A computational enzymatic optimization for fixing carbon dioxide to starch

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Abstract. Carbon dioxide is fixed and processed into starch by the plants’ photosynthesis through complicated molecular pathways. While planting and cultivating crops are the major ways to harvest starch, an artificial anabolic pathway has recently been realized in China. Traditional crop production demands extended harvest periods, extensive land, and substantial water use. In contrast, the artificial pathway enhances starch synthesis efficiently, using fewer resources for a more sustainable approach. In 2021, Chinese researchers reported the anabolic starch artificial pathway(ASAP) to synthesize starch in vitro. Although the previous research established a milestone, steps need to be optimized. In this work, enzymatic starch synthesis is chosen to be further engineered, building mutants with similar catalytic functions. Computational tools are used to build an iterative docking-mutating simulation (IDMS). It can automatically finish the cycle of protein mutations and docking. Autodock and Rosetta are used in the coding. 445 different protein mutants are generated and analyzed in silico, among which the best five were chosen for experimental investigation. In the experimental analysis, mutant E shows nearly the same catalytic efficiency as the wild-type in the first hour, with a 2.5-fold expression rate.