

Call for Applications for a Master's Thesis on „Elucidation of Key Performance Indicators of Catalytic Peptides in Deep Eutectic Solvents“

Background and Research Objective

Natural Deep eutectic solvents (NADESs) are a class of low-cost, tunable, and environmentally friendly ionic liquid analogues formed by mixing a salt with a hydrogen bond donor, offering a valuable alternative in (bio)catalysis. While aqueous solutions have a limited solubility for many chemically relevant compounds and organic solvents are toxic to the environment and the catalyst, DES have been shown to (i) promote substrate loading, (ii) support catalyst stability, and (iii) can be constructed from renewable sources. Considering their obvious benefits, their molecular interaction with the catalyst remains enigmatic, rendering their application in biocatalysis limited and require the need for further characterization. Only few examples of catalysts were reported that perform very well under non-aqueous conditions, but the majority require at least minimal presence of water to allow their catalytic reaction to occur. For instance, the horse radish peroxidase-catalyzed oxidation of 4-aminoantipyrine in choline chloride-based DES was performed in 80-90 % (w/w) water. To better understand this behavior, catalytic peptides, *i.e.*, the catalytic backbone of a protein, will be used to mimic a solvent-exposed active site of enzymes. This project therefore aims to elucidate and characterize the relationship between the peptides and the solvents for future improvements.

Content of the Thesis

This project elucidates the direct interaction of different DES and catalytic peptides by means of biochemical investigation and the determination of key performance indicators (KPIs) such as catalytic efficiency, total turnover number, product titer, volumetric productivity, among others. These parameters will be obtained by UV-Vis spectroscopy from the oxidation of colorimetric substrates, *e.g.*, ABTS, TMB, and DMP. Additionally, esterification and ester hydrolysis will be investigated in 2 in 1 DES in which one or both DES components can act as substrates. Activity of the peptides is monitored by chromatographic methods, such as gas and liquid chromatography. The thorough parameterization of this interaction may inform the design of catalytic peptide sequences that perform under non-aqueous conditions with improved KPIs compared to conventional solvents.

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