COMPUTATIONAL ENZYME DESIGN FOR INDUSTRIALLY RELEVANT REACTIONS

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Key Words: computational enzyme design, asymmetric reactions, regioselectivity, *de novo* enzyme activity

Cognition of life from the perspective of synthetic biology centers on the design, construction, and characterization of novel biological systems using engineering design principles. Most catalytic functions in living organisms are achieved by enzymes, which serve as key components in synthetic biology. While the amino acid sequence makes up the primary structure of the protein, the chemical/biological properties of the protein are dependent on the three-dimensional or tertiary structure. In the nascent field of synthetic biology, researchers are striving to engineer novel biological functionality based on the structures. The development of computational enzyme design algorithms can provide large amounts of prototype molecules for the synthetic biological devices, especially for new catalytic devices, and also provide templates and guidelines for important components of synthetic biology. As the performance of computational algorithms and design strategies continue to improve, protein designers can construct enzymes from scratch and even create highly proficient biocatalysts. This talk provides a brief overview of design principles of proteins and highlights the latest examples of using computational methods to create enzymes for industrially viable applications.

References:

1. R. Li et al. Computational redesign of enzymes for regio-and enantioselective hydroamination, *Nature chemical biology*, 14 (7), 664 (2018).
2. Y. Bu et al. Engineering improved thermostability of the GH11 xylanase from *Neocallimastix patriciarum* via computational library design, *Applied microbiology and biotechnology*, 102 (8), 3675-3685 (2018).
3. B. Wu et al. Versatile peptide C-terminal functionalization via a computationally engineered peptide amidase. *ACS Catalysis* 6 (8), 5405-5414 (2016).