OptFlux: a software for metabolic engineering

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OptFlux is an open-source, user-friendly and modular software aimed at being the reference computational tool for metabolic engineering applications. It allows the use of stoichiometric models of microbial metabolism for simulation and optimization purposes.
Metabolic engineering deals with designing organisms with enhanced capabilities regarding the productivities of desired compounds[1]. This field has received increasing attention within the last few years due to the extraordinary growth in the adoption of white or industrial biotechnological processes for the production of bulk chemicals, pharmaceuticals, food ingredients and enzymes, among other products.
Many different approaches have been used to aid in metabolic engineering efforts that take available models of metabolism together with mathematical tools and/or experimental data to identify metabolic bottlenecks or targets for genetic engineering.
However, the rational design of microbial strains has been limited to the developers of the computational or mathematical techniques, since a platform that provides a user friendly interface to perform such tasks was not yet available.
Towards the purpose of changing this scenario, we introduce the *OptFlux*, whose main features are the following:
- Open-source – it allows all users to use the tool freely and invites the contribution of other researchers;
- User-friendly – facilitates its use by users with no/little background in modelling/informatics;
- Modular – facilitates the addition of specific features by computer scientists
- Compatible with standards –compatibility with the Systems Biology Markup Language (SBML)[2] and the layout information of CellDesigner[3].
At the present version, the main methods implemented in OptFlux for the simulation of both wild-type and mutant organisms are Flux Balance Analysis[1], Minimization of Metabolic Adjustment (MOMA)[4], and Regulatory on/off Minimization of Metabolic flux changes (ROOM)[5].
The optimization tasks, i. e., the identification of metabolic engineering targets can be performed with Evolutionary Algorithms, Simulated Annealing and Local Search methods [6,7].
Other features like the calculation of Elementary Flux Modes[8] and Metabolic Flux Analysis[1] will be added to the present platform in the near future as new modules
The software is made available, together with other resources, in the home page: http://www.optflux.org

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