OptFlux3: an improved platform for in silico design of cellular factories

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The rational design of cellular factories for industrial biotechnology aims to create optimized organisms for the production of bulk chemicals, pharmaceuticals, food ingredients and enzymes, among others. Metabolic engineering (ME) plays a key role in this process, supported by the latest advances in genetic engineering in combination with computational tools to define targets for strain improvement. OptFlux is an open-source reference computational platform for the optimization of cellular factories by the application of in silico ME methods, designed for non-computational experts by providing a user-friendly interface. It allows to load genome-scale models from several sources to be used in the prediction of cellular behavior and identification of metabolic targets for genetic engineering. Its latest version, OptFlux3, allows to perform the simulation of wild type and mutant strains (allowing the simulation of gene/ reaction deletion and over/under expression). Regarding strain optimization, the new architecture opts for a multi-objective framework, allowing users to easily add different goals as optimization targets in a flexible way. Specialized multi-objective algorithms, co-exist with traditional single objectives algorithms to be applied for each case. Also, OptFlux3 includes a new visualization framework for metabolic models and phenotype simulations and a new plug-in management interface that allows to install and remove plug-ins in execution time. Currently available plug-ins include the calculation and visualization of elementary modes, topological analysis and the ability to add reactions/ pathways to existing models. OptFlux is made freely available for all major operating systems, together with suitable documentation in www.optflux.org.