

## Green chemistry: Quantumzyme case study on biocatalytic approaches for enzyme engineering

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### Abstract:

Active pharmaceutical ingredient (API)s form the significant number of marketed drugs in the pharmaceutical industry. These ingredients are usually present in enantiomeric form and in most cases one enantiomeric form may be harmful or inactive while the other form is the intended active ingredient for the drug. Therefore, it is imperative that the intended active pharmaceutical intermediate is present in pure form in the drug.

Enzymes are versatile bio-catalysts, which have attracted a lot of industrial attention in last few years. Many industrial chemical processes are not friendly to the environment and, enzymes – a natural counterpart – could be a friendly substitute in some of these processes. Enzymes exhibit exceptional specificity for natural substrate, but may not act on the substrates currently in use. Consequently, they need to be modified to extend their applicability to different purposes under different conditions. This process of enzyme modifications tailored to suit the given conditions, is known as **enzyme engineering**.

While green chemistry is everyone's desire, it is not within everyone's reach to adopt biotransformation as a process of API synthesis.

Though there are various protein engineering techniques to construct an enzyme with improved activity, stability, specificity; *in-silico* enzyme design approaches have several advantages over other approaches. In this article, we present a comprehensive overview of the strategies and computational methodologies employed for enzyme engineering to catalyse chemical reactions. We are introducing our QZyme WorkBench™ - an in-house protocol for enzyme engineering approach with examples.