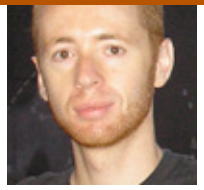

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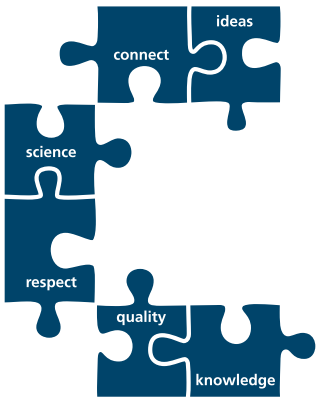
# Modelling allosteric regulation for prediction of flux control in the central carbon metabolism of E. coli

Rational strain design is a fundamental step in the development of microbial cell factories. Multiple genetic manipulations are often required in order to redirect the metabolic flux towards a product of industrial interest. Most manipulation targets are focused on central carbon metabolism, which provides the molecular precursors and the energy required for other biochemical pathways. However, the complex regulation of those pathways is still not completely unraveled. Recent studies have shown that central carbon metabolism is mostly regulated at post-transcriptional levels. In this work, we explore the role of allosteric regulation in the control of metabolic fluxes. We begin by expanding a metabolic network reconstruction of the central carbon metabolism of E. coli with allosteric interaction information from relevant databases. This model is used to integrate a multi-omic dataset for this organism. We analyze the coordinated changes in enzyme, metabolite and flux levels between multiple experimental conditions, and observe cases where allosteric regulators have a major contribution in the metabolic flux changes. We then develop a method for systematic prediction of potential cases of allosteric control for given metabolic perturbations. This is a valuable approach for predicting coordinated flux changes that would not be predicted with a purely stoichiometric model representation.

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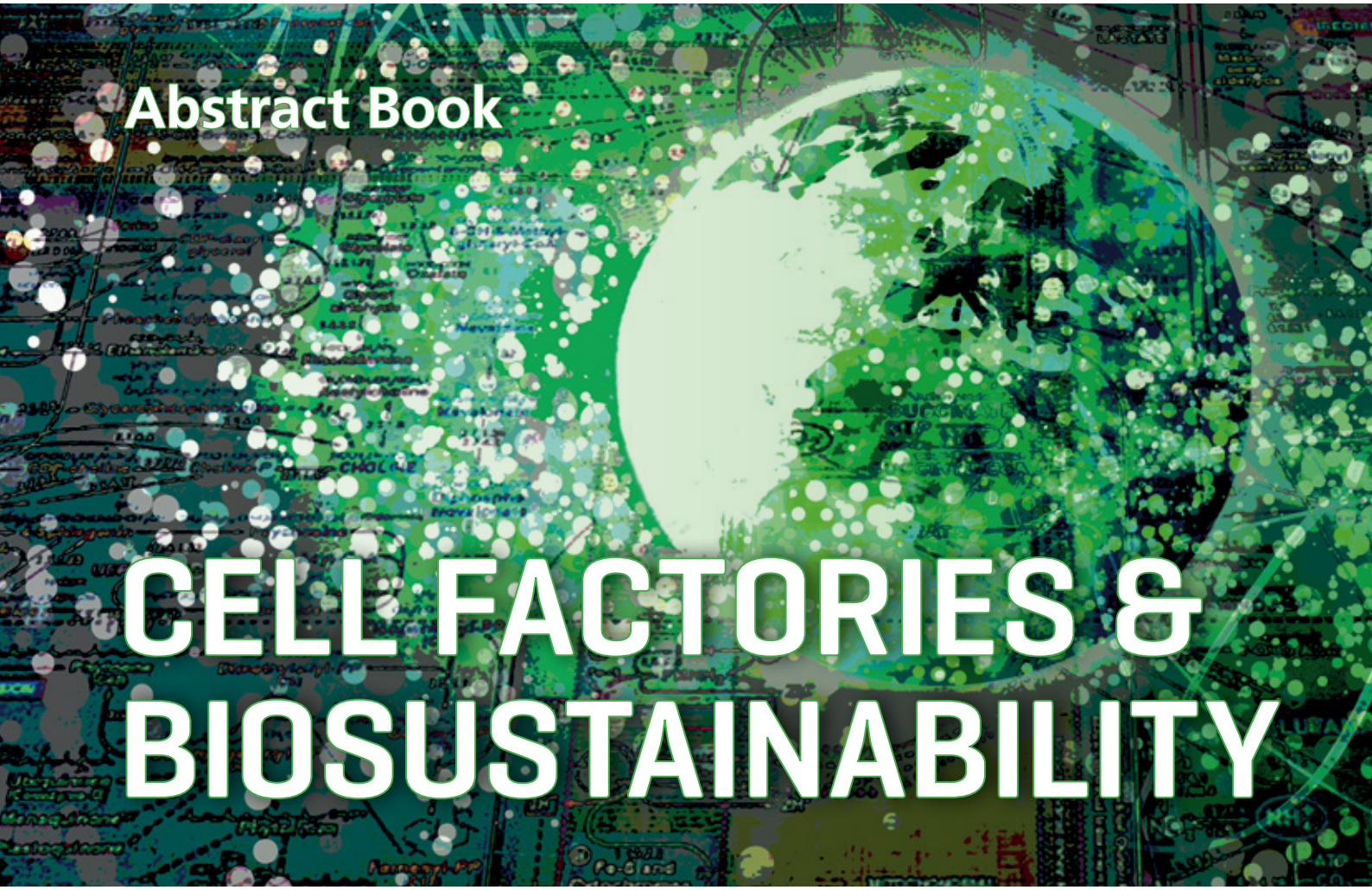


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