mec.2020.e00133]

Hansen, T., Elferink, H., van Hengst, J. M., Houthuijs, K. J., Remmerswaal, W. A., Kromm, A., Berden, G., van der Vorm, S., Rijs, A. M., Overkleeft, H. S., Filippov, D. V., Rutjes, F. P., van der Marel, G. A., Martens, J., Oomens, J., Codée, J. D., Boltje, T. J. **Characterization of glycosyl dioxolenium ions and their role in glycosylation reactions** (Nature Communications, 1 Dec 2020)[https://doi.org/10.1038/s41467-020-16362-x]

Gallant, J. L., Heunis, T., Sampson, S. L., Bitter, W. **ProVision: a web-based platform for rapid analysis of proteomics data processed by MaxQuant** (Bioinformatics (Oxford, England), 8 Dec 2020)[https://doi.org/10.1093/bioinformatics/btaa620]