A Computationally Designed Protein Enables Efficient Regeneration Of A Biomimetic Cofactor To Support Diverse Redox Chemistries

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BRIEF DESCRIPTION

Production of chiral chemicals through biotransformation requires an oxidoreductase enzyme and an efficient redox cofactor system comprising electron donors coupled to a dehydrogenase enzyme to regenerate the reduced cofactors.The researchers at the University of California, Irvine (UCI), provide a way to computationally design and optimize hydrogenase enzyme interaction with biomimetic cofactor analogs to improve increase enzymatic efficiency. The group has produced the modified enzyme and show that it is capable of a diverse range of chemical biotransformation.

FULL DESCRIPTION

Enzymatic biotransformation is a convenient way to manufacture chiral chemicals.Typically, an enzymatic biotransformation requires an enzyme, such as oxidoreductase, and a redox cofactor system to mediate the regeneration of the enzyme.Unfortunately, natural redox cofactors can be expensive and unstable.Although simple and efficient redox cofactor analogs, also known as biomimetics, have been synthesized, native enzymes seem to display low activities towards these simple biomimetic cofactor analogs. The researchers at the University of California, Irvine, have computationally designed a modified dehydrogenase enzyme to improve the shape and electrostatic complementary of the binding pocket of the modified enzyme towards the synthesized cofactor biomimetics.When the produced enzyme was compared to the wild type, there was 1000-fold improvement in enzymatic activity.The design strategies incorporated in this work clearly shows a novel utility in protein engineering and modeling of biomimetic cofactor analogs.

SUGGESTED USES

- Synthesize chiral compounds via enzymatic biotransformation
- *In silico* design

ADVANTAGES

- Simple and Cheap
- Efficient and Stable
- Environmentally Friendly
- 1000-fold more activity than wild-type

PATENT STATUS

Country	Type	Number	Dated	Case

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OTHER INFORMATION

CATEGORIZED AS

- **Biotechnology**
  - Industrial/ Energy
- **Materials & Chemicals**
  - Chemicals
- **Medical**
  - Research Tools

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