Prediction of novel metabolic pathways for industrially valuable chemicals

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A plenty of systematic platforms have been researched and developed in the past decades to make the metabolic pathways for efficient production of desired chemicals. For this reason, we developed the systematic framework to design biosynthetic pathways and select enzyme candidates through filtering process. The framework is composed of route generation and prioritization process. Route generation step designs pathways by reaction operators constructed by the logics acquired from analysis of reaction transformation pattern. Next, binding site covalence, chemical similarity, thermodynamic favorability, pathway distance and organism specificity are considered for the feasibility. Novel pathways for isobutanol, 3-hydroxypropionate (3HP) and butyryl-CoA were predicted. This systematic framework should play a role of valuable asset for the application of metabolic engineering. [This work was supported by the Technology Development Program to Solve Climate Changes on Systems Metabolic Engineering for Biorefineries from the Ministry of Science, ICT and Future Planning (MSIP) through the National Research Foundation (NRF) of Korea (NRF-2012M1A2A2026556 and NRF-2012M1A2A2026557).]