BIOTRANS
LA ROCHELLE 2023

N°304 / PC
TOPIC(s) : Enzyme discovery and engineering

Engineering of an EneIRED for direct synthesis of asymmetric conjugate reduction-reductive amination products

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PURPOSE OF THE ABSTRACT

Due to their ability to catalyse the synthesis of asymmetric amines, IREDs have many potentially useful applications in synthesis of agrochemicals and APIs, where enantiopure products are often desirable. Chemically synthesising enantiomerically pure compounds can be challenging, often requiring costly resolution processes of racemic mixtures, therefore utilising enantioselective biocatalysts to avoid these extra steps is favourable. Following the discovery of an IRED capable of catalysing conjugate reduction in tandem with reductive amination in a two-step mechanism, the wild-type substrate scope was investigated and was found to favour reactions between unhindered substrates. Rational design principles were applied alongside mutagenesis and directed evolution in an attempt to broaden the existing substrate scope and facilitate acceptance of sterically bulky substrates that were not previously accepted by the wild-type.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

EneIRED | Engineering | Directed Evolution

BIBLIOGRAPHY