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Reconstruction of metabolic networks from *in silico* labeled substrates

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Abstract

Metabolism transforms compounds to produce energy and building blocks. Metabolic network reconstruction allows better understanding of the metabolism and the catabolism of living cells and is commonly available at the metabolite level. Atom-level representation of the pathways could yield many insights into the exact mechanisms of enzymatic reactions. The ability to trace the fate of individual atoms through the metabolic pathways will also be very useful in many applications of metabolic engineering, systems biology and drug discovery. So far, the atom mappings in enzymatic reactions have not been studied in depth and most of the metabolic databases do not contain comprehensive information on atom tracing through biochemical pathways. *KEGG RPAIR* database contains such information between single metabolite pairs; however, it would be difficult to extend these mappings for every pathway and in every organism.We developed a computational framework for the *in silico* atom labeling and tracking through metabolic pathways. This framework analyzes all atom transitions based on enzymatic reaction rules by tracking the movement of every single atom through metabolic pathways. Our method allows a straightforward and computationally efficient means for the observation of all possible fluxes in a proposed network model based on atom biotransformation.

We demonstrate the usefulness of our framework through a case study of biosynthesis of 3-Hydroxypropanoate (3HP) in *E,coli* and we compare the efficiency of different pathways in terms of the fate of the labeled atoms of substrates.

Biography

Noushin Hadadi is currently a PhD student and research assistant in the group of Professor Vassily Hatzimanikatis at the Laboratory of Computational Systems Biotechnology (LCSB) at EPFL. Noushin earned his B.Sc. in Chemical Engineering at University of Tehran, Iran, in 2007. In 2008, Noushin joined EPFL as a Master student. She received her Master's degree in Biochemical Engineering in 2011, and started her PhD right afterwards. Noushin's research interests include the development of computational frameworks for better understanding the metabolic networks of model organisms such as *E,coli*. Having full description of enzymatic reactions in metabolic networks helps for the discovery of novel metabolic pathways for the microbial production of valuable chemicals.