A system framework to identify promising enzyme candidates to synthesize novel pathways to produce desired biochemical

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We propose a systematic approach and related framework with the aim of predicting novel synthetic pathways for desired chemicals at a reliable level. To allow applications to in vivo or in vitro systems, we considered factors that can affect the novel pathways. There are five factors that evaluate three types of abilities: similarity, thermodynamics, and coexpression. The five factors are binding site covalence, chemical similarity, thermodynamic favorability, pathway distance, and organism specificity. We suggest a method to evaluate these factors and obtain priority scores which rank identified pathways. The factors are evolutionary fitted and thus the system is optimized itself. Our approach will enhance the production of high value added chemicals and biofuels.

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