ChemPager: Greener Processes through Data Analysis

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ChemPager[1-2] is a freely available data analysis tool for analyzing, comparing and improving synthetic routes. The talk aims to provide a hands-on experience on the functionalities offered by ChemPager which extend way beyond Green Chemistry into scenario planning and cost analysis.

We also present an expansion of this application that makes use of the functionality of the PMI Predictor, which the ACS Green Chemistry Institute Pharmaceutical Roundtable has recently published as a web application[3]. This addition enables ChemPager to predict the cumulative process mass intensity of chemical routes, irrespective of their development status, by comparison with a set of reactions executed on large scale. The prediction of this core green chemistry metric will help improve existing routes and the decision-making process among route alternatives without the need for experimental data.

[1] H. Loureiroa, M. Prem, G. Wuitschik, *Chimia*, **2019**, *accepted*.
[2] D. Kaiser, J. Yang, G Wuitschik, *Org. Process Res. Dev.,* **2018**, 22, 9, 1222
[3] a) A. Borovika, J. Albrecht, J. Li, A. S. Wells, C. Briddell, B. R. Dillon, L. J. Diorazio, J. R. Gage, F. Gallou, S. G. Koenig, M. E. Kopach, D. K. Leahy, I. Martinez, M. Olbrich, J. L. Piper, F. Roschangar, E. Sherer, M. D. Eastgate, ChemRxiv 2019, DOI: 10.26434/chemrxiv.7594646.v1; b) J. Albrecht, J. Li, A. Borovika, M. D. Eastgate, PMI Predictor, https://www.acsgcipr.org/tools-for-innovation-in-chemistry/process-mass-intensity-prediction-calculator/