A computational framework for automated enzyme selection using structural information

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To produce a variety of valuable chemicals including pharmaceuticals, biofuels, and commodity chemicals, it is necessary to introduce known heterologous reactions from biochemical databases or to design novel biosynthetic pathways. However, identifying the enzymes to catalyze each metabolic reaction steps is often challenging and depends primarily on the expert knowledge. Here, we present MELI-3D (Mechanism-based Enzyme Ligand Interactions), a computational method that predicts the promiscuous enzymes of orphan or novel reactions based on enzyme-substrate interactions using structural information. Our method verified the performance of the predictive model through cross-validation tests on the in-house reference datasets. Further, we performed massive application studies on the identification of enzyme sequences for orphan enzymes and novel designed pathways [This work was supported by the Technology Development Program to Solve Climate Changes on Systems Metabolic Engineering for Biorefineries from the Ministry of Science and ICT through the National Research Foundation (NRF) of Korea (NRF-2012M1A2A2026556 and NRF-2012M1A2A2026557)].