De novo enzymes by computational design.

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Abstract

Computational enzyme design has emerged as a promising tool for generating made-to-order biocatalysts. In addition to improving the reliability of the design cycle, current efforts in this area are focusing on expanding the set of catalyzed reactions and investigating the structure and mechanism of individual designs. Although the activities of de novo enzymes are typically low, they can be significantly increased by directed evolution. Analysis of their evolutionary trajectories provides valuable feedback for the design algorithms and can enhance our understanding of natural protein evolution.

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Details

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