# OPTFLUX: AN OPEN-SOURCE SOFTWARE PLATFORM FOR *IN SILICO* 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 (ME) applications. It allows the use of stoichiometric metabolic models for phenotype simulation and strain optimization purposes.

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) and the layout information of CellDesigner.

At the present version, the main methods implemented in OptFlux for the simulation of both wild-type and mutant organisms are Flux Balance Analysis, Minimization of Metabolic Adjustment (MOMA), and Regulatory on/off Minimization of Metabolic flux changes (ROOM).

Besides SBML, the software supports importing and exporting to several flat file formats used in the community. OptFlux has also a visualization module that allows the analysis of the model structure and the superimposition of simulation results with the model graph.

The optimization tasks, i. e., the identification of metabolic engineering targets can be performed with Evolutionary Algorithms, Simulated Annealing and Local Search methods. Metabolic Flux Analysis and Elementary mode analysis have also been recently implemented.

The software is made available, together with documentation and other resources, in the project's home page: http://www.optflux.org. Given its plug-in based architecture it can be easily extended with new functionalities. Currently, a number of plug-ins are being developed to enlarge its features, including network topology analysis tools, elementary modes calculation and analysis, integration with Boolean network based regulatory models, among others.

Systems Biology, Human Health, and Emerging
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# Metabolic Engineering VIII:
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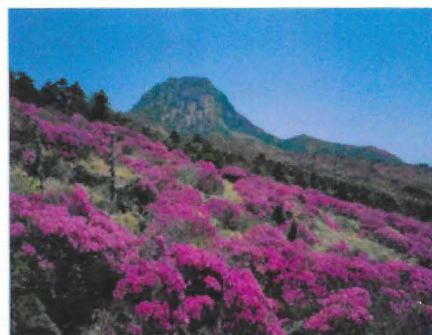### June 13 – 17, 2010

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