# AIMMS publication report for: 2020-11-09

### New papers: 2020-10/11

Bugatti, K., Bruno, A., Arosio, D., Sartori, A., Curti, C., Augustijn, L., Zanardi, F., Battistini, L. **Shifting Towards αVβ6 Integrin Ligands Using Novel Aminoproline-Based Cyclic Peptidomimetics** (Chemistry - A European Journal, 21 Oct 2020)[https://doi.org/10.1002/chem.202002554]

Salvito, D., Fernandez, M., Jenner, K., Lyon, D. Y., de Knecht, J., Mayer, P., MacLeod, M., Eisenreich, K., Leonards, P., Cesnaitis, R., León-Paumen, M., Embry, M., Déglin, S. E. **Improving the Environmental Risk Assessment of Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials** (Environmental toxicology and chemistry, 1 Nov 2020)[https://doi.org/10.1002/etc.4846]

van Beek, L. F., Surmann, K., van den Berg van Saparoea, H. B., Houben, D., Jong, W. S., Hentschker, C., Ederveen, T. H., Mitsi, E., Ferreira, D. M., van Opzeeland, F., van der Gaast–de Jongh, C. E., Joosten, I., Völker, U., Schmidt, F., Luirink, J., Diavatopoulos, D. A., de Jonge, M. I. **Exploring metal availability in the natural niche of Streptococcus pneumoniae to discover potential vaccine antigens** (Virulence, 5 Oct 2020)[https://doi.org/10.1080/21505594.2020.1825908]

Marino, S. D., Gerolin, A. **An Optimal Transport Approach for the Schrödinger Bridge Problem and Convergence of Sinkhorn Algorithm** (Journal of Scientific Computing, 1 Nov 2020)[https://doi.org/10.1007/s10915-020-01325-7]

Adihou, H., Gopalakrishnan, R., Förster, T., Guéret, S. M., Gasper, R., Geschwindner, S., Carrillo García, C., Karatas, H., Pobbati, A. V., Vazquez‐Chantada, M., Davey, P., Wassvik, C. M., Pang, J. K. S., Soh, B. S., Hong, W., Chiarparin, E., Schade, D., Plowright, A. T., Valeur, E., Lemurell, M., Grossmann, T. N., Waldmann, H. **A protein tertiary structure mimetic modulator of the Hippo signalling pathway** (Nature Communications, 1 Nov 2020)[https://doi.org/10.1038/s41467-020-19224-8]

Grimmel, S. A., Teodoro, T. Q., Visscher, L. **Is it worthwhile to go beyond the local-density approximation in subsystem density functional theory?** (International Journal of Quantum Chemistry, 1 Nov 2020)[https://doi.org/10.1002/qua.26111]