



## **Systems Biology, Bioinformatics and Metabolic Engineering**

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This research line covers the topics of genome-scale metabolic model re-construction, biological text mining and metabolic engineering with the ultimate aims of designing improved cell factories for the application in industrial biotechnology processes and of improving our understanding of important human pathogens.

In Metabolic Engineering problems, it is often difficult to predict the effects of genetic modifications on the resulting phenotype, owing to the complexity of metabolic networks. Consequently, the task of identifying the modifications that will lead to an improved microbial phenotype is a quite complex one, requiring robust mathematical and computational tools. Part of our effort is therefore dedicated to the generation of better mathematical models of microbial metabolism, applying Bioinformatics tools like Data Mining and Biological Text Mining.

We have also developed algorithms for identifying gene knockouts that can improve productivities in strains using stoichiometric metabolic models and have been focusing our attention on the possibility of indicating other genetic modifications such as gene additions and over-expressions. Furthermore, we have developed an open-source software tool, called OptFlux, aiming at being the reference metabolic engineering platform.

The tasks of model re-construction and the interpretation of the results obtained by *in silico* metabolic engineering approaches are difficult if not impossible to achieve without a proper contextualization with available literature information.

Our main text mining software tool, called @Note, offers as major functional contributions the ability to process abstracts and full-texts; an information retrieval module enabling PubMed search and journal crawling; a pre-processing module with PDF-to-text conversion, tokenisation and stopword removal; a semantic annotation schema; a lexicon-based annotator; a user-friendly annotation view that allows to correct annotations and a text mining module supporting dataset preparation and algorithm evaluation.