



Modeling Enzymes: From Basics to Bacterial Resistance

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NOVEMBER 14-17, 2024

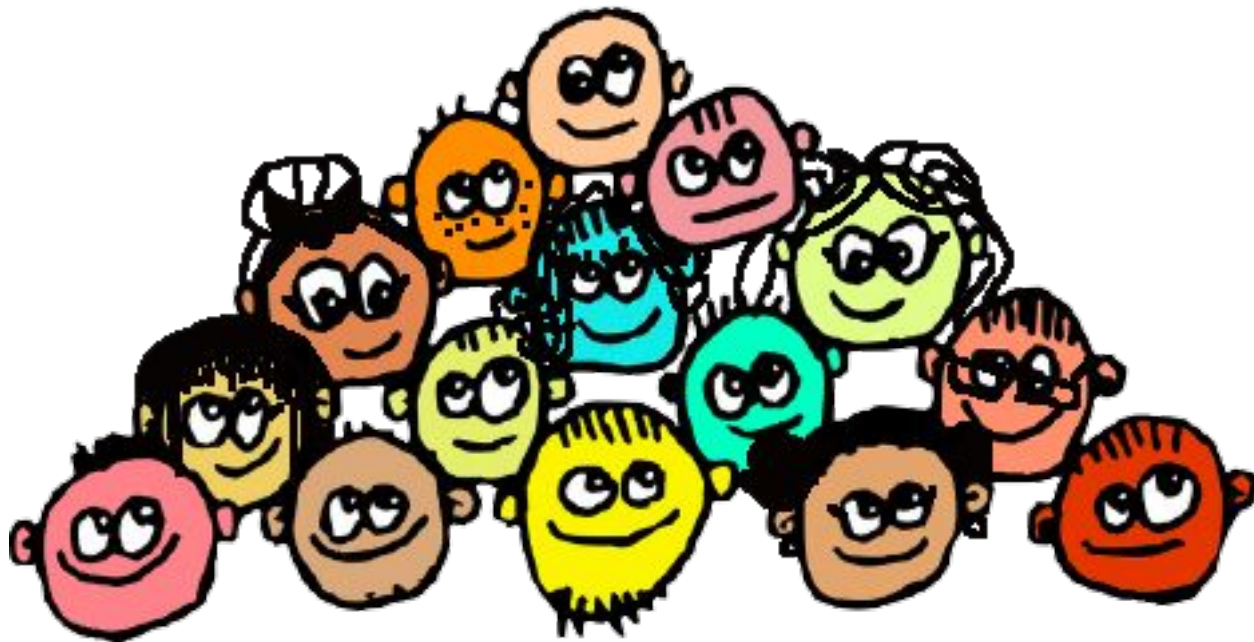
Who am I?



3D Molecular Designs



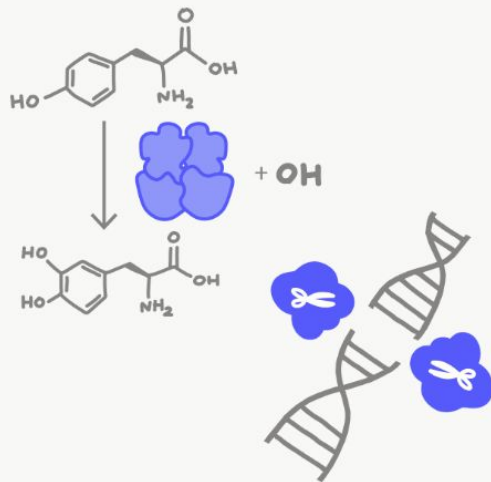
Who are you?



What do your students need to know about enzymes?



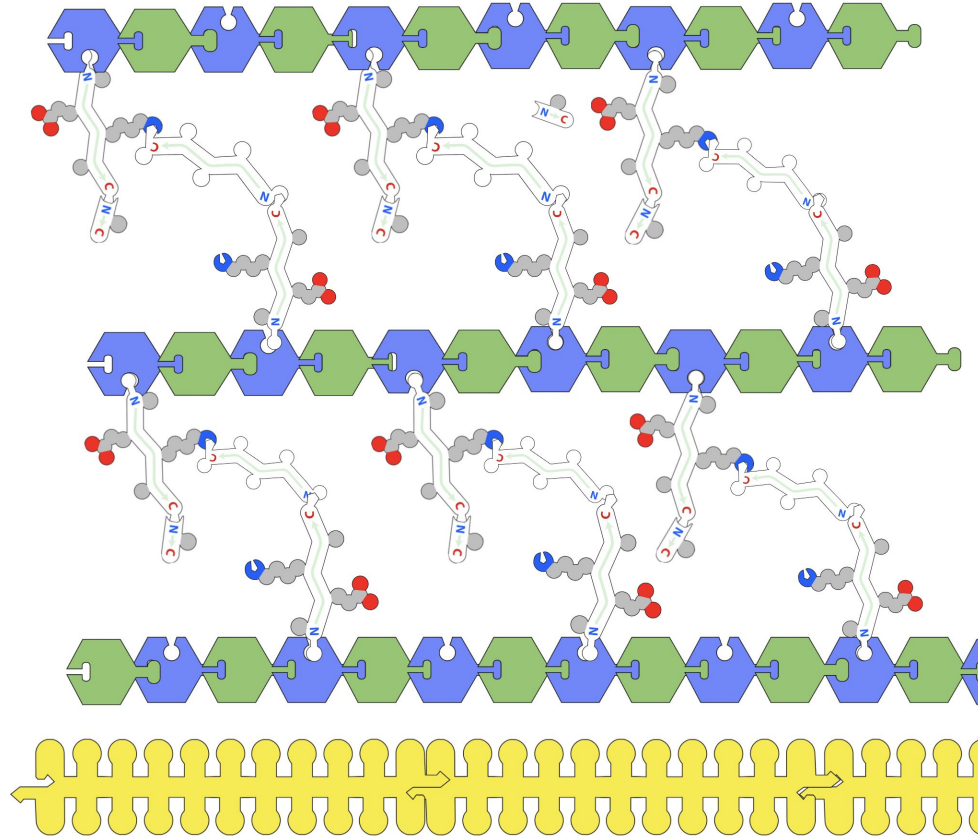
Enzyme



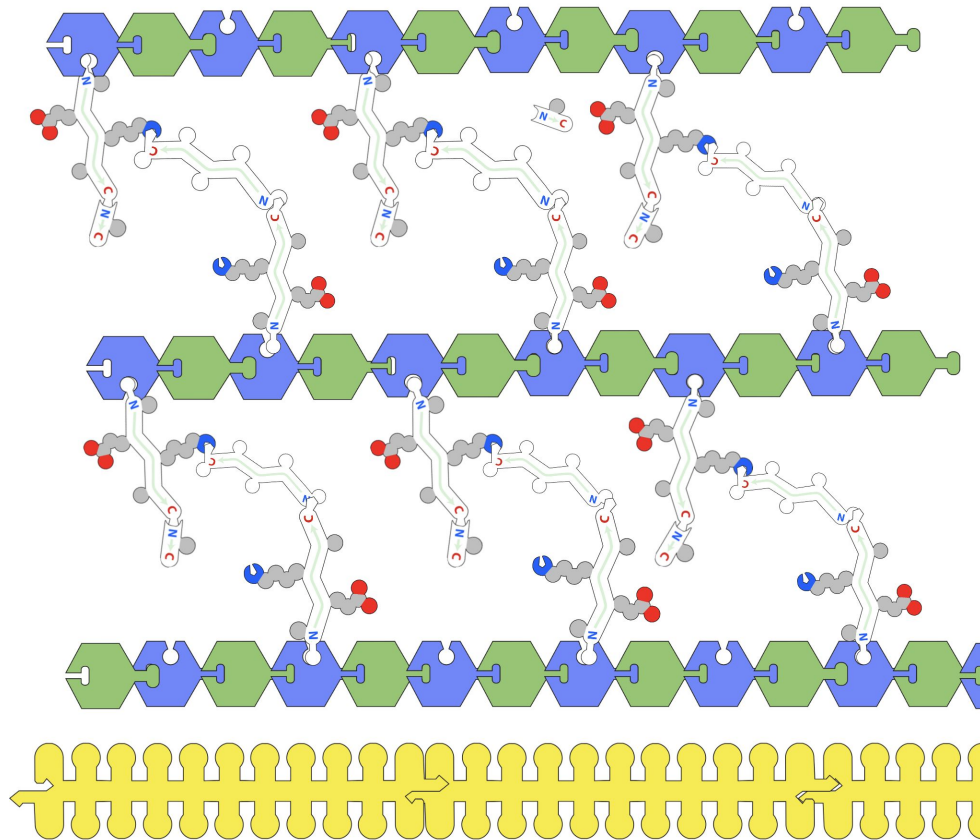
A molecule, typically a protein, that causes or catalyzes a chemical change. Usually an enzyme's name describes a molecule involved in the activity it performs and ends with the suffix -ase. For example, lactase is a well-known enzyme that breaks down lactose, a sugar found in milk. Cas9 is a nuclease, an enzyme that breaks apart the backbone of nucleic acids (RNA or DNA).

« [Back to Glossary Index](#)

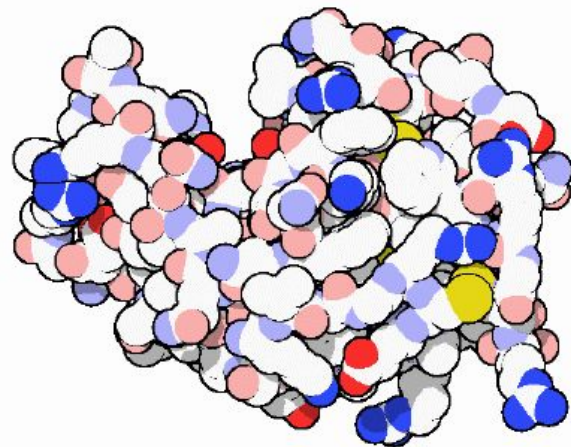
Our natural defenses against bacteria include enzymes!



Our natural defenses against bacteria include enzymes!



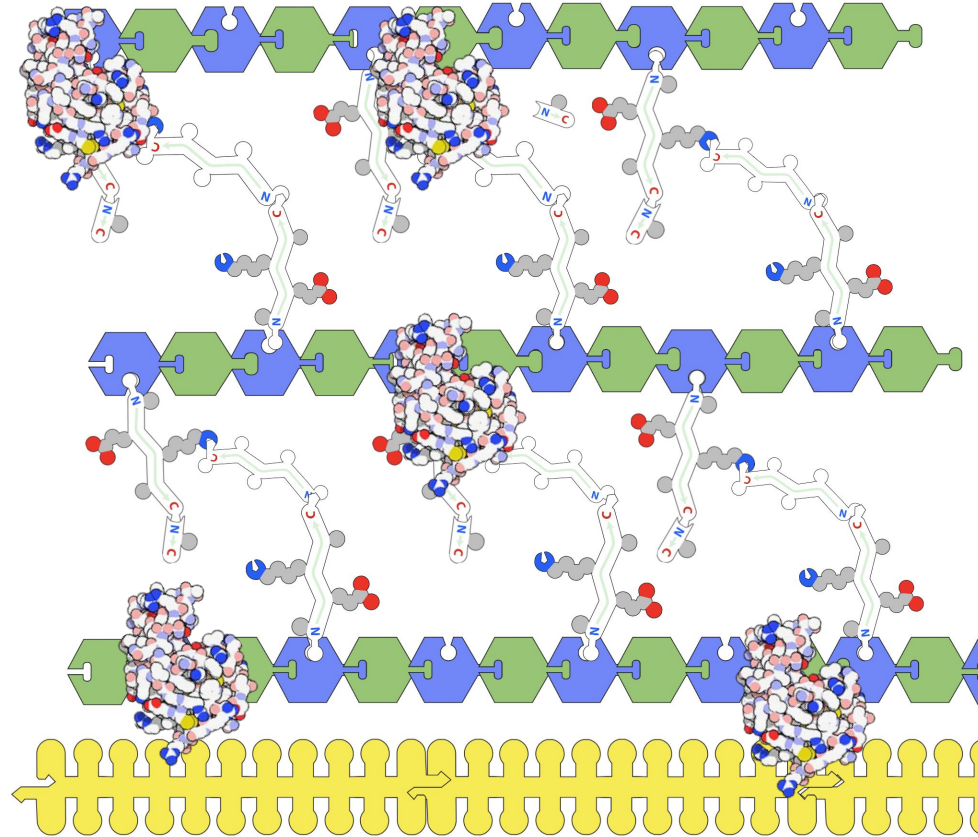
<https://pdb101.rcsb.org/motm/9>



Lysozyme

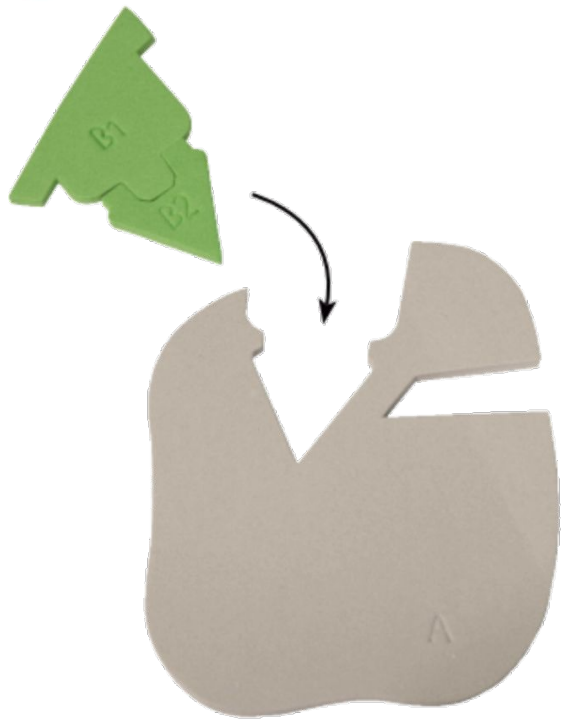


Our natural defenses against bacteria include enzymes!



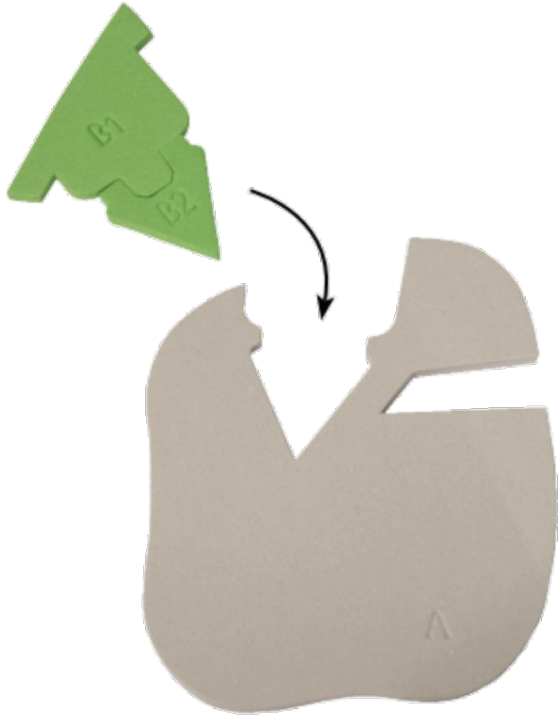
Let's Play! In two dimensions.



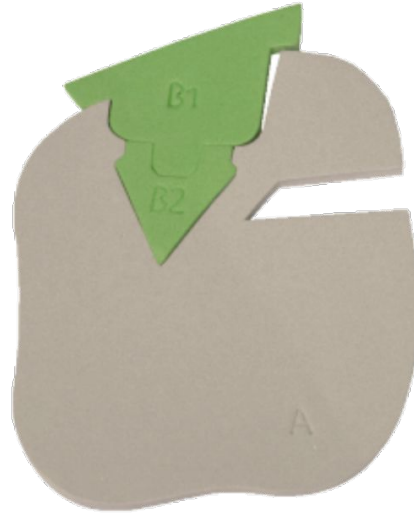


Step 1

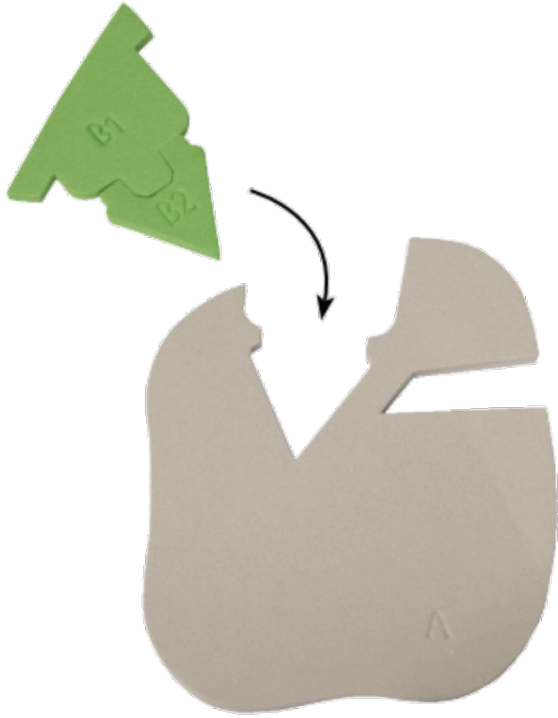




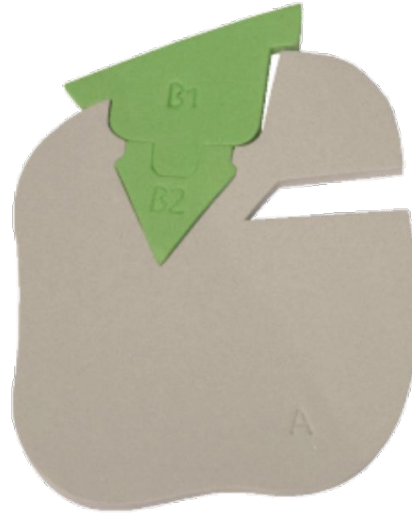
Step 1



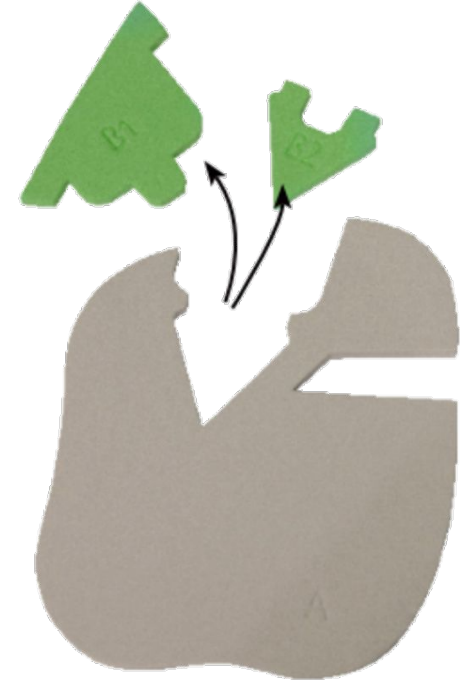
Step 2



Step 1

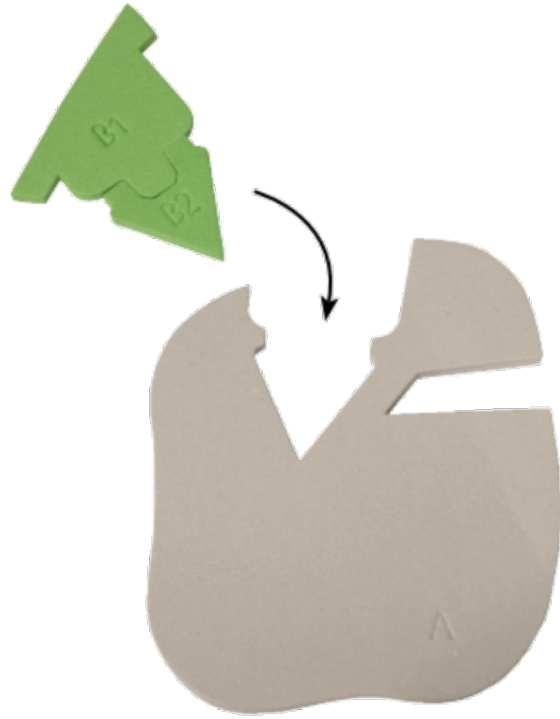


Step 2

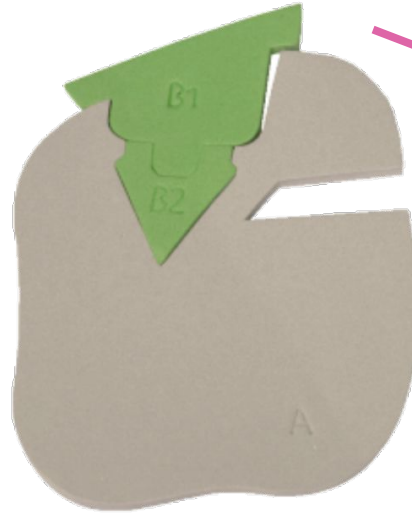


Step 3

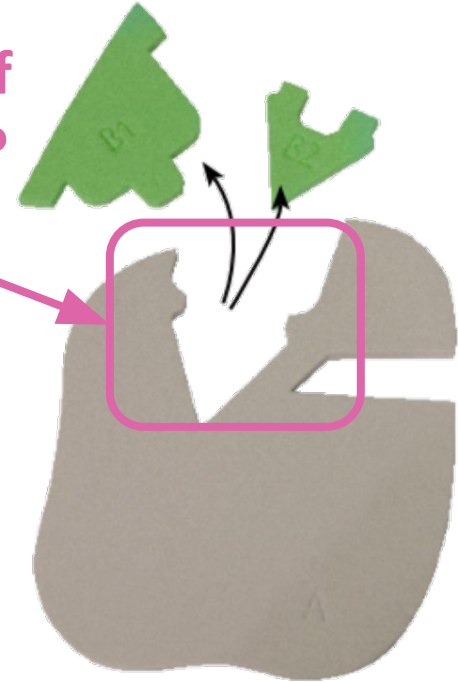
Catabolic process - breaks the substrate into smaller products



Step 1



Step 2



Step 3

What did you notice about the behavior of the active site?

Catabolic process - breaks the substrate into smaller products





Let's Play Again!



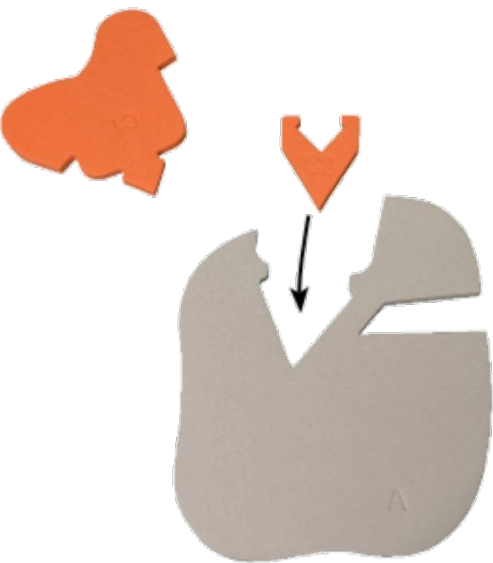


Let's Play Again!



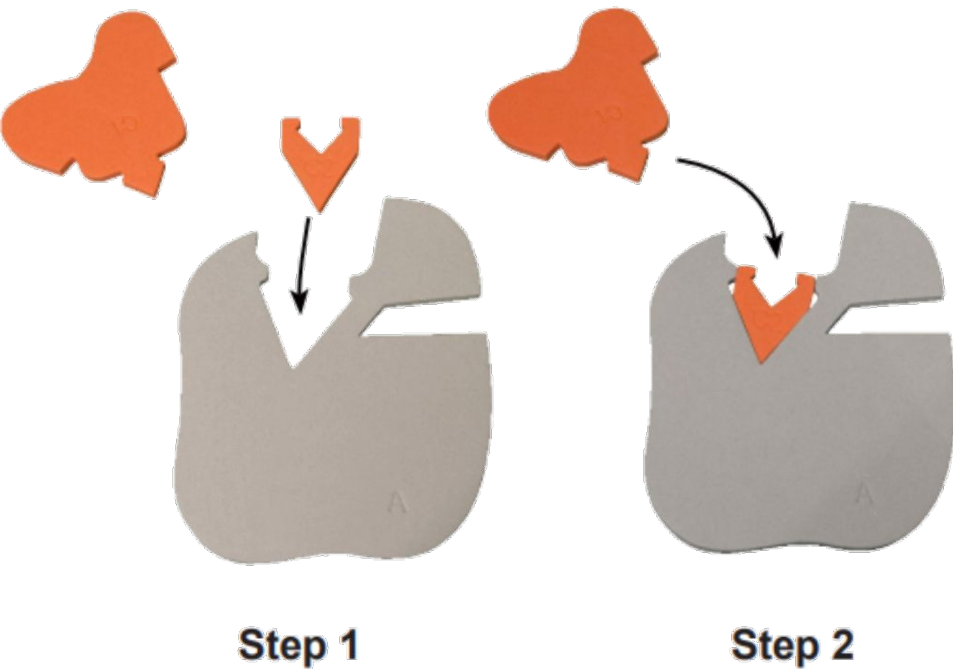
What did you discover?

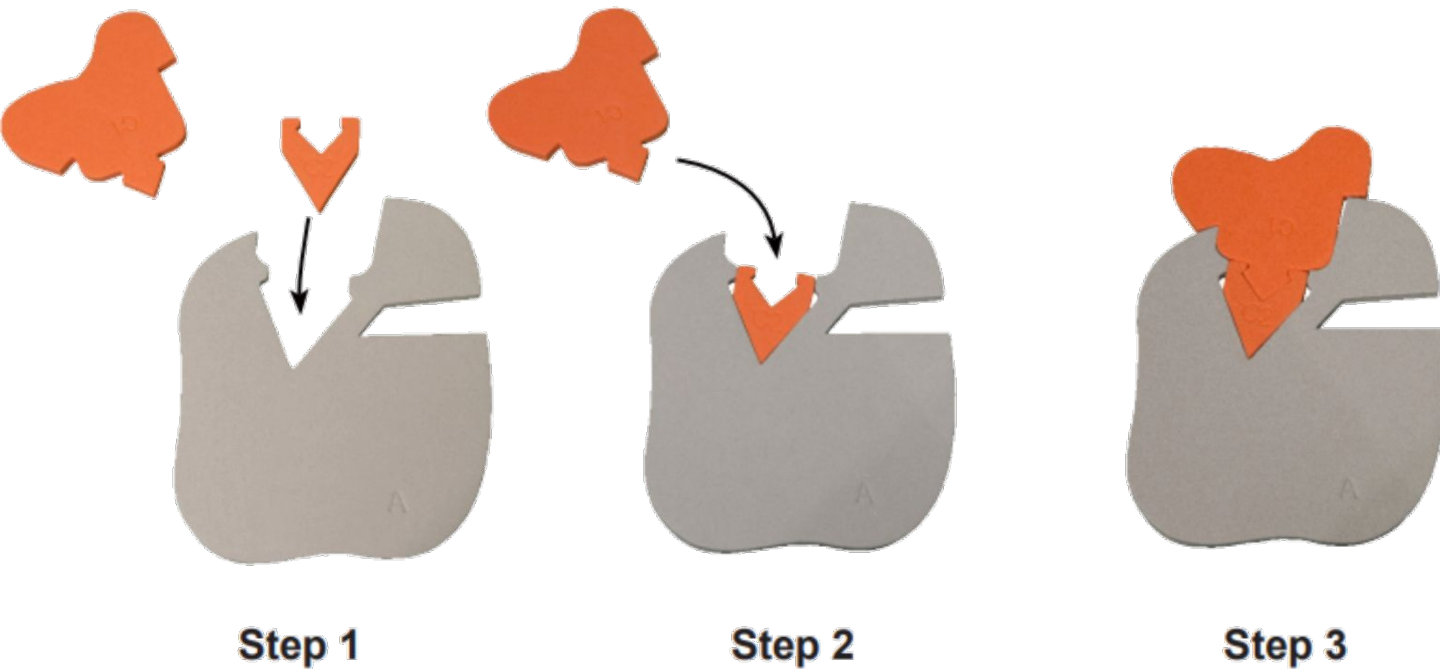


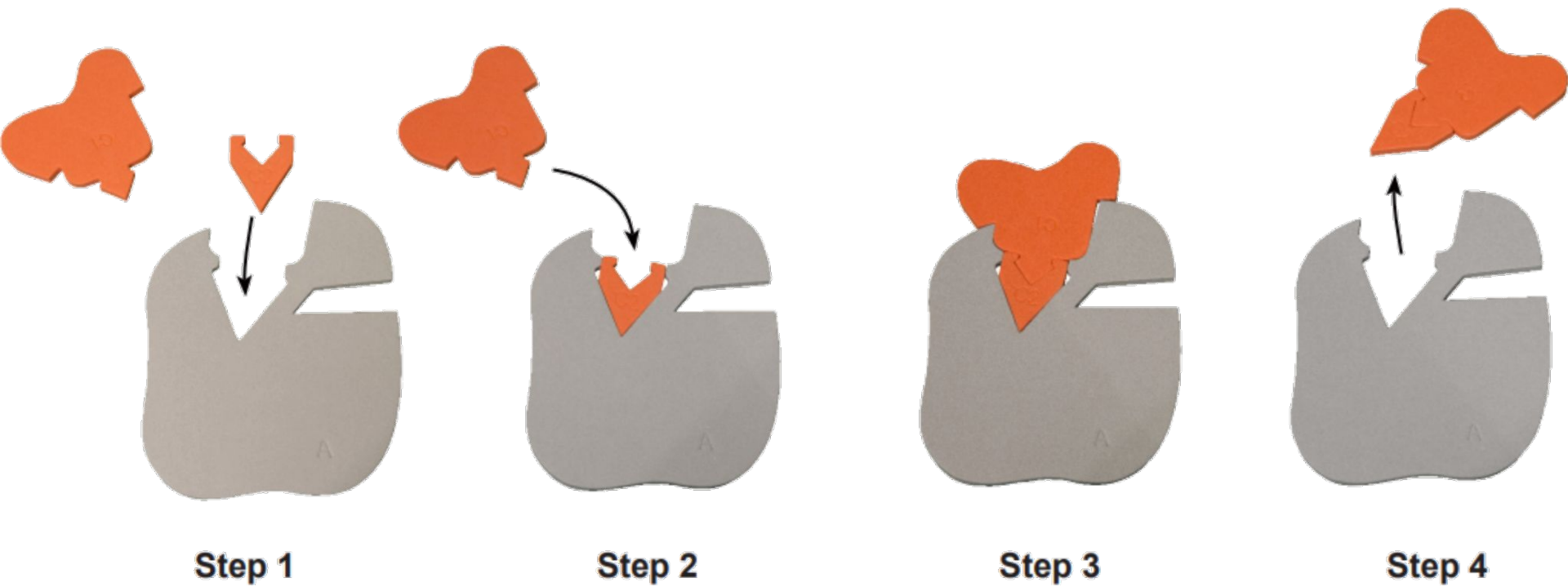


Step 1







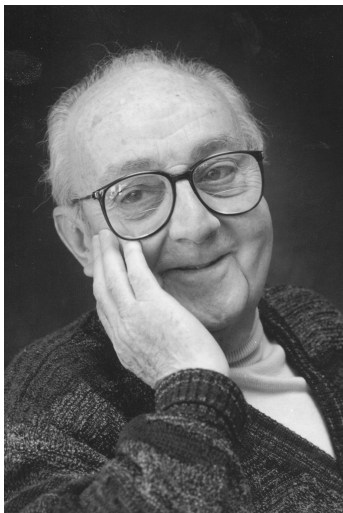




What can students learn from these pieces?



Let's focus again on the active site

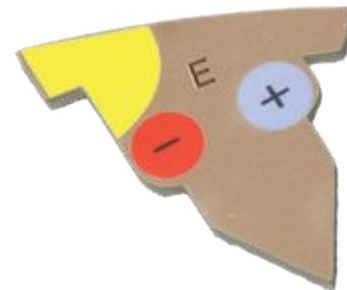
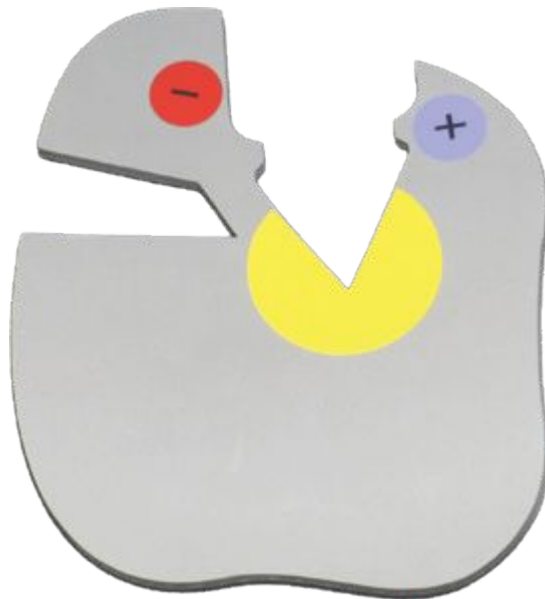


<https://commons.wikimedia.org/wiki/File:GeorgeEPBox.jpg>

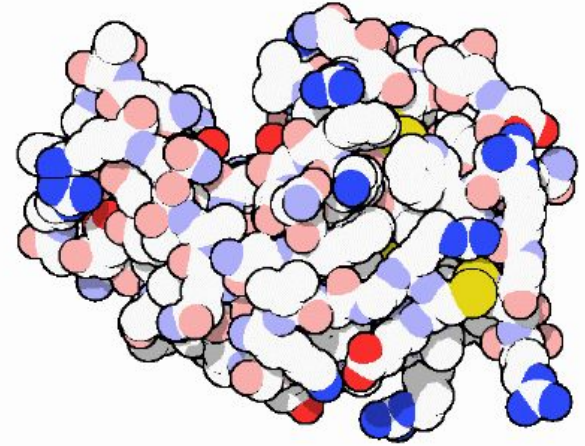
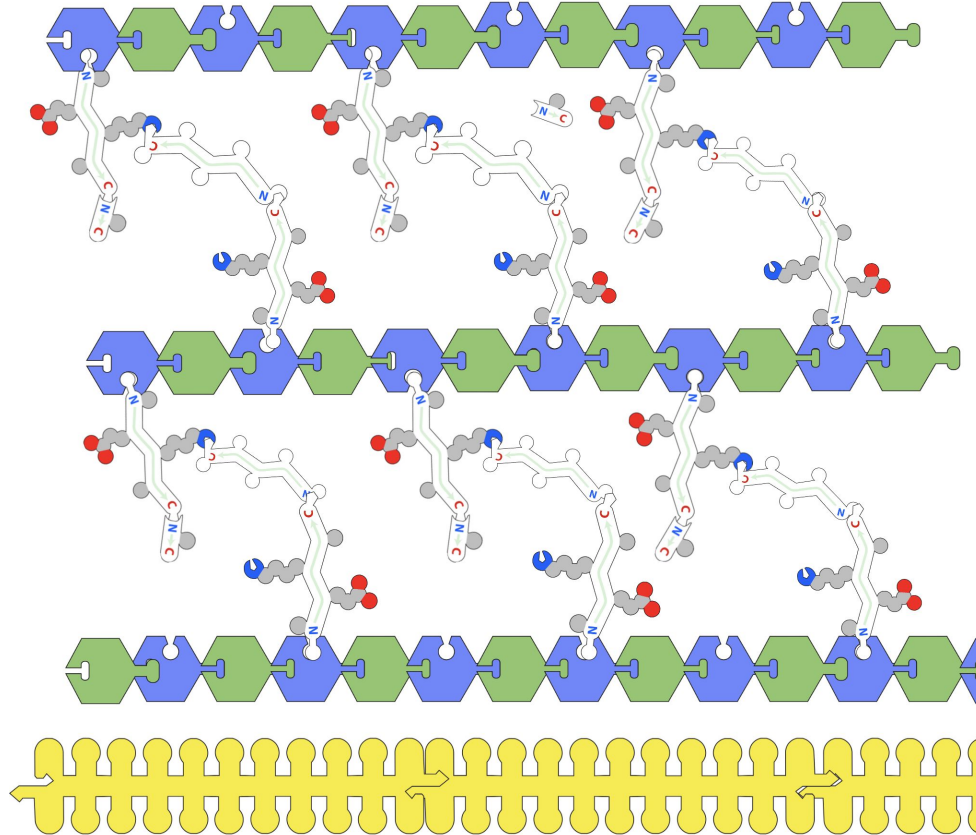
“All models are wrong,
some are useful.”
-George Box



Is shape really the only thing?

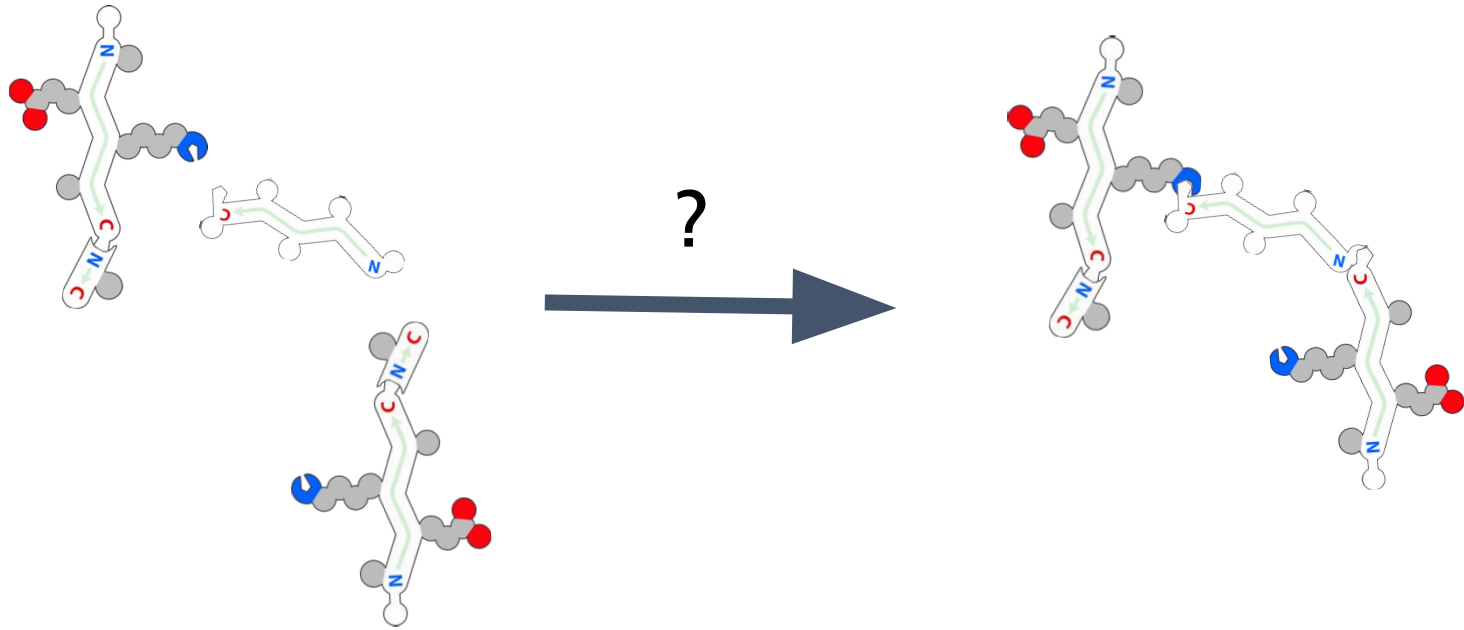


Let's get back to bacterial infections.

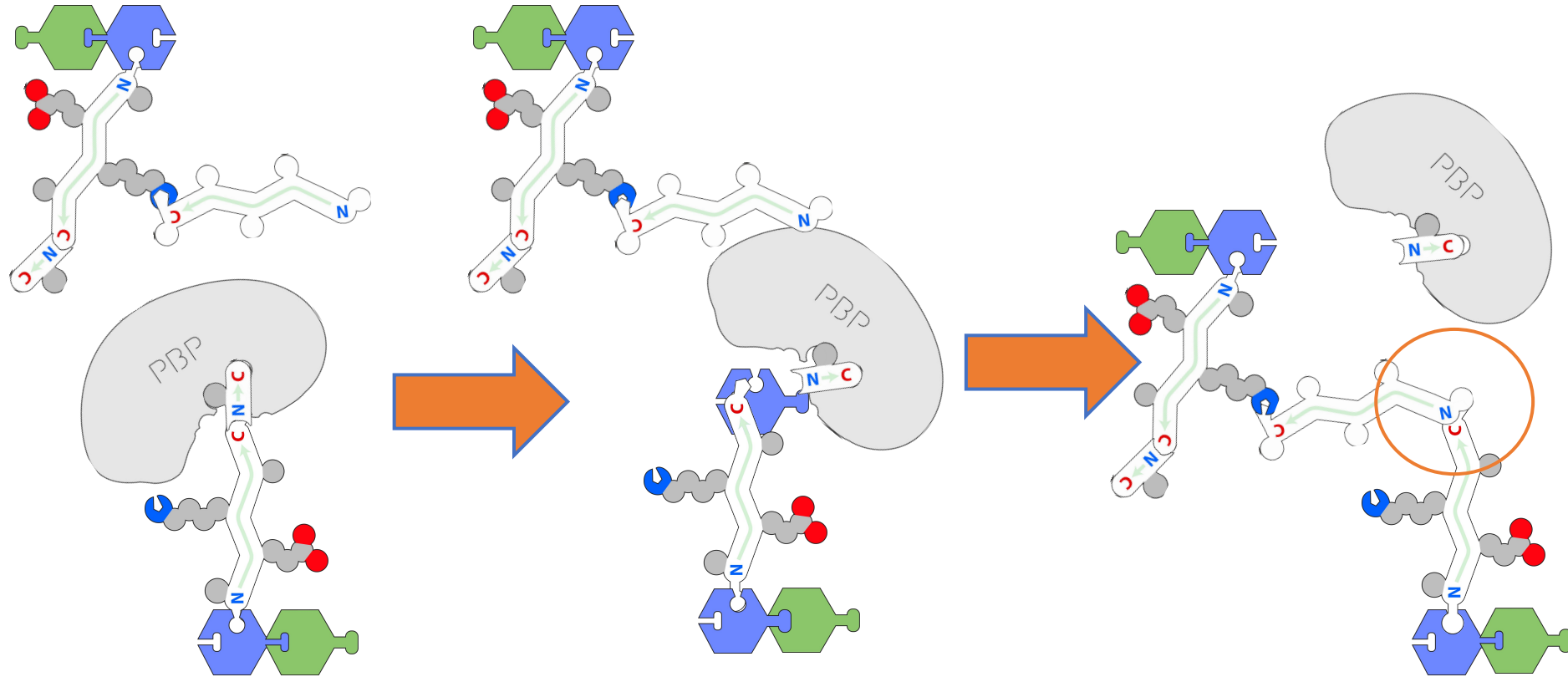


Lysozyme

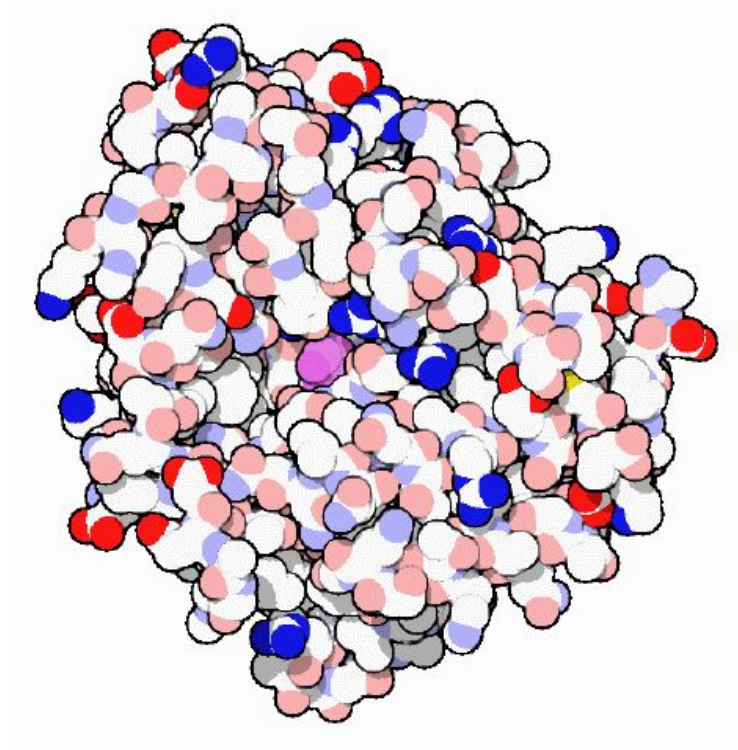
Back to peptidoglycan and it's assembly...



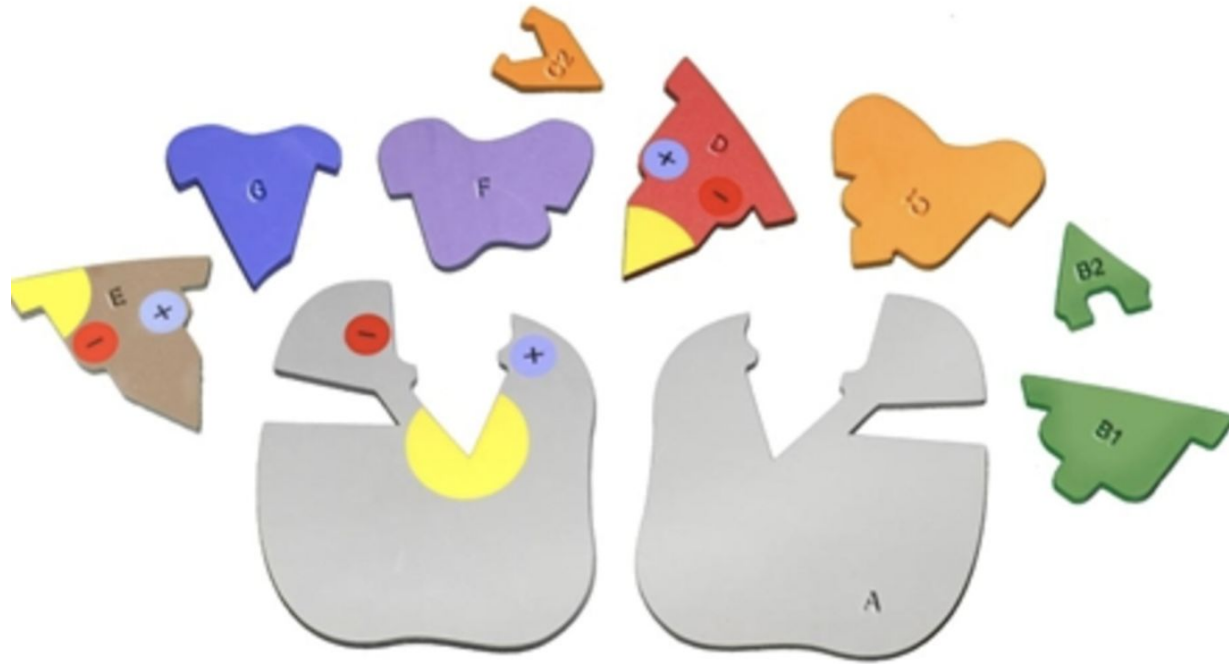
D-alanyl-D-alanine peptidase



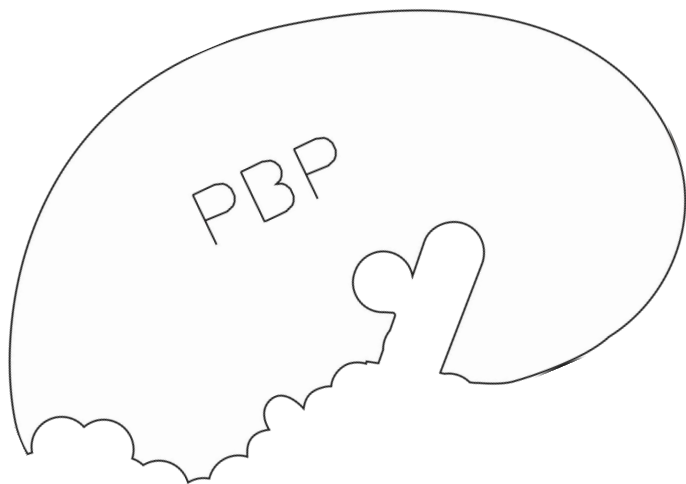
D-alanyl-D-alanine peptidase



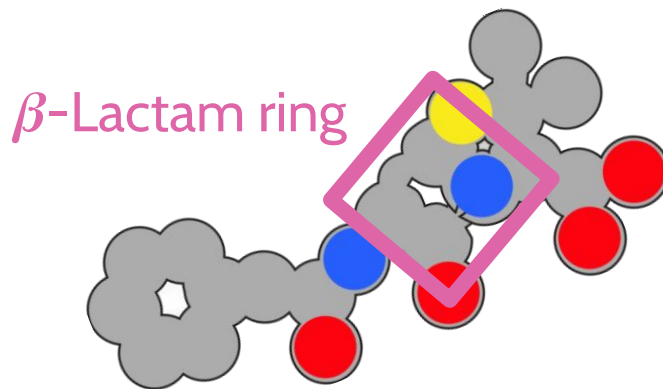
Given what you have learned, how could we inhibit PBPs?



Binding Battles: The Evolutionary Tale of Enzymes and Antibiotics

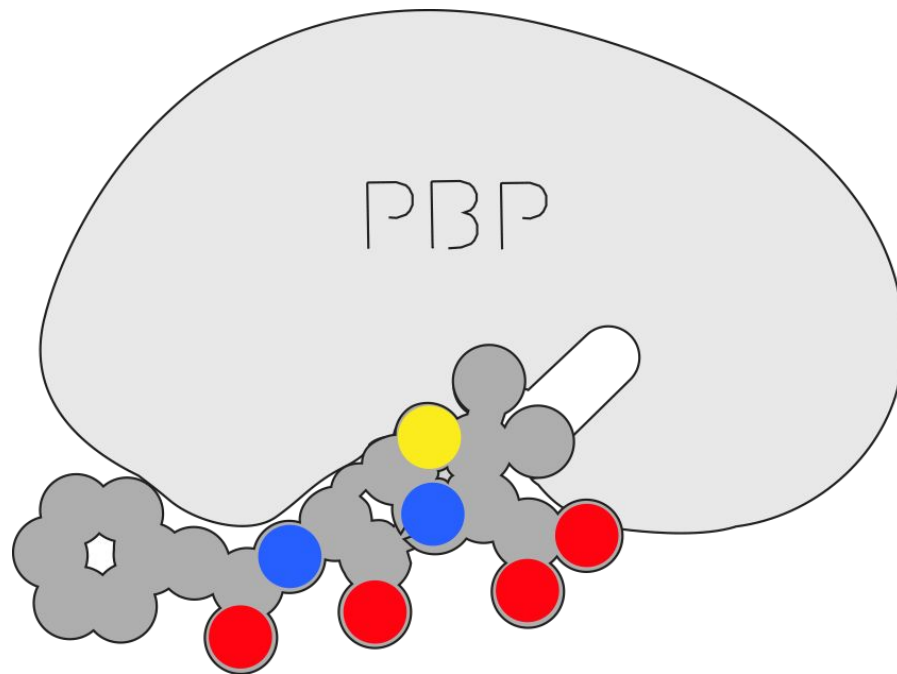


“Penicillin Binding Protein”



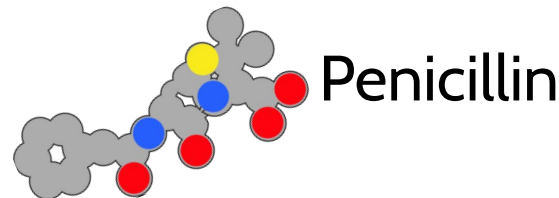
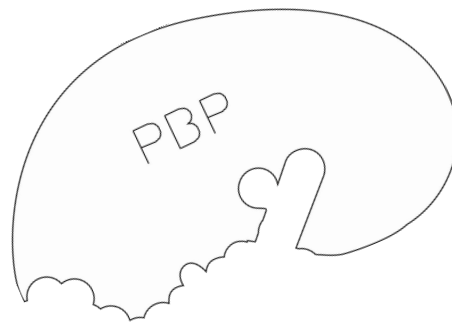
Penicillin

Were you right?



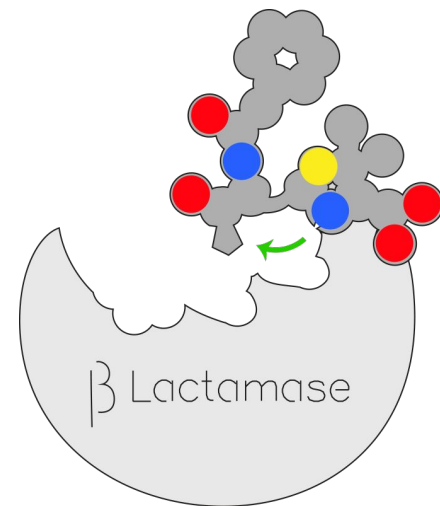
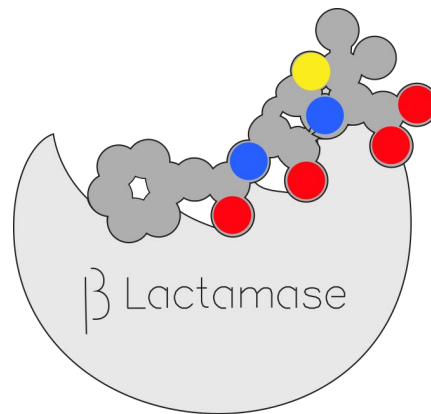
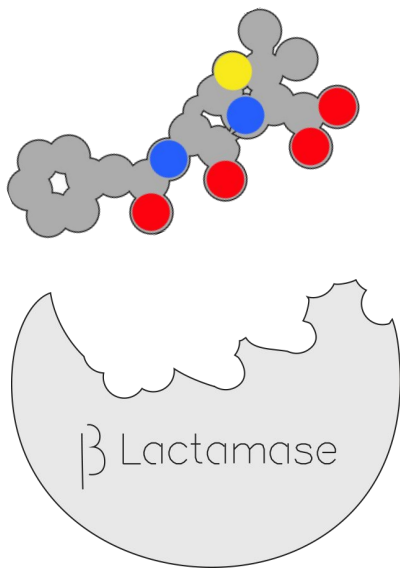
How might evolution respond to the presence of penicillin?

DISCUSS.
DECIDE.

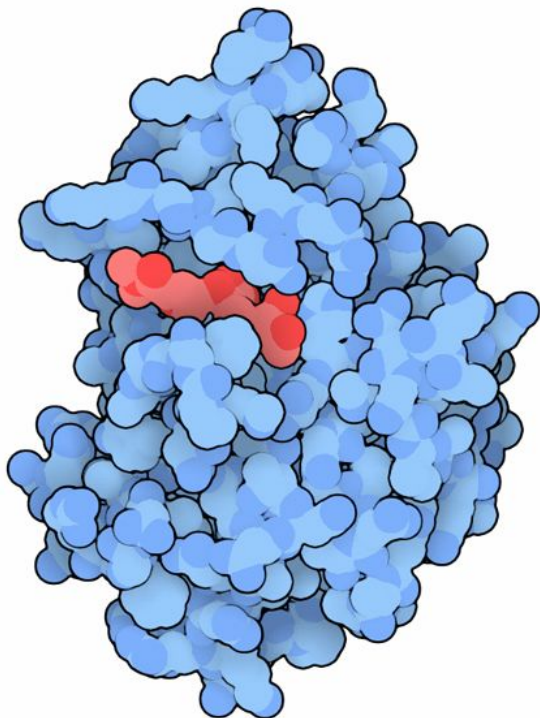


Binding Battles: The Evolutionary Tale of Enzymes and Antibiotics

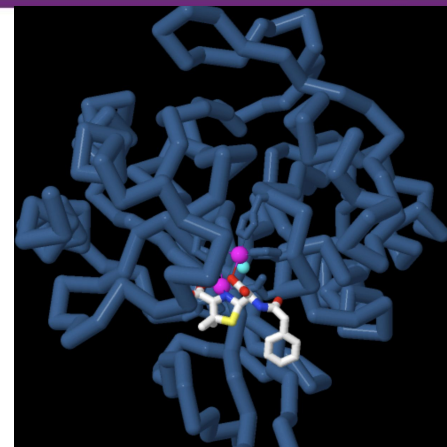
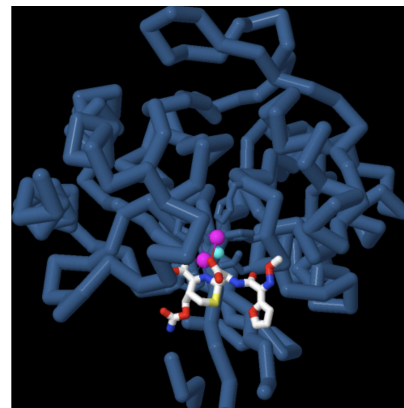
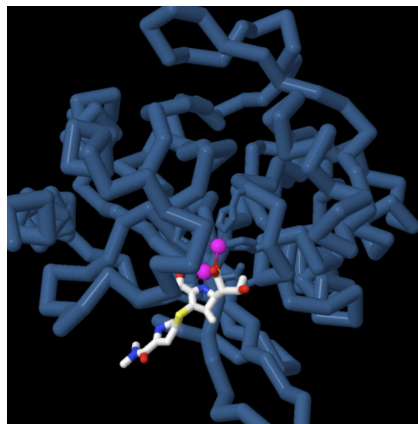
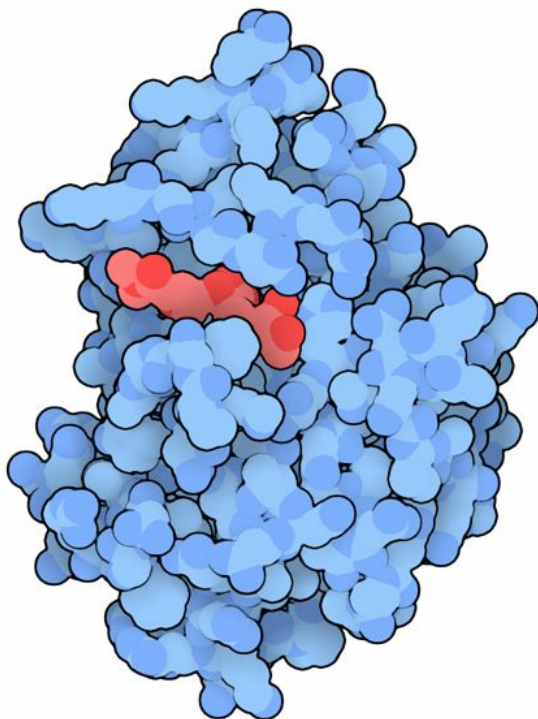
Evolutionary response 1:



Beta Lactamase: New Delhi Metalo variant

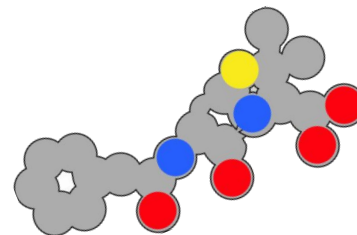
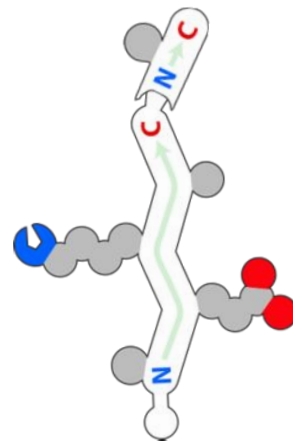
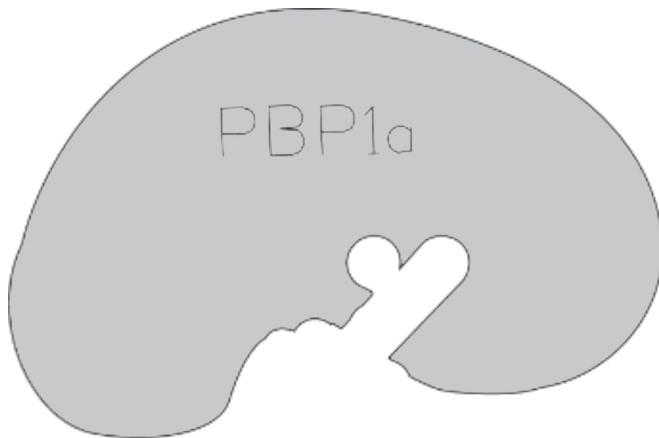


New Delhi metallo-variant- β -lactamase



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Evolutionary response 2: What happened here?



Time for questions!





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