# Bioinformatics Open Days

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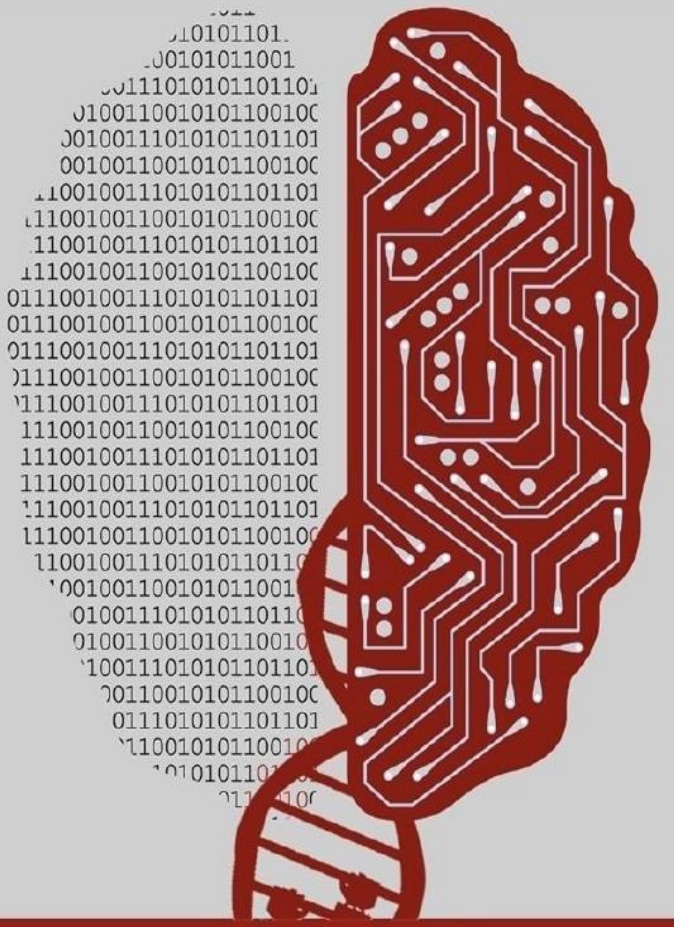

# BOOK OF ABSTRACTS

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NEBIUM

# BIOINFORMATICS OPEN DAYS

Campus de Gualtar, Universidade do Minho

18th and 19th of February 2016

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## Development of pathway analysis based algorithms for strain optimization

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Current *in silico* approaches for the optimization of microbial strains with industrial relevance make extensive use of constraint-based models (CBMs) of cell metabolism. Such approaches, usually divided in constraint-based (CB) and pathway analysis (PA), are used to find metabolic engineering strategies to fulfill an industrial objective. PA methods are less biased than CB ones, but their use depends on the complexity and scale of the model, unlike CB methods.

The aim of this work is to extend the usage of PA methods to genome-scale models and compare the performance and results provided by PA methods with CB methods. To this end, a novel implementation of the MCSEnumerator algorithm and routines for enumeration of constrained minimal cut sets using it were developed and integrated in the OptFlux metabolic engineering platform [2]. The developed routines and their output were validated with previously determined examples.

A case study involving succinate production on *Saccharomyces cerevisiae* was developed, for which knockout strategies were determined using both PA methods. Clustering analysis of the solutions (knockout sets) and predicted phenotypes was performed, highlighting different mechanisms of product synthesis. Finally, the structure and production robustness were compared with strategies from CB methods, showing that PA methods enable more robust product synthesis, but involve more knockouts as they are usually supersets of other CB strategies.

**References**

[1] von Kamp, A., & Klamt, S. (2014). Enumeration of Smallest Intervention Strategies in Genome-Scale Metabolic Networks. *PLoS Computational Biology*

[2] Rocha, I., Maia, P., Evangelista, P., Vilaça, P., Soares, S., Pinto, J. P., ... Rocha, M. (2010). OptFlux: an open-source software platform for in silico metabolic engineering. *BMC Systems Biology*

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