Expanding Metabolic Capabilities Using Novel Pathway Designs: Computational Tools and Case Studies

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Design and selection of efficient metabolic pathways is critical for the success of metabolic engineering endeavors. Convenient pathways should not only produce the target metabolite in high yields but also are required to be thermodynamically feasible under production conditions, and to prefer efficient enzymes. To support the design and selection of such pathways, different computational approaches have been proposed for exploring the feasible pathway space under many of the above constraints. In this review, an overview of recent constraint-based optimization frameworks for metabolic pathway prediction, as well as relevant pathway engineering case studies that highlight the importance of rational metabolic designs is presented. Despite the availability and suitability of in silico design tools for metabolic pathway engineering, scarce?although increasing?application of computational outcomes is found. Finally, challenges and limitations hindering the broad adoption and successful application of these tools in metabolic engineering projects are discussed.