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Description

The sustainability of plastic materials implies attaining a renewable origin and recyclable nature. Unfortunately, both conditions are far from being fulfilled by the current industry. In the polyester sector, PET [poly(ethylene- terephthalate)], one of the most common plastics, has a petrochemical origin. Happily, PEF [poly(ethylene-furandicarboxylate)] is emerging as a biobased alternative to PET. Moreover, enzymatic biocatalysis can contribute to the industrial and environmental feasibility of bioplastics with next-generation technologies for the synthesis and recycling of both building blocks and polymers. For PEF and other furanic polymers, esterase-type enzymes can be tailored for ad hoc depolymerization reactions. Moreover, oxidase-type enzymes are called to provide selective and environmentally-friendly alternatives to convert HMF (5-hydroxymethylfurfural) from biomass sugars into the PEF building-block FDCA (2,5-furandicarboxylic acid).

Despite this potential, some of the most relevant enzymes such as HMF oxidases and aromaticpolyesterases are not optimally suited to oxidize or hydrolyze plastic compounds (since they naturally evolved to act on their natural counterparts). Therefore, protein engineering is mandatory to optimize them in terms of substrate specificity and operational conditions. In this process, rational engineering will be possible when supported by extensive computational simulations of the access, accommodation and reaction of target substrates at the active site of the selected enzymes. For these studies, advanced software simulating substrate binding by the enzymes and their engineered variants needs to be used. This will be combined with datasets of relevant enzymes and predictive models by regression simulation and machine learning. Some commercial enzymes, such as catalases and lipases, can be directly used by the polymer industry, taking advantage of the wide repertoire available. However, the production of new enzymes or engineered variants of key enzymes (HMF oxidases and esterases) is still to be optimized, using heterologous expression hosts, adequate fermentation technologies and process intensification. Finally, the biotechnological processes for the production of both plastic polymers (from FDCA) and building blocks (from HMF) are also to be optimized in terms of reaction

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