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Case Study 2 - Greener Plastics: Addressing Single-Use Plastics
Week 3: End-of-Life Part 2

Scenario:

Your team works as scientific advisors for your local congressperson. An NPR podcast has recently caused an uproar for your boss' constituency. The podcast highlighted the shortcomings of the current recycling programs for single-use plastics. The constituency is demanding action from the congressperson.

Understanding the limitations of their knowledge of the problem, the congressperson has tasked their scientific advisors (you and your group) to develop a **Policy Paper**. The paper should provide **background information on what plastics are**, the **scope of the plastic pollution problem**, and evidence used to argue in support of **one of two competing legislative proposals** (shown below):

1) Fixing problems associated with the **beginning-of-life (synthesis and sourcing)** of single-use plastic polymers.
2) Addressing problems with the **end-of-life (recycling/disposal)** of single-use plastic polymers.

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Overall Goals for Case Study 2

During Case Study 2, your group will engage in a number of science and engineering practices using your knowledge of chemistry and the tools and data we have provided. Over the next four weeks, you will accomplish each of the following:

1. **Construct a molecular-level explanation of how and why** each polymer-forming reaction scheme occurs using your understanding of chemistry.
2. **Define the beginning-of-life problem** faced by the **polymer manufacturing** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
3. **Define the end-of-life problem** faced by the **chemical recycling** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
4. **Define the end-of-life problem** faced by the **chemical decomposition** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.
5. **Design a solution** to the congressperson's problem and communicate your group's solution through a **Policy Paper** that outlines an **evidence-based argument** of your choice of **which legislative proposal to support**.

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Goals for Case Study 2 Week 3

Defining the Problem and Evaluating Solutions

4. **Define the end-of-life problem** faced by the **chemical decomposition** companies and **evaluate the strengths and weaknesses** to possible solutions to the problem.

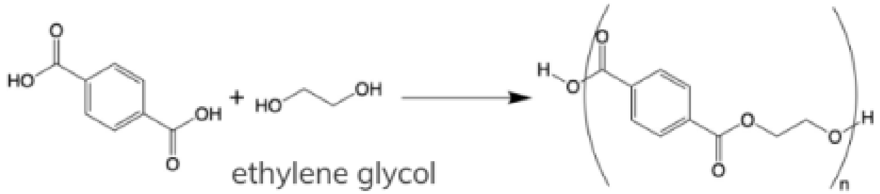
In Case Study 2 Week 1, you explored the science and sustainability of monomer sourcing, the beginning-of-life solution. **In Case Study 2 Weeks 2 and 3, you are exploring end-of-life solutions: recycling or decomposition**.

Poly(ethylene terephthalate) (PET):

- Traditional plastic for single-use drink bottles
- Oil based monomers
- Non-renewable feedstocks

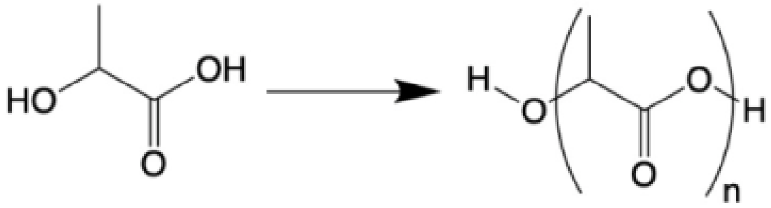
Poly(lactic acid):

- Potential PET replacement
- Monomer is isolated from plants like corn and sugarcane
- renewable feedstocks



ethylene glycol

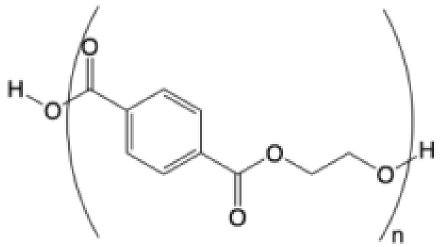
terephthalic acid



lactic acid

Evaluating Solutions for End-of-Life

Not all plastics can be composted. For plastics that are isolated from petroleum products or other non-renewable sources, efficient recycling is important. The discovery of bacteria capable of "eating" plastic has spurred an interest in identifying enzymes that can perform the depolymerization reactions. The enzymes closest to commercialization catalyze the depolymerization of PET.



Many carboxylic acid derivatives can be formed and hydrolyzed in biological systems (i.e., amides in proteins). **Why would it make sense that an enzyme could evolve to perform the depolymerization (hydrolysis) of the esters in PET?**

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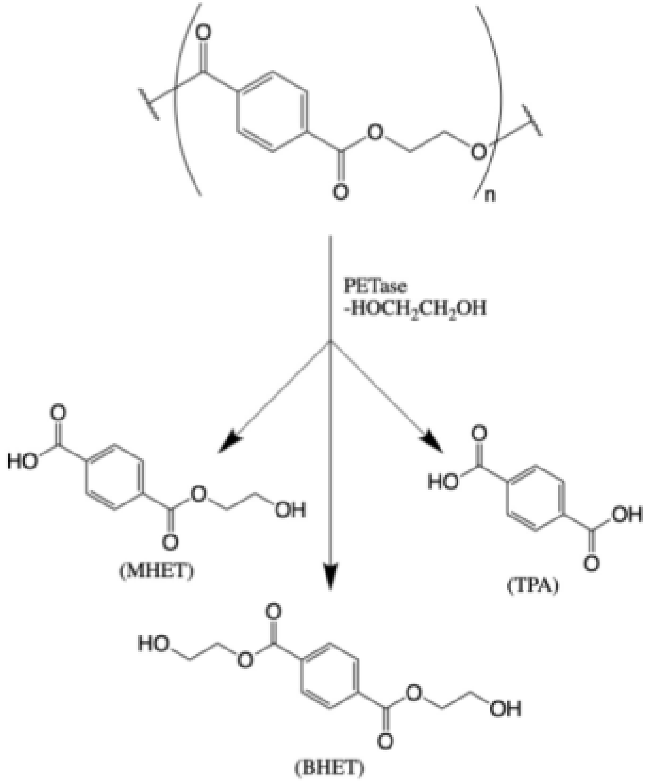
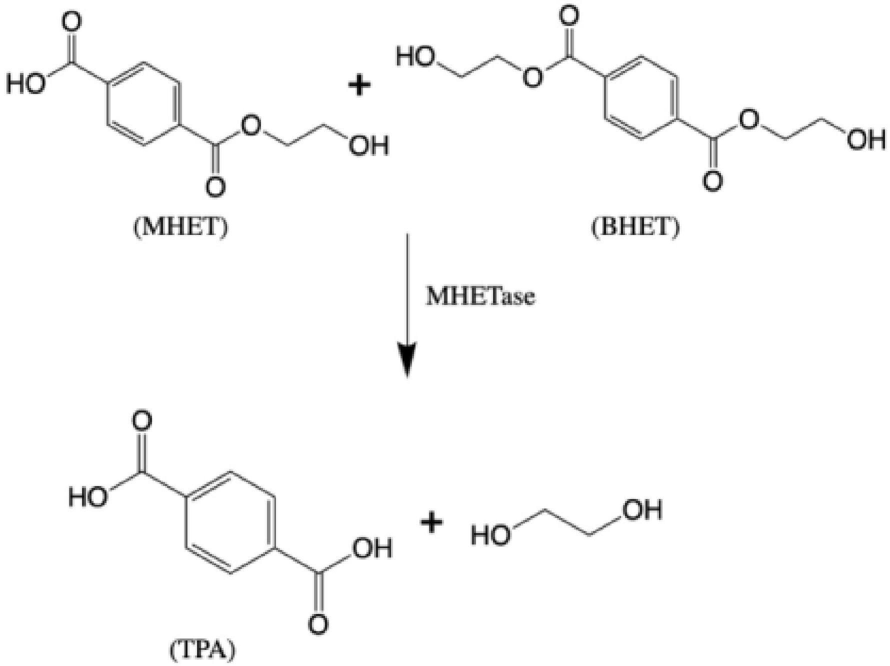
Recently researchers have reported a two enzyme system. In the scheme below, the first enzyme (PETase) catalyzes the following reaction.





Then, the second enzyme (MHETase) catalyzes the removal of remaining ethylene glycol molecules.

The active site of both enzymes contains a Serine-Histidine-Aspartate catalytic triad (**Figure 1**). Similar to most proteases, the key residue is the serine.

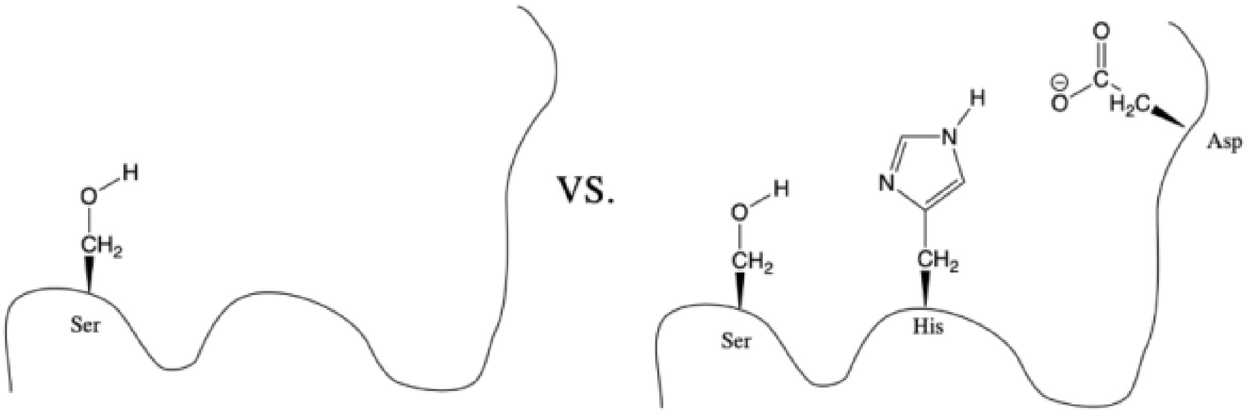
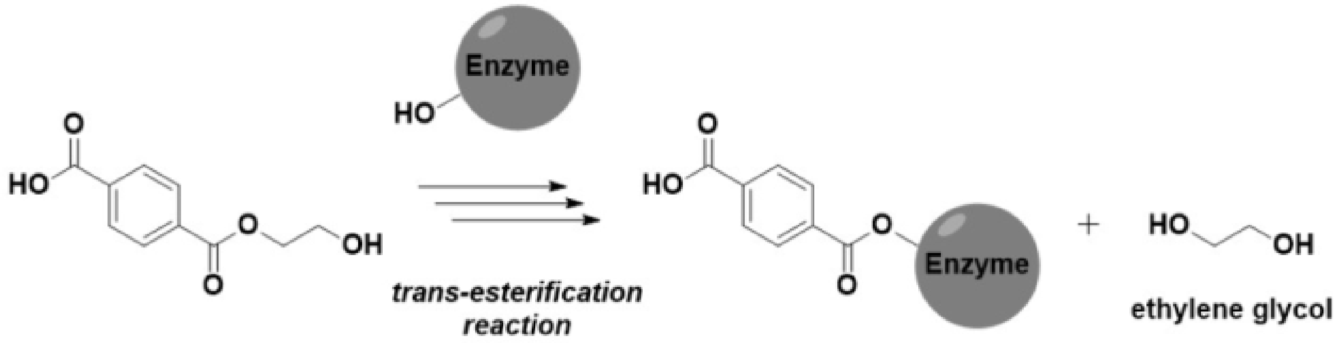
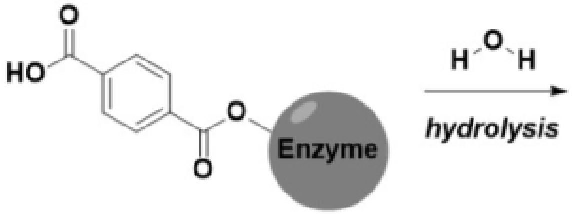


Figure 1: A theoretical active site with only Ser (left) vs. the catalytic triad of Ser/His/Asp (right).

The release of the terephthalic acid and ethylene glycol monomers starts with a **trans-esterification reaction** to release ethylene glycol (step 1, shown below). This is followed by hydrolysis of the resulting ester bond between the enzyme and terephthalic acid (step 2). In the green box below, **draw the mechanism for this final hydrolysis step (step 2), which releases the terephthalic acid monomer.** Hint: **water acts as a nucleophile** under these biological conditions.





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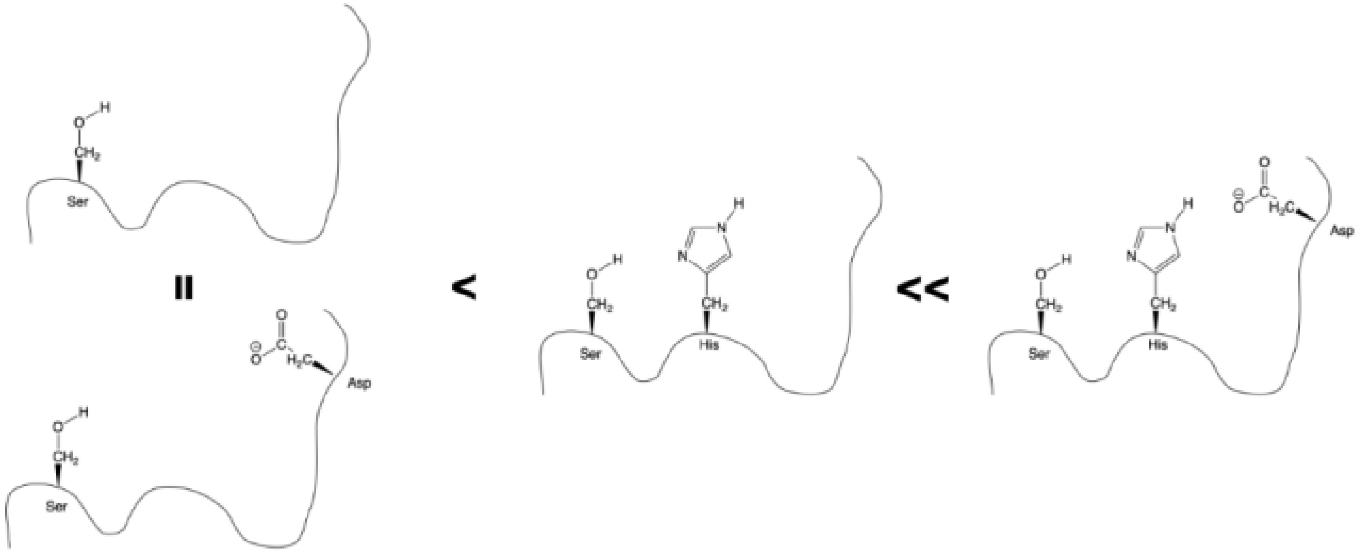
While **Serine is the key residue that actually interacts with the ester**, the **neighboring amino acids around Serine influence the rate of this reaction**. Experimentally, we have determined that the reaction rate follows this pattern:

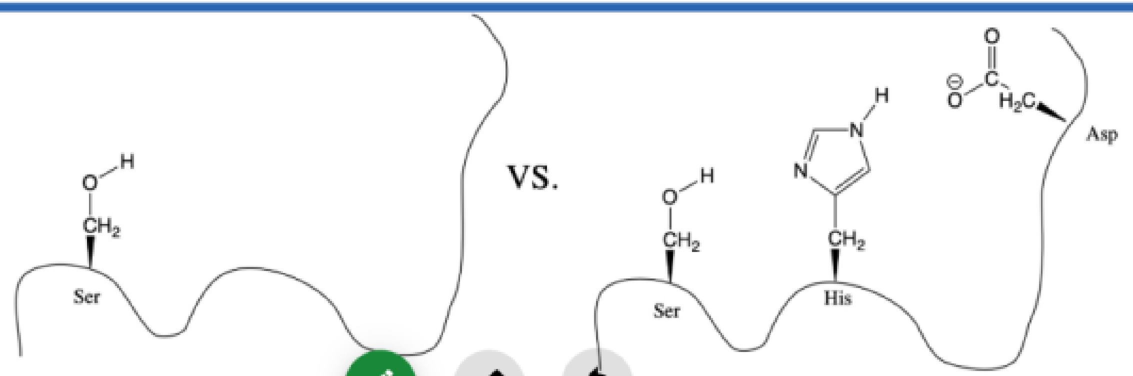
Serine only ~ Serine-Aspartate < Serine-Histidine << Serine-Histidine-Aspartate



Based on this information, does the presence of the Histidine and Aspartate amino acid residues make Serine a better or worse nucleophile?

- ☐ Better Nucleophile
- ☐ No Difference in Nucleophilicity
- ☐ Worse Nucleophile

In the **blue box** below, **annotate the drawing with mechanistic arrows** to highlight how these residues interact. *Hint: think about acid-base reactions.*



In the **green box** below, **explain how and why the Histidine and Aspartate residues have this effect on Serine**. Consider how they c**hange the nucleophilicity of Serine**.

Although this is a promising technology, just putting the PET into a solution containing both enzymes (PETase and MHETase) does **NOT** depolymerize PET at a **fast enough rate to be commercially viable**. Research is heavily focused on ways to further **increase the rate of depolymerization.** One research group has made the **enzymes with a linker chaining the two enzymes together** (**Figure 2**).

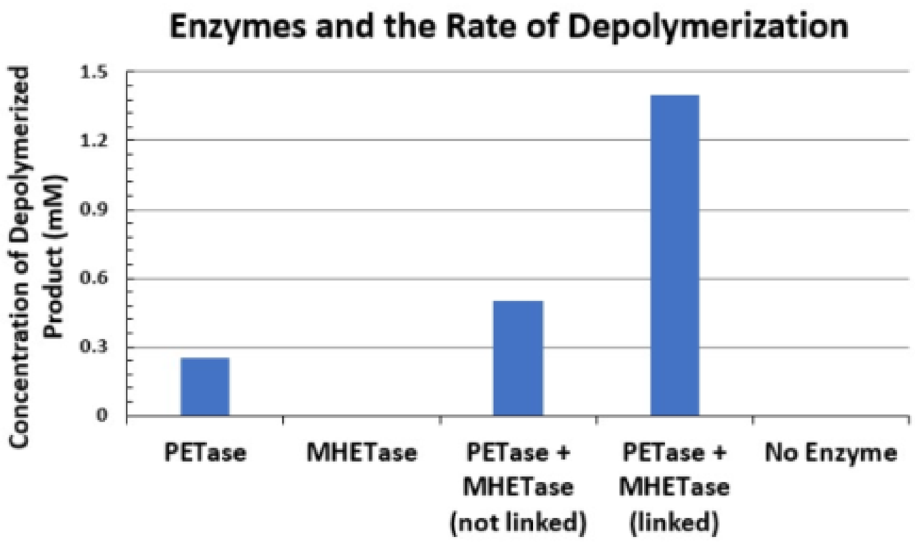
Figure 2: Examples of linking chains for the PETase and MHETase enzymes.

What effect do you predict the **linker will have on the rate of depolymerization**?

- ☐ Increase in Rate of Depolymerization
- ☐ No Change in Rate of Depolymerization
- ☐ Decrease in Rate of Depolymerization

Enzymatic Depolymerization

The graph (see left) shows example data for the rate of depolymerization of PET in the presence of various enzymes (see Slide 4 as a refresher on these enzymes). The **y-axis** shows the **"Concentration of Depolymerized Product (mM)"** where a **higher concentration value signifies a greater degree of depolymerization**. The **x-axis** shows the different **options of enzymes** that could be used for depolymerization, including **PETase and MHETase either with or without a linker chaining the enzymes together** (as described on the previous slide).



Do the data shown above **support your prediction from the previous slide**? Your previous prediction is shown below on the left.

- ☐ Increase in Rate of Depolymerization
- ☐ No Change in Rate of Depolymerization
- ☐ Decrease in Rate of Depolymerization

- ☐ Yes, the data support my prediction.
- ☐ No, the data do **NOT** support my prediction.

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As you can see on the previous slide, the **linked enzymes** resulted in almost **triple the rate of depolymerization of PET**. In the green box below, **explain why the linked enzymes lead to this increased rate of depolymerization**. *Hint: think about the conditions needed for molecules to react. Remember, molecules need to collide with the proper energy and orientation.*

Defining the Problem

In the green box below, **describe the end-of-life problem with decomposition** in Case Study 2 and **why it is a problem**. In your response, **identify the physical system** (in which the problem is embedded) and **its components**, **specify the stakeholders of interest** to the problem and match each stakeholder to the **criteria/constraints that are important** to consider when designing an acceptable solution.

Case Study 2 Week 3

List the **team names, MSU emails, and CEM section numbers** of everyone in your group who participated in this week's Case Study activity.

Leave this blank if you DO NOT intend to turn this in.

Team Member 1	MSU Email	Section Number
Team Member 2	MSU Email	Section Number
Team Member 3	MSU Email	Section Number
Team Member 4	MSU Email	Section Number

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You must hit "Complete" to earn credit for the assignment.

Once you hit "Complete" your answers will be submitted to your instructor so make sure they reflect your final responses before hitting "Complete"