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Automatic reconstruction and modeling of biocatalyst systems for the production of specific biochemical compounds

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The knowledge of organisms and their metabolic pathways allowed constructing biological systems for the production of chemicals and pharmaceuticals such as antibiotics and biofuels. Synthetic biology expands the number of these biological systems by the assembly of artificial metabolic pathways, called synthetic pathways, not present in natural organisms. Synthetic pathways could be integrated in modified micro-organisms or in biocatalyst systems. A biocatalyst system is an *in vitro* assembly composed only of purified enzymes and metabolites that are useful for the production of a desired metabolic compound through a biochemical reaction network. This *in vitro* assembly, as compared to cellular system, has several advantages, such as the production of only desired metabolites and a great engineering flexibility. We explored an *in silico* approach to identify and analyze new biocatalyst systems for the production of target metabolic compounds. This approach proceeds in several steps. The first step is the enumeration of several biocatalyst systems that could synthesize a target product from a desired starting substrate. Next, a selection based on several criteria is applied to choose a biocatalyst system among the group of biocatalyst systems identified in the enumeration step. The last step is the modeling of the selected biocatalyst system to evaluate the production rate and the yield of the target product. This communication explains in more detail the *modus operandi* for the different steps of our *in silico* approach.

Biography

Frederic Cadet is Vice President in Research & Development of the company Peacel. He has a PhD in Protein Engineering, Data Mining and Biosimulation. From 2004 to 2008, as an Executive School, University & Research Commissioner, he managed a budget of 1.3 billion Euros and was responsible for 32,000 employees. He is Former Chairman of the ERA Nets (European Research Area Networks) NetBIOME. He has developed pioneering research activities in bioinformatics. He is author of over 70 publications and Referee for 17 international scientific journals. He is Organizing Committee Member for 2nd International Conference on Genetic and Protein Engineering, November 14-16, 2016 Atlanta, USA.

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