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Computational and enzymatic experimental strategies for polymers circularity

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PURPOSE OF THE ABSTRACT

The interest in polymers derived from renewable sources has amplified as demonstrated by the large number of recent patents and publications. The material and polymer sectors are facing the challenge of integrating the sustainability of both processes and products, including their management after disposal [1,2]. Biocatalysis can boost such innovation, leveraging on enzymes that overcome the limitations of conventional chemical strategies by catalyzing, under highly selective and mild conditions, the targeted modification, synthesis or degradation of polymers and, most importantly, biobased polymers . Hydrolases, such as lipases and cutinases, were successfully used for in vitro polycondensation of bio-based diacids and polyols, leading to biodegradable polyesters with controlled structures. In parallel the capacity of several cutinases and lipases to degrade polyesters was evaluated by several groups [3,4]. The possibility to correlate structural features of a polymer with the catalytic properties of an enzyme would allow the rational design of environmentally safe new tailor-made biodegradable polymers.
The RenEcoPol project aim was to develop alternative routes for recyclable polyester synthesis based on biobased building blocks using green processes such as biocatalysis. Within RenEcoPol a computational procedure able to analyze and evaluate the ability of different hydrolases to interact and to accept short chain substrates either for synthetic or degradative processes. In this respect specific modelling software's for proteins and protein-ligands interactions such as molecular dynamics and docking were selected and integrated into an automatic workflow. A series of bio-based monomers and enzymes were screened up to now and the computational studies results were correlated with some available experimental data and the results indicate that ability of enzymes to hydrolyze or synthesize polyesters can rationally selected by integrating different computational tools. The pipeline, here implemented in modeFRONTIER software allows to select, from a pool of enzymatic structures, the optimum biocatalyst for catalyzing the synthesis and/or the hydrolysis of polyesters. The new biobased polyesters will be characterized in detail by several analytical techniques for structure confirmation and assessment of the physico-chemical properties. In the third step the biodegradability and ecotoxicity in different natural and synthetic conditions of the synthesized materials was evaluated and in the last step a strategy for the recoverment of the components was demonstrated as proof of concept.

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FIGURES

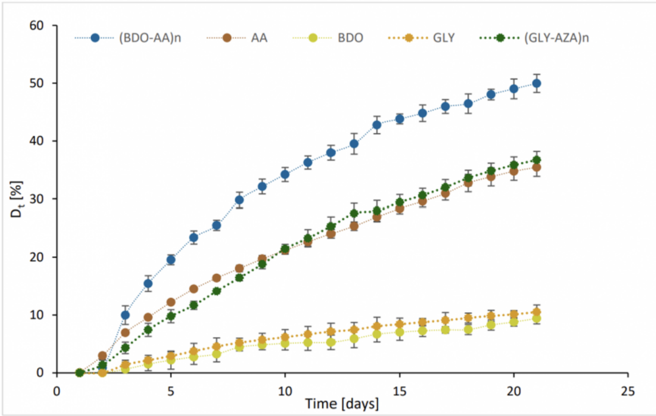

FIGURE 1

Figure 1

Workflow used for the automatic in-silico screening of hydrolases including docking and molecular dynamics steps

FIGURE 2

Figure 2

Degree of degradation of the oligoesters after 21 days of incubation in a marine environment; the data were normalized by subtracting the values of the control samples

KEYWORDS

rational design | degradation | lipases | cutinases

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