

QM/MM MD STUDIES OF POLYESTER SYNTHESIS/HYDROLYSIS

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The world is suffering the consequences of plastic pollution, however modern societies remain heavily reliant on plastics. More sustainable alternatives are actively being sought-after. Enzymatic synthesis can offer a more sustainable route for polyester synthesis. Nevertheless, there are still limitations, such as limited activity and selectivity for some monomers, unfavorable compatibility in chemoenzymatic reactions and low stability under harsh reactions conditions. We have studied the catalytic mechanisms for polycaprolactone hydrolysis/synthesis by the wildtype enzymes *Archaeoglobus fulgidus* carboxylesterase (AfEST) and *Candida antarctica* lipase B (CaLB) and respective enzyme variants by performing Quantum Mechanics/Molecular Mechanics Molecular Dynamics simulations [1-3]. Our results give important insights towards the design of new enzyme variants combining good activity with high thermostability.

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