3-D Molecular Designs
...where molecules become real ™

MSOE UNIVERSITY Center for BioMolecular Modeling

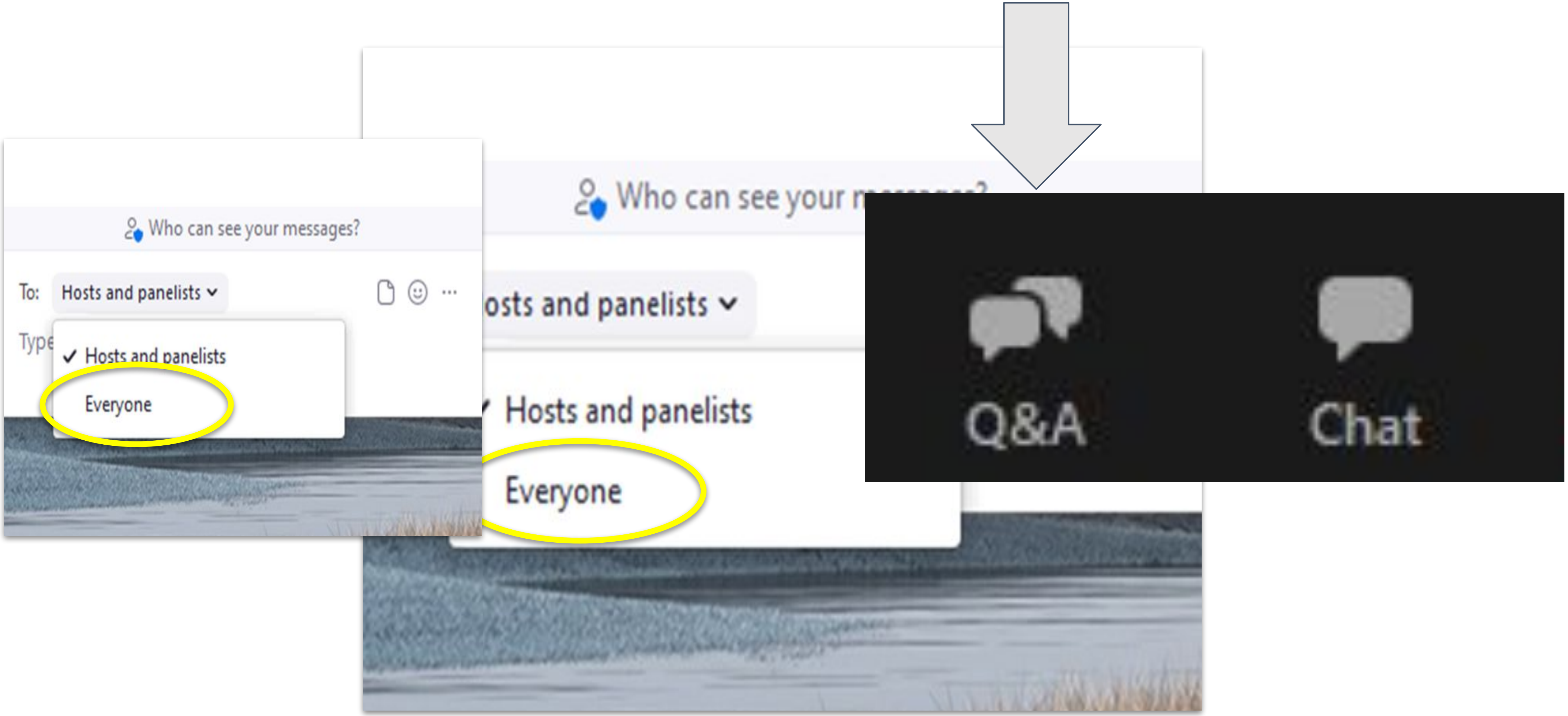
MODELING MARVELS
2022 EDUCATORS WEBINARS

- **RUTH HUTSON, MSSE**
  Demystifying Protein Dimensionality & Exploring Enzymes
- **TIM HERMAN, PhD**
  Protein Folding Problem Nevermore

PROTEINS WEBINAR
TUESDAY | MARCH 1 6:30 - 8 PM CST

Welcome to MAPS!

Modeling a Protein Story


Who can see your messages?
To: Hosts and panelists
Type
Hosts and panelists
Everyone
Who can see your
osts and panelists
Hosts and panelists
Everyone
Q&A
Chat

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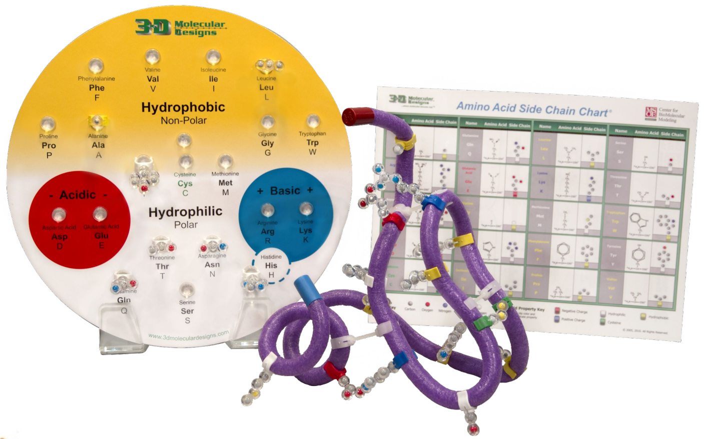
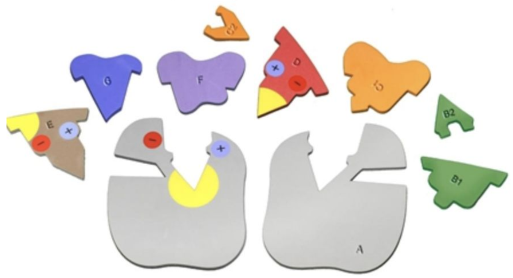
Protein Student Modeling Pack

Amino Acid Starter Kit©
Protein-Folding Kit





Enzymes in Action Kit

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PROTEINS WEBINAR

TUESDAY | MARCH 1 6:30 - 8 PM CST

PRESENTER:

RUTH HUTSON, MSSE

Blue Valley High School, Randolph, KS

Demystifying Protein Dimensionality & Exploring Enzymes

MODELING MARVELS
2022 EDUCATORS WEBINARS

Workshop Learning Goals

- Demonstrate how the unique properties of the 20 amino acids determine the final shape of the protein
- Demonstrate how modifications to the enzyme active site affect its reactivity
- Apply knowledge of enzymes to explain the results of the catalase lab

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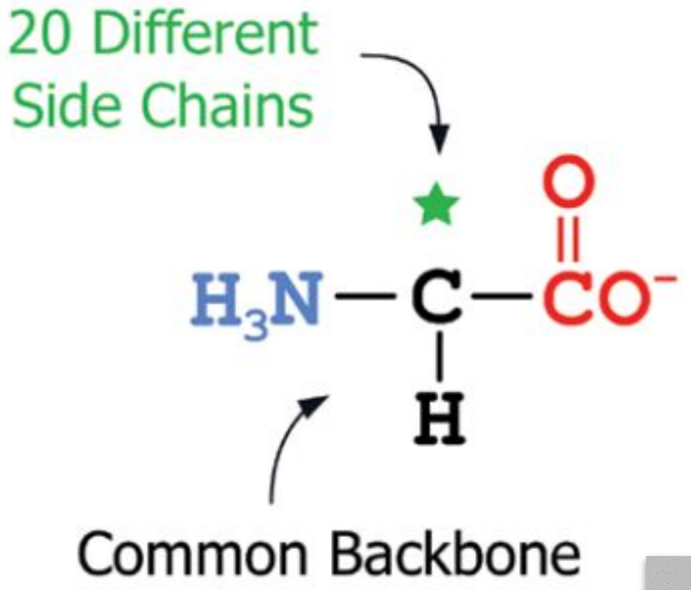
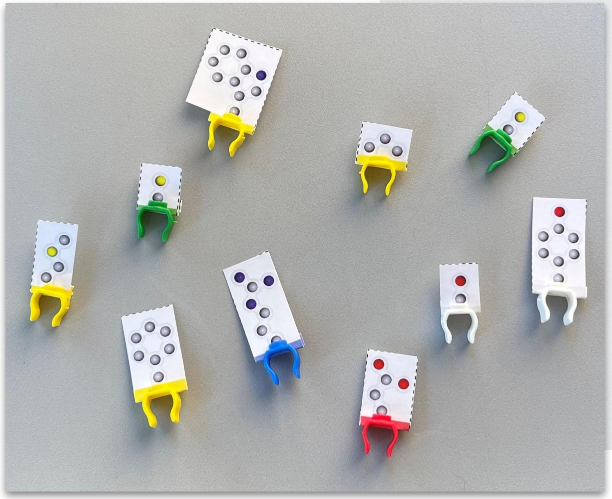

20 Different Side Chains
$H_3N-C-CO^-$
O
H
Common Backbone



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I notice	I wonder

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I notice	I wonder

WHAT PATTERNS DO YOU SEE AMONG THE SIDE CHAINS?

WHAT QUESTIONS DO YOU HAVE?

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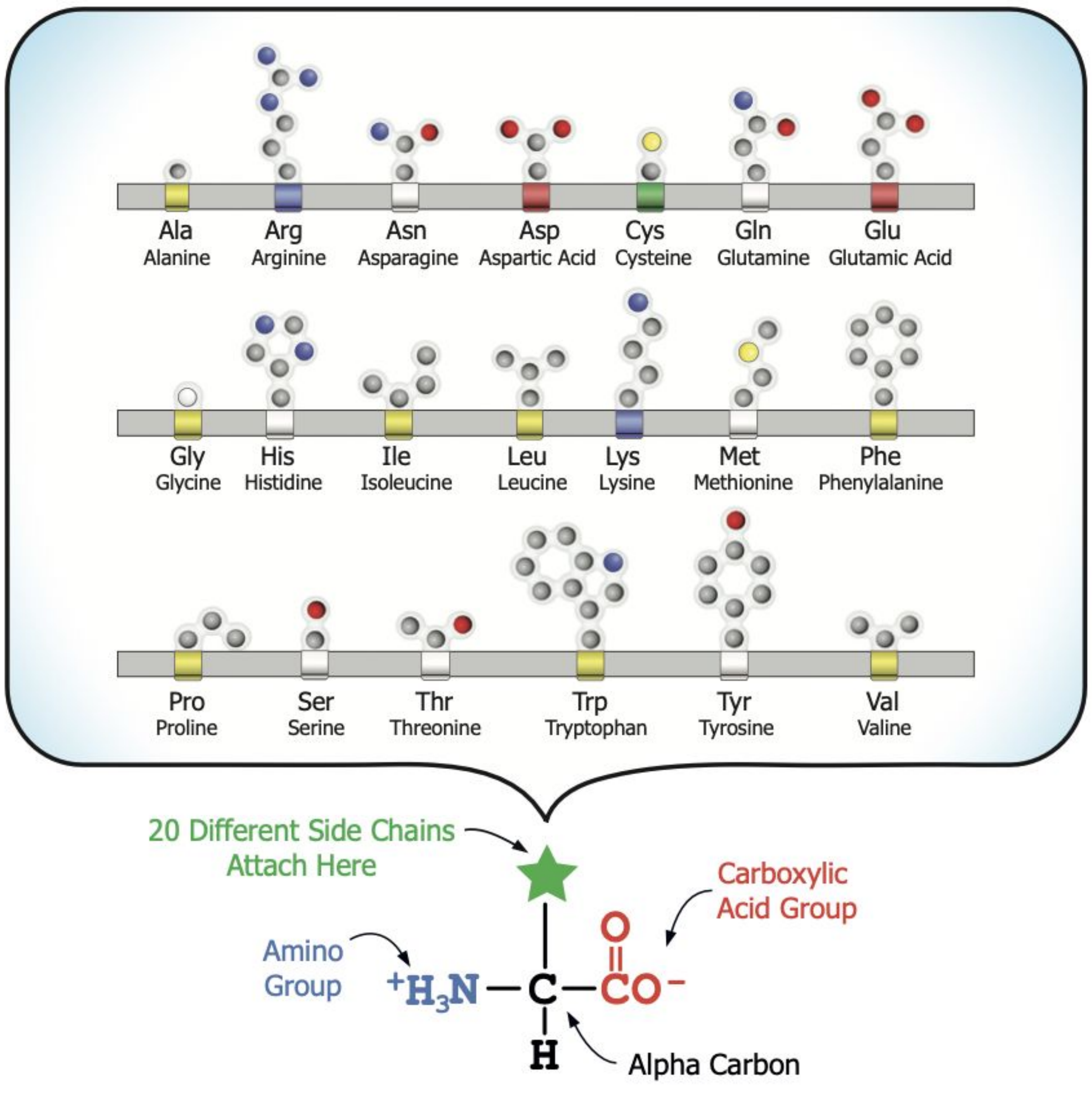
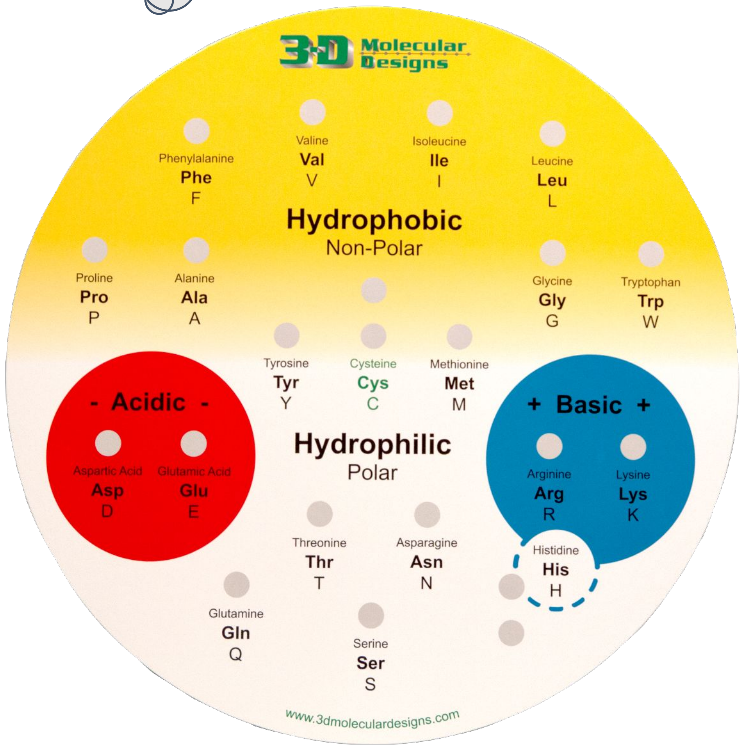
CHAT WATERFALL

Notice	Wonder
The clips are different colors.	Why are the clips different colors? Does it mean something?
Carbon is gray. Oxygen is red. Nitrogen is blue. Sulfur is yellow. Hydrogen is white.	Are all the atoms shown?
Some side chains are more complex than others.	



Ala
Alanine
Arg
Arginine
Asn
Asparagine
Asp
Aspartic Acid
Cys
Cysteine
Gln
Glutamine
Glu
Glutamic Acid
Gly
Glycine
His
Histidine
Ile
Isoleucine
Leu
Leucine
Lys
Lysine
Met
Methionine
Phe
Phenylalanine
Pro
Proline
Ser
Serine
Thr
Threonine
Trp
Tryptophan
Tyr
Tyrosine
Val
Valine
20 Different Side Chains Attach Here
Carboxylic Acid Group
Amino Group
^+H_3N
C
CO^-
O
H
Alpha Carbon

WHAT ARE THE DIFFERENCES BETWEEN THE HYDROPHOBIC AMINO ACIDS AND THE HYDROPHILIC AMINO ACIDS?



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Some side chains are more complex than others.	
Hydrophobic side chain have more carbon; if they have other atoms, ~~they~~ are less hydrophobic	How does this repel water?
Acidic side chains contain 2 oxygen atoms	What purpose?
Basic side chains contain nitrogen atoms	What purpose?
	Why two cysteines? Why two histidines?
Non-polar / polar is a spectrum. Some things are more polar than other things	

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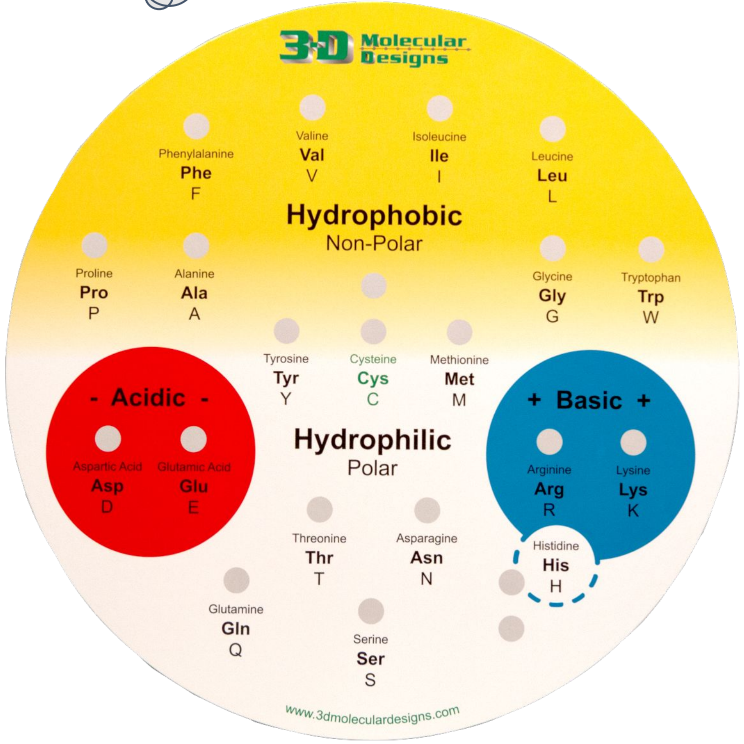

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CHAT WATERFALL

WHAT CAUSES PROTEINS TO FOLD INTO THEIR 3-D SHAPES? MAKE A PREDICTION

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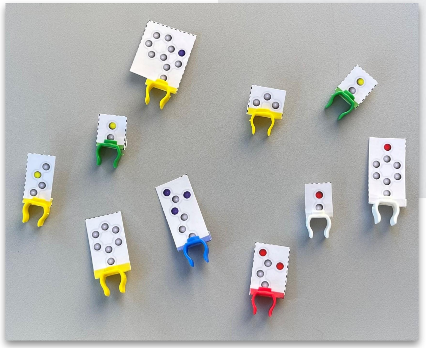

KEY

Hydrophobic Side Chains are Yellow

Hydrophilic Side Chains are White

Acidic Side Chains are Red

Basic Side Chains are Blue

Cysteine Side Chains are Green

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KEY

Hydrophobic Side Chains are **Yellow**

Hydrophilic Side Chains are **White**

Acidic Side Chains are **Red**

Basic Side Chains are **Blue**

Cysteine Side Chains are **Green**

SIX HYDROPHOBIC

THREE HYDROPHILIC

TWO ACIDIC

TWO BASIC

TWO CYSTEINE

A TOTAL OF FIFTEEN SIDE CHAINS

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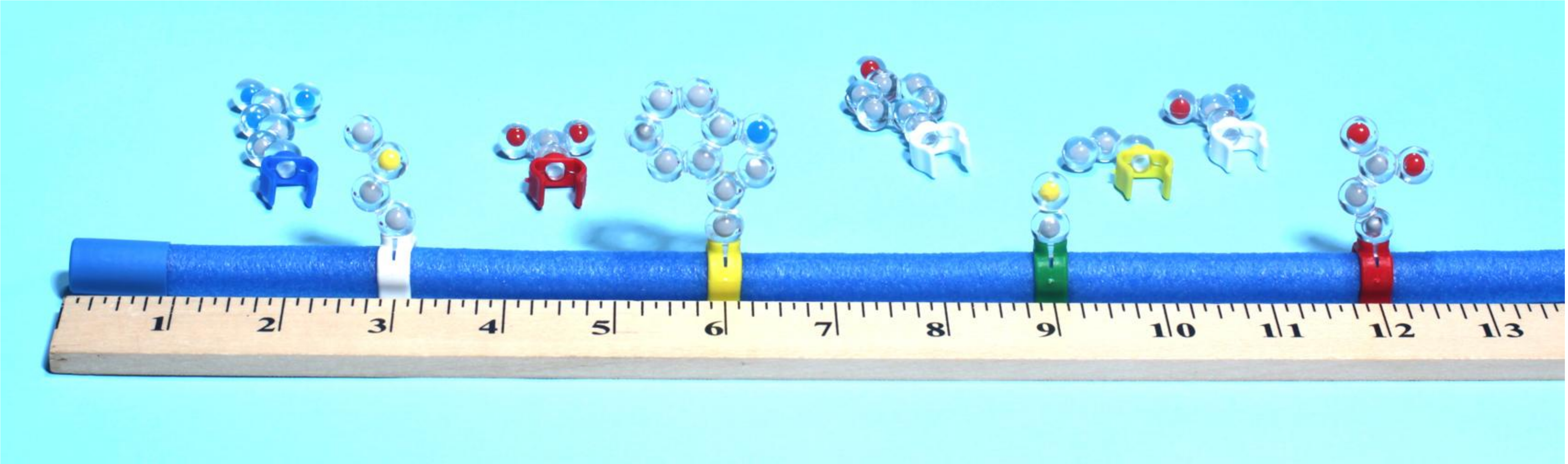
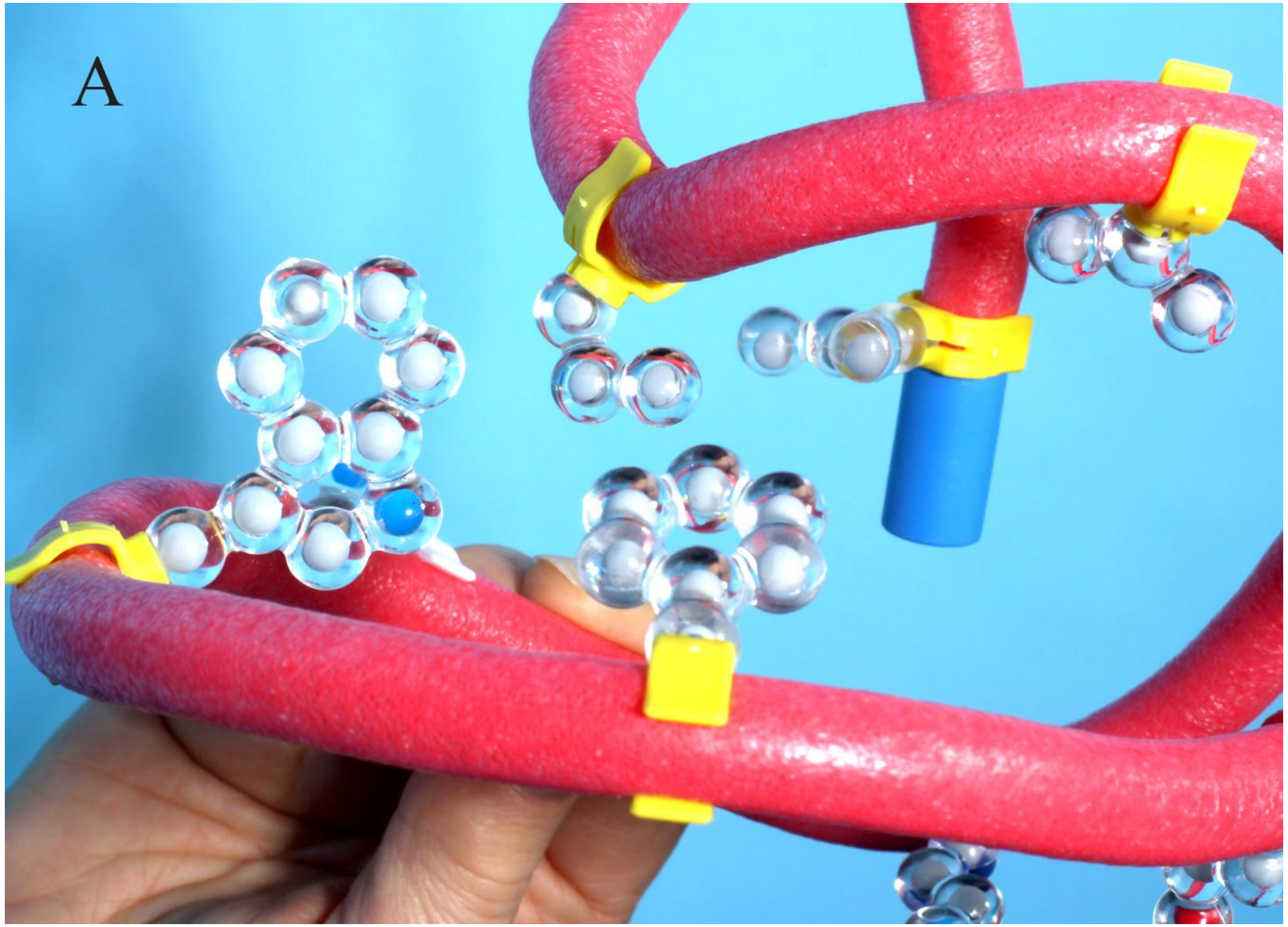
IN ANY ORDER ARRANGE YOUR AMINO ACIDS EQUIDISTANT FROM EACH OTHER.

YOU HAVE MADE A POLYPEPTIDE.



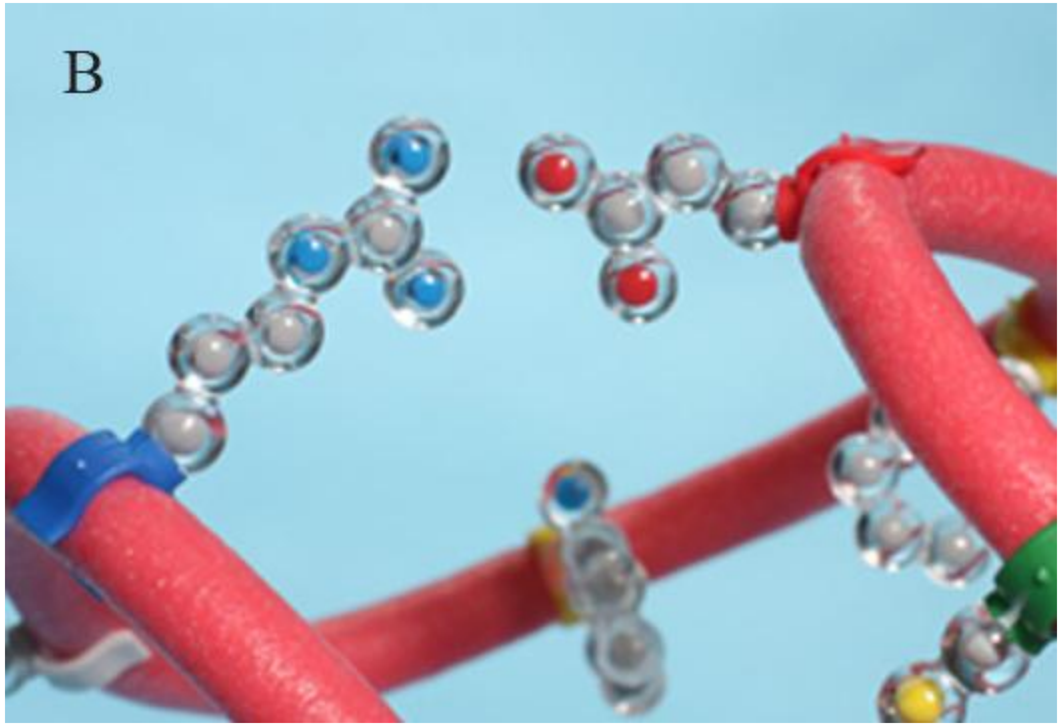
LET'S "FOLD" IT INTO A PROTEIN

ROTATE THE HYDROPHOBIC AMINO ACIDS TO THE INSIDE



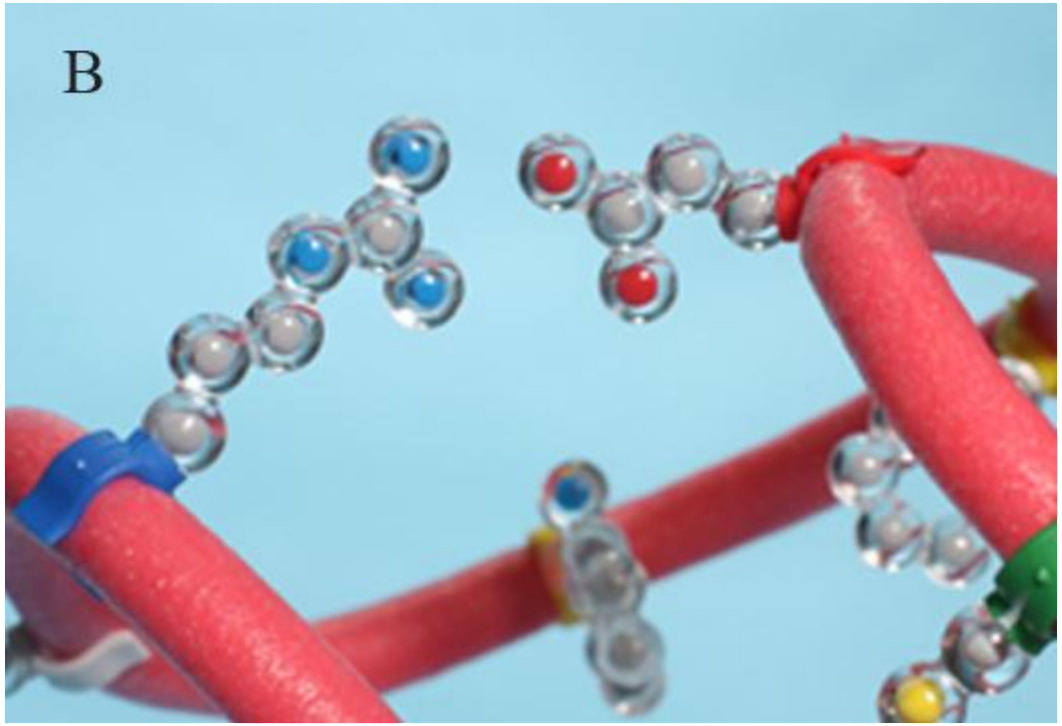
CONTINUE "FOLDING"

BRING THE ACIDIC AND BASIC SIDE CHAINS UNTIL THEY ARE TWO CM FROM EACH OTHER



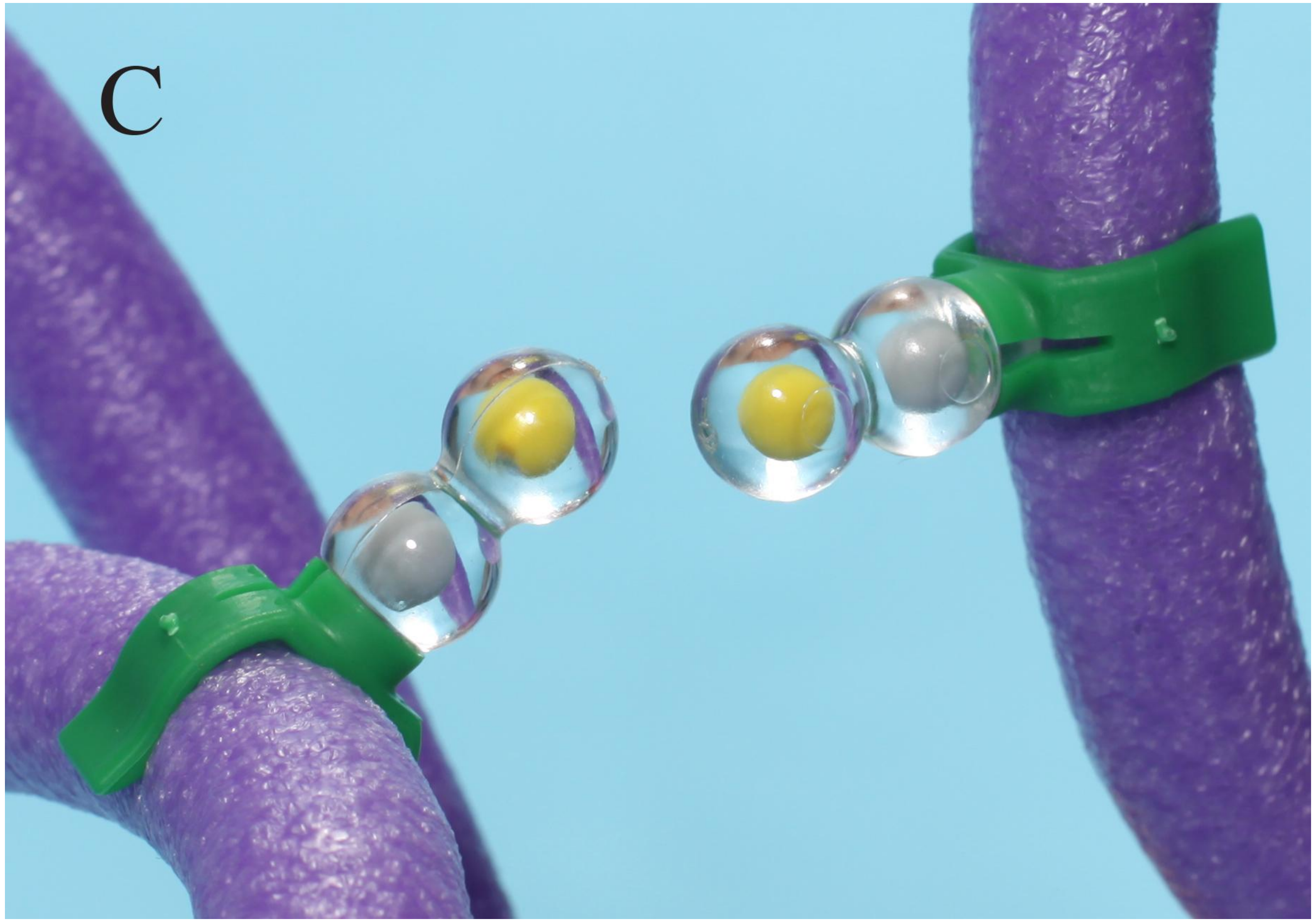
MAKE SURE THAT YOU ALSO ROTATE ANY HYDROPHOBIC SIDE CHAINS THAT MOVE OUT OF PLACE.

THROUGHOUT THIS WHOLE EXERCISE FIND A SHAPE IN WHICH ALL THE PROPERTIES APPLY.



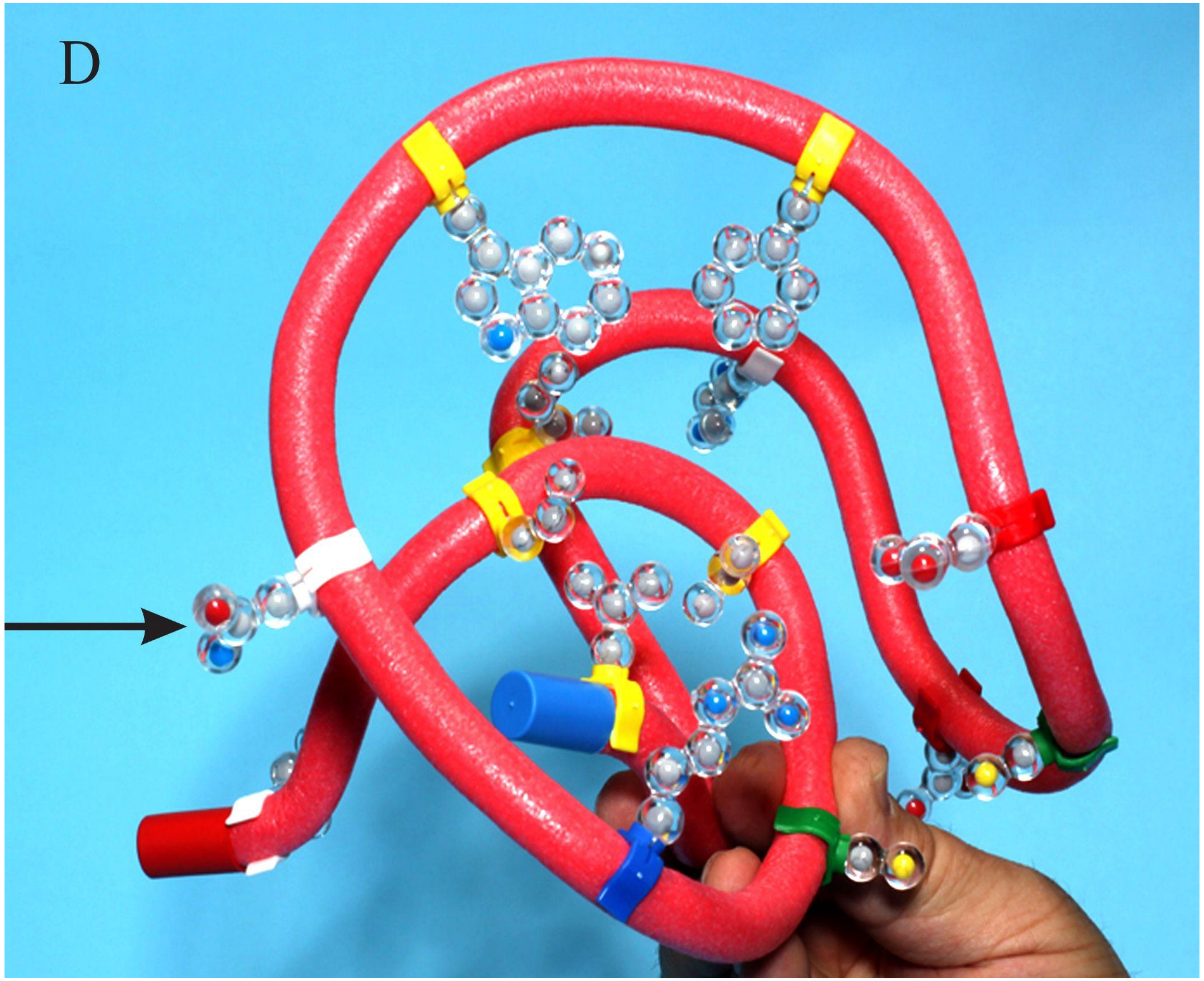
CONTINUE "FOLDING"

POSITION THE CYSTEINES SO THEY ARE OPPOSITE EACH OTHER.

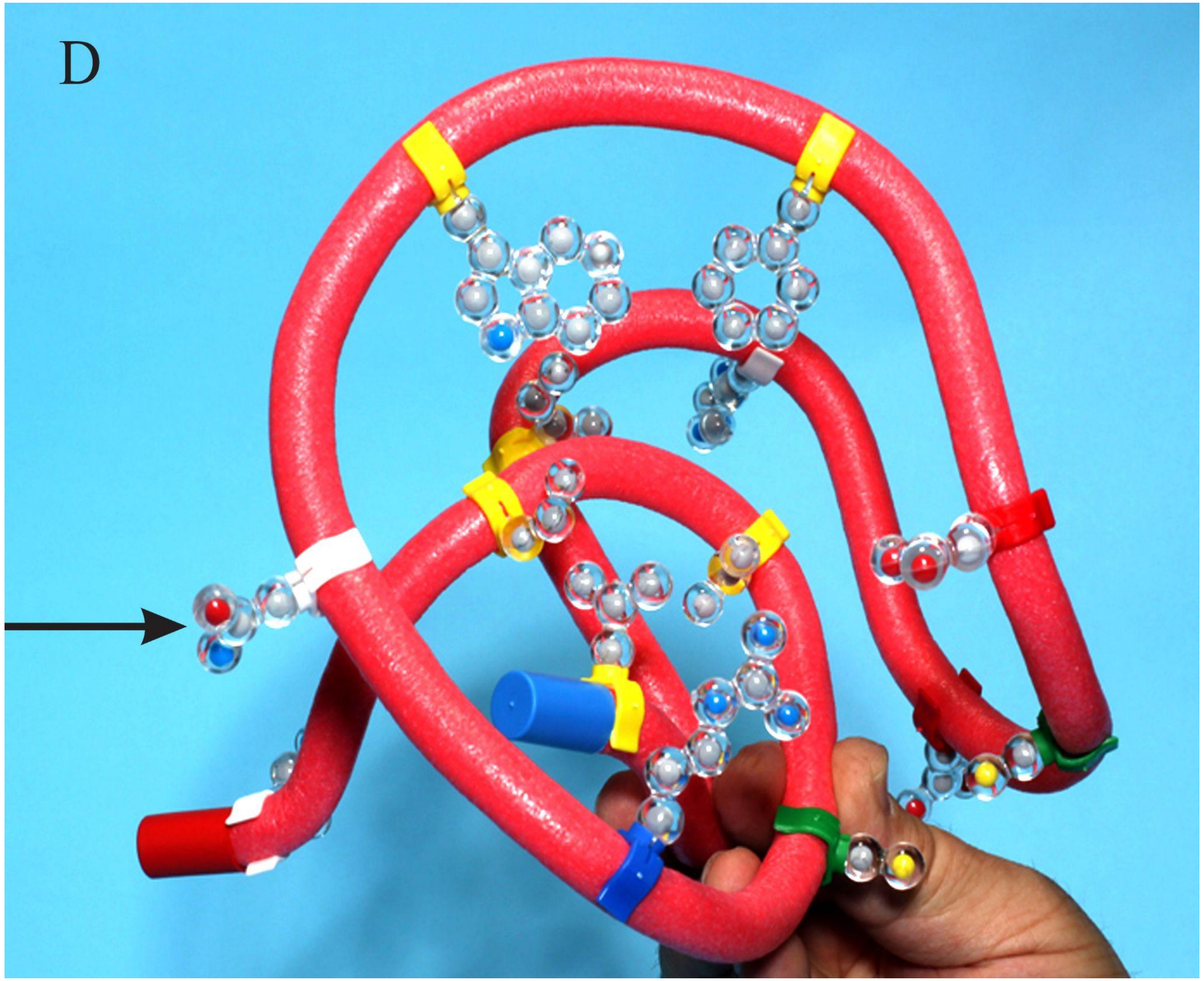


CONTINUE “FOLDING”

FINALLY ROTATE THE HYDROPHILIC SIDE CHAINS SO THEY ARE ON THE OUTER SURFACE



THE FINAL SHAPE OF THE PROTEIN IS CALLED THE TERTIARY STRUCTURE



WHY DIDN'T YOUR PROTEINS ALL LOOK THE SAME?

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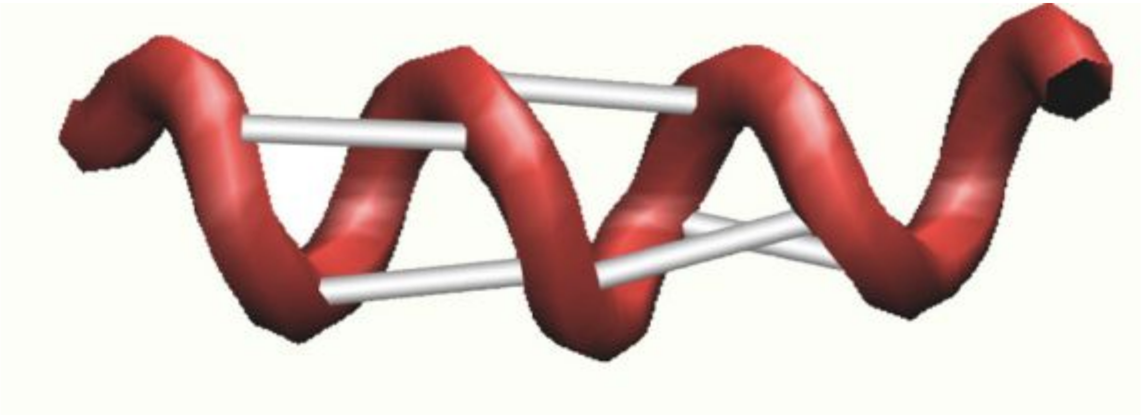
CHAT WATERFALL

THE IMPORTANCE OF SECONDARY STRUCTURE

ALPHA HELIX



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THE IMPORTANCE OF SECONDARY STRUCTURE

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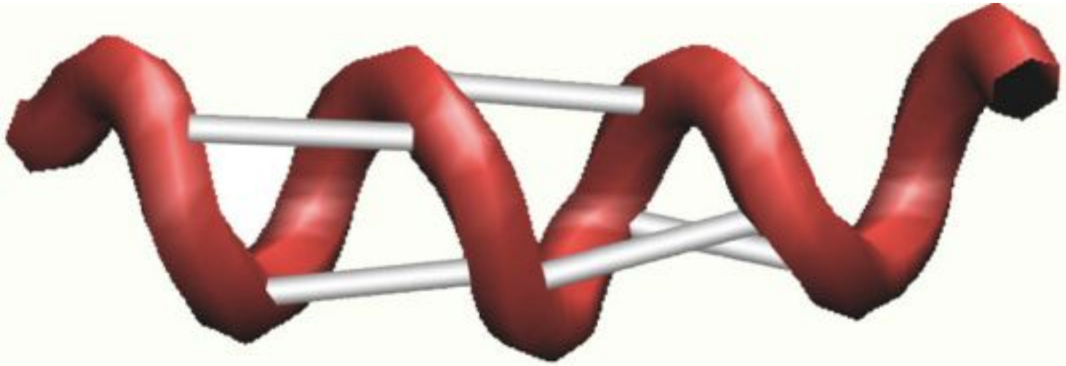
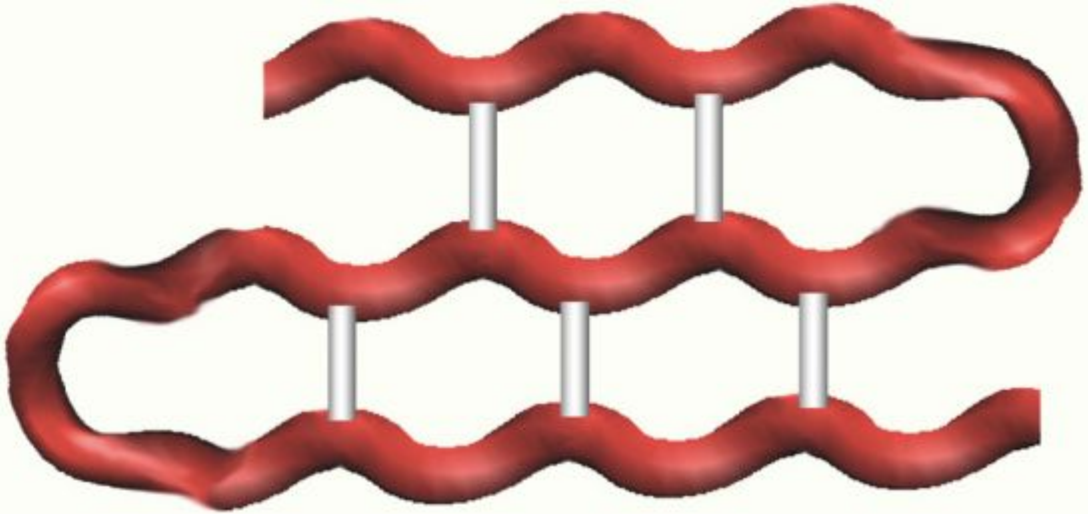


BETA SHEET



THE IMPORTANCE OF SECONDARY STRUCTURE

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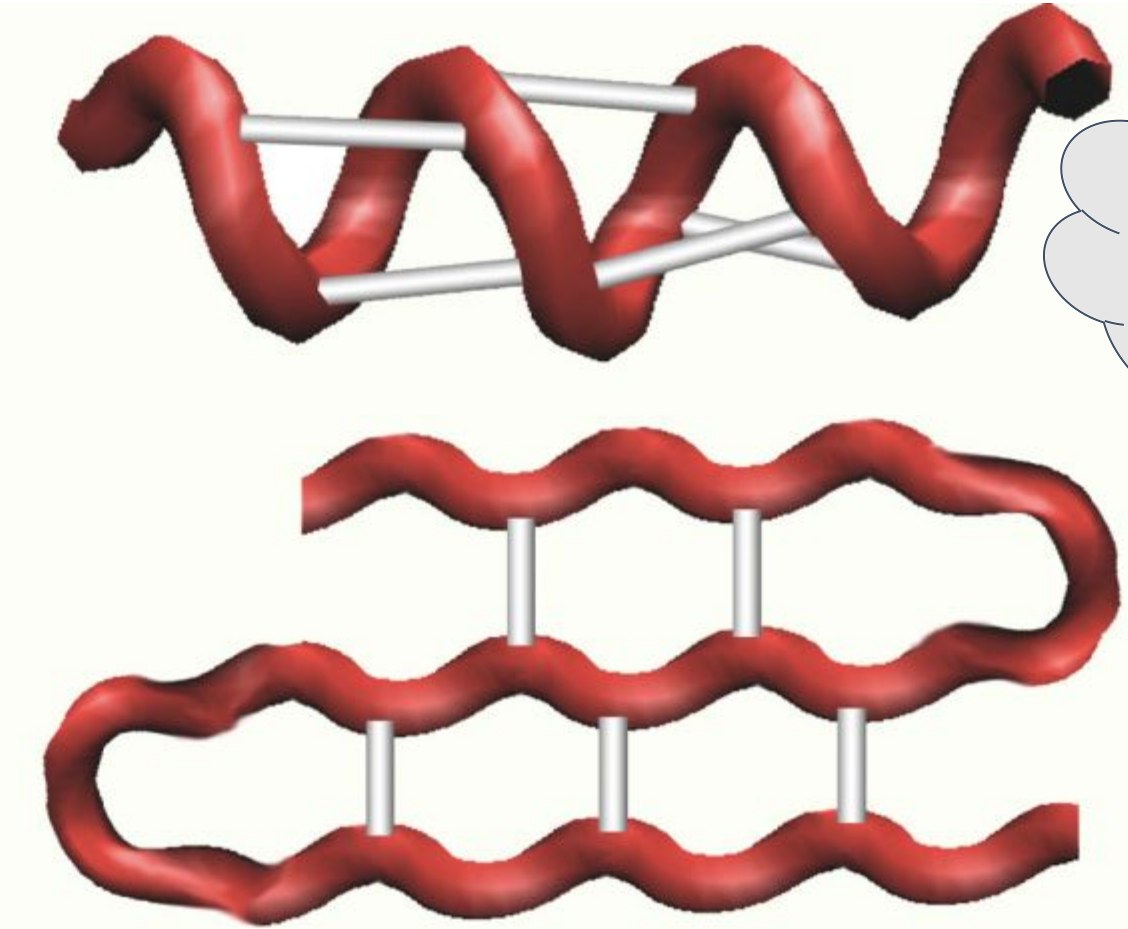
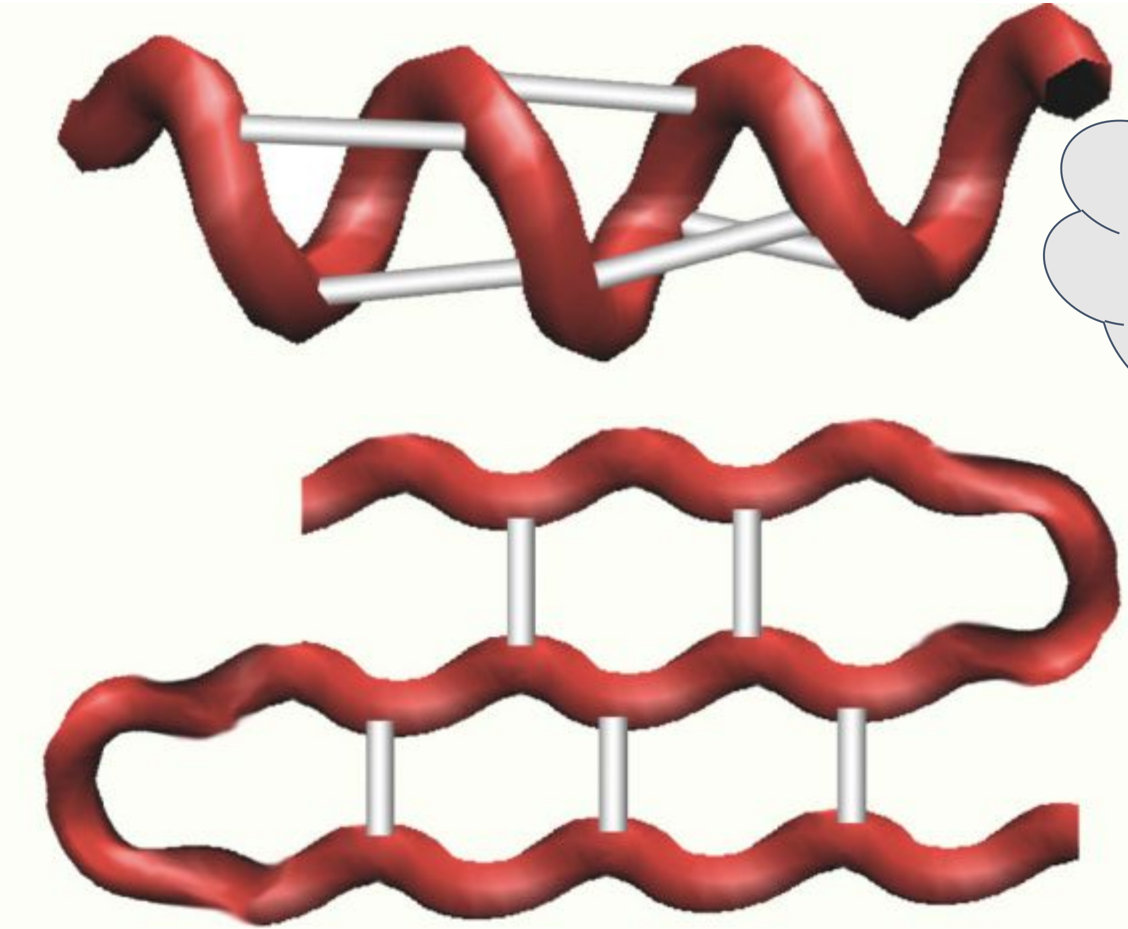


BETA SHEET

HOW DO SECONDARY STRUCTURES STABILIZE A PROTEIN?

THE IMPORTANCE OF SECONDARY STRUCTURE

ALPHA HELIX



BETA SHEET

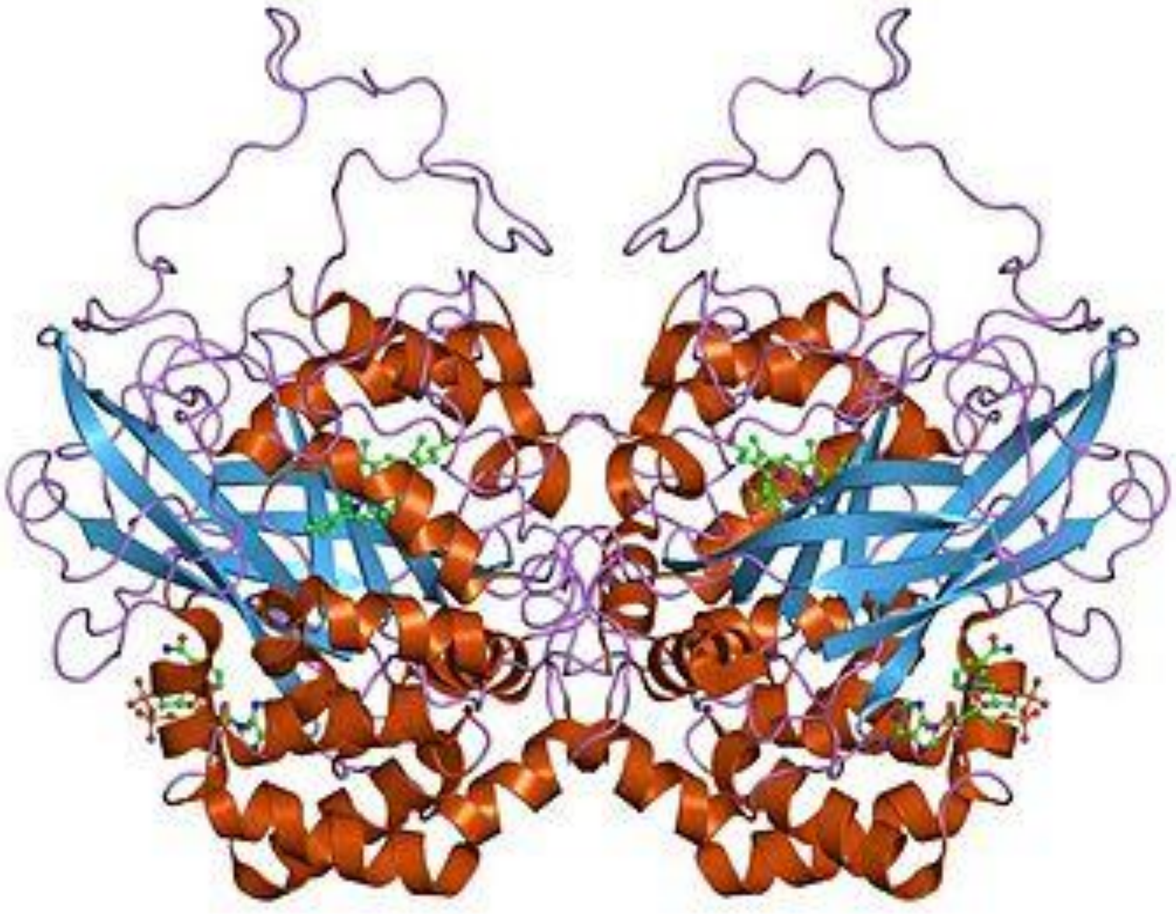
HOW DO SECONDARY STRUCTURES STABILIZE A PROTEIN?

CHAT WATERFALL

WHAT ABOUT QUATERNARY STRUCTURE?

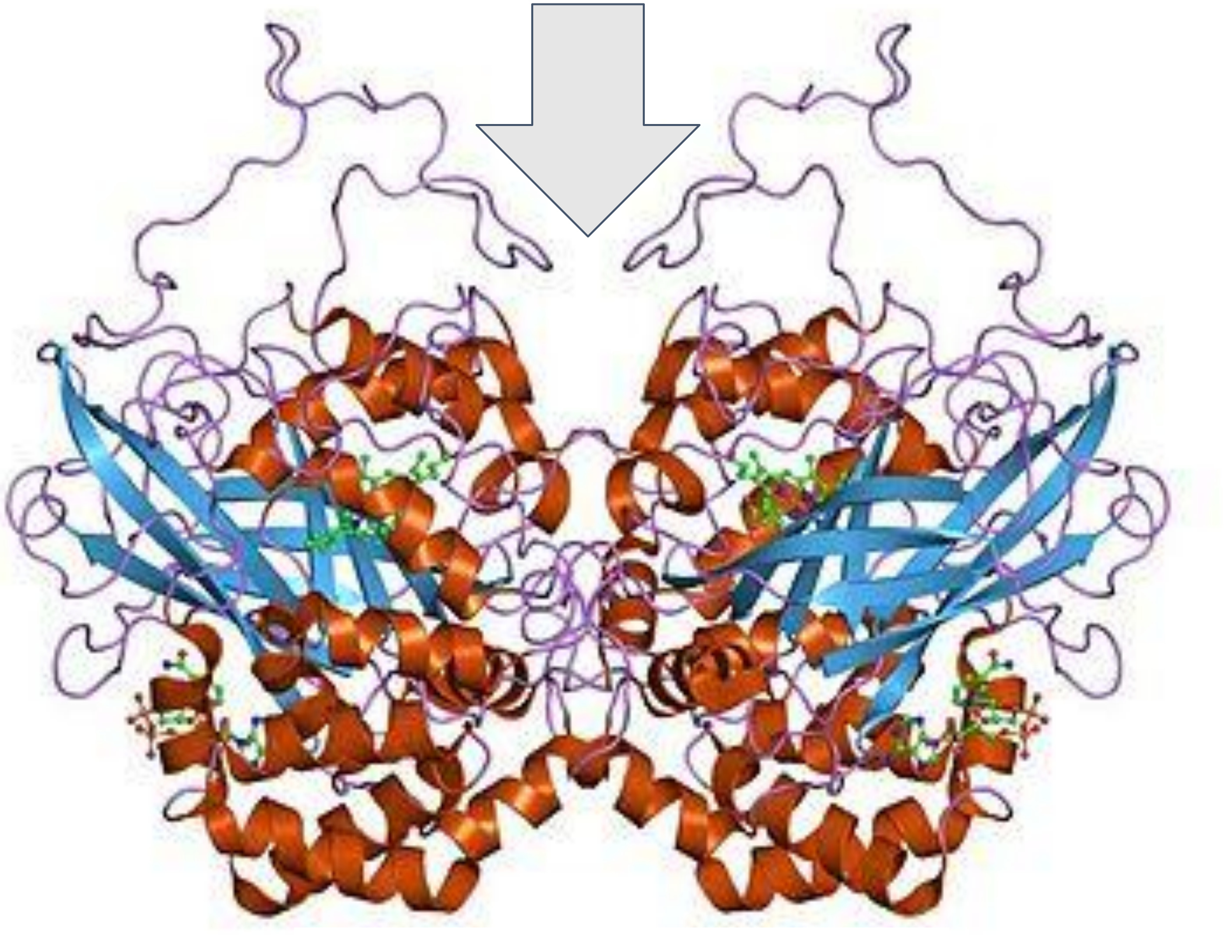
Catalase

Case study and a multi-day wet lab that allows students to explore and manipulate enzyme actions



Catalase Lab

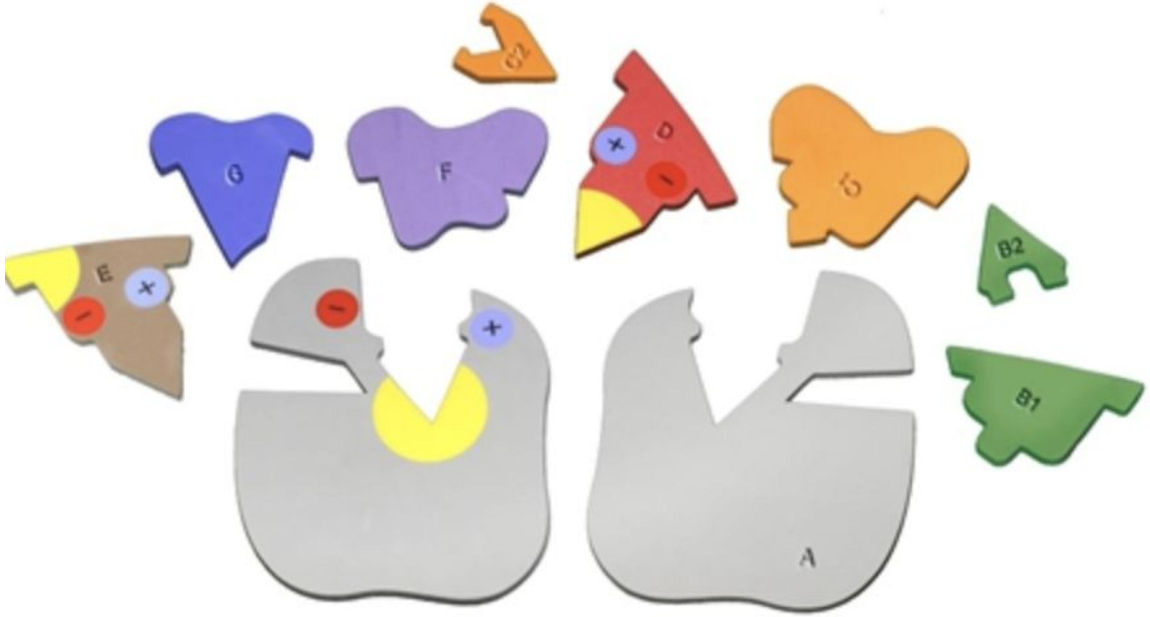
Case study and a multi-day wet lab that allows students to explore and manipulate enzyme actions



$$2H_2O_2 \rightarrow 2H_2O + O_2$$

Enzymes in Action - Student Modeling Pack

Enzymes in Action Kit



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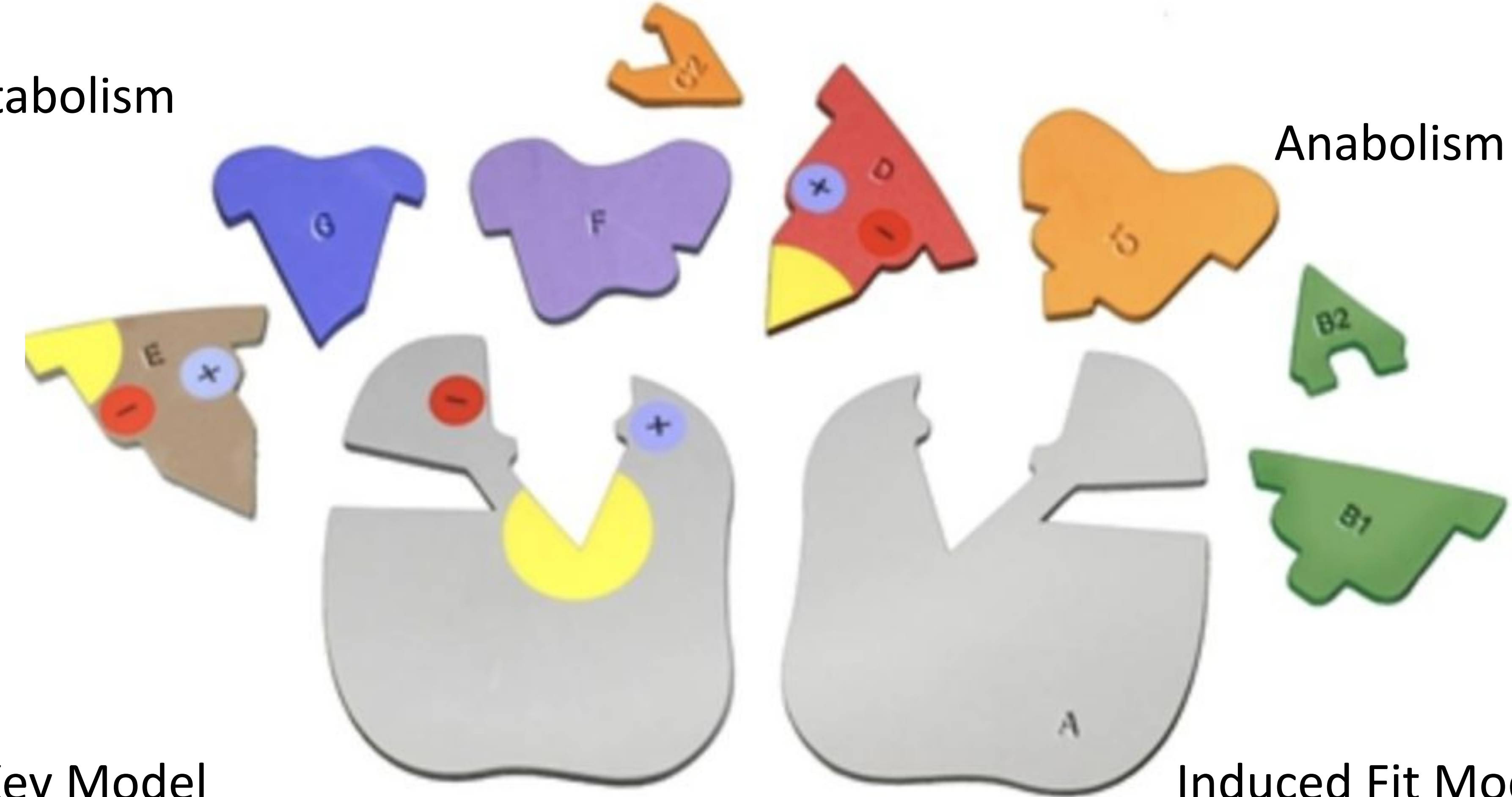
Catabolism

Anabolism

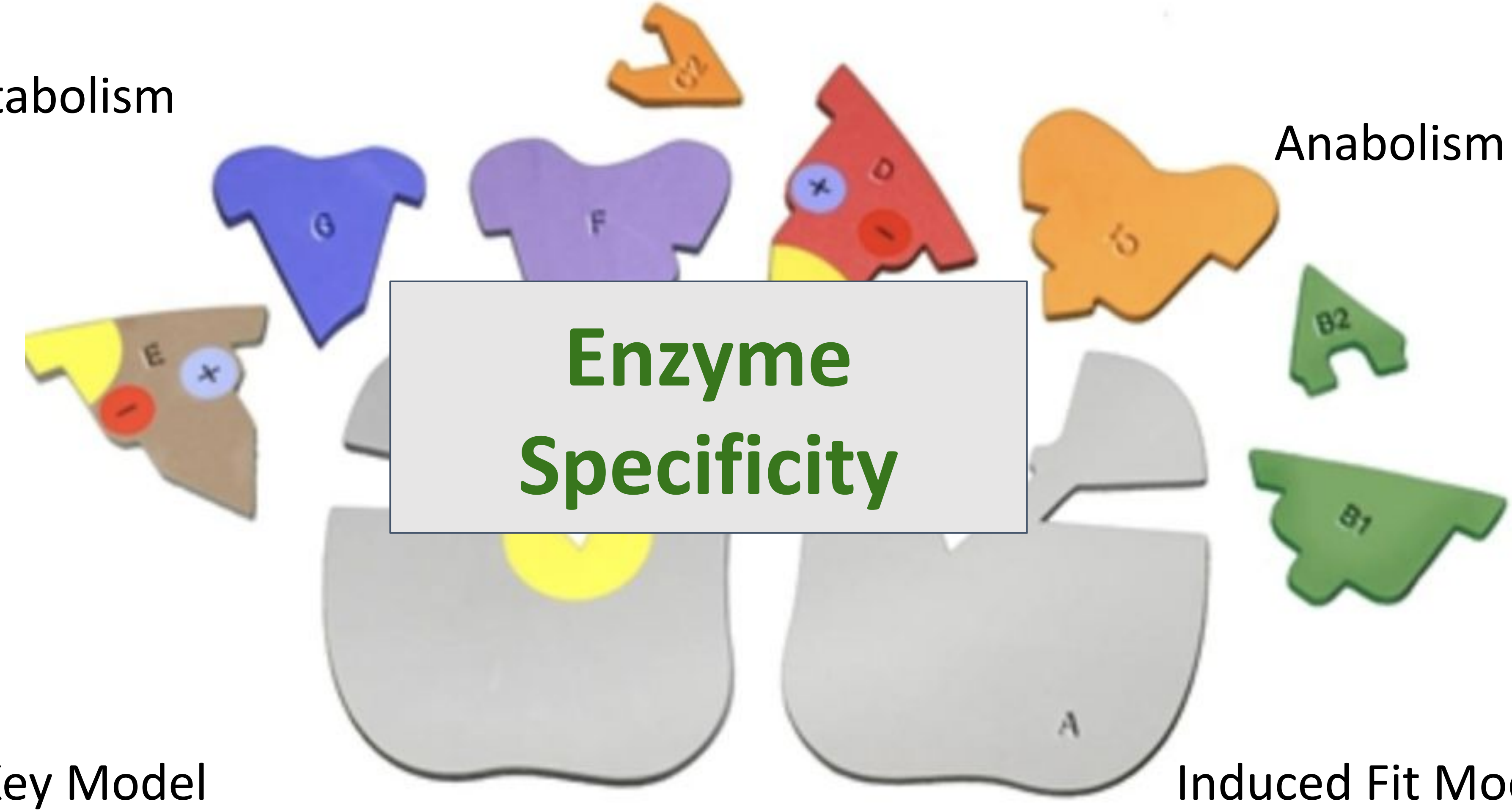


Lock and Key Model

Induced Fit Model

Catabolism

Anabolism



Enzyme Specificity

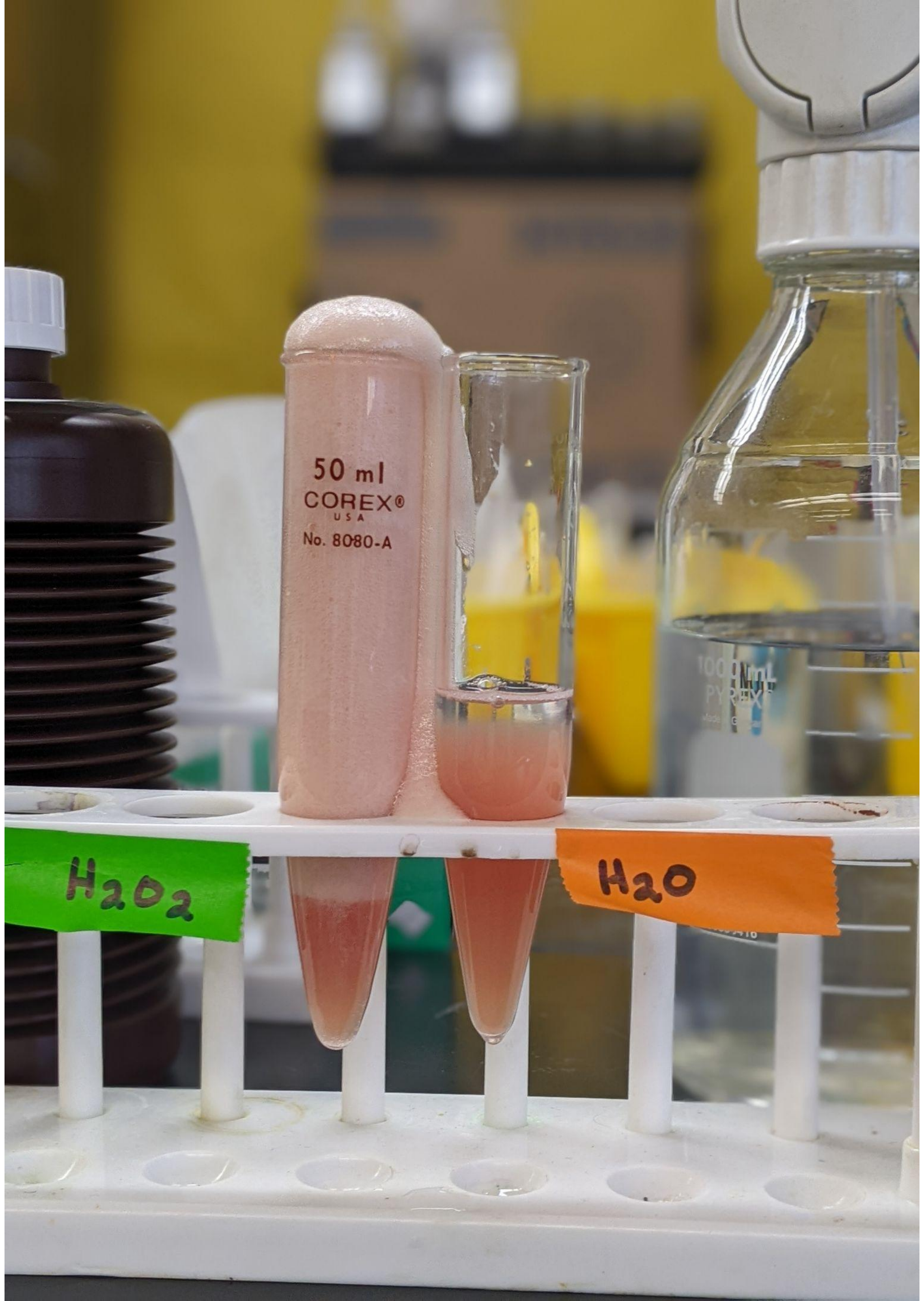
Lock and Key Model

Induced Fit Model

HYDROGEN PEROXIDE

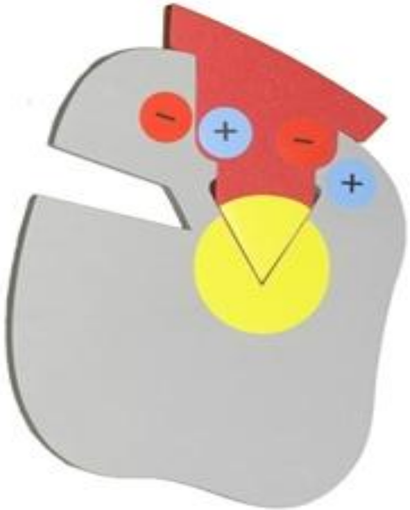
WATER

HYDROGEN PEROXIDE



WATER

HYDROGEN PEROXIDE



WATER

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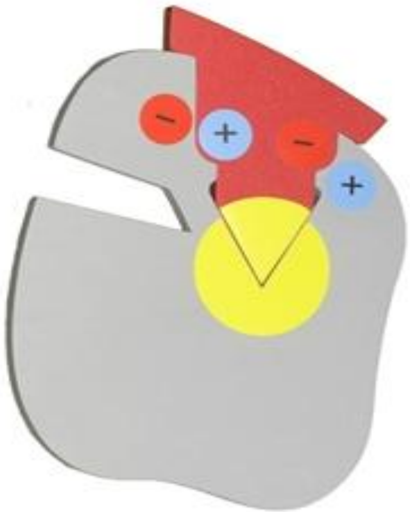
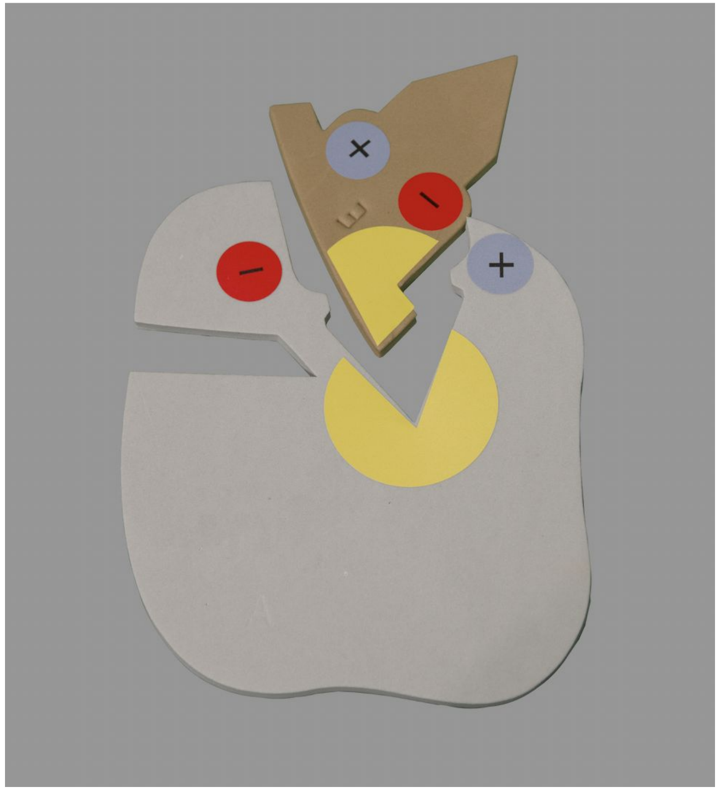
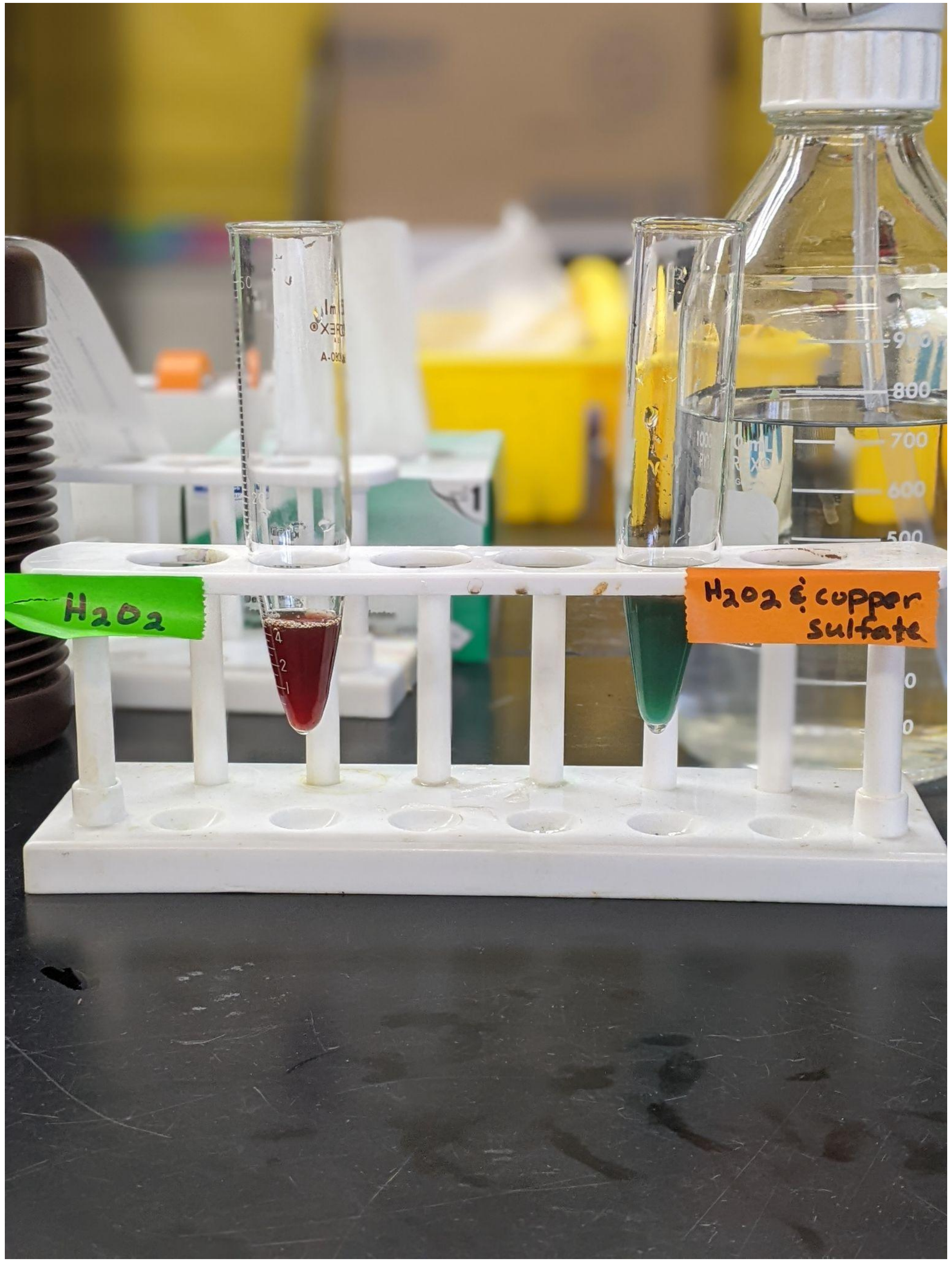


WATER



Competitive Inhibition

NO TREATMENT



COPPER SULFATE

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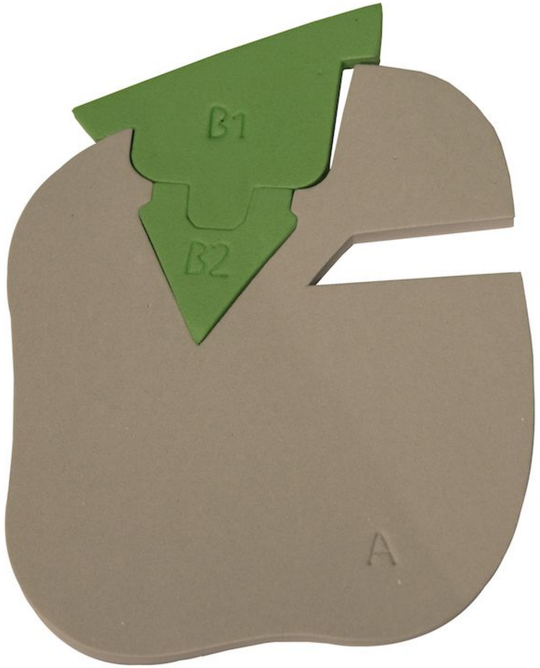

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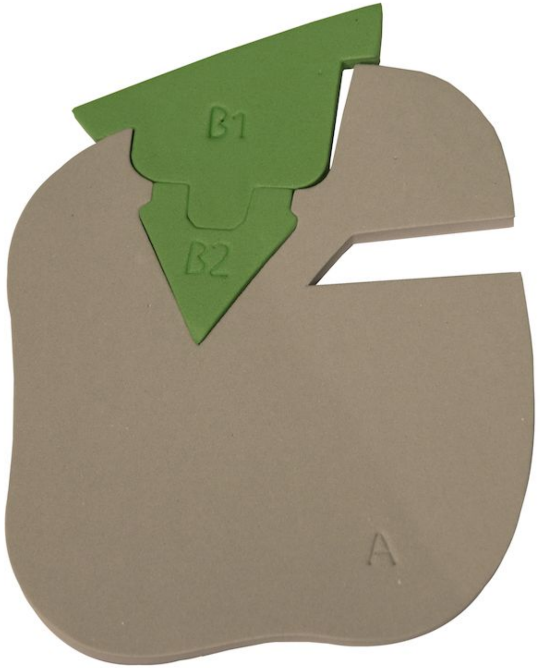

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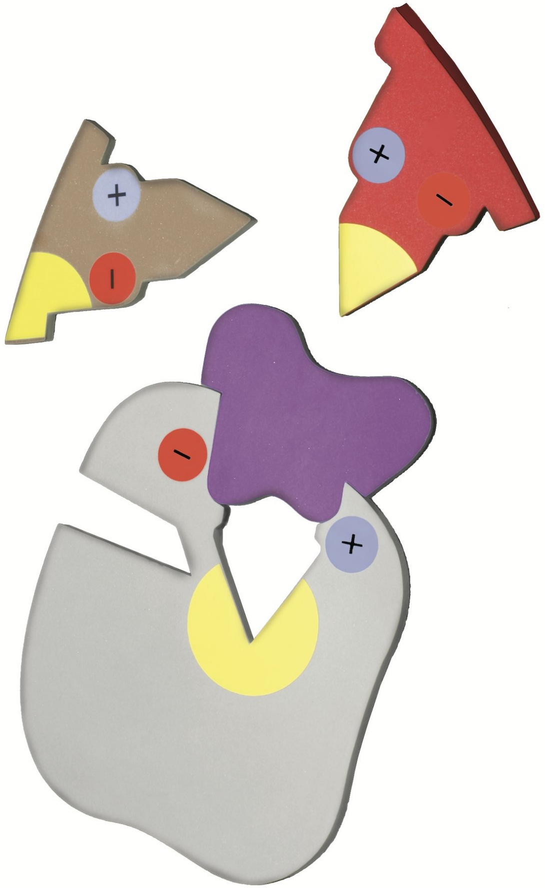
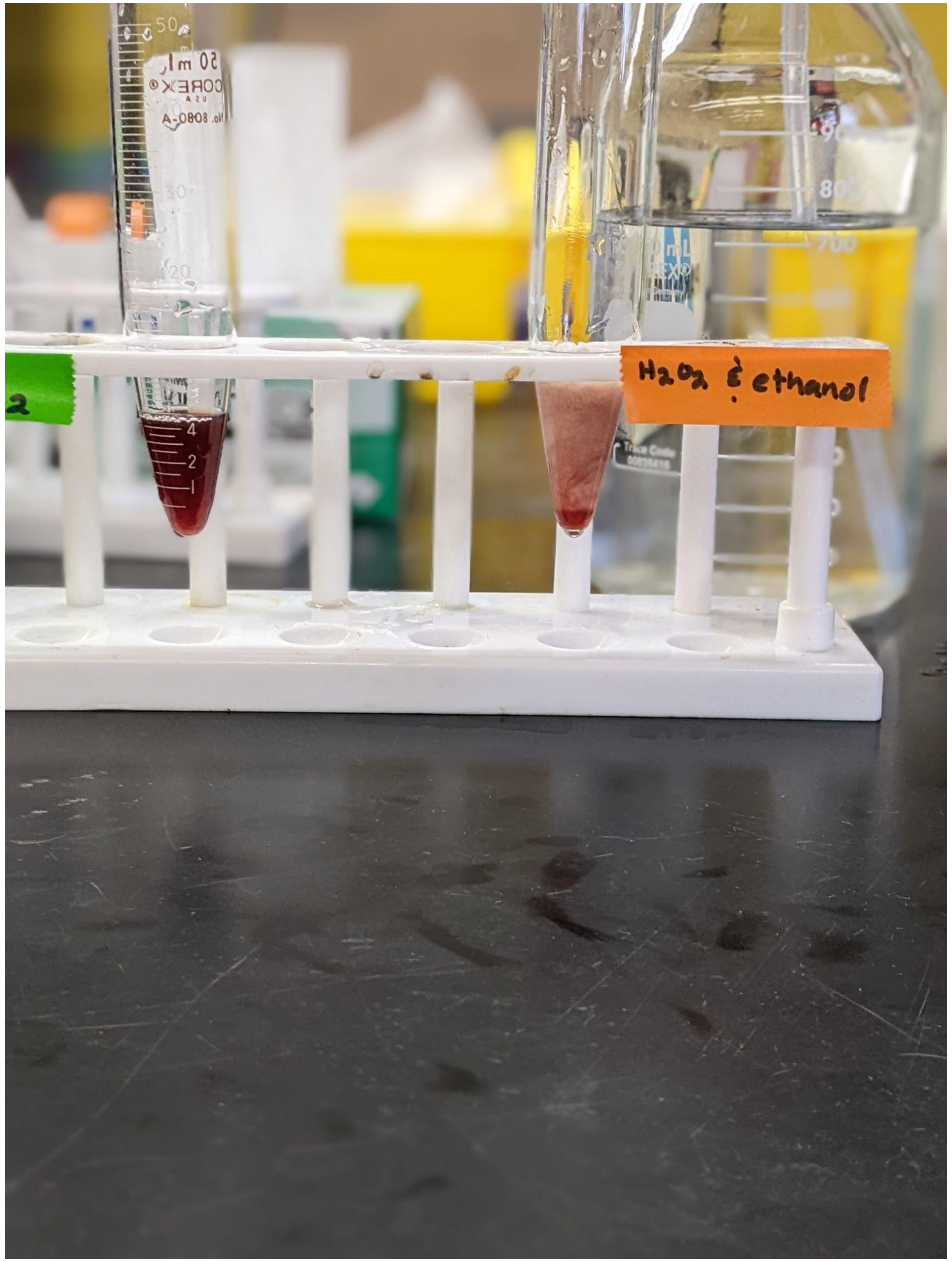


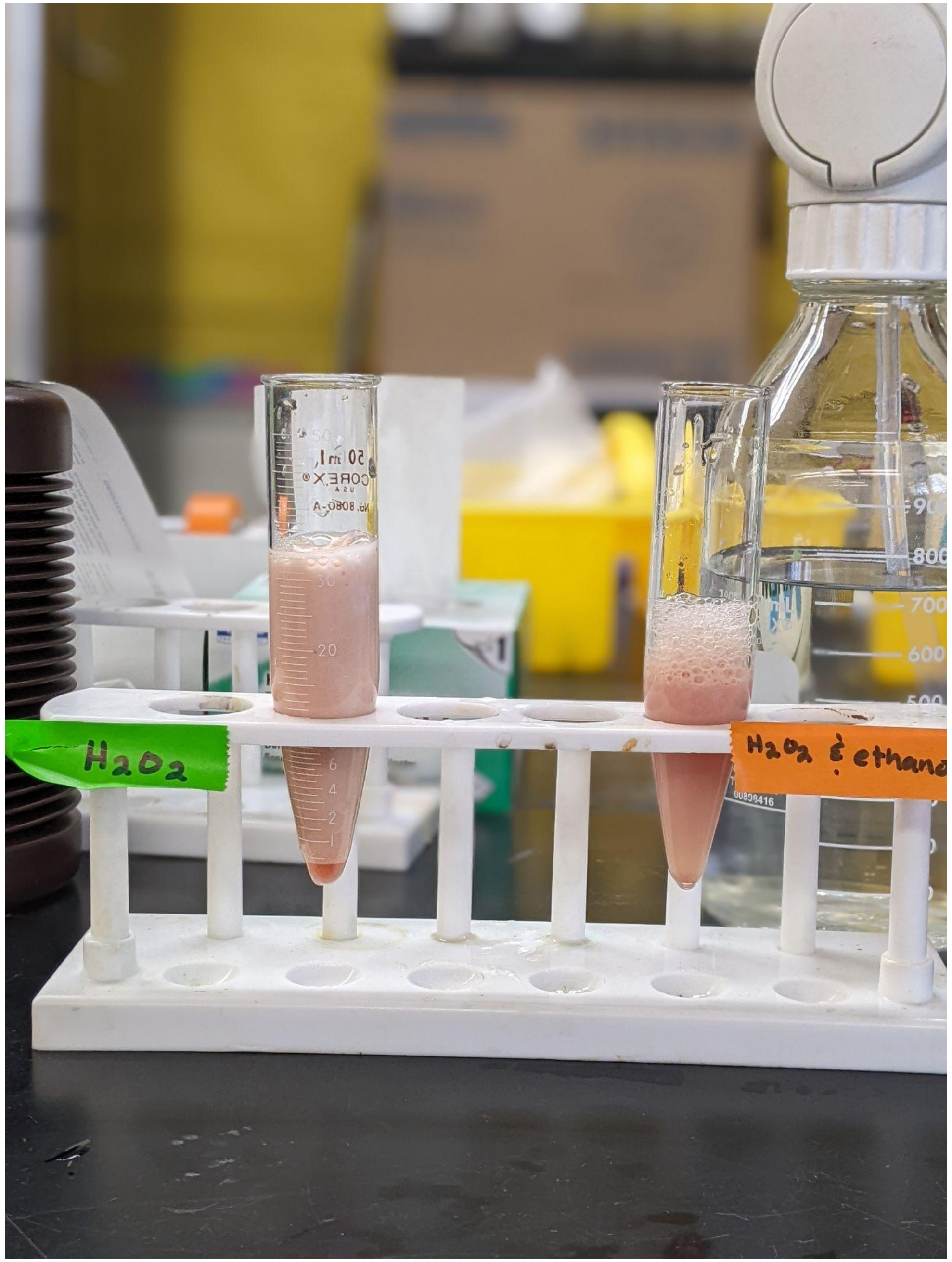
Non-competitive Inhibition

NO TREATMENT



ETHANOL
or
EDTA

NO TREATMENT



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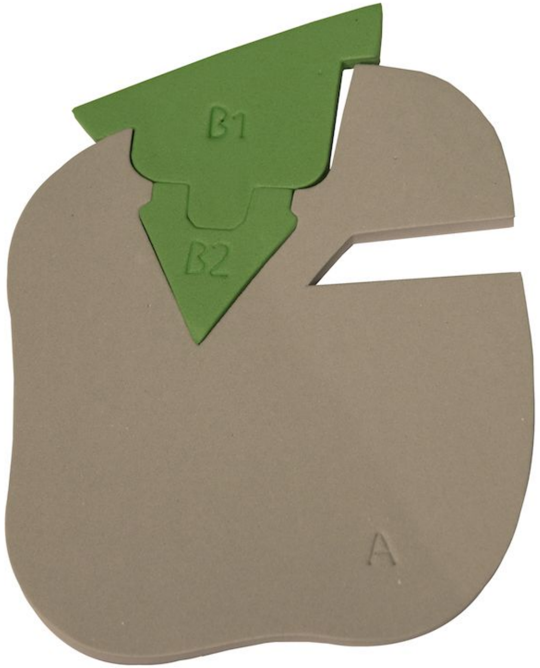

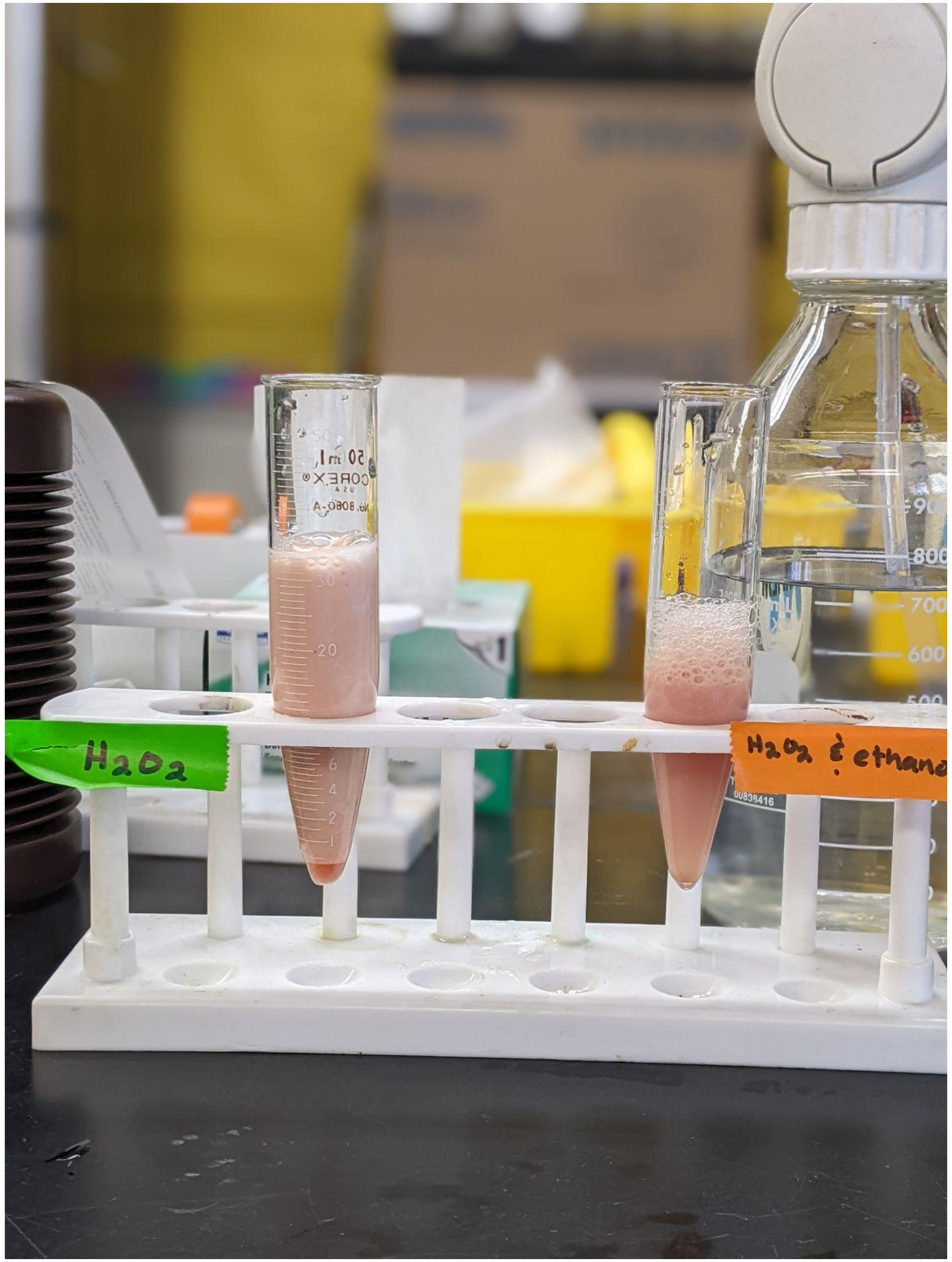

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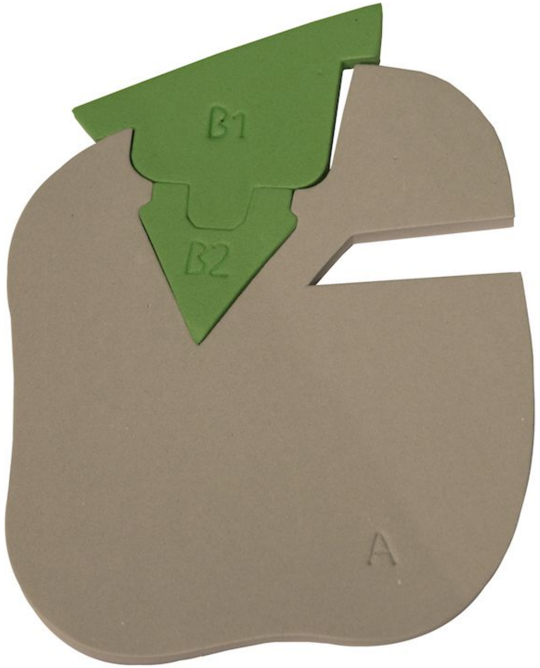

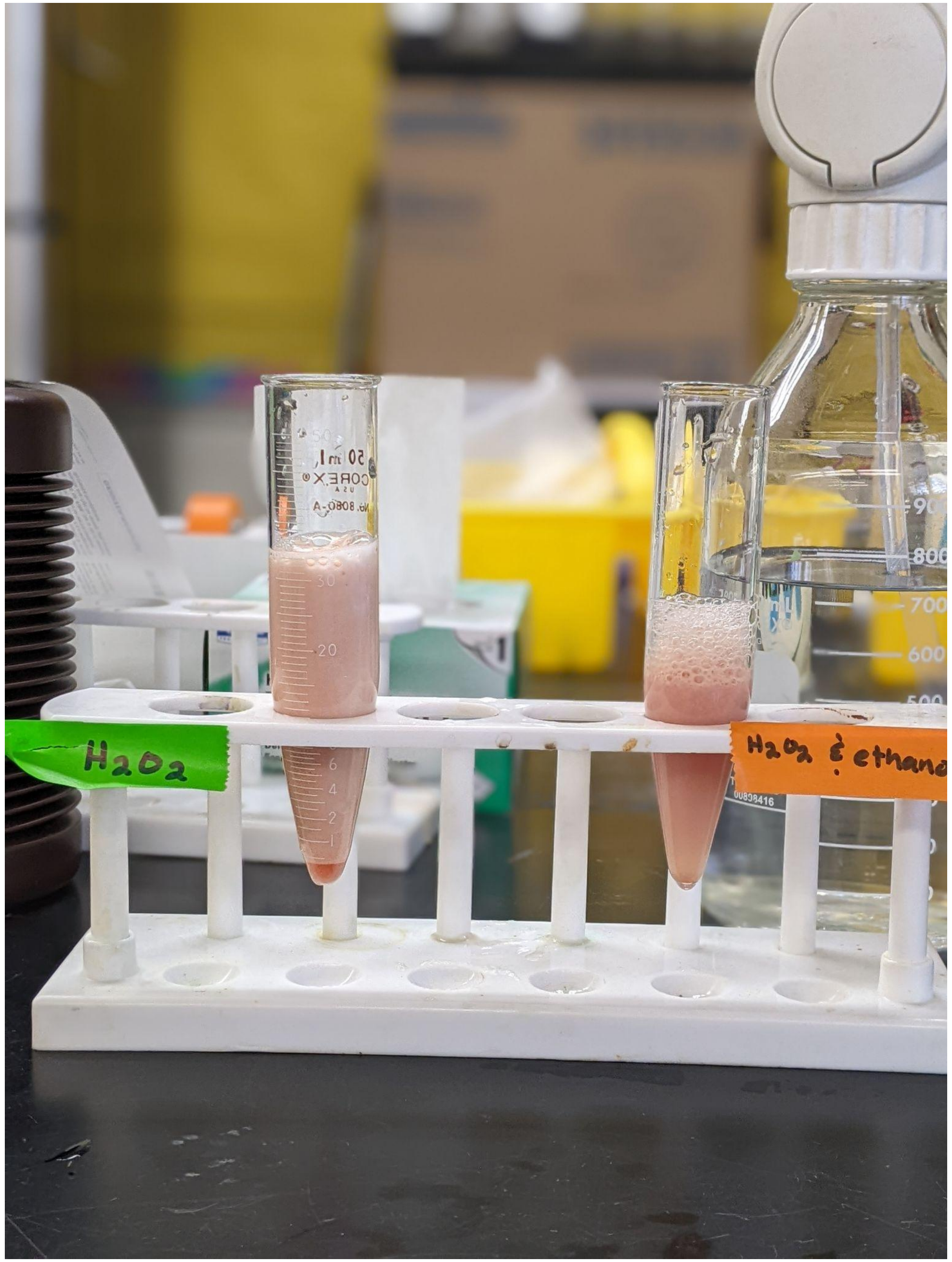

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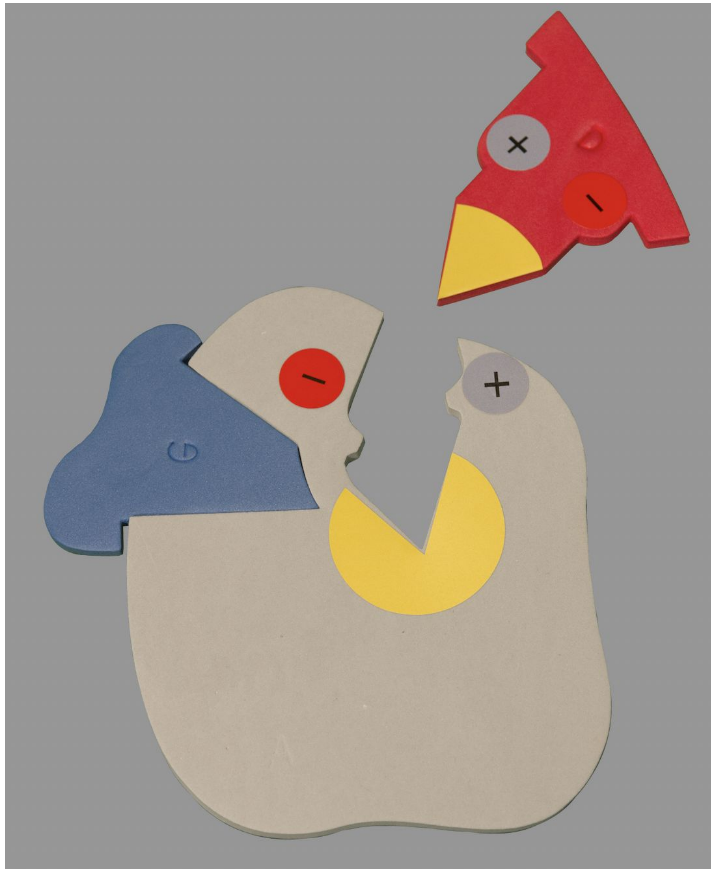

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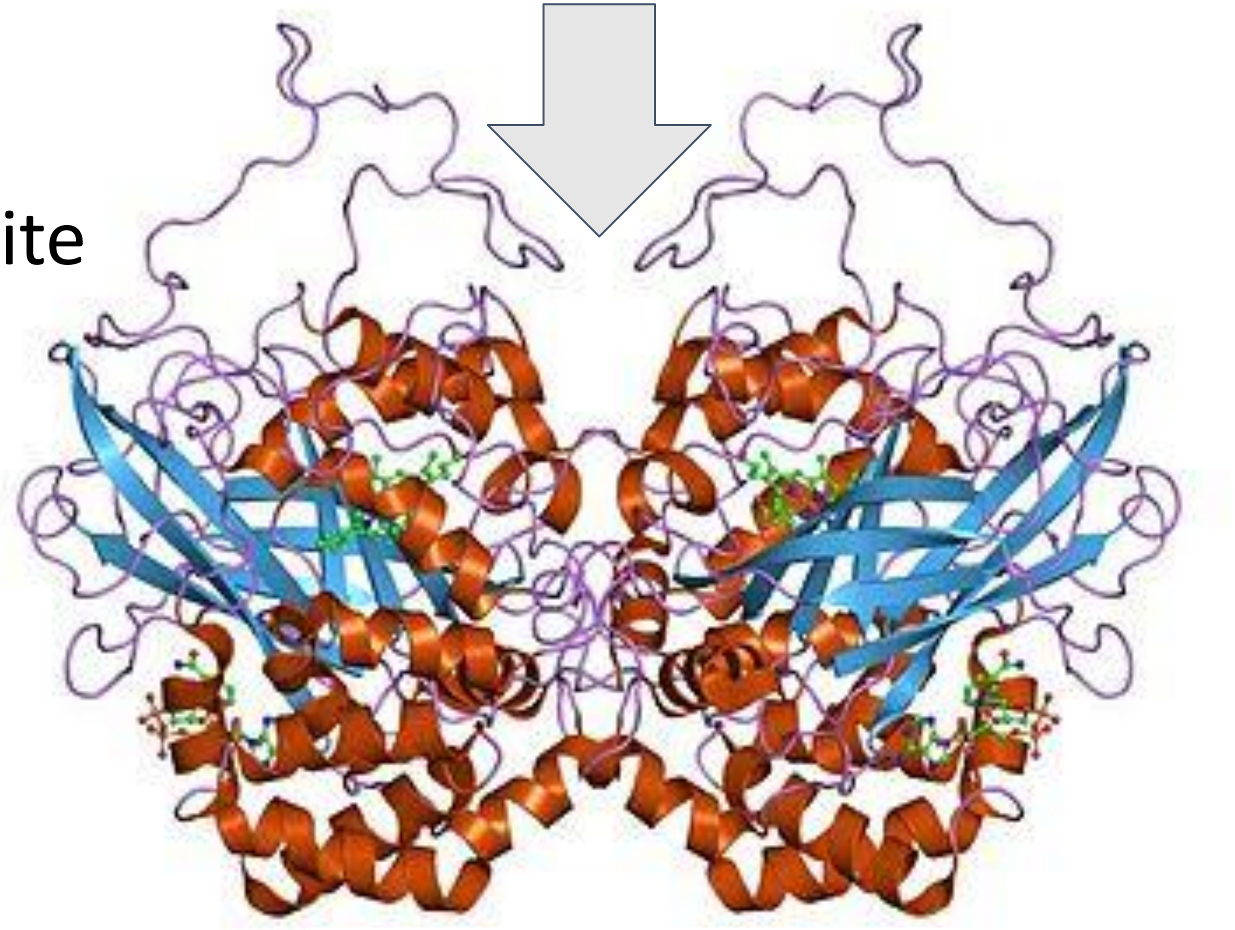
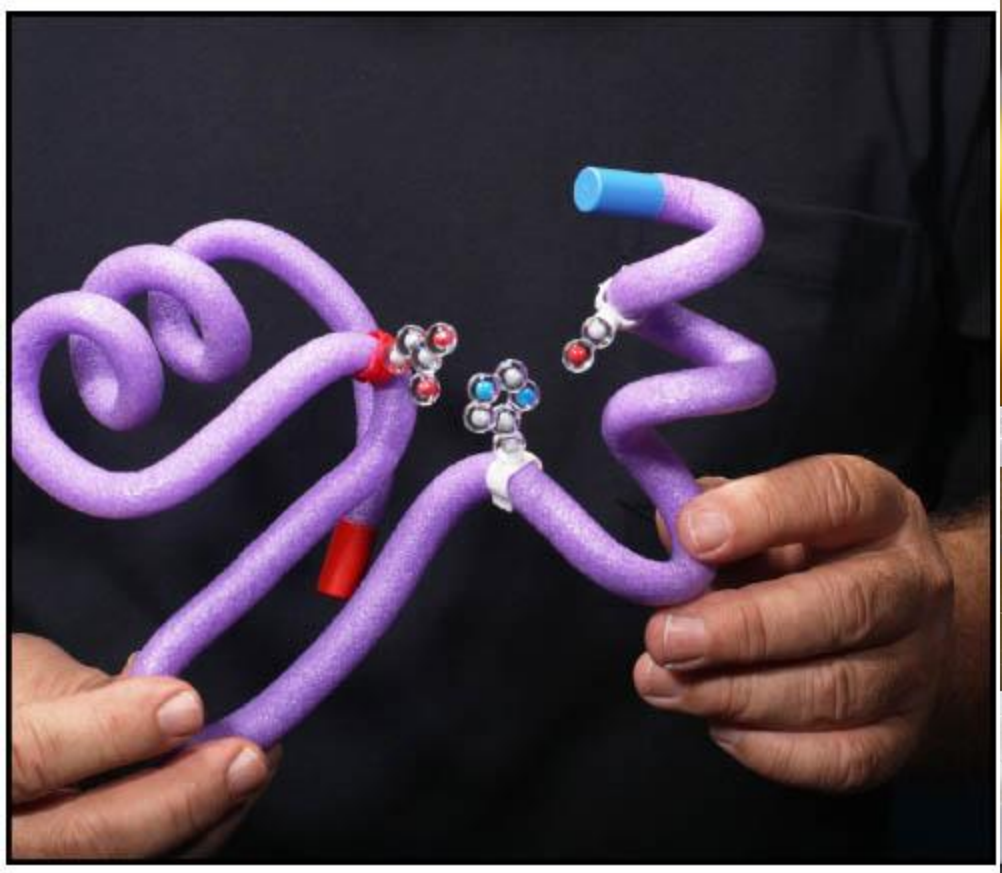
Modeling Catalase's Active Site



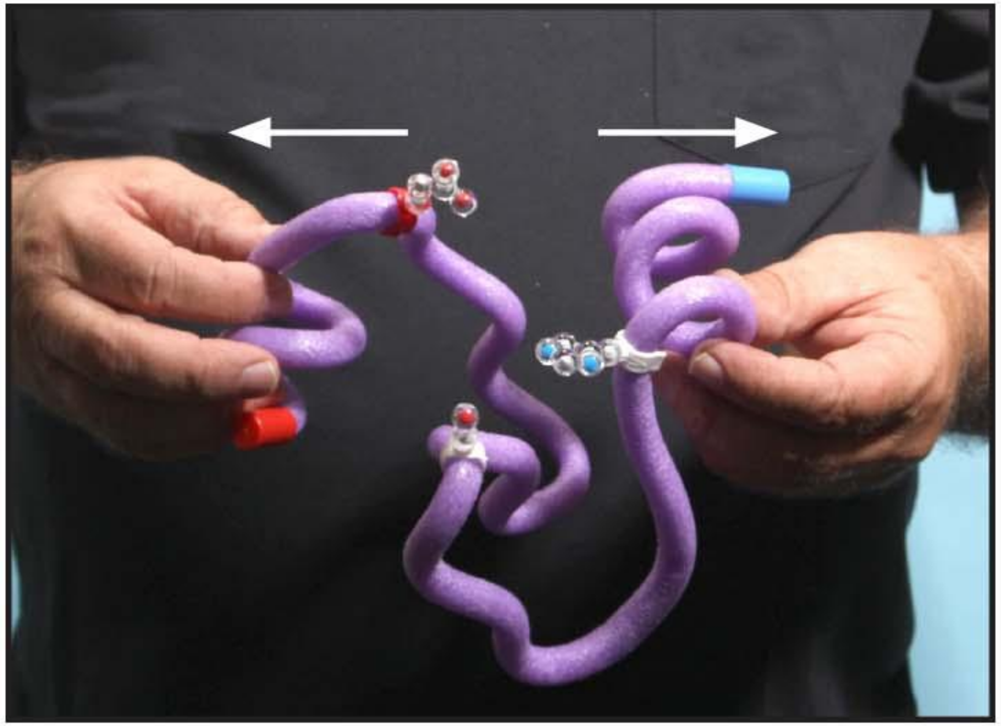
$$2H_2O_2 \rightarrow 2H_2O + O_2$$

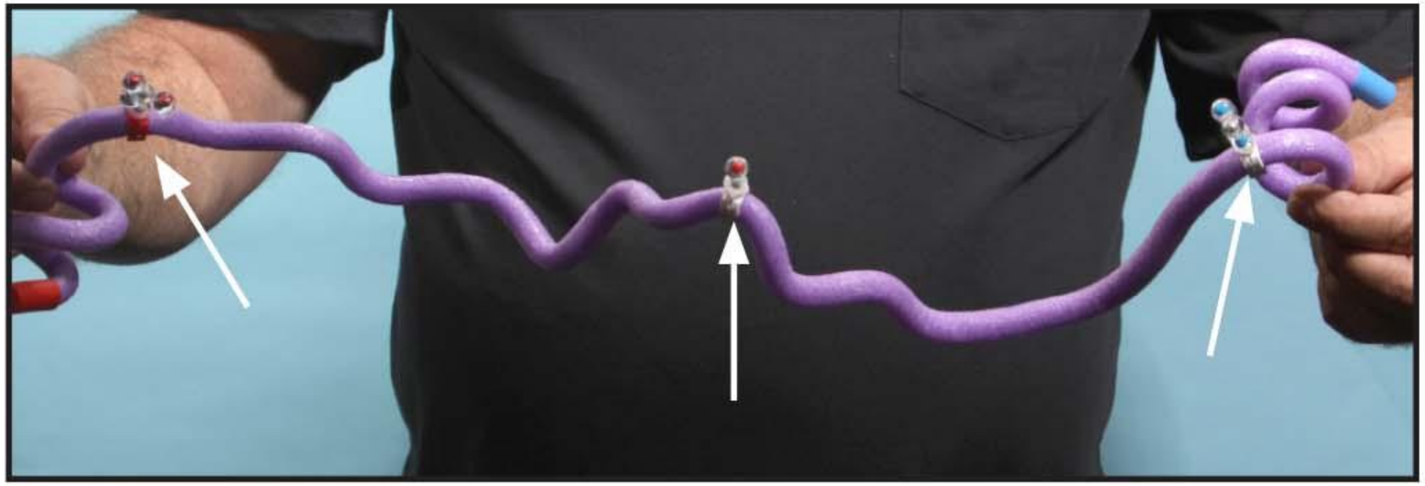
COMPARING ACIDS AND BASES

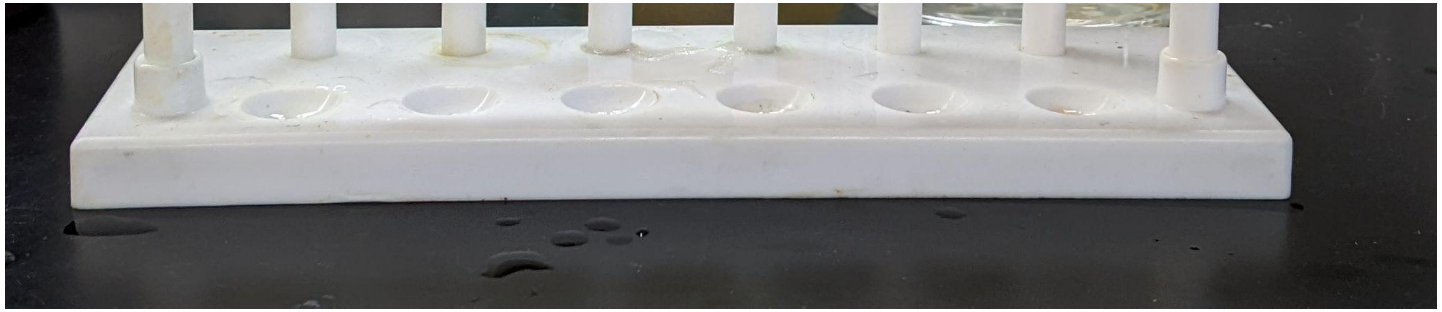
COMPARING ACIDS AND BASES



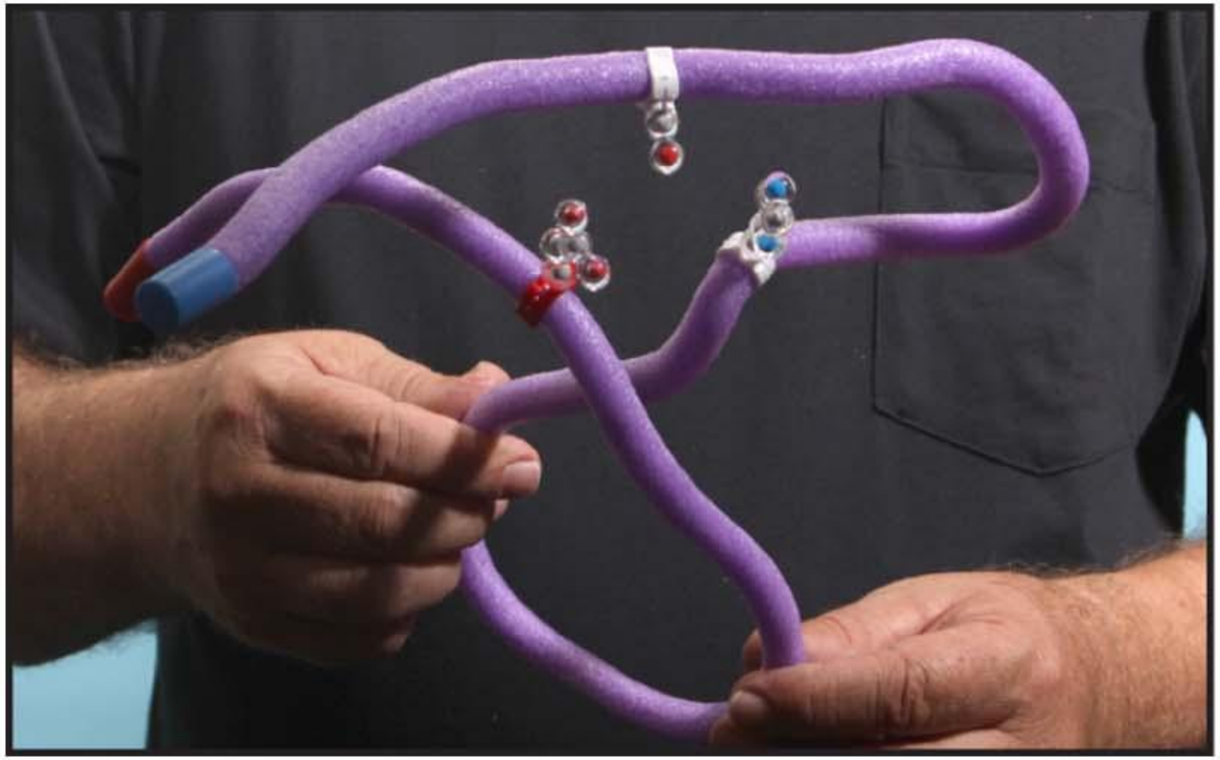
COMPARING ACIDS AND BASES

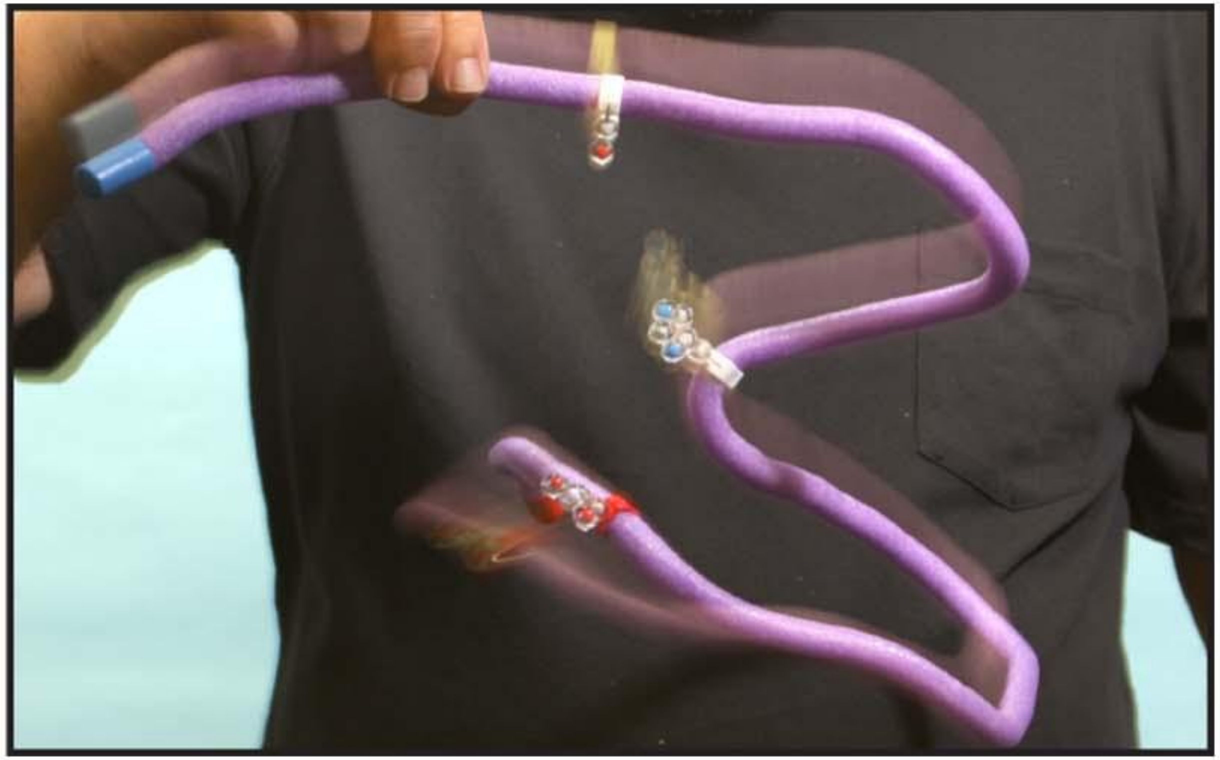


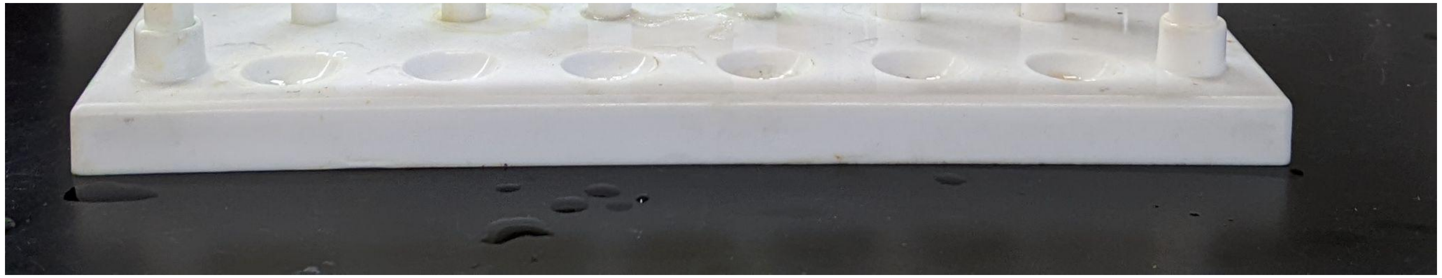




COMPARING ACIDS AND BASES

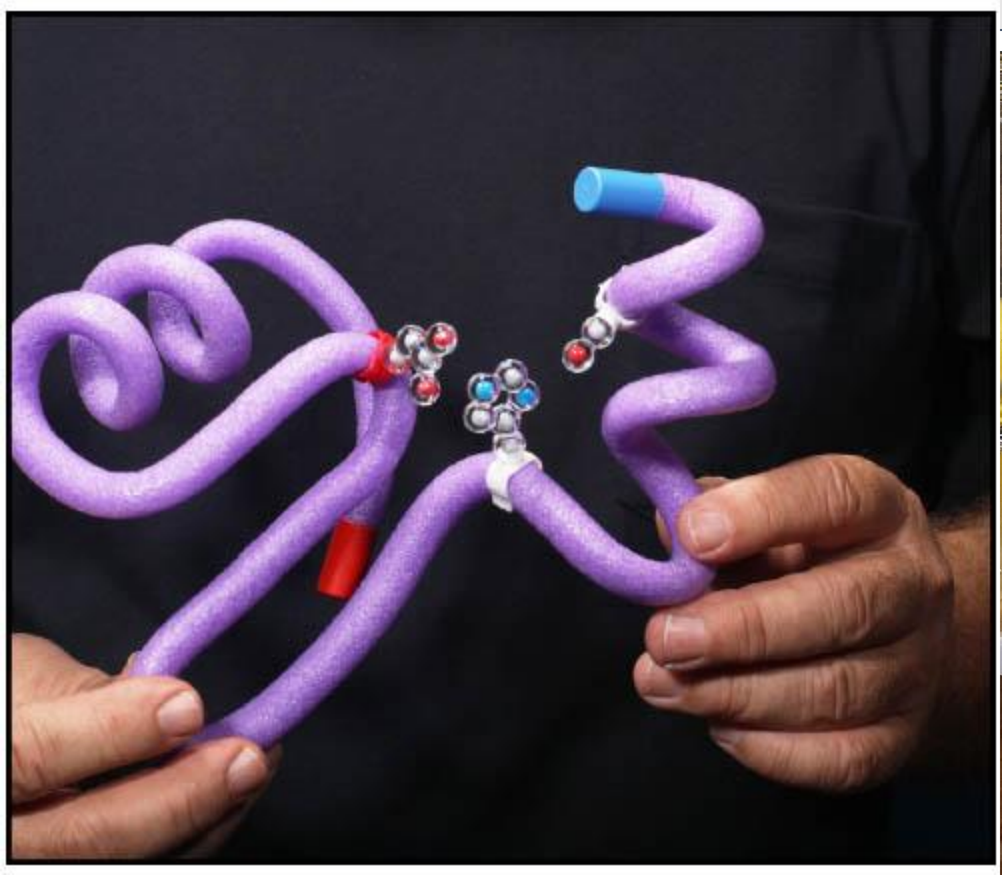


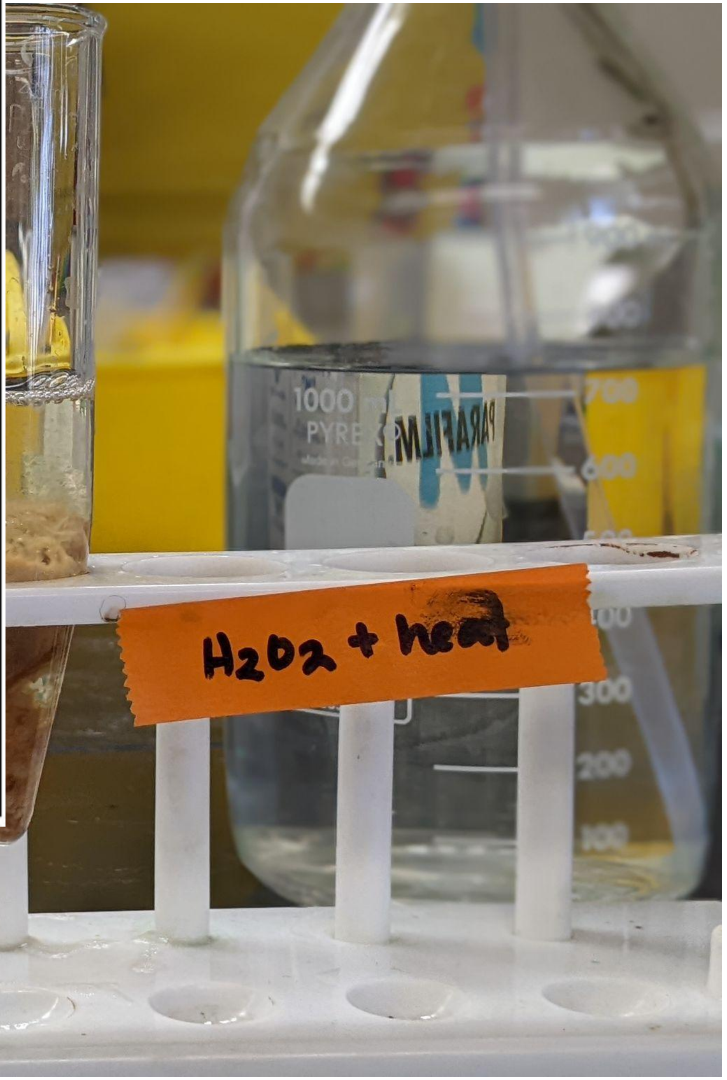




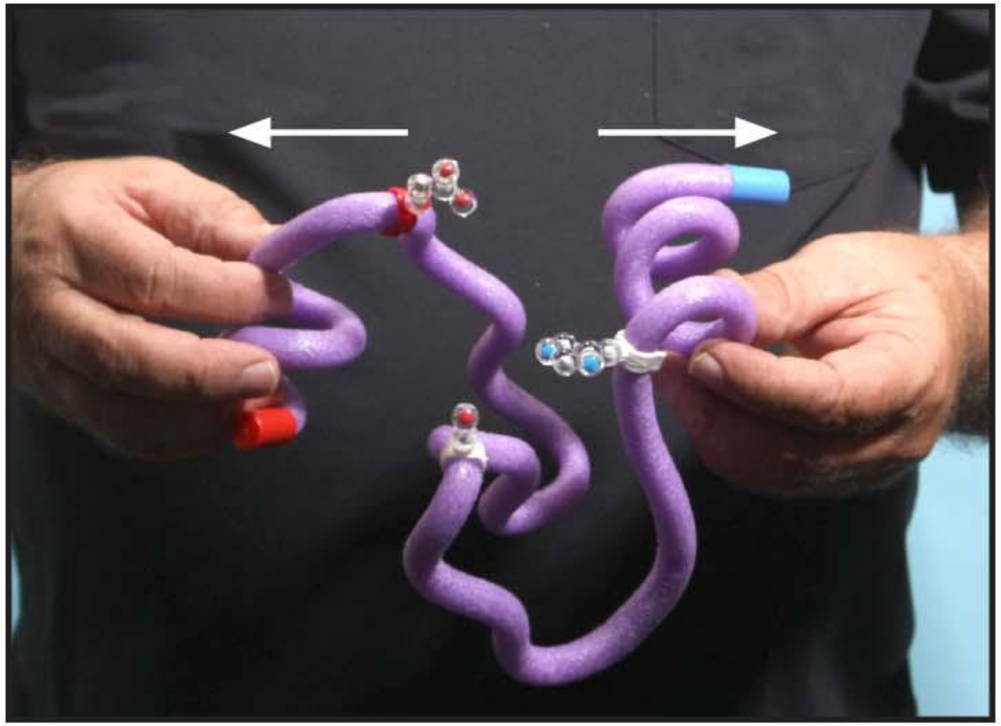
COMPARING COLD AND HEAT

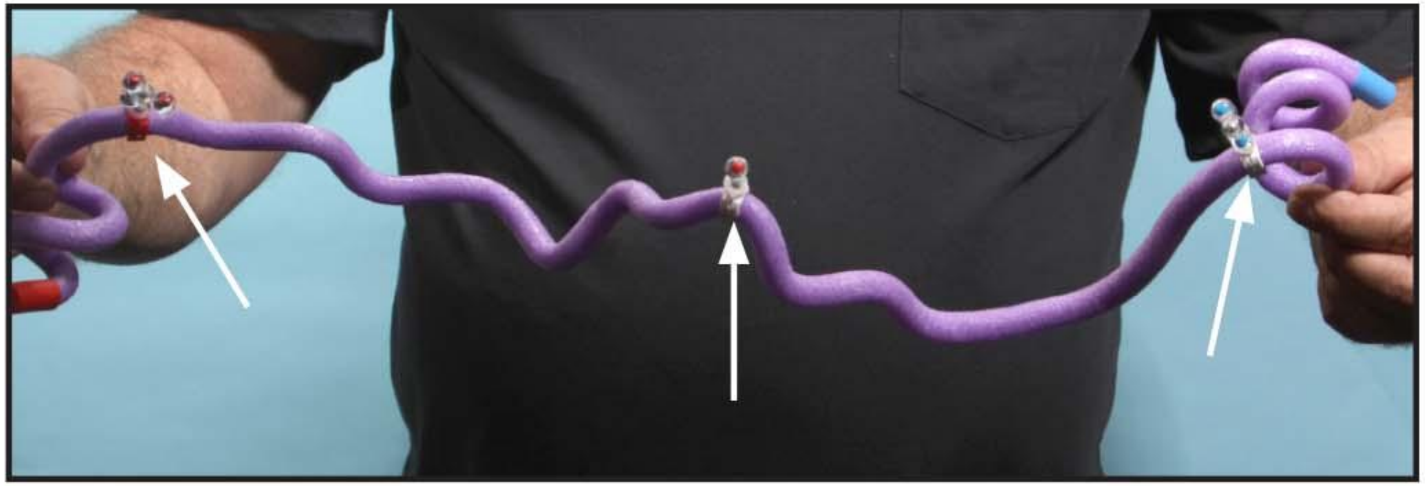
COMPARING COLD AND HEAT



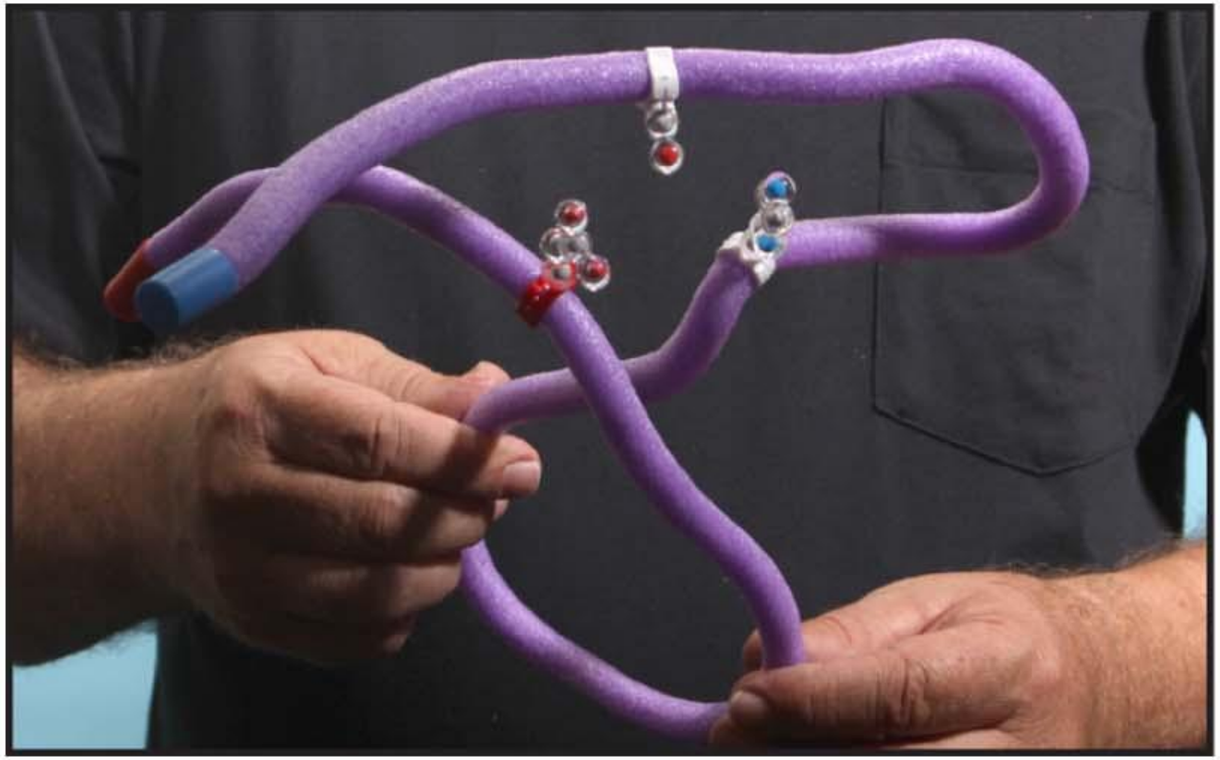


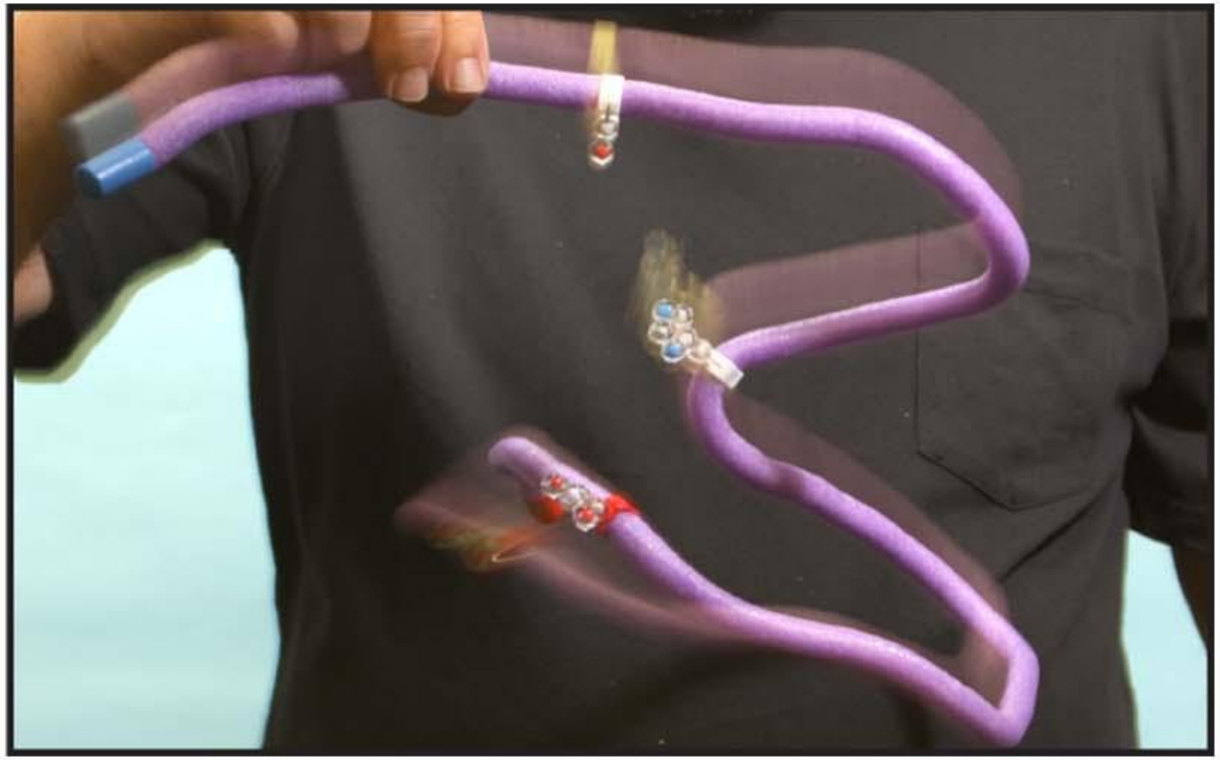
COMPARING COLD AND HEAT

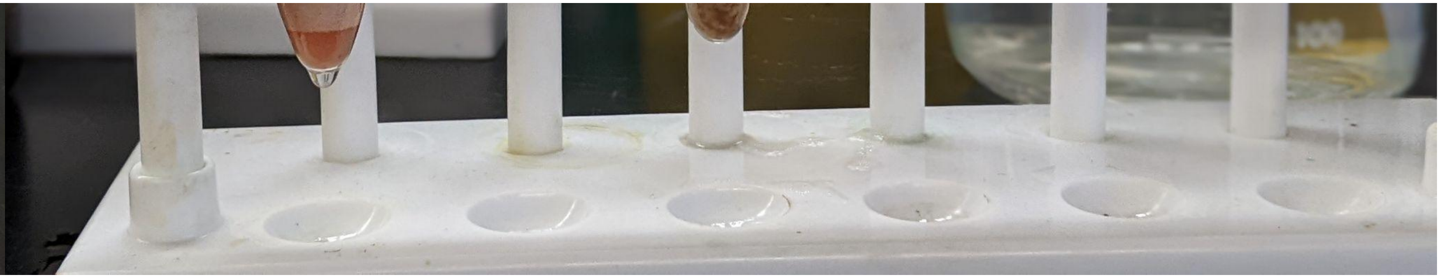




COMPARING COLD AND HEAT







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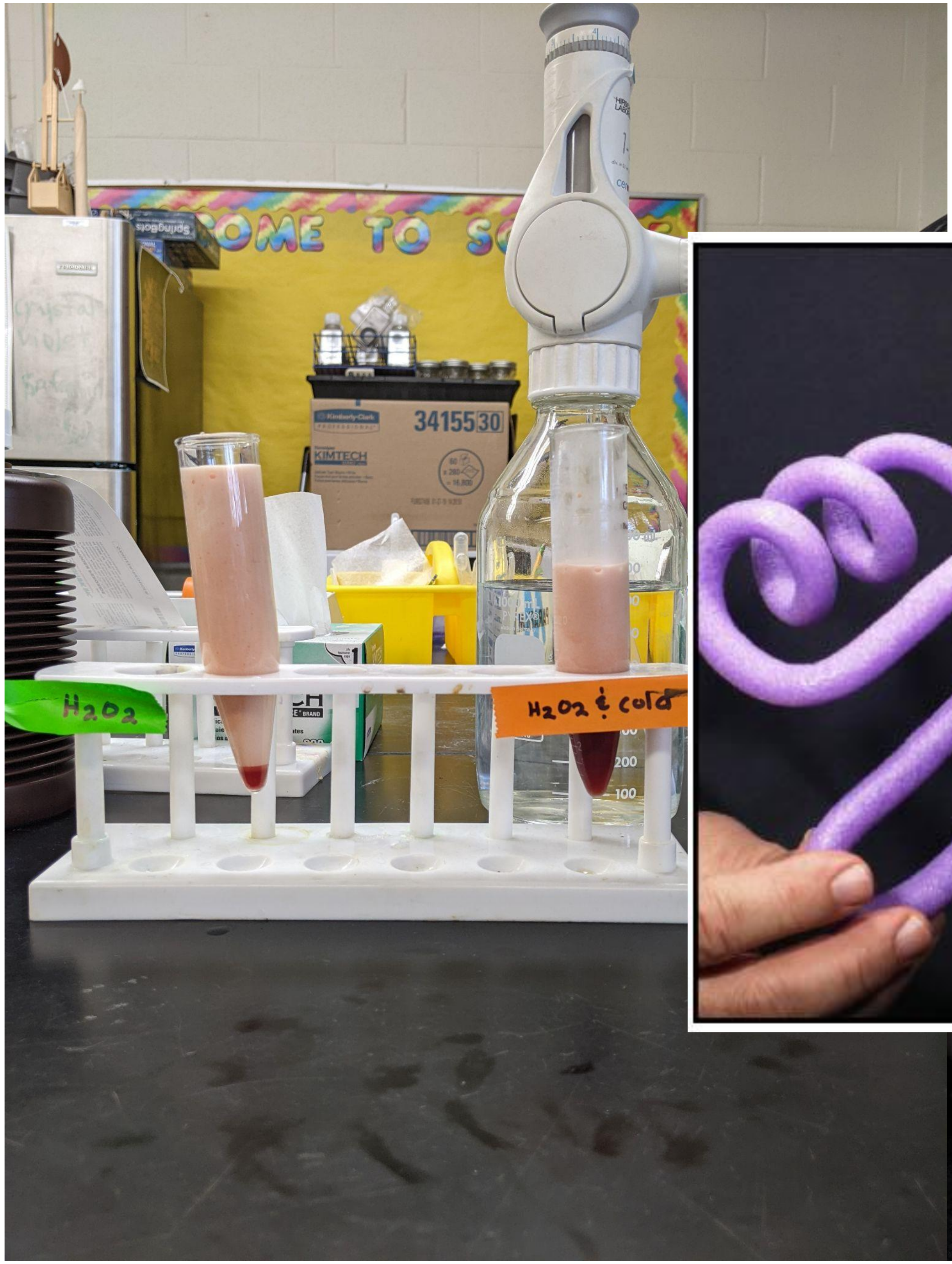
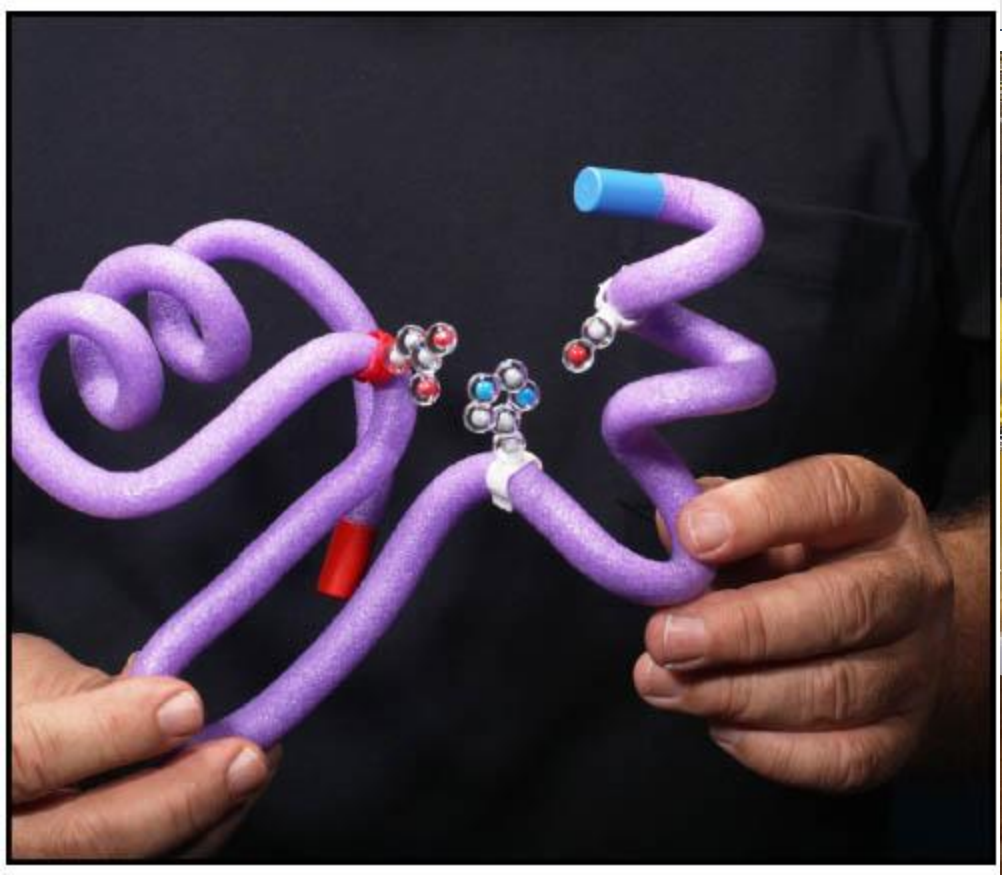
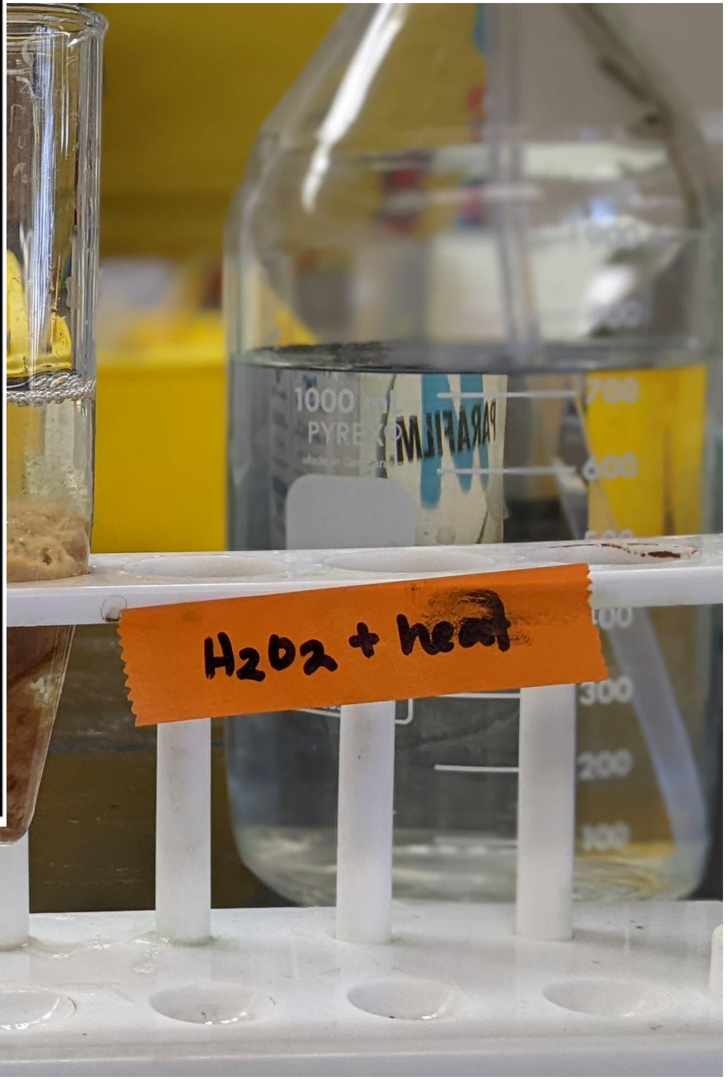
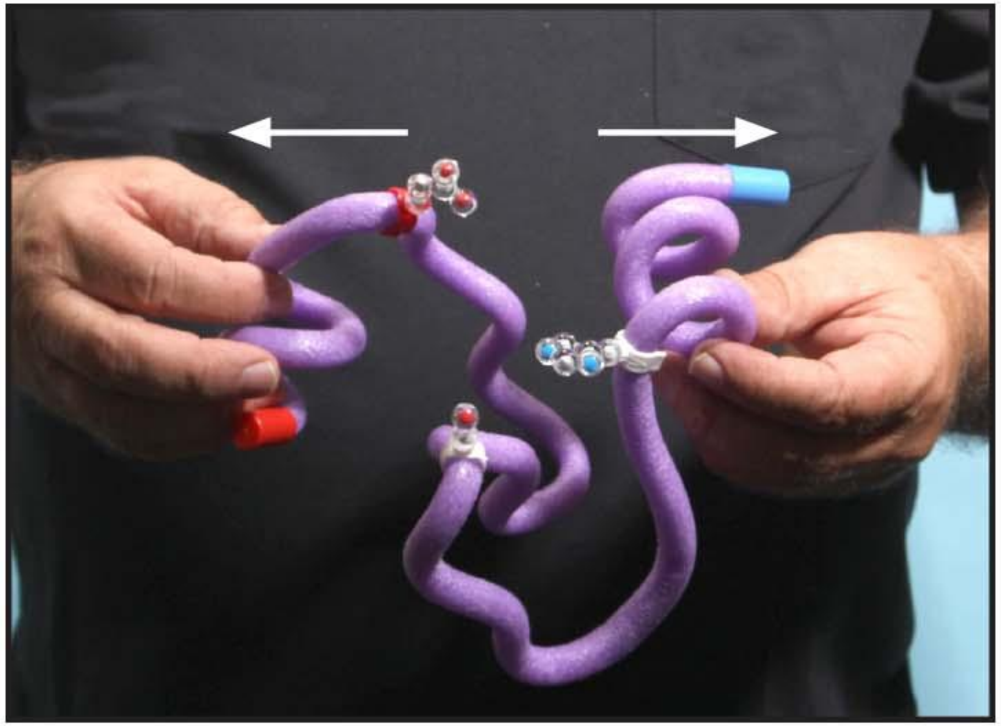
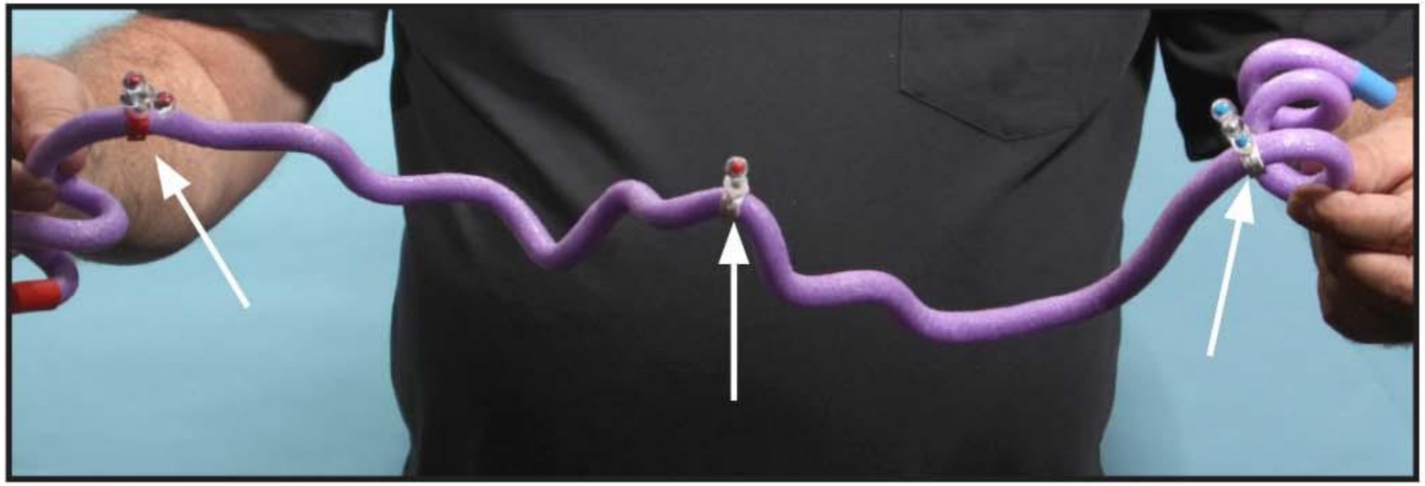


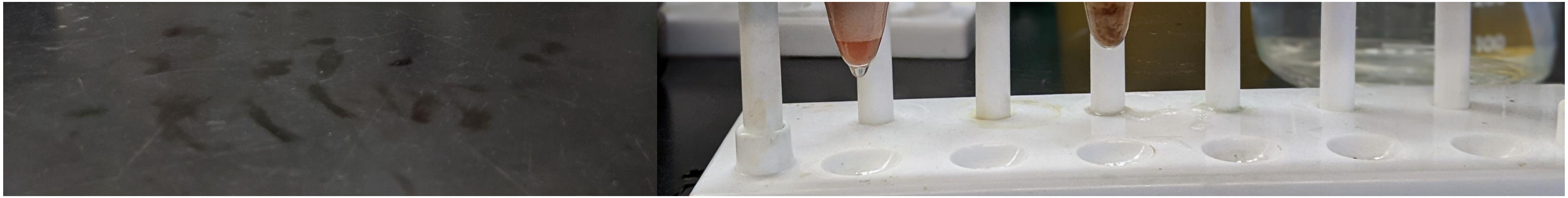




COMPARING COLD AND HEAT







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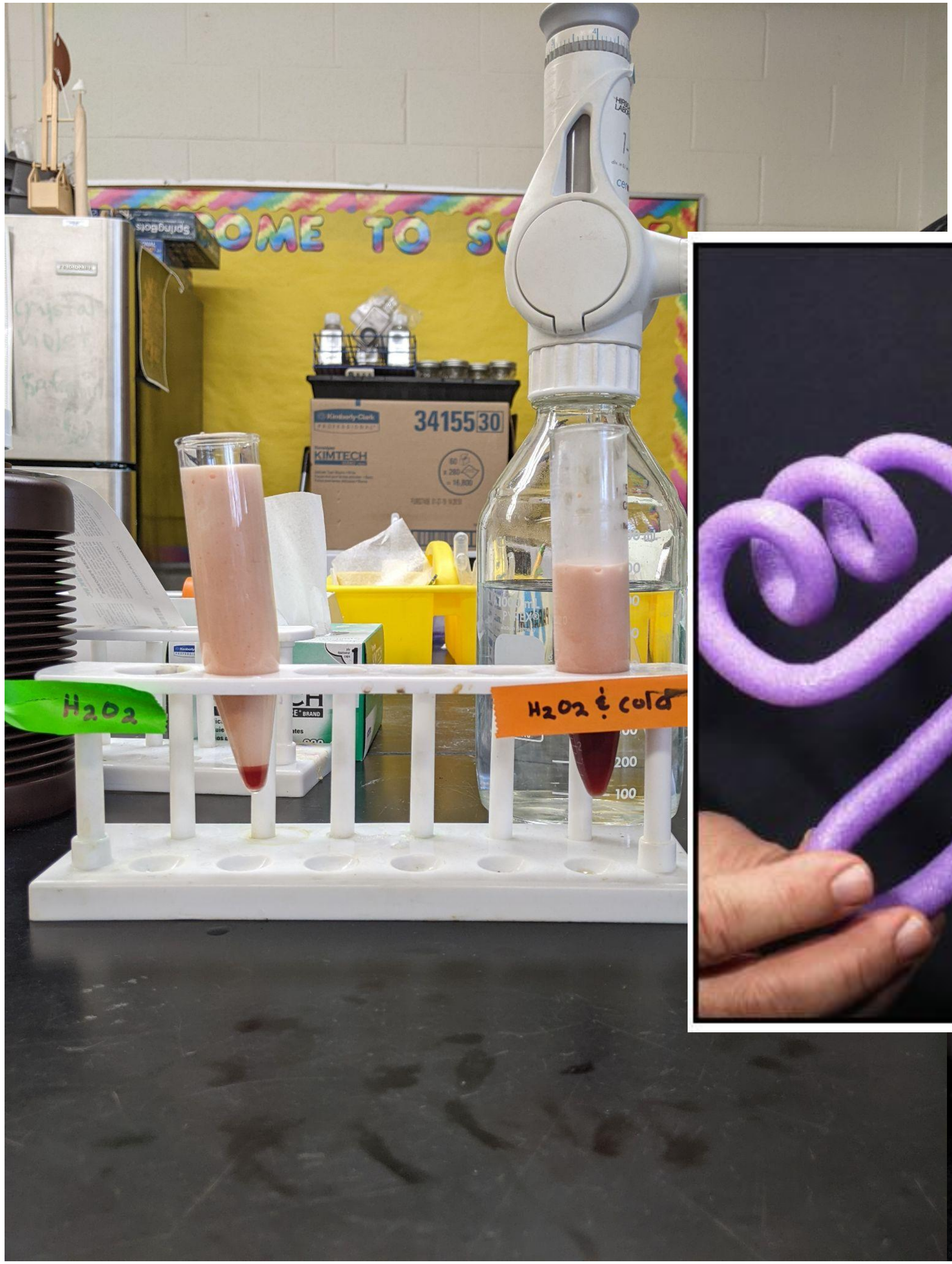
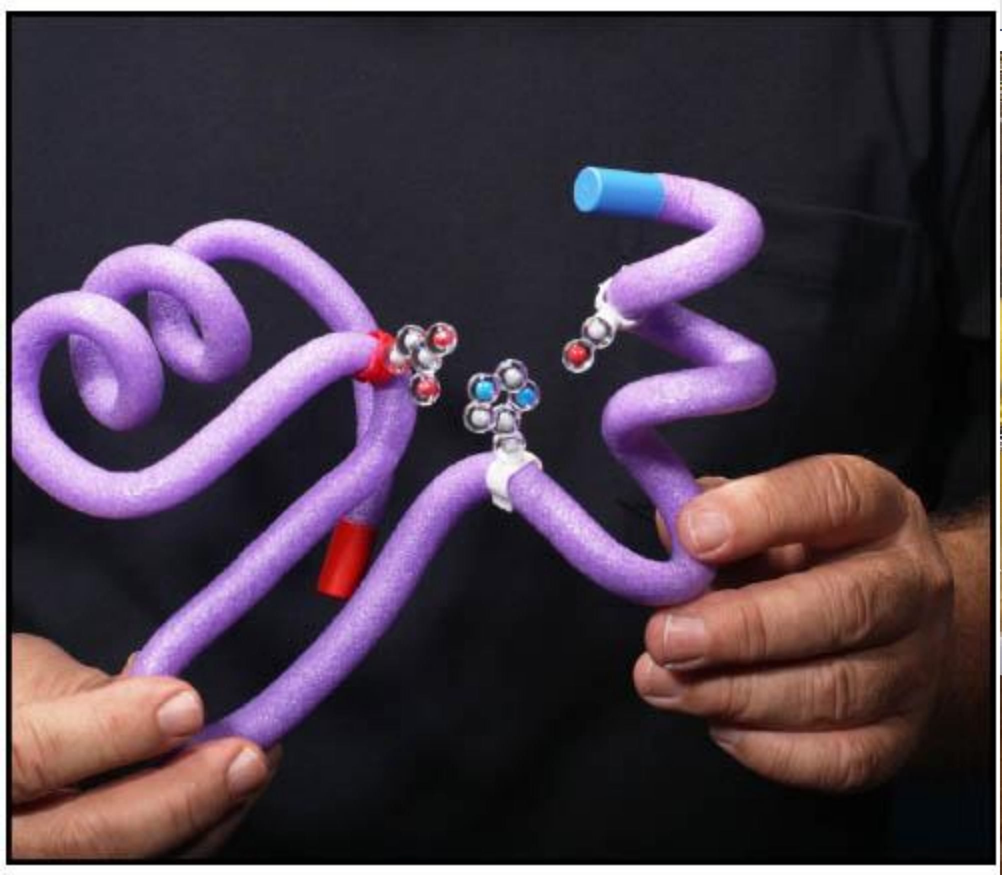
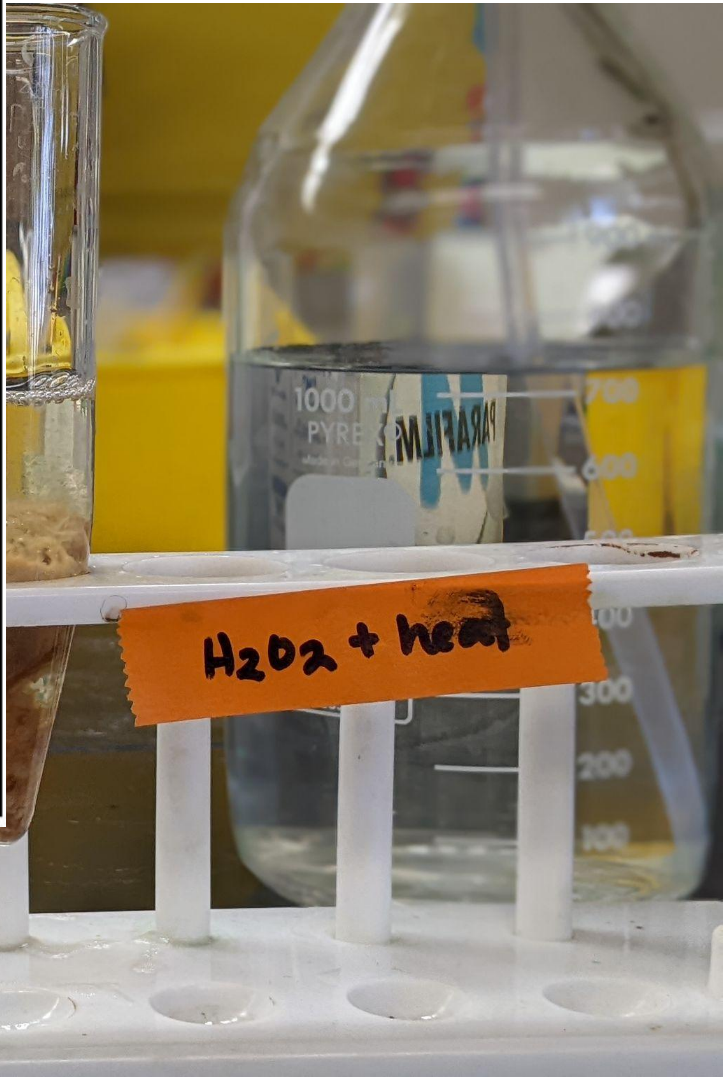


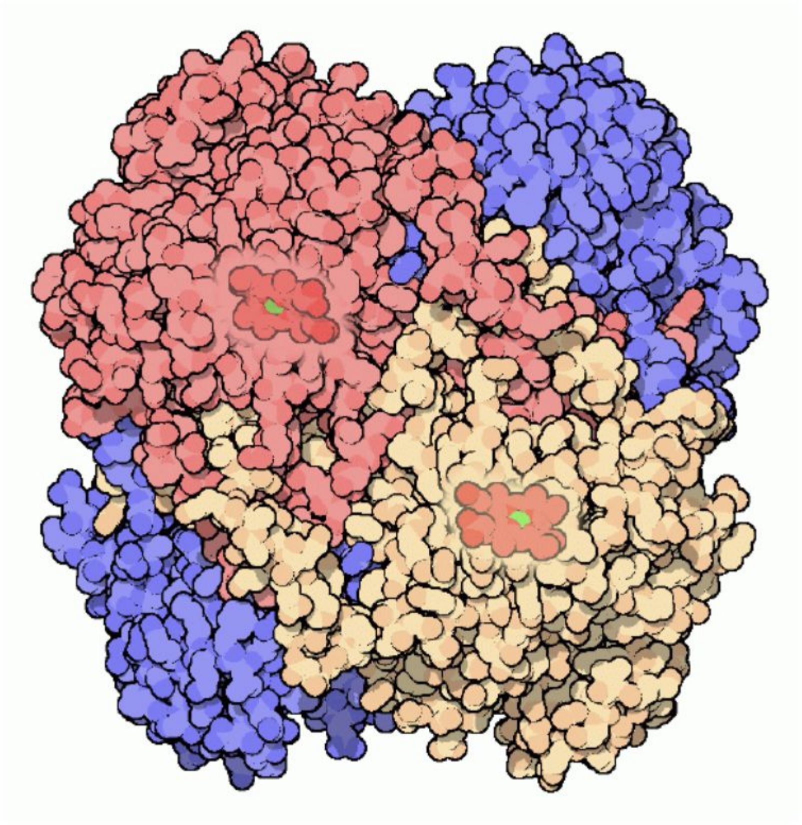




Catalase

Catalase protects us from dangerous reactive oxidizing molecules

Living with oxygen is dangerous. We rely on oxygen to power our cells, but oxygen is a reactive molecule that can cause serious problems if not carefully controlled. One of the dangers of oxygen is that it is easily converted into other reactive compounds. Inside our cells, electrons are continually shuttled from site to site by carrier molecules, such as carriers derived from riboflavin and niacin. If oxygen runs into one of these carrier molecules, the electron may be accidentally transferred to it. This converts oxygen into dangerous compounds such as superoxide radicals and hydrogen peroxide, which can attack the delicate sulfur atoms and metal ions in proteins. To make things even worse, free iron ions in the cell occasionally convert hydrogen peroxide into hydroxyl radicals. These deadly molecules attack and mutate DNA. One theory, still controversial, is that this type of oxidative damage accumulates over the years of our life, causing us to age.



Catalase, with the heme in red and the central iron in green.

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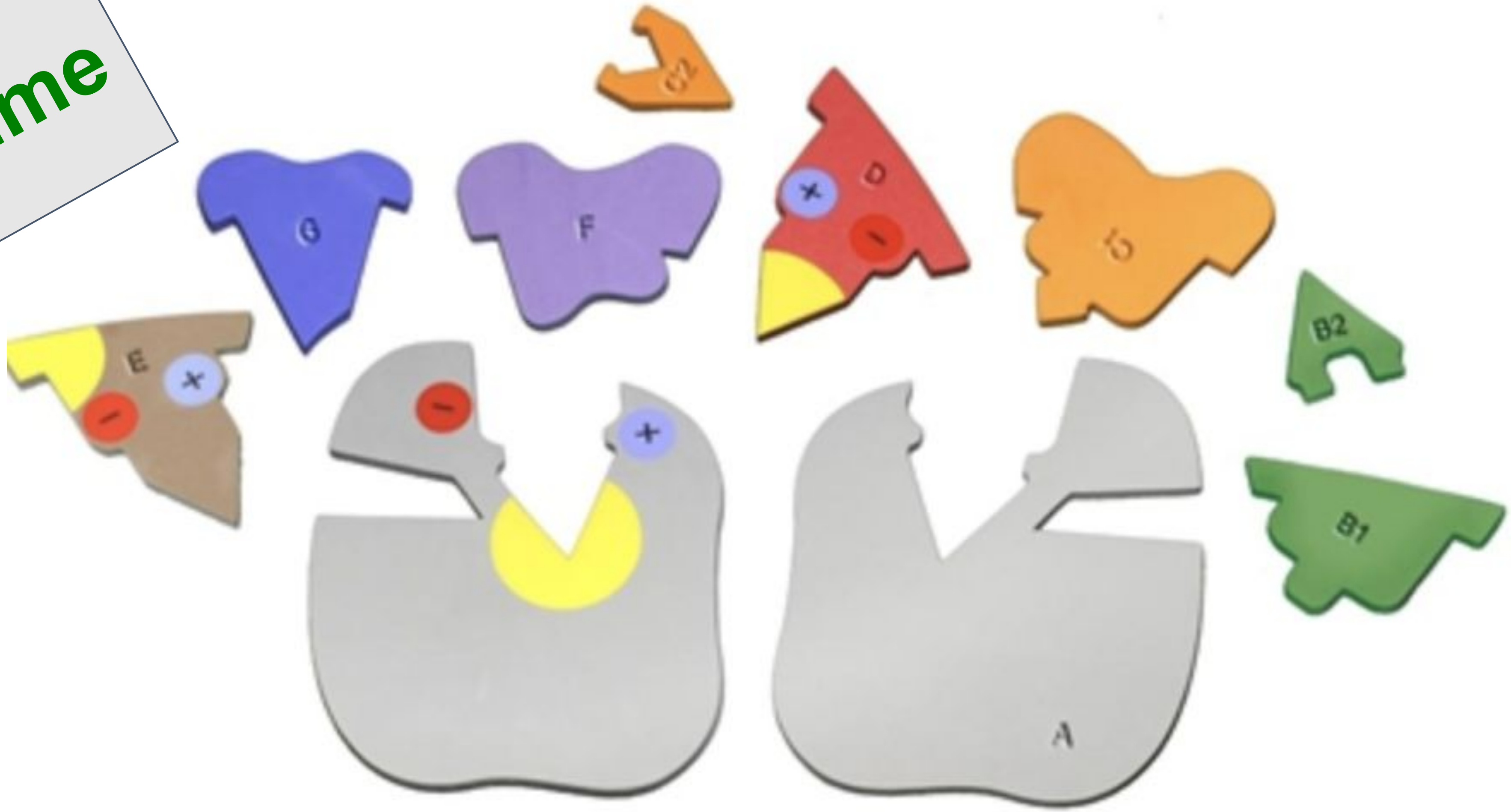
Antioxidants to the Rescue

Fortunately, cells make a variety of antioxidant enzymes to fight the dangerous side-effects of life with oxygen. Two important players are superoxide dismutase, which converts superoxide radicals into hydrogen peroxide, and catalase, which converts hydrogen peroxide into water and oxygen gas. The importance of these enzymes is demonstrated by their prevalence, ranging from about 0.1% of the protein in an Escherichia coli cell to upwards of a quarter of the protein in susceptible cell types. These many catalase molecules patrol the cell, counteracting the steady production of hydrogen peroxide and keeping it at a safe level.

Better, Stronger, Faster

Catalases are some of the most efficient enzymes found in cells. Each catalase molecule can decompose millions of hydrogen peroxide molecules every second. The cow catalase shown here (PDB entry 8cat) and our own catalases use an iron ion to assist in this speedy reaction. The enzyme is composed of four identical subunits, each with its own active site buried deep inside. The iron ion, shown in green, is gripped at the center of a disk-shaped heme group. Catalases, since they must fight against reactive molecules, are also unusually stable enzymes. Notice how the four chains interweave, locking the entire complex into the proper shape.

Assessment Time



Workshop NGSS Connections

SEPs	CCCs	DCIs
Asking Questions	**Patterns**	**HS-LS1-1**
Developing and Using Models	**Cause and Effect**	**HS-LS1-2**
Constructing Explanations	**Structure and Function**	**LS-1A**
	Stability and Change	**LS-1C**
	Scale, Proportion, and Quantity	**LS-1D**

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TUESDAY | MARCH 1 6:30 - 8 PM CST

PRESENTER:

TIM HERMAN, PhD

MSOE Center for BioMolecular Modeling &
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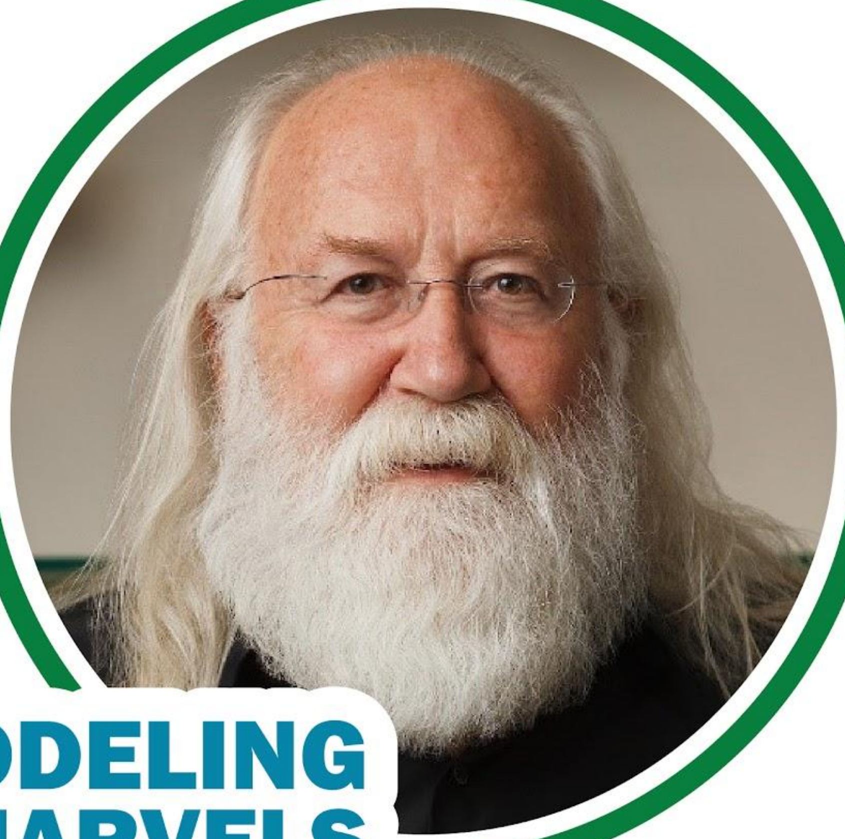
Protein Folding Problem Nevermore



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