

## On the Quest for Plastic-degrading Enzymes: Modern Problems Require Computational Solutions

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Plastics are ubiquitous in the global economy due to their chemical/physical stability and low-cost production. Consequently, this promoted a massive production/use of this type of material. As a consequence of poor waste management, a significant environmental accumulation was propagated and became a major problem of the modern world. Polyurethane (PU) is one of the types of recalcitrant plastics with the fastest-growing market due to its versatility (it has been ranked as the 6th most used polymer in 2018). Thus, its management is of global interest. Nowadays, there is a demand to develop efficient and environmentally-friendly PU-recycling methods. Biodegradation is a promising route as it is a microorganism and/or enzyme centered process which does not require high temperatures (unlike the currently implemented recycling methods). Moreover, some studies have already demonstrated the potential use of enzymes to degrade plastic polymers (*e.g.*, PETase and MHETase). Concerning the PU family, an enzymatic degrading activity has already been observed towards the clearance of Impranil (a simple polyester-PU colloid) by *Pseudomonas sp.* lipase. In addition, the structure of *Pseudomonas sp.* MIS38 lipase (a representative of this type of bacterial enzymes) has already been solved. This opened the door to computational studies regarding the use of this type of enzyme towards PU degradation. Throughout the presentation, it is going to be demonstrated in what manner computational methods can aid the quest for discovering interesting plastic-degrading enzymes. Moreover, examples of the study of *Pseudomonas sp.* MIS38 lipase cleavage of the urethane bond will be given.