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Deep eutectic solvents enable robust hydroxylation of fatty acids: A correlation between water activity and thermostability of FA-HY1

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PURPOSE OF THE ABSTRACT

This work aims to explore the performance and application of fatty acid hydratases in green and sustainable deep eutectic solvents (DESs). As the first case, a robust system with the combination of fatty acid hydratase-1 (FA-HY1) from Lactobacillus Acidophilus and DESs for biocatalytic hydroxylation of fatty acids was developed. The results indicated that the catalytic performance of FA-HY1 was mainly determined by the composition of DESs. Especially water molecules, as the co-substrate of hydroxylation reactions, have been proven as the key factor of the thermostability of FA-HY1 in DESs systems as well. By varying the water activity of DESs, we found that FA-HY1 displayed improved thermostability at lower water activity. In particular, the half-life time of FA-HY1 increased 6-fold in choline chloride/sorbitol system with water activity (aw = 0.84) compared to aqueous (Kpi) system. Moreover, the thresholds of water activity in betaine/glycerol and choline chloride/sorbitol systems were determined as 0.64 and 0.75, respectively. We further investigated the recyclability of FA-HY1 in choline chloride/sorbitol system, after three rounds of recycling, the hydroxylation efficiency of 83.2% was still observed. However, the conversion dropped to only 8.3% in aqueous system. In addition, molecular dynamics simulation was performed in DESs and aqueous systems by determining the RMSD, RMSF, Rg, and RDF values, which revealed the mechanistic features of the thermostability of FA-HY1 in DESs.

FIGURES

FIGURE 1

Figure 1

Graphic Abstract

FIGURE 2

KEYWORDS

Deep eutectic solvents | Fatty acid hydroxylation | Hydratase | Thermostability

BIBLIOGRAPHY