

Structural insights into polyethylene terephthalate (PET) hydrolase from *Ideonella sakaiensis* in the context of PET bio-degradation

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INTRODUCTION

The invention of plastic has revolutionized the world's industrial market and now it is one of the most used substance with a wide range of applications in many fields. It has become one of the key raw materials for the synthesis of basic household commodities to large industrial storage units or research lab materials etc. Its durability strength and moldability have made it the material of choice for many products.

Along with its advantages, plastic also has equally potential disadvantages that have turned out as global problem - plastic waste management. As human dependency grew stronger year by year on plastics, it has also significantly risen the plastic waste accumulation on land and in oceans. Plastic degradation takes many years, which is why plastics are a threat to the environment.

In 2016, in Japan, a bacterium called *Ideonella sakaiensis*, which is capable of consuming and breakdown of Polyethylene terephthalate (PET) as sole carbon and energy source was discovered. It is found to have an enzyme called PETase that potentially degrades PET.

PET is a high molecular weight polymer composed of ester bond linked terephthalate and ethylene glycol. Its physical and chemical properties have made it one of the most extensively used type of plastic. However, usage of large amounts of these plastics have led to accumulation of these in the environment. Specifically, *Ideonella sakaiensis* adheres to PET surface and produces a unique enzyme called PETase which degrades PET by hydrolyzing it.

PETase enzymes belong to class of esterases which catalyze polyethylene terephthalate (PET) plastic to monomeric mono-2-hydroxyethyl terephthalate.

$(\text{ethylene terephthalate})_n + \text{H}_2\text{O} \rightarrow (\text{ethylene terephthalate})_{n-1} + \text{MHET}$

Non enzymatic PET degradation takes hundreds of years to get completed whereas PETases can degrade PET in a matter of days.

The structure analysis of three dimensional structure of PETase was performed in order to understand the enzyme stability and its catalytic action.

EXPERIMENTALS

In order to understand the overall organization of the PETase enzyme a three dimensional structural analysis was performed using Computational tools. The three dimensional structure of PETase was downloaded from the protein data bank (PDB ID : 6ILW). The secondary structural analysis (α -helices and β -strands) and ligand interactions was performed using PYMOL software.



Fig1 : Three dimensional structure of PETase showing α -helices and β -strands

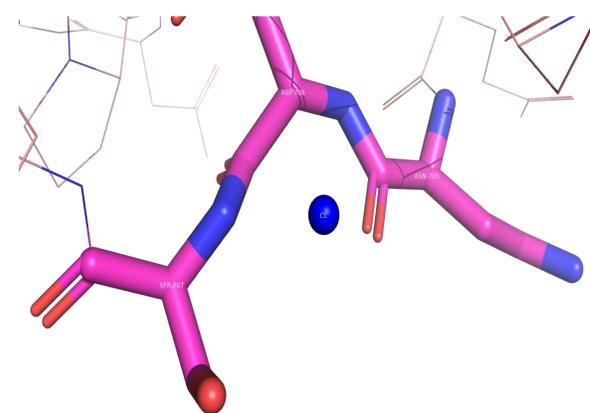


Fig2 : Interaction of Chlorine (CL) ligand with the residues in PETase

RESULTS & DISCUSSION

Based on the computational analysis done by using PYMOL software, the following analysis was done. The three dimensional secondary structure of PETase (PDB ID : 6ILW) was observed to have 7- alpha helices and 8 beta strands in it (Fig:1). When observed for ligand interactions, PETase shows two unique ligands interactions. They are one with chlorine (Cl) atom (Fig:2) and another with sodium (Na) atom (Fig:3).

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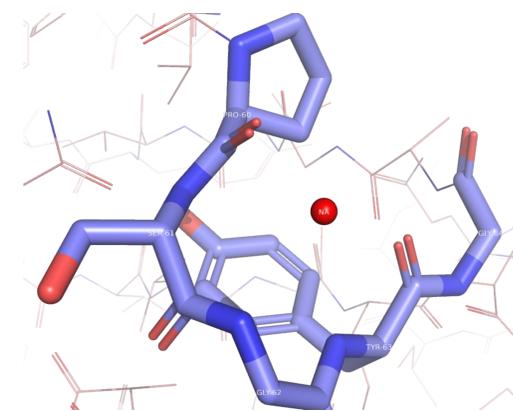


Fig3 : Interaction of Sodium (Na) ligand with the residues in PETase

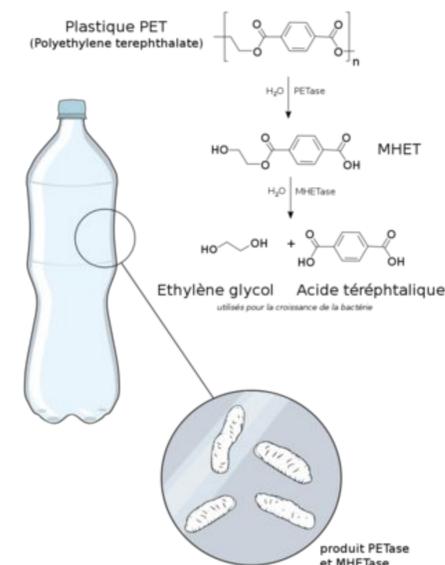


Image ref : Allison Chan (2016). "The Future of Bacteria Cleaning Our Plastic Waste"(PDF)

Fig4 : Activity of PETase secreted by *Ideonella sakaiensis* on PET surface