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Holistic understanding of alcohol dehydrogenase catalysis in deep eutectic solvents through experimental and computational approaches

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PURPOSE OF THE ABSTRACT

Biocatalysis starts a transition phase from default aqueous media to non-aqueous media in the spirit of Green Chemistry. The use of oxidoreductases (EC1) in non-conventional media is particularly vital for the synthesis of value-added chiral chemicals.[1] Deep eutectic solvents (DES) have emerged as a new class of sustainable solvents with tremendous tunability and biocompatibility.[2,3] Redox biocatalysis in DESs combines the best of two worlds: enzymes' selectivity and DESs' designability.[4] Design redox biocatalysis in DESs requires an in-depth understanding of DES's impact on enzymes. This stimulates us to study DESs' effects on oxidoreductases by assessing the catalytic performance of alcohol dehydrogenases (ADHs) in DES-water mixtures with the aid of molecular dynamics (MD) simulations.[5?7] Enzymes' activity was found positively correlated to water activity (?W) due to the changes in solvation layers surrounding enzymes.[6?7] Individual DES components were first revealed to have discrepant effects on enzymes, e.g., positive (Gly) or negative (ChCl), promoting the knowledge-oriented design of a new enzyme-compatible eutectic mixture (ChCl-Gly, 1:9).[7] We will deepen the study with experimental analyses and in silico simulations (Fig. 1).
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FIGURES

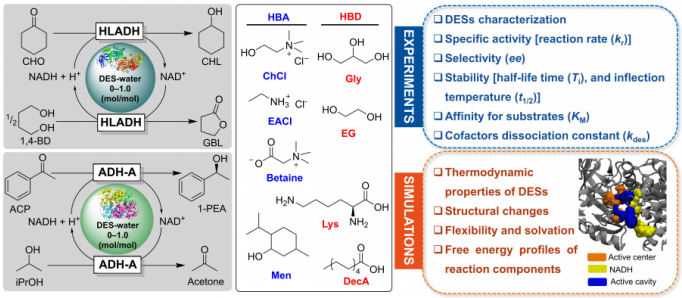

FIGURE 1

Fig.1

Reduction of cyclohexanone (CHO) and acetophenone (ACP) catalyzed by horse live ADH (HLADH) and ADH-A in various DES-water mixtures. HBA: hydrogen bond acceptor, HBD: hydrogen bond donor.

FIGURE 2

KEYWORDS

redox biocatalysis | non-aqueous media | deep eutectic solvents | alcohol dehydrogenase

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