3d molecular designs
Transforming Science Learning

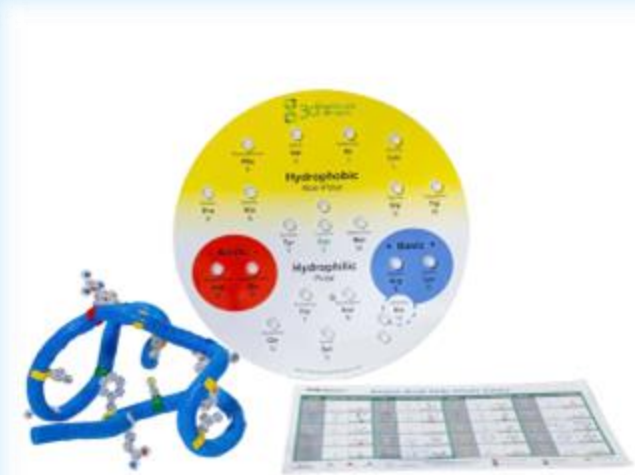
Georgia Science Teachers Association

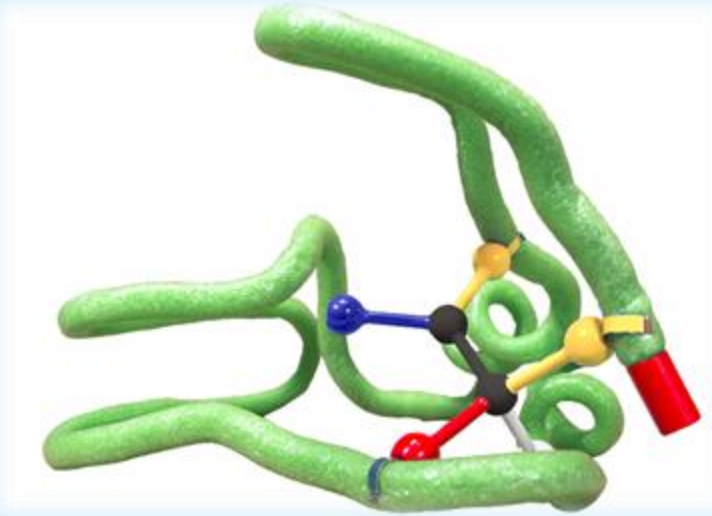
Enzyme Explorations: Real-world Connections with Wet Labs

Ruth Hutson, MSSE

3d molecular designs

Trans*forming* Science Learning



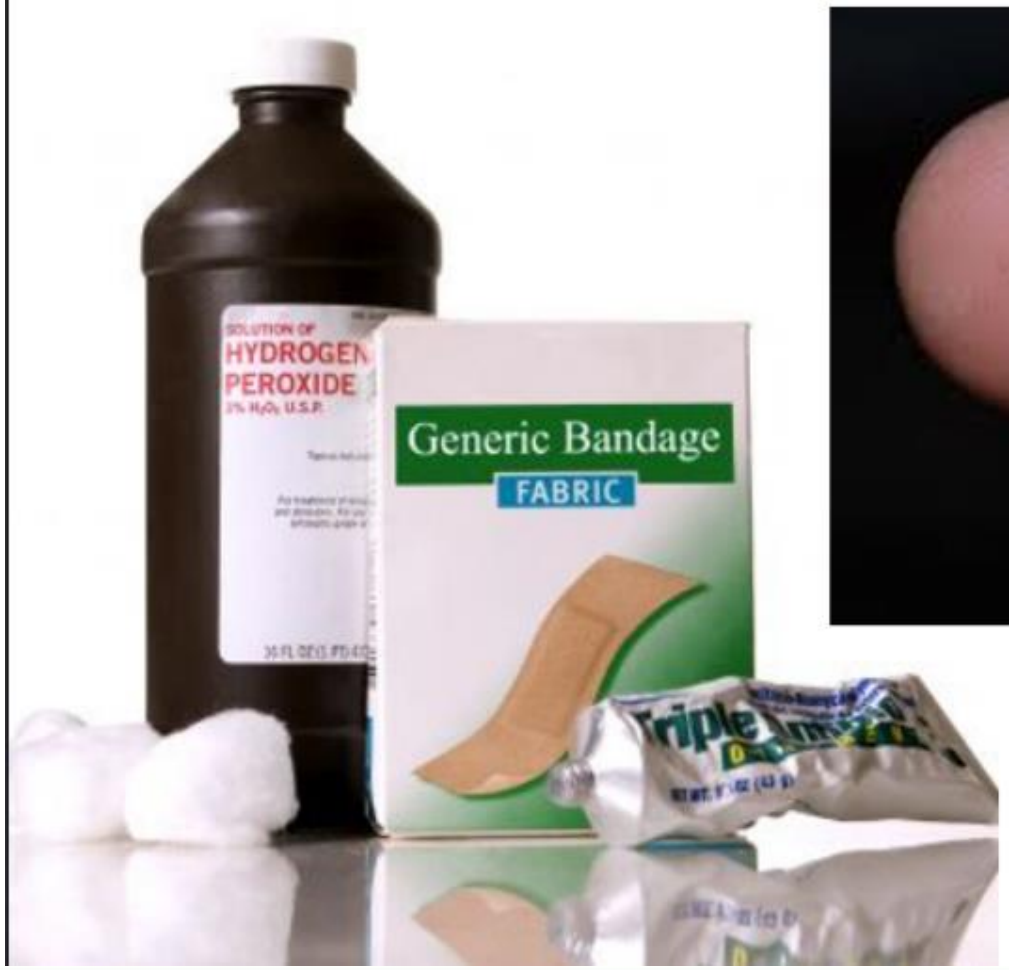


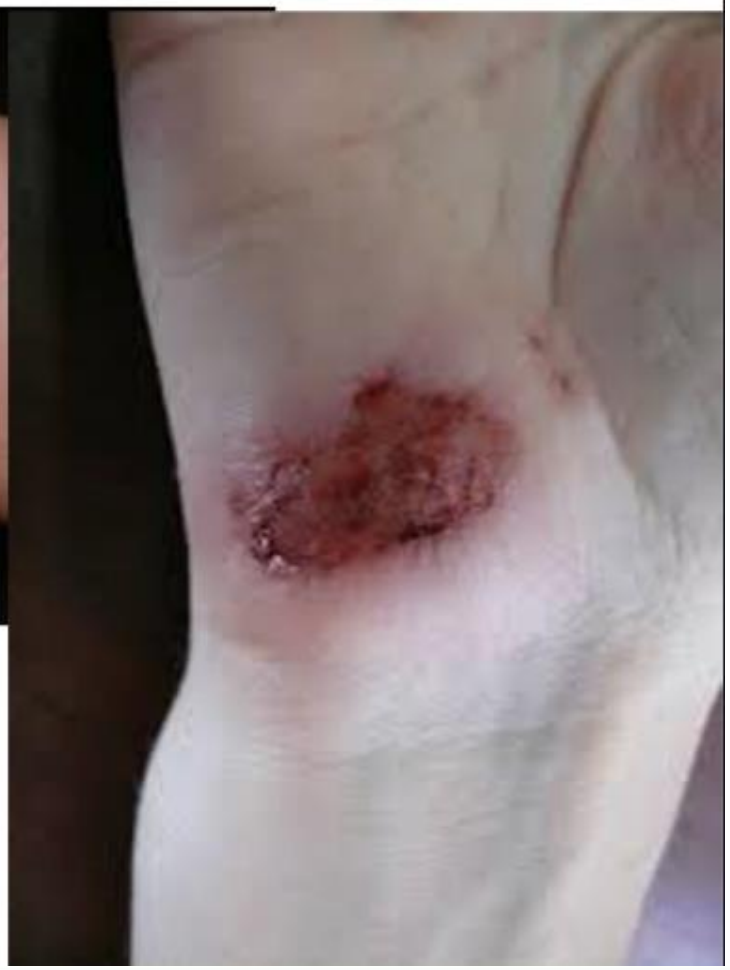
Workshop Outcomes

- Construct an enzyme active site.
- Explore what happens to protein structure when environmental conditions are perturbed.
- Make predictions and compare them to wet labs results.

Phenomenon:

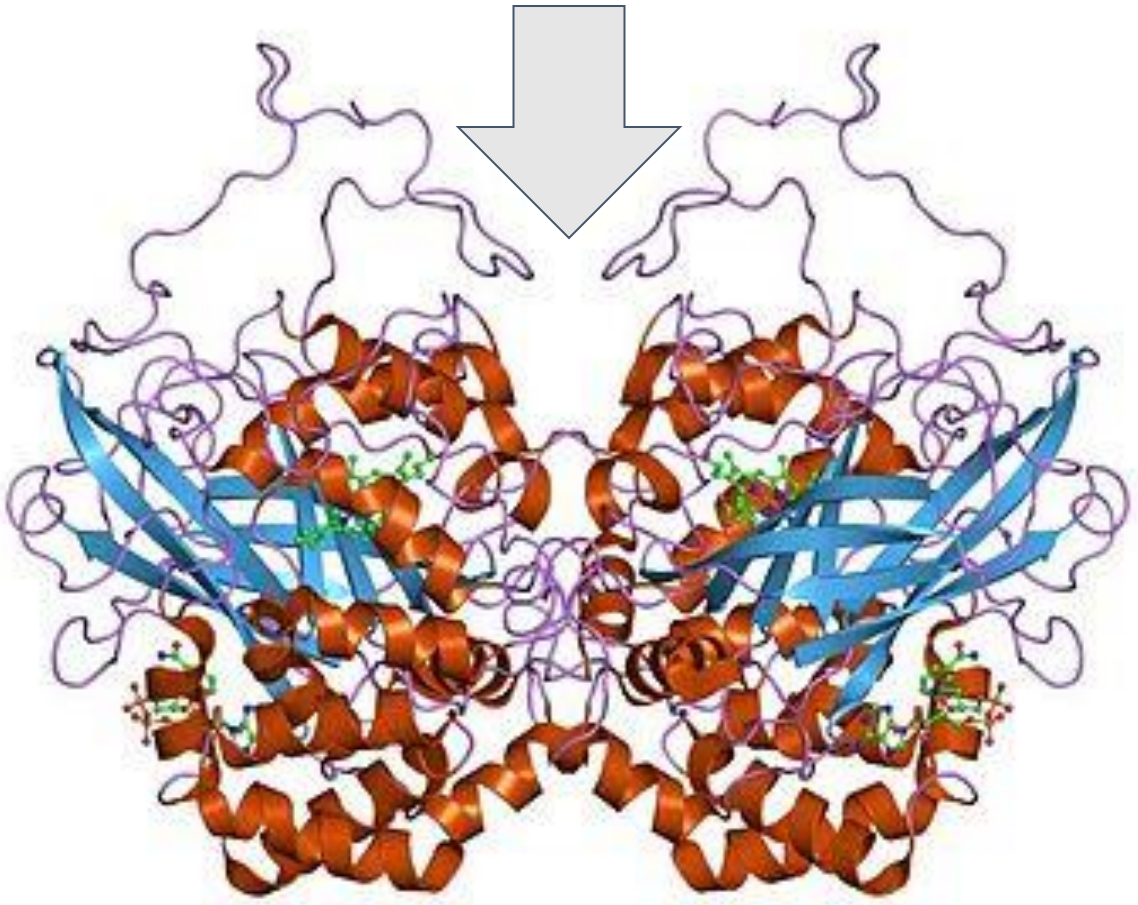
Hydrogen Peroxide Bubbles when put on a cut.





Catalase Lab

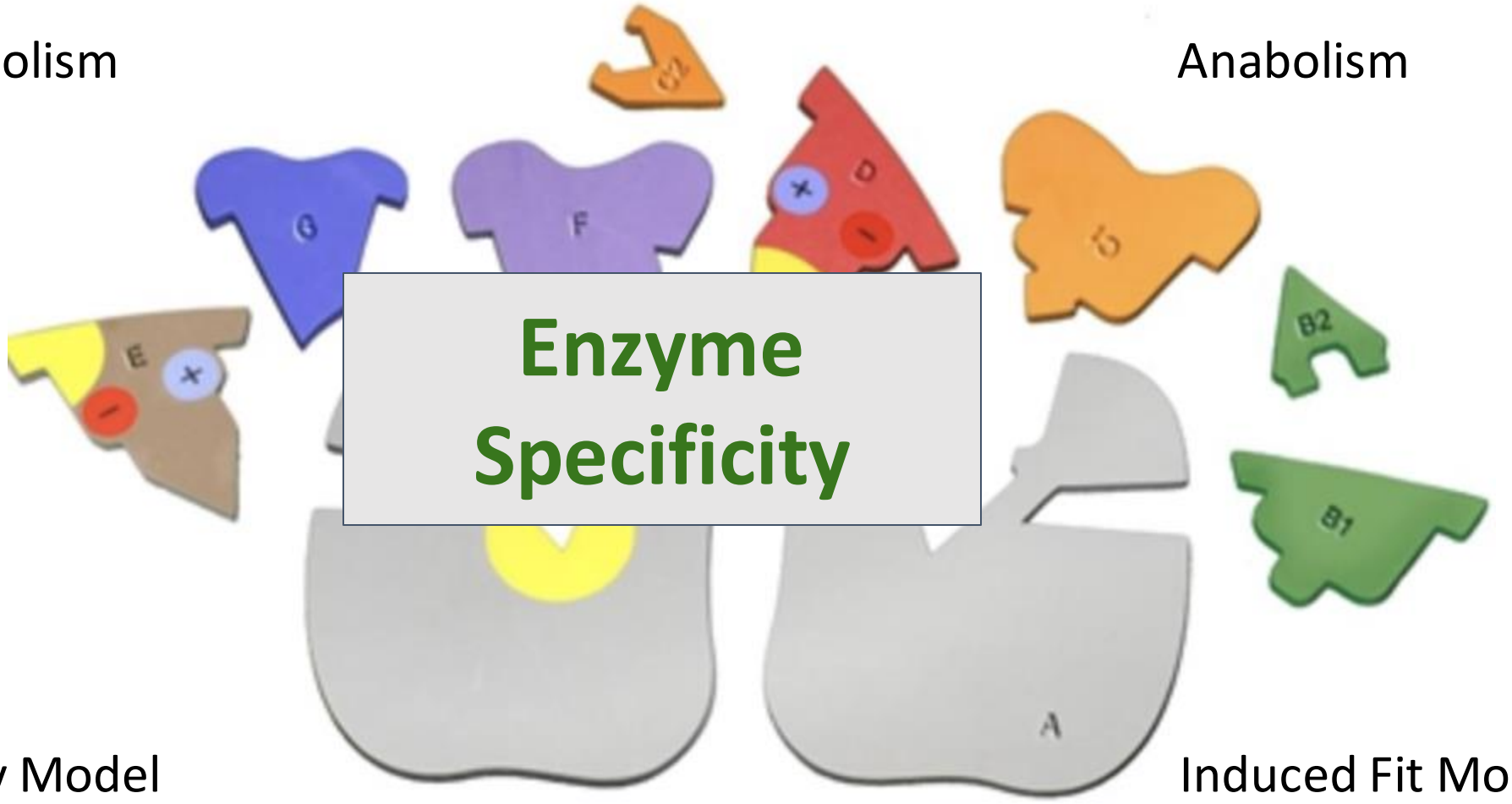
Case study and a multi-day wet lab that allows students to explore and manipulate enzyme actions



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

Catabolism

Anabolism



Enzyme Specificity

Lock and Key Model

Induced Fit Model

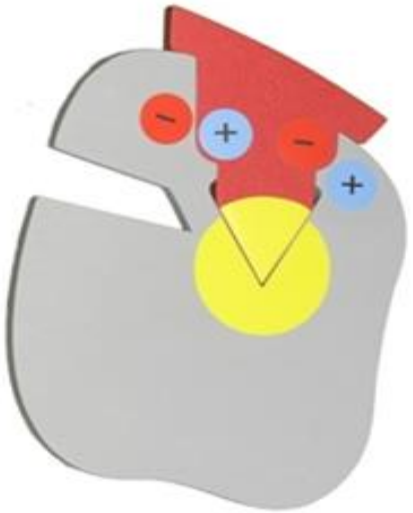
HYDROGEN PEROXIDE

WATER

HYDROGEN PEROXIDE

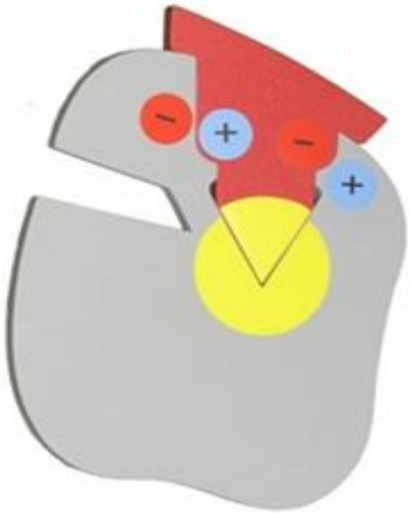
WATER

HYDROGEN PEROXIDE

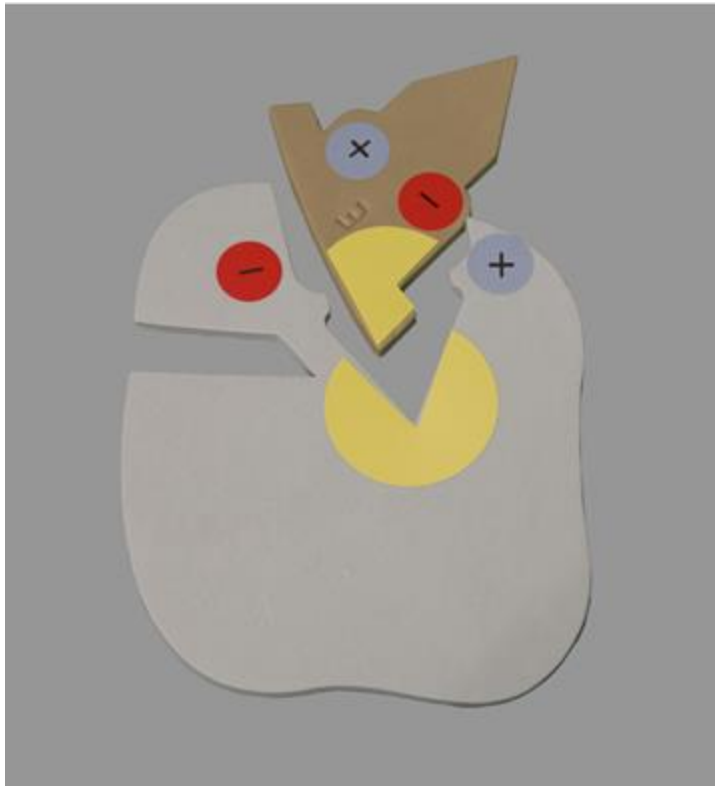


WATER

HYDROGEN PEROXIDE



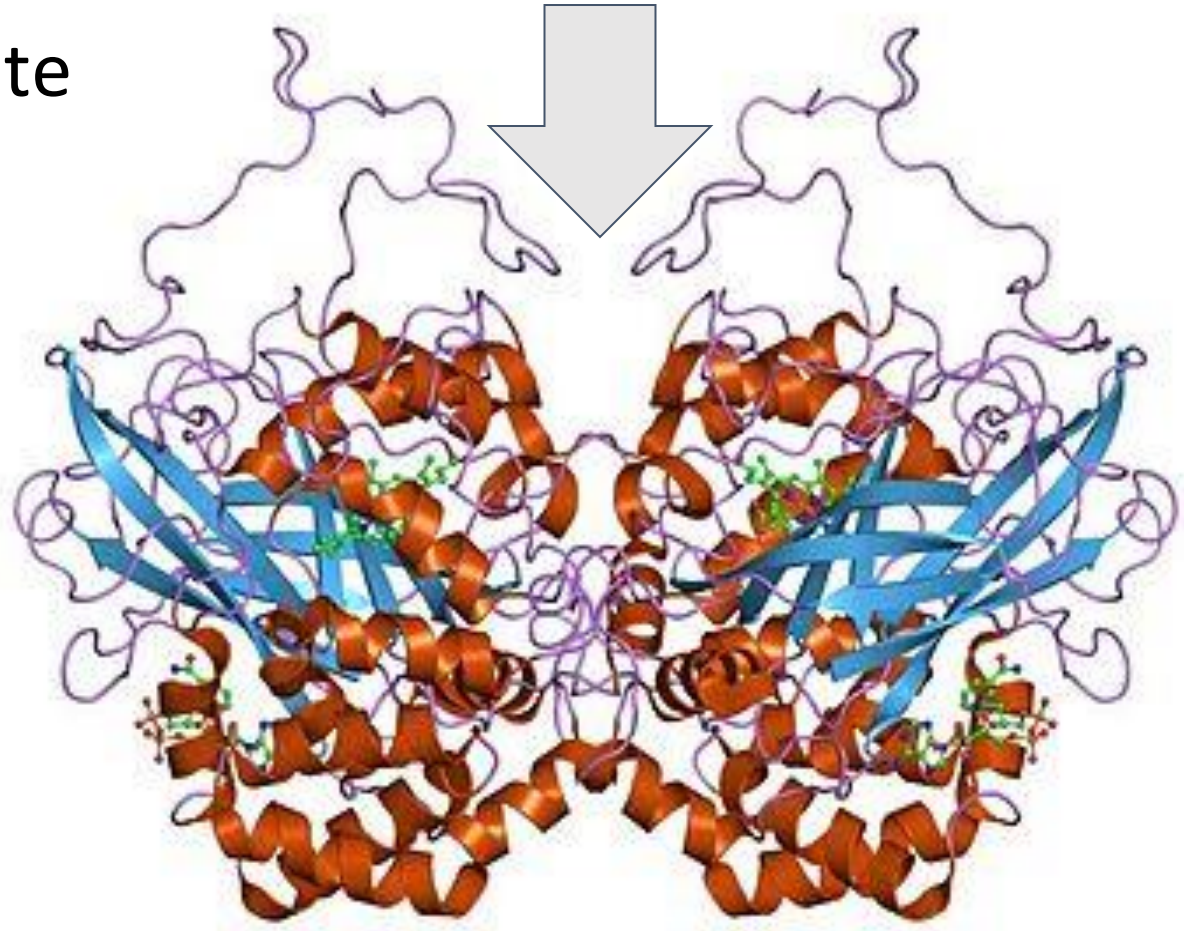
WATER



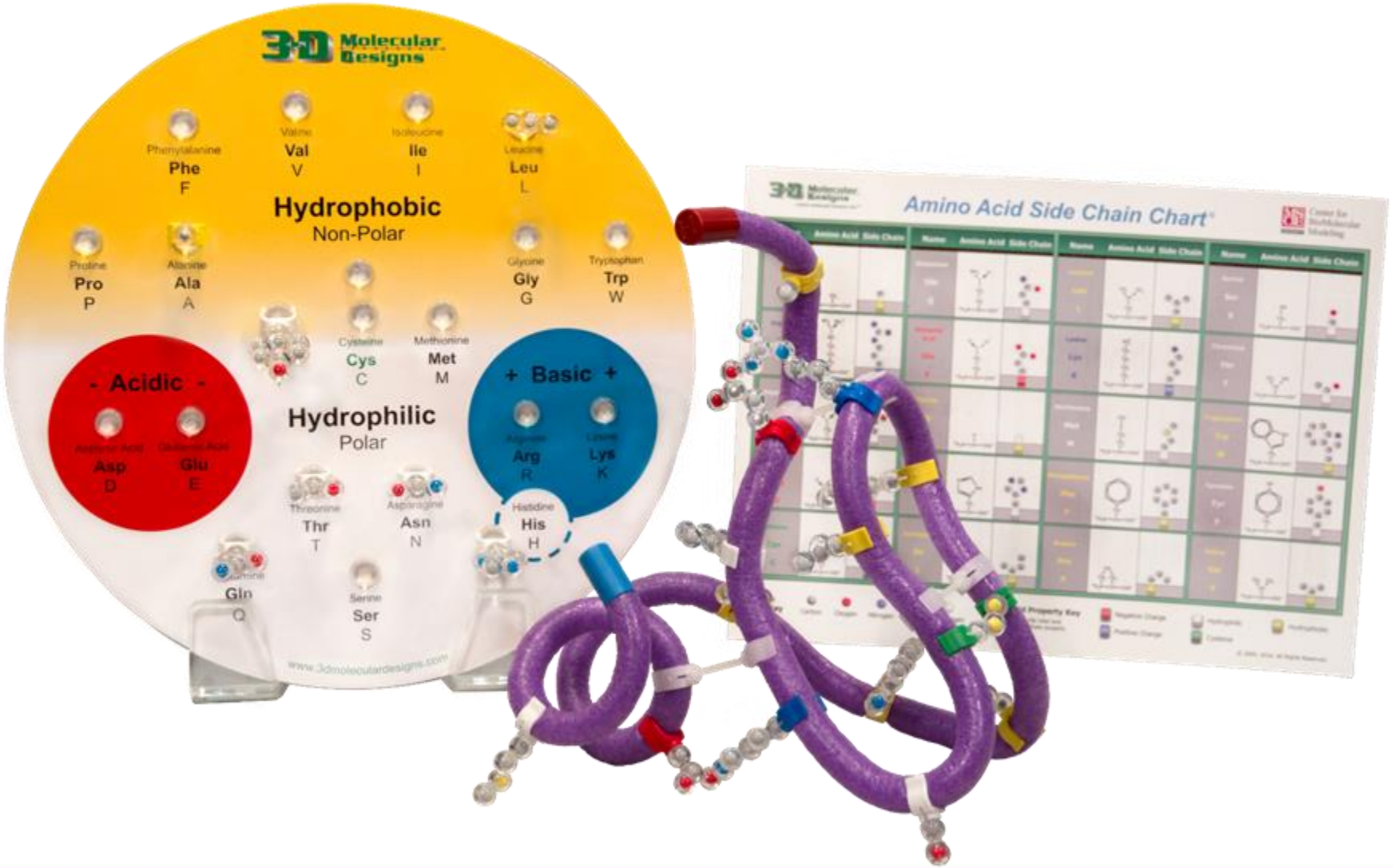
COMPARING ACIDS AND BASES

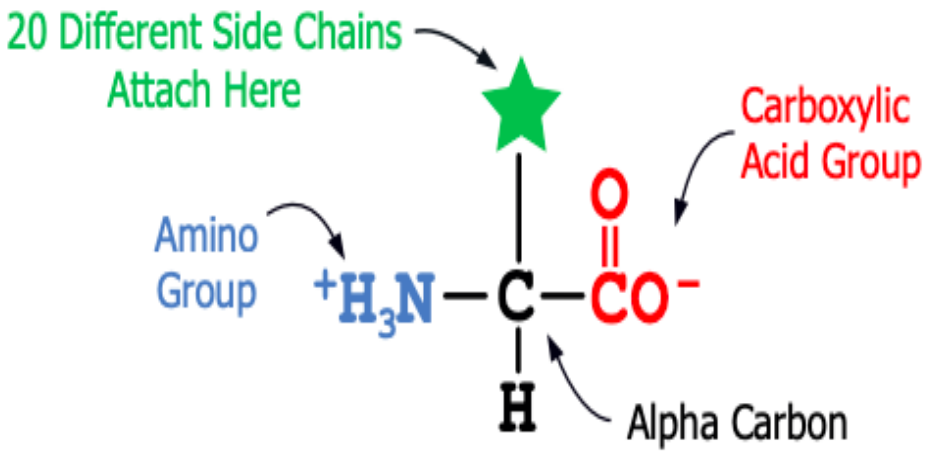
COMPARING COLD AND HEAT

Modeling Catalase‘s Active Site



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

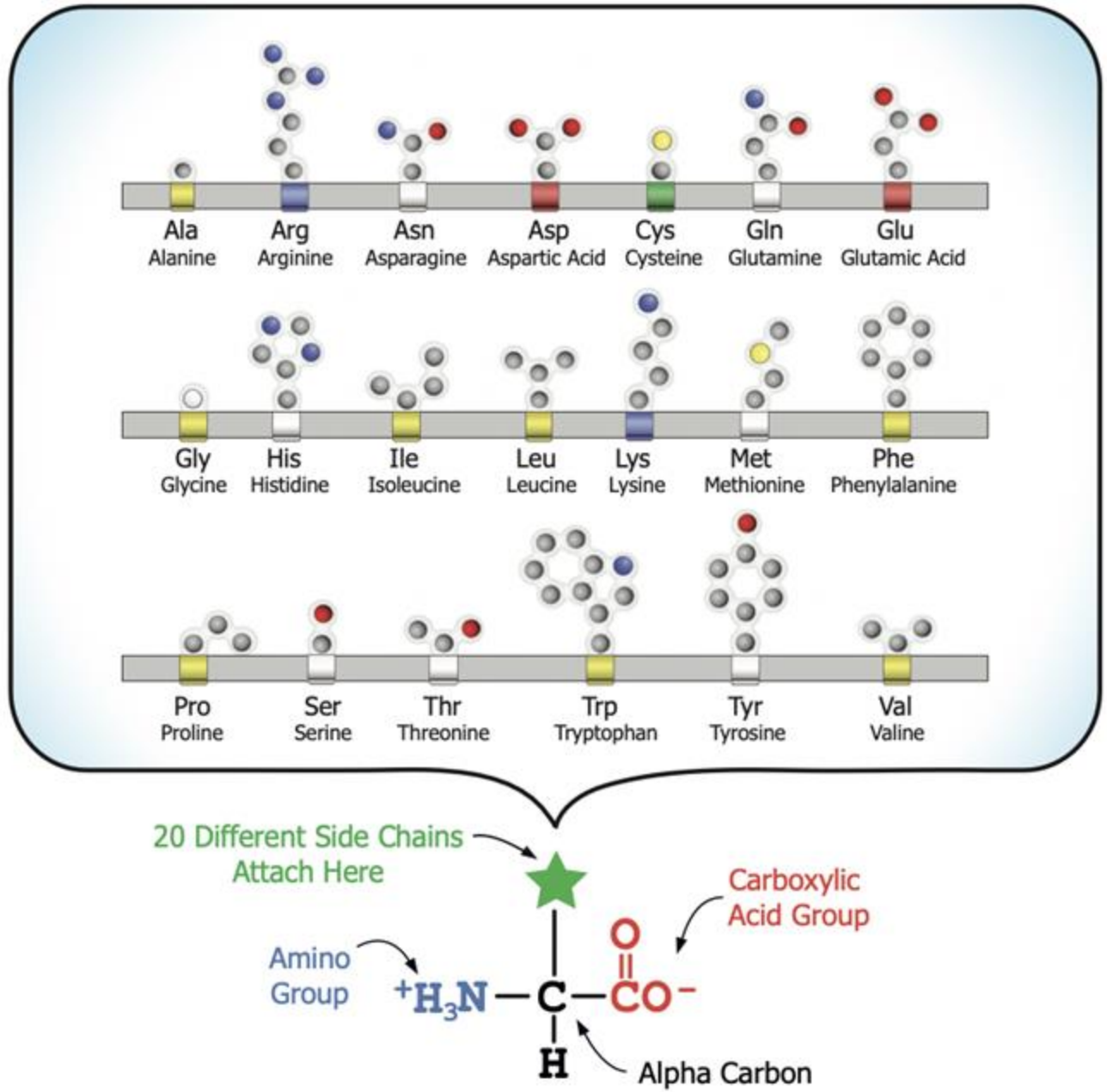

3-D Molecular Designs
Phenylalanine
Phe
F
Valine
Val
V
Isoleucine
Ile
I
Leucine
Leu
L
Hydrophobic
Non-Polar
Proline
Pro
P
Alanine
Ala
A
Glycine
Gly
G
Tryptophan
Trp
W
Cysteine
Cys
C
Methionine
Met
M
- Acidic -
Aspartic Acid
Asp
D
Glutamic Acid
Glu
E
Hydrophilic
Polar
+ Basic +
Arginine
Arg
R
Lysine
Lys
K
Threonine
Thr
T
Asparagine
Asn
N
Histidine
His
H
Glutamine
Gln
Q
Serine
Ser
S
www.3dmoleculardesigns.com
Amino Acid Side Chain Chart

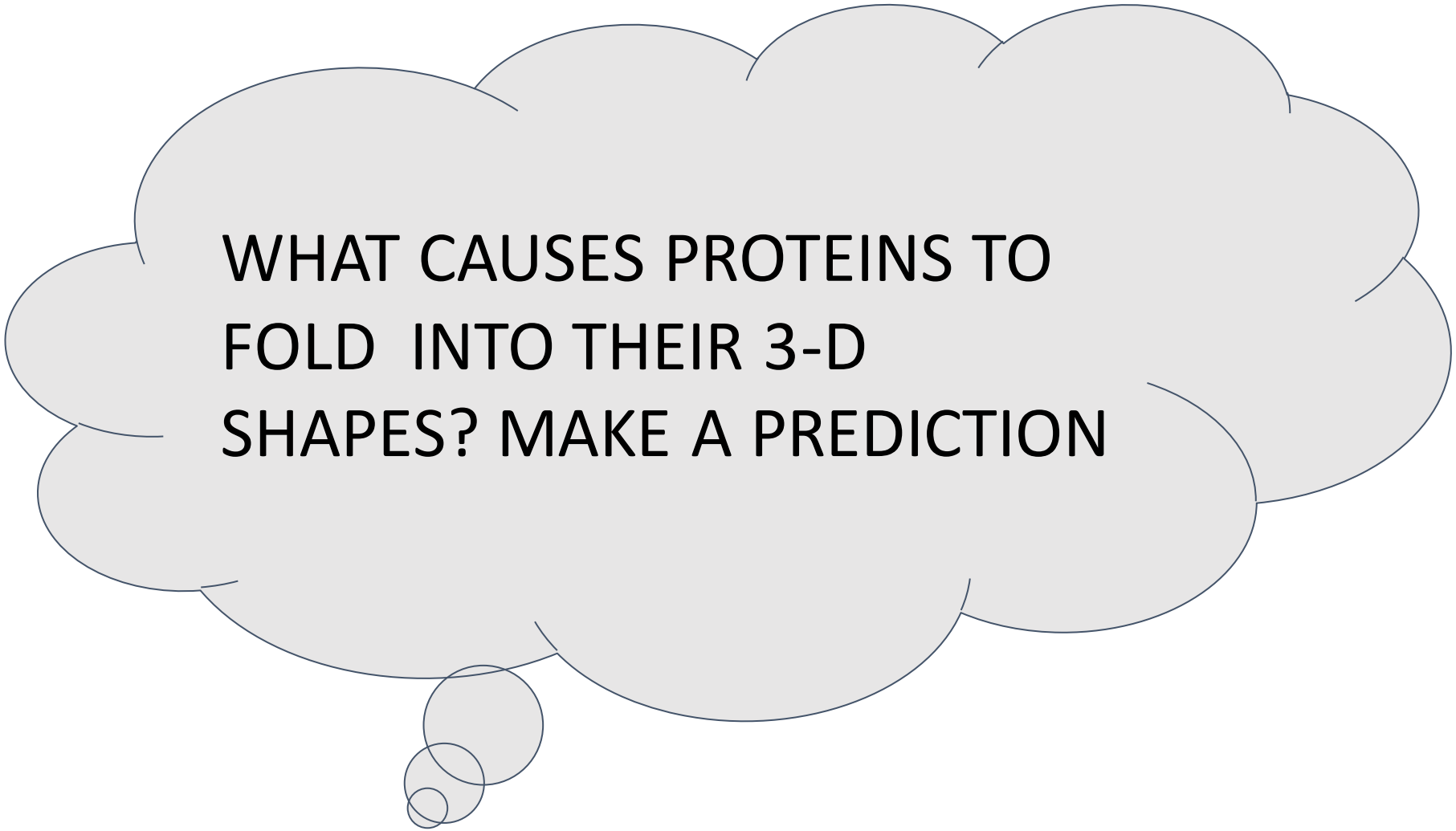

20 Different Side Chains
Attach Here
Carboxylic
Acid Group
Amino
Group
+H3N
C
CO-
O
H
Alpha Carbon

I notice	I wonder

WHAT PATTERNS DO YOU SEE AMONG THE SIDE CHAINS?

WHAT QUESTIONS DO YOU HAVE?


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
O
CO^{-}
H
Alpha Carbon


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

3d molecular designs

KEY

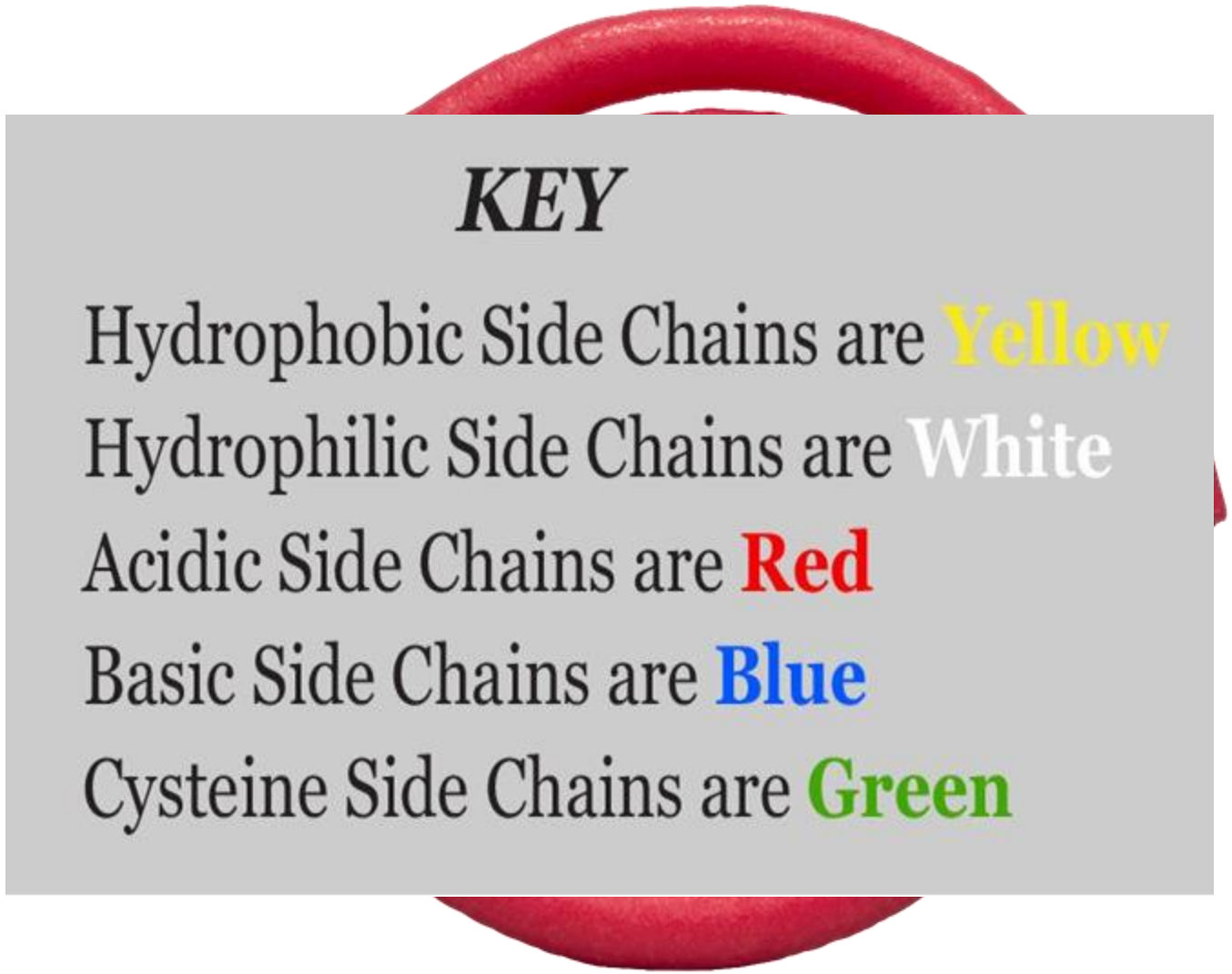
Hydrophobic Side Chains are **Yellow**

Hydrophilic Side Chains are **White**

Acidic Side Chains are **Red**

Basic Side Chains are **Blue**

Cysteine Side Chains are **Green**



SIX HYDROPHOBIC

THREE HYDROPHILIC

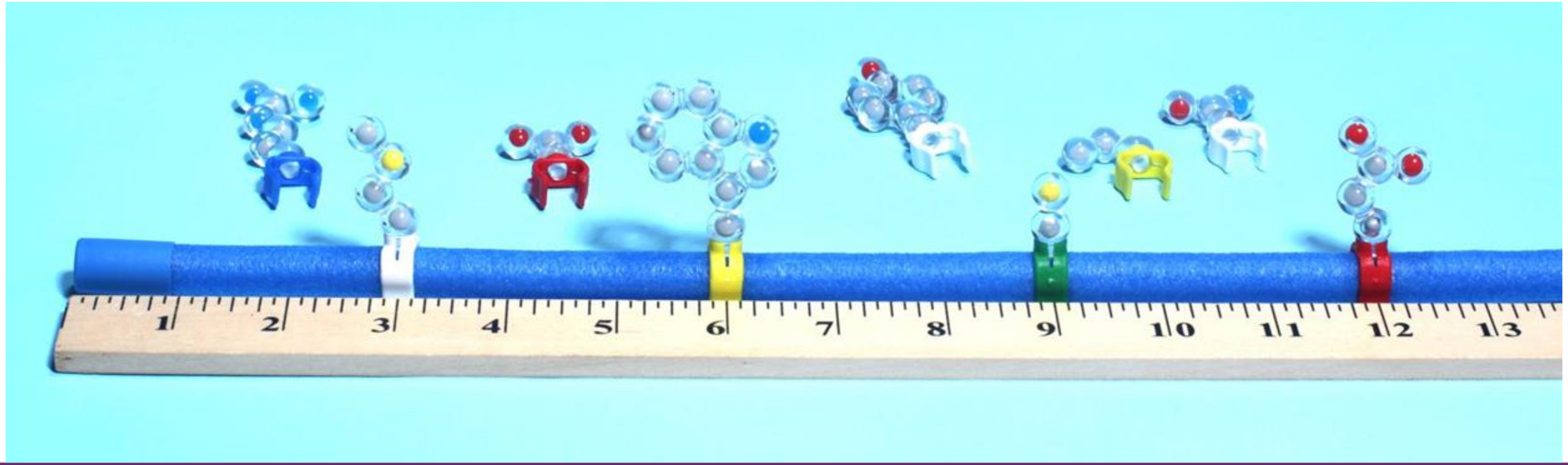
TWO ACIDIC

TWO BASIC

TWO CYSTEINE

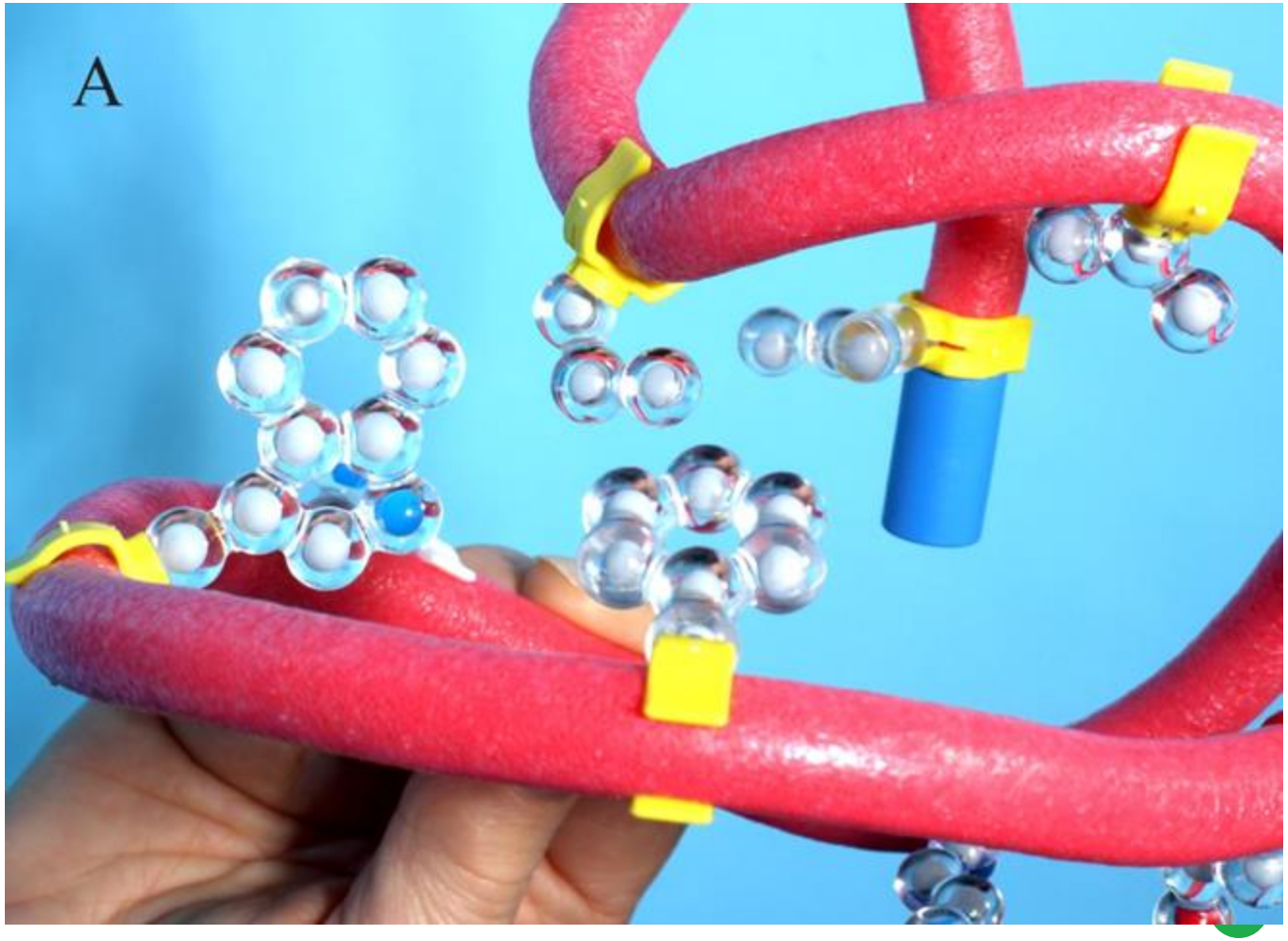
A TOTAL OF FIFTEEN SIDE CHAINS

IN ANY ORDER ARRANGE YOUR AMINO ACIDS
EQUIDISTANT FROM EACH OTHER.
YOU HAVE MADE A POLYPEPTIDE.



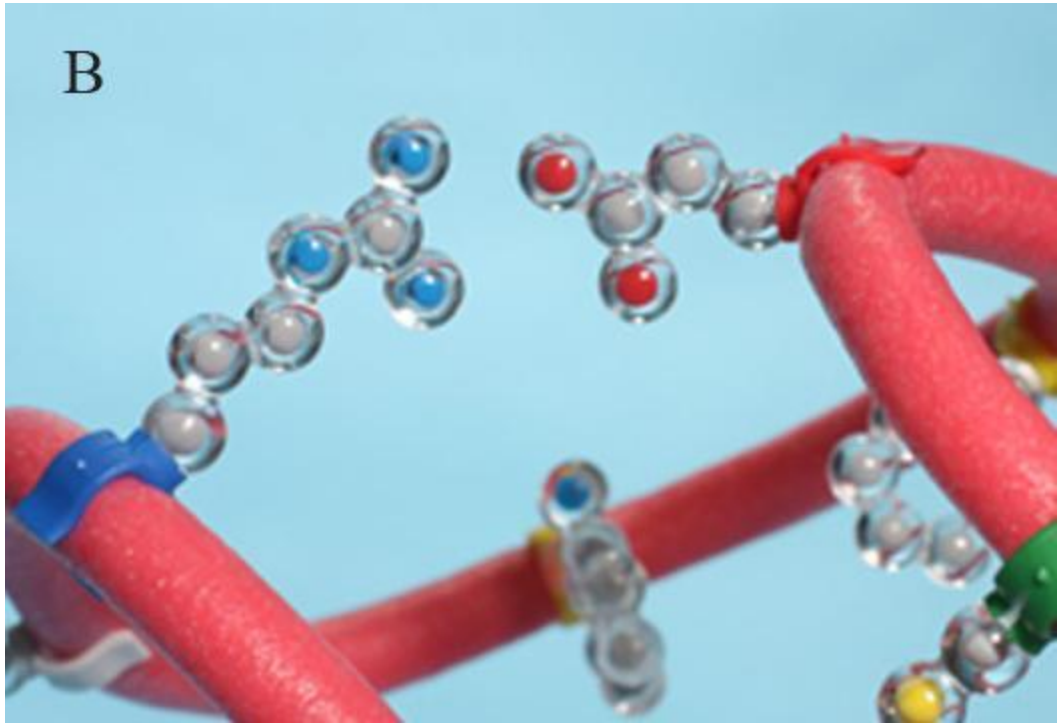
LET’S “FOLD” IT INTO A PROTEIN

ROTATE THE HYDROPHOBIC AMINO ACIDS TO THE INSIDE



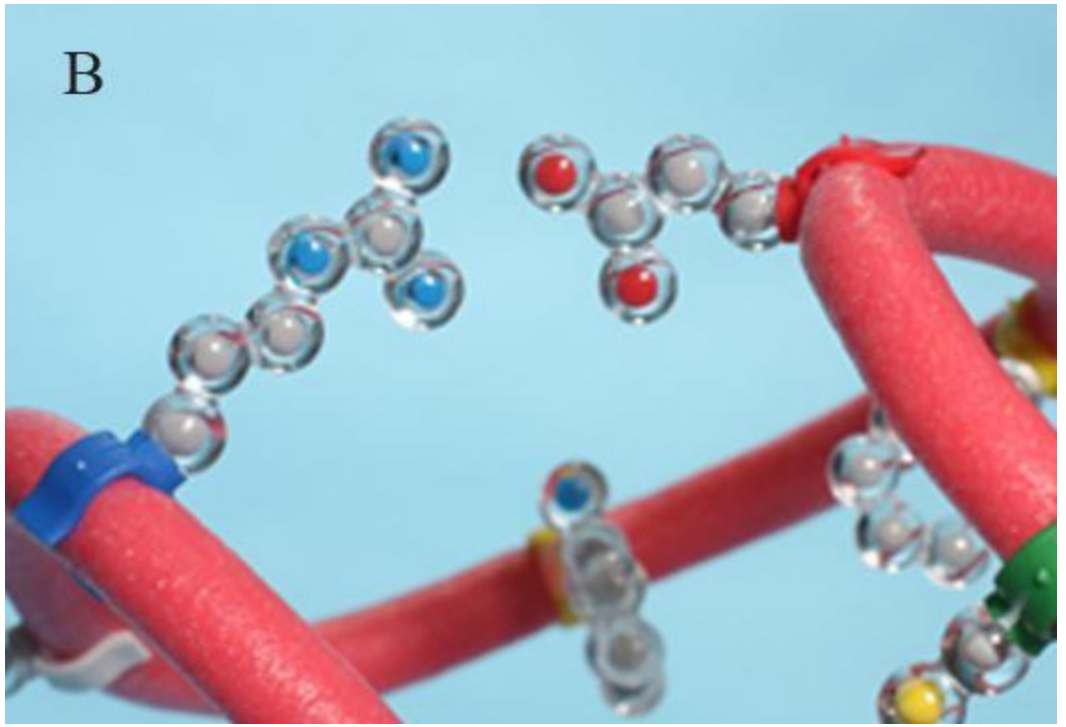
CONTINUE “FOLDING”

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



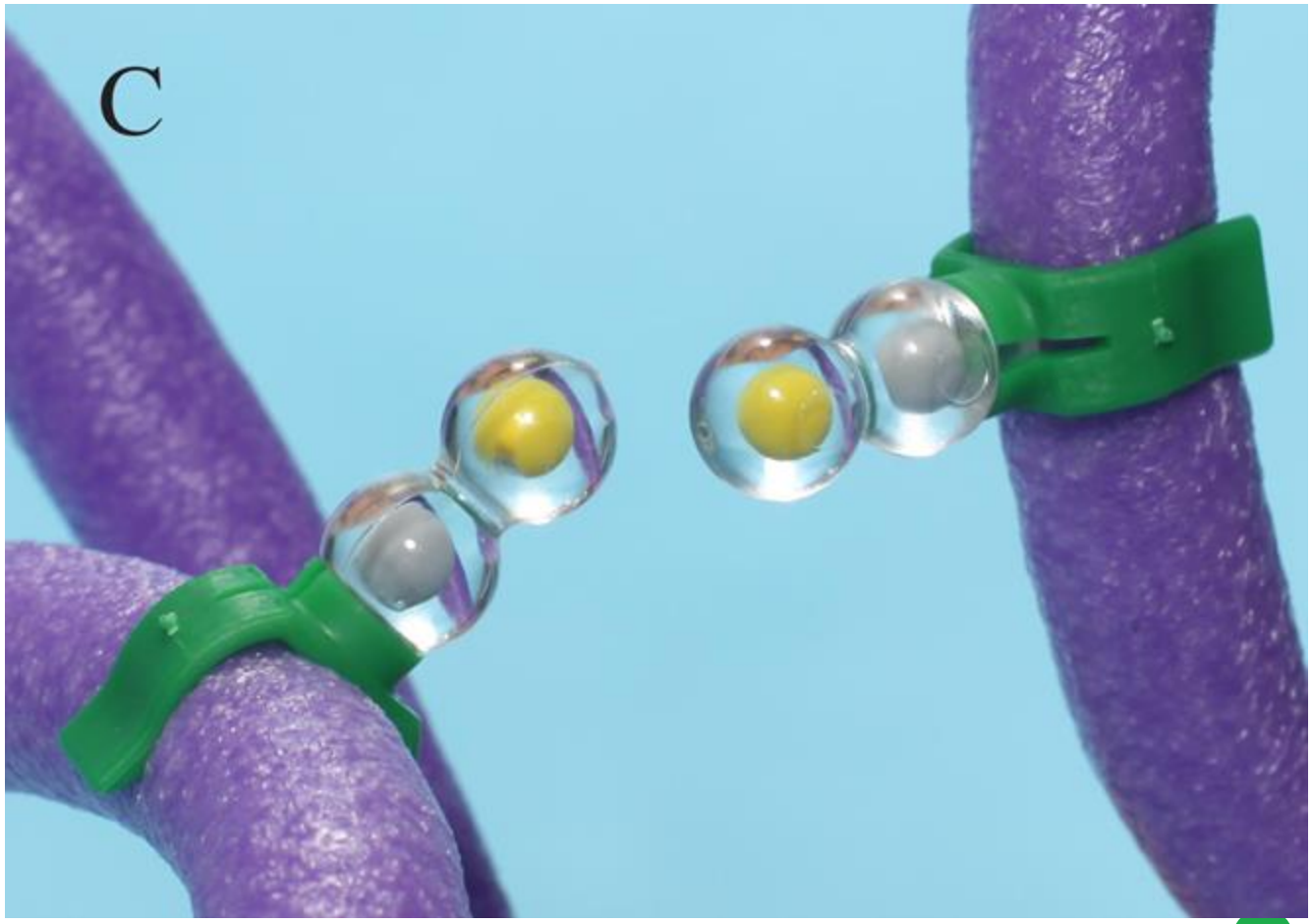
MAKE SURE THAT YOU ALSO ROTATE ANY HYDROPHOBIC SIDE CHAINS THAT MOVE OUT OF PLACE.

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



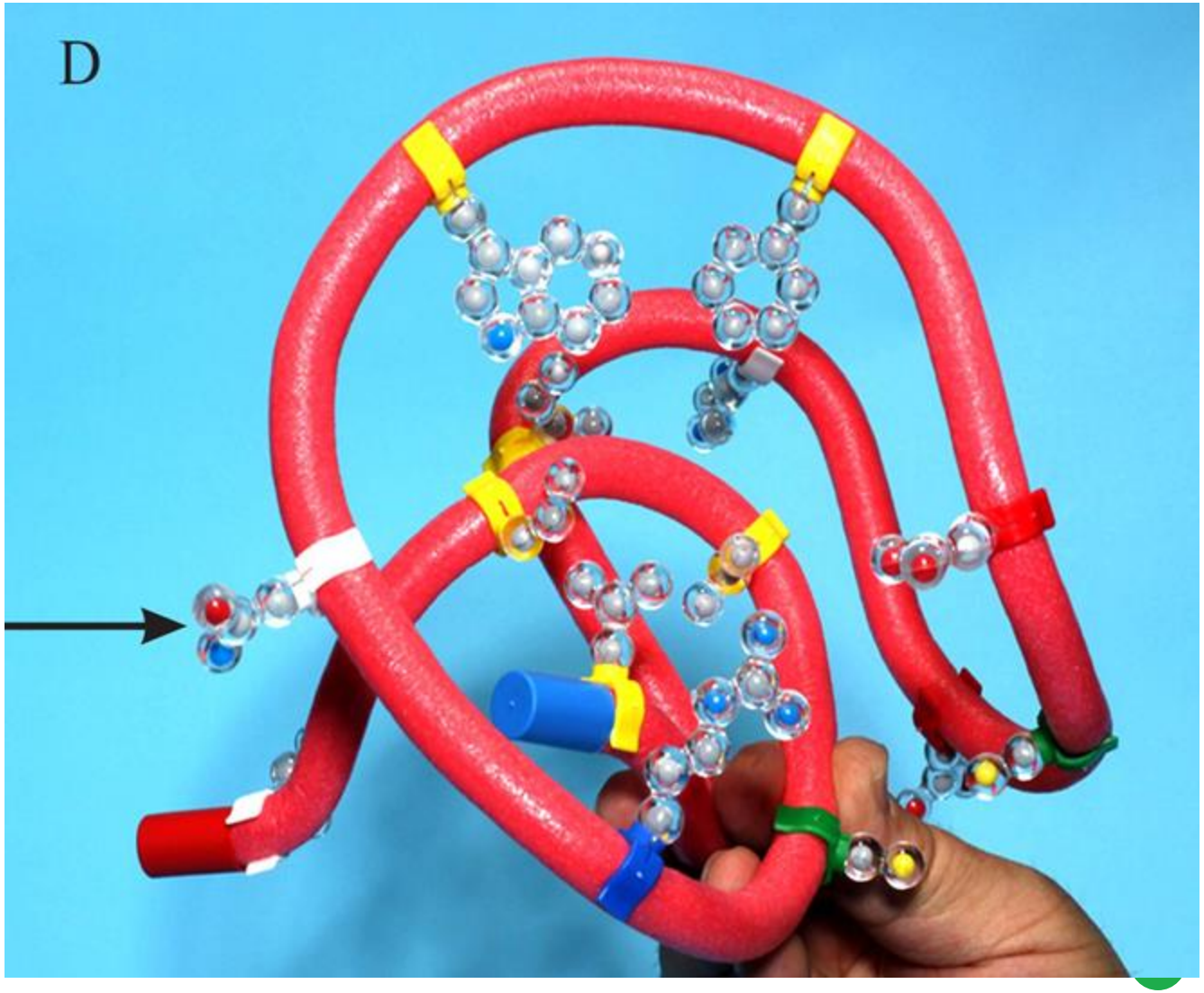
CONTINUE “FOLDING”

POSITION THE CYSTEINES SO THEY ARE OPPOSITE EACH OTHER.

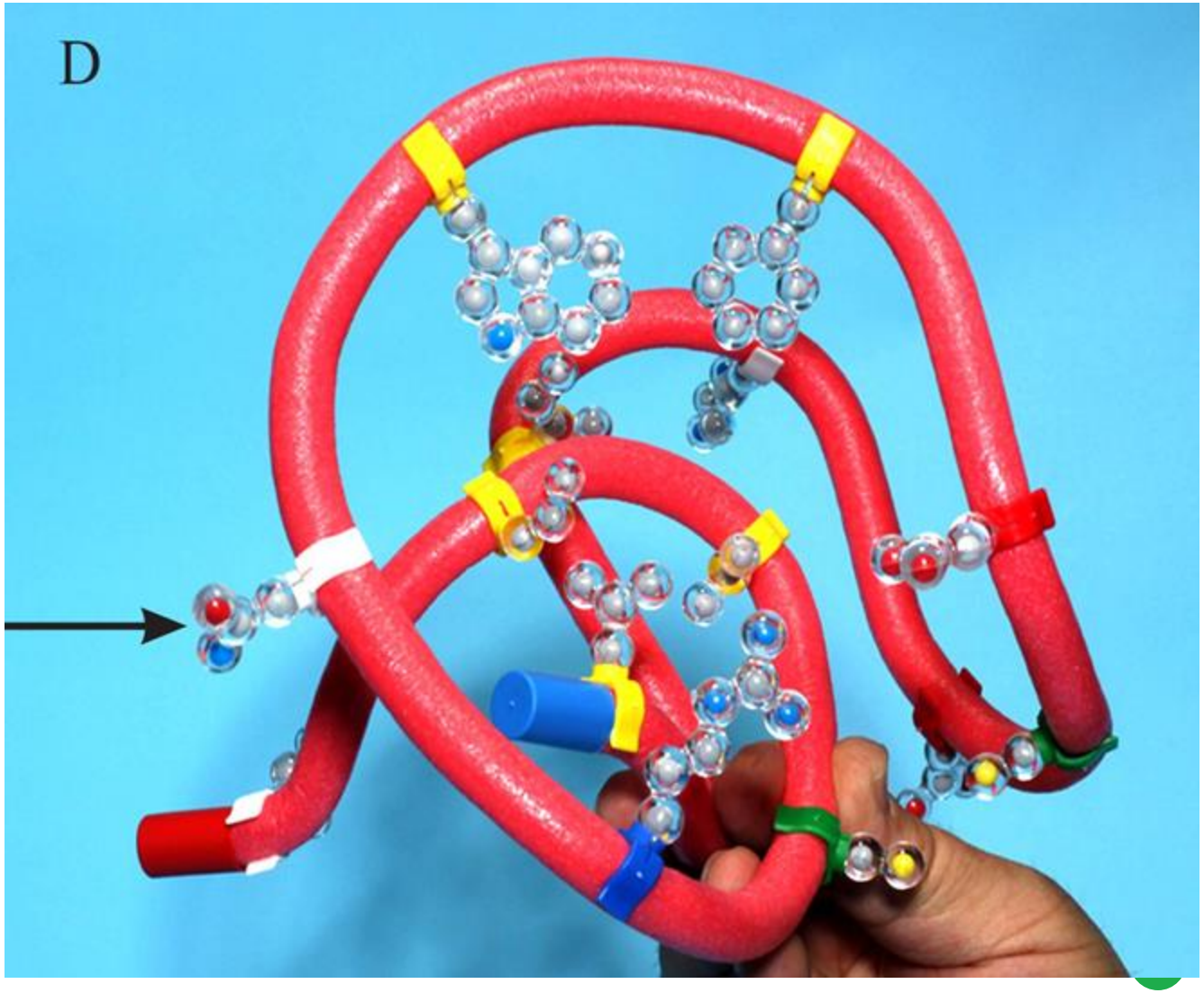


CONTINUE “FOLDING”

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



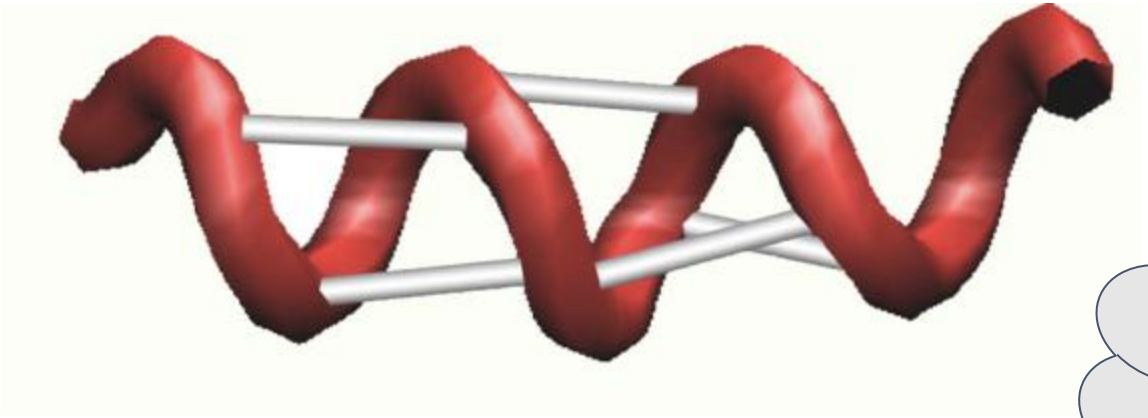
THE FINAL SHAPE OF THE PROTEIN IS CALLED THE TERTIARY STRUCTURE



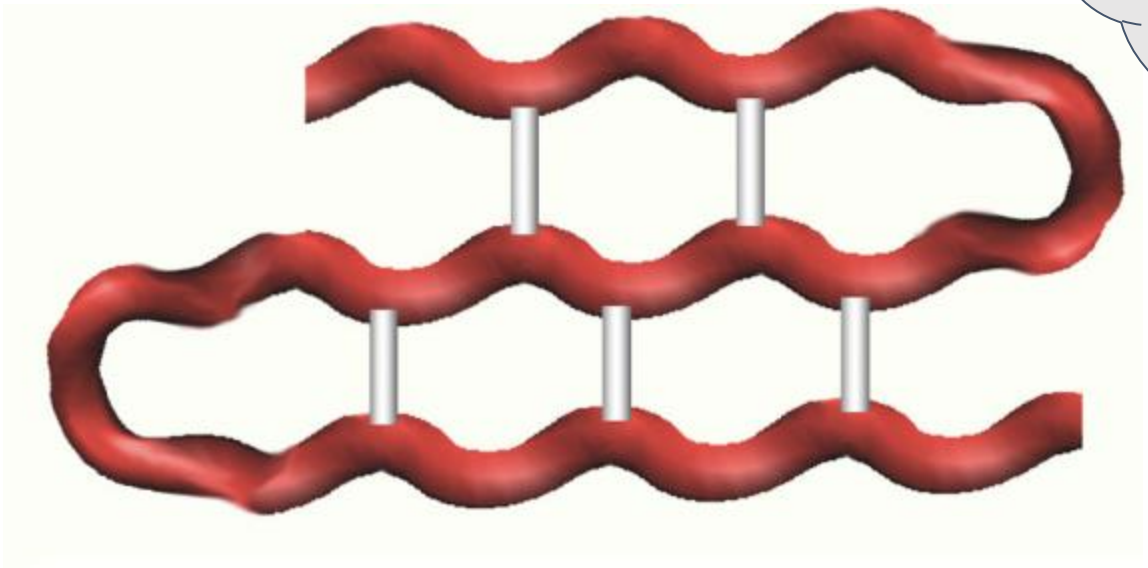

WHY DIDN’T YOUR PROTEINS ALL LOOK THE SAME?

THE IMPORTANCE OF SECONDARY STRUCTURE

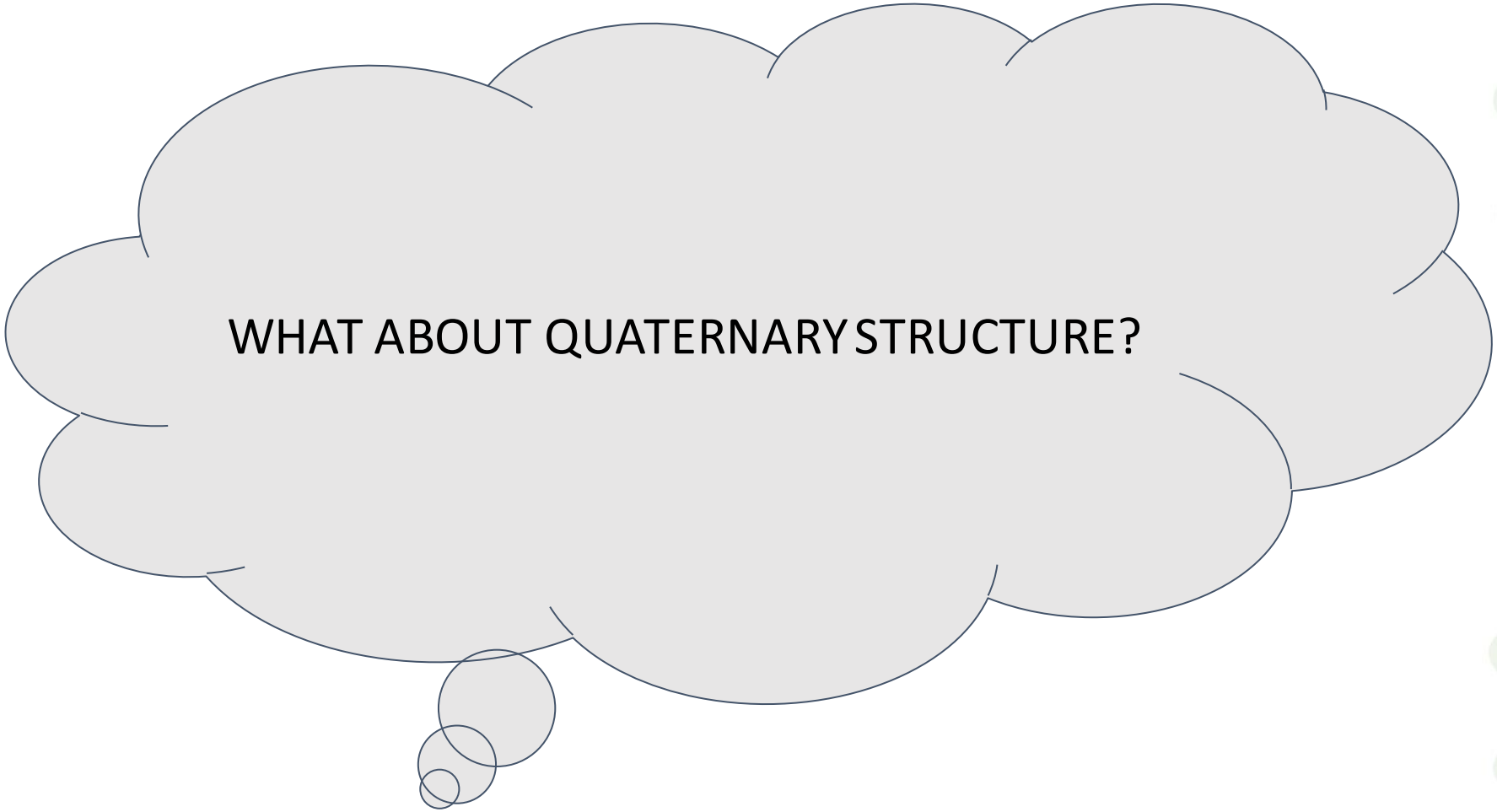
ALPHA HELIX



BETA SHEET

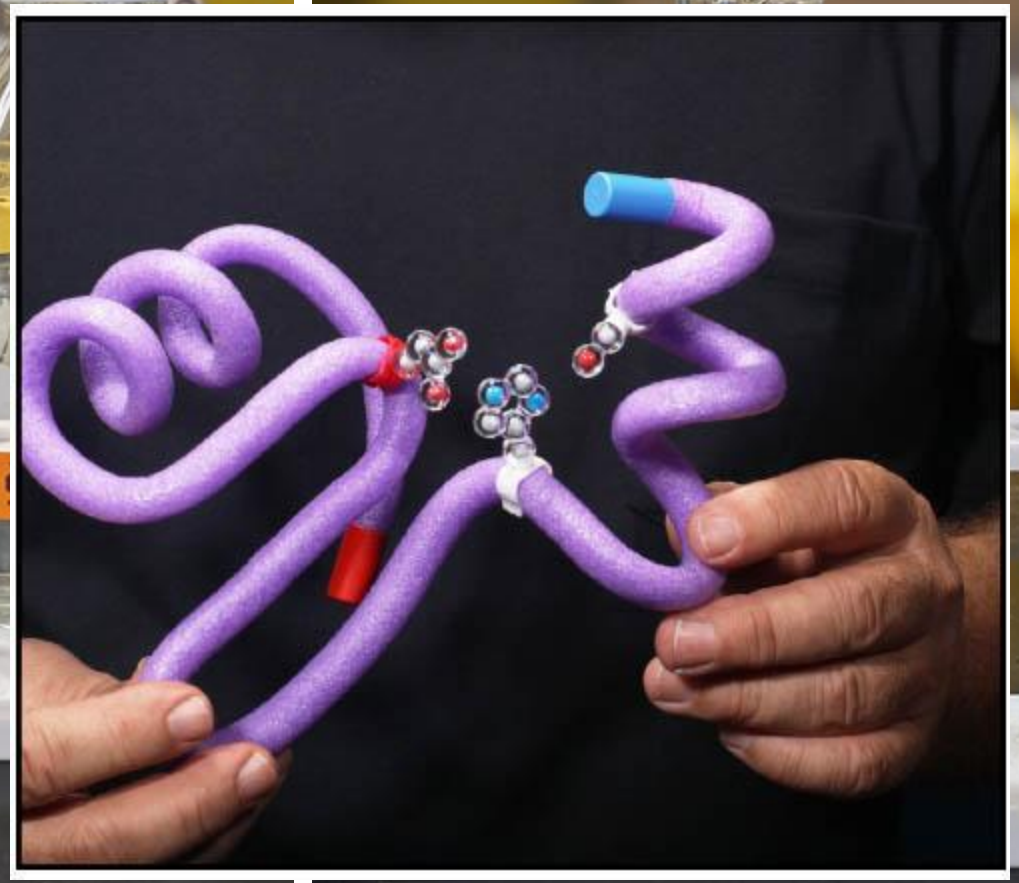


HOW DO SECONDARY STRUCTURES STABILIZE A PROTEIN?

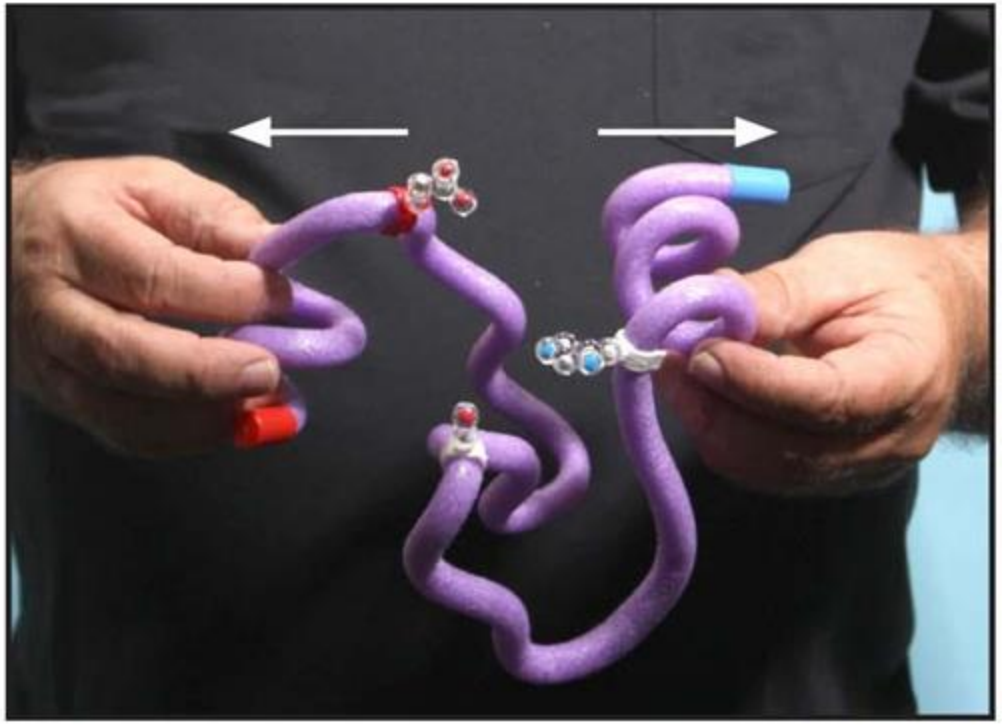

WHAT ABOUT QUATERNARY STRUCTURE?

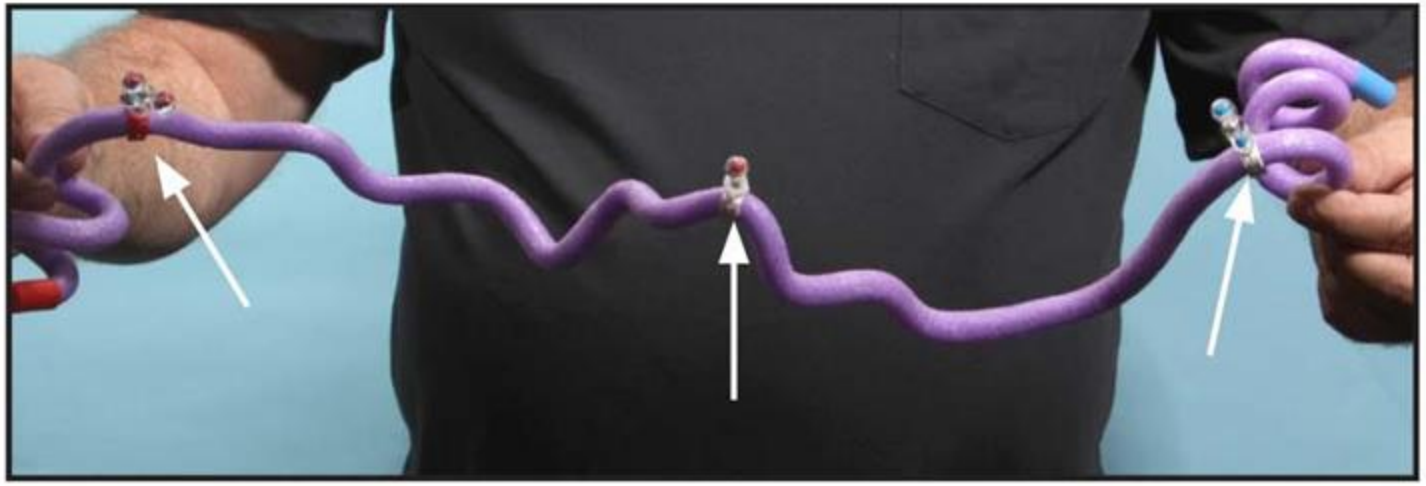
COMPARING ACIDS AND BASES

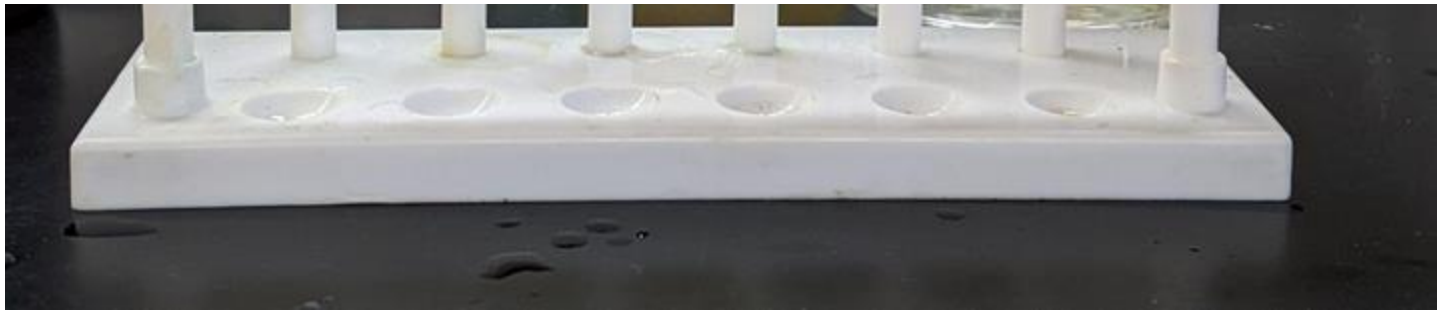
COMPARING ACIDS AND BASES



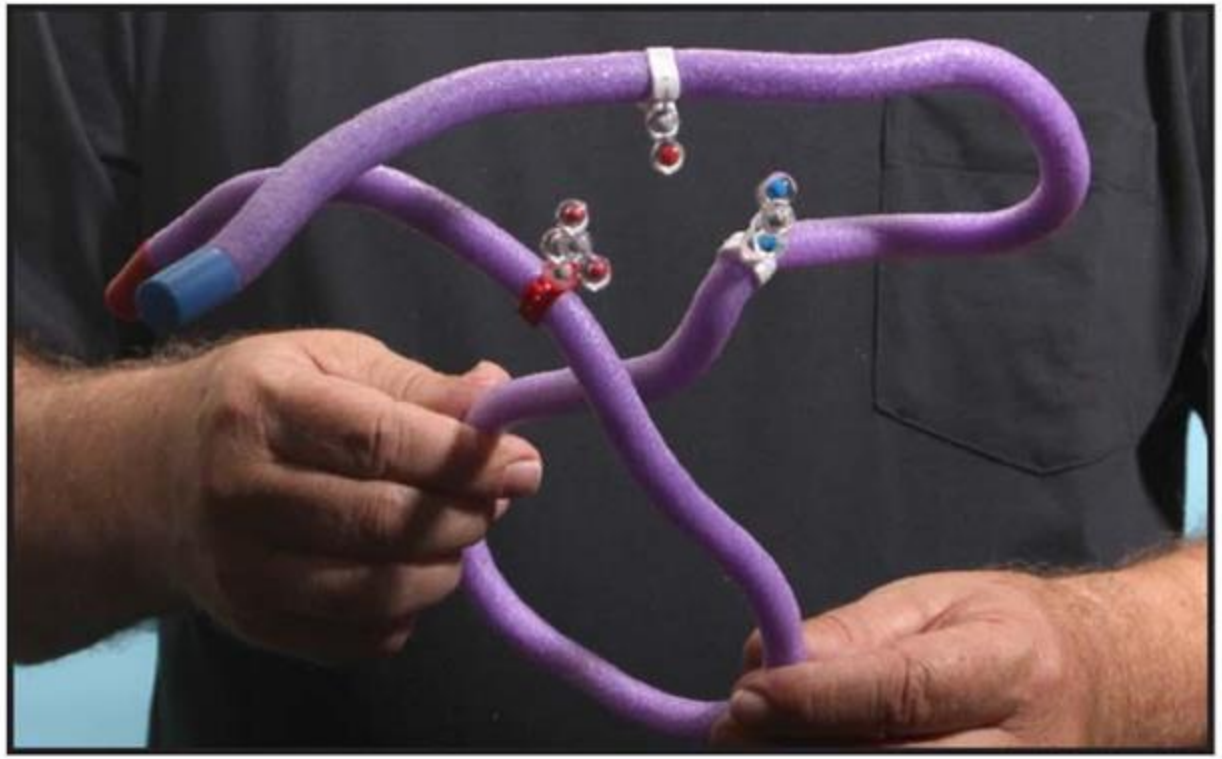
COMPARING ACIDS AND BASES

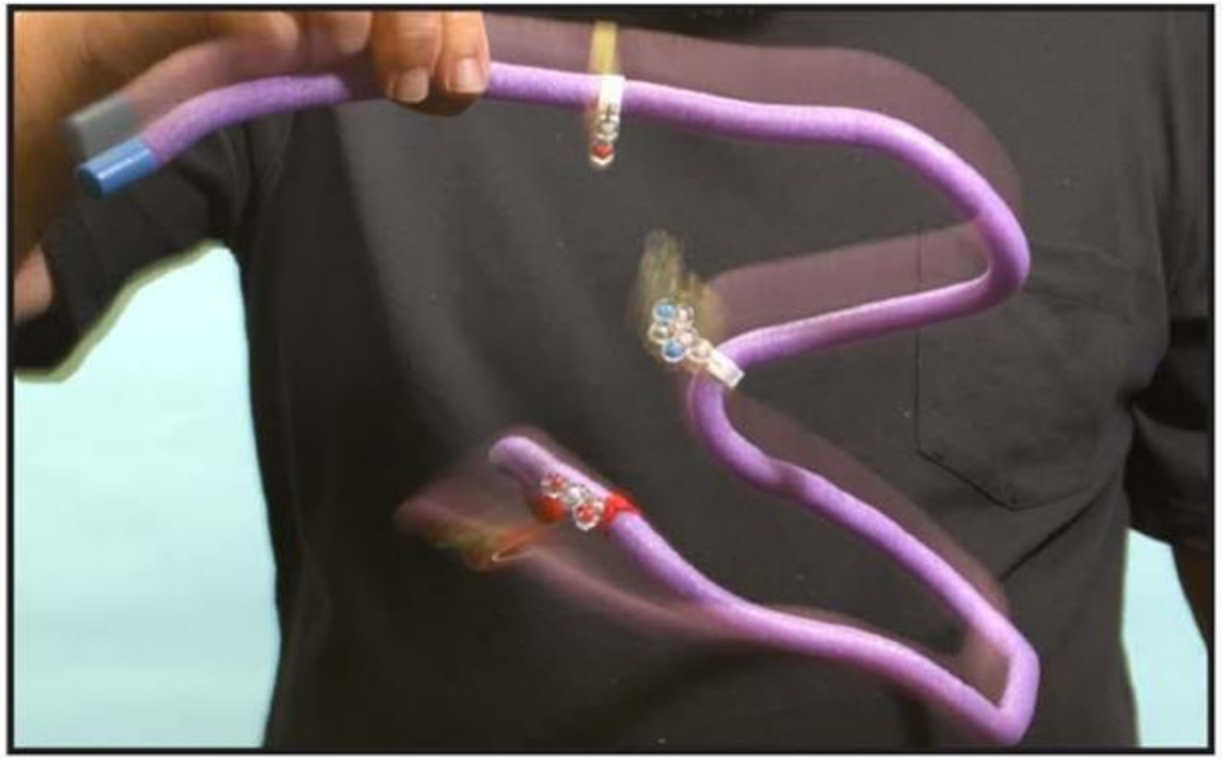






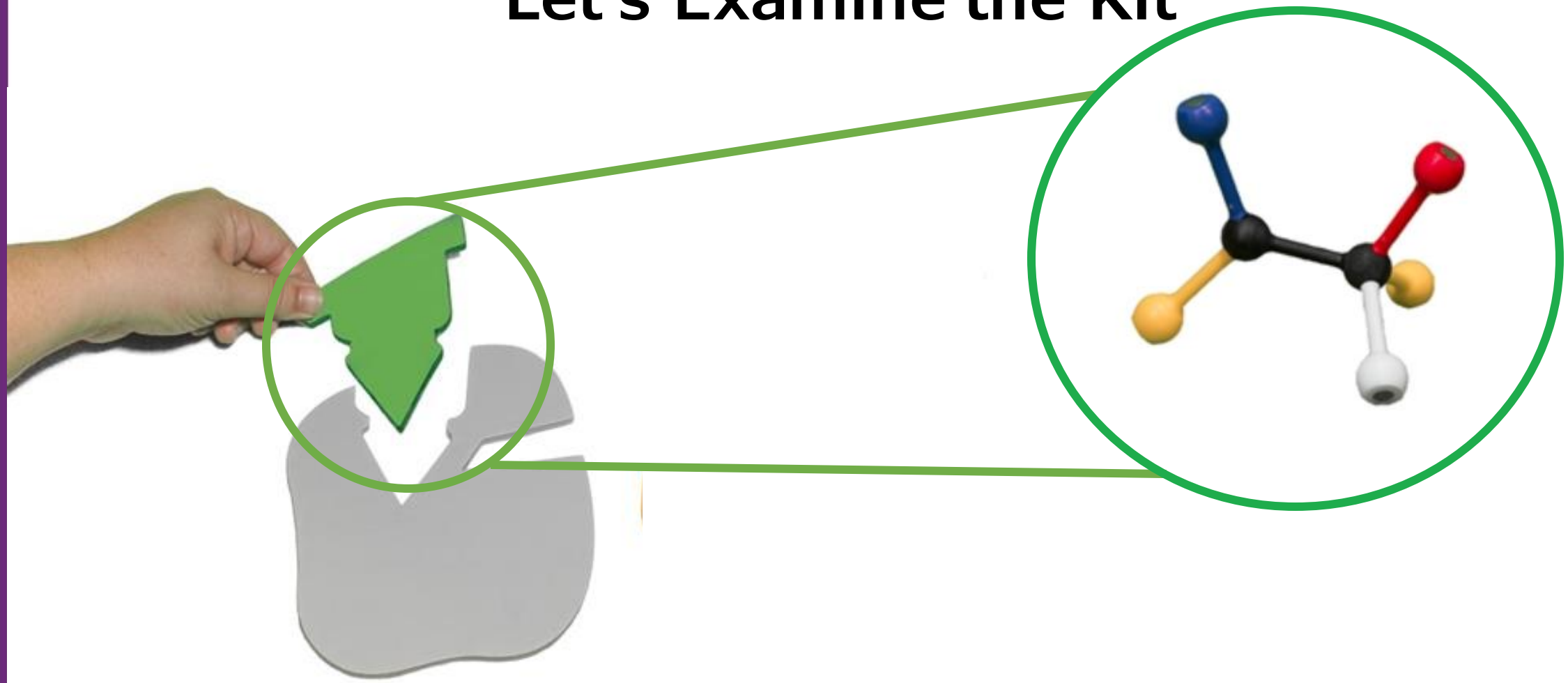
COMPARING ACIDS AND BASES



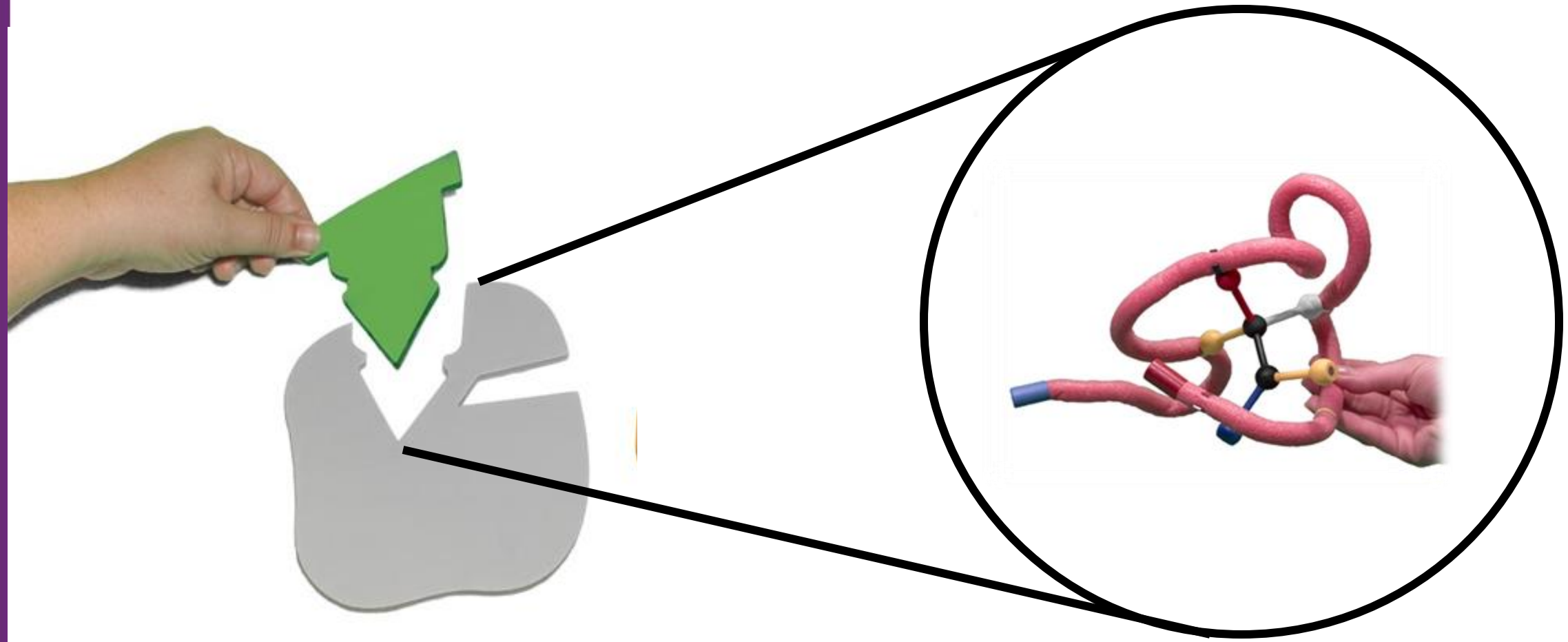


COMPARING COLD AND HEAT

Let's Examine the Kit

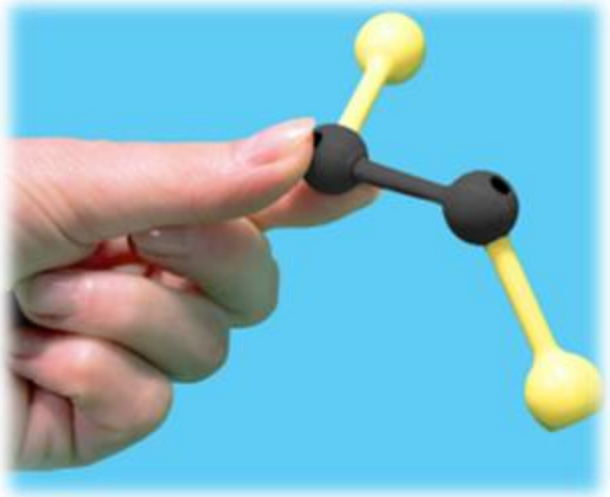


Let's Examine the Kit



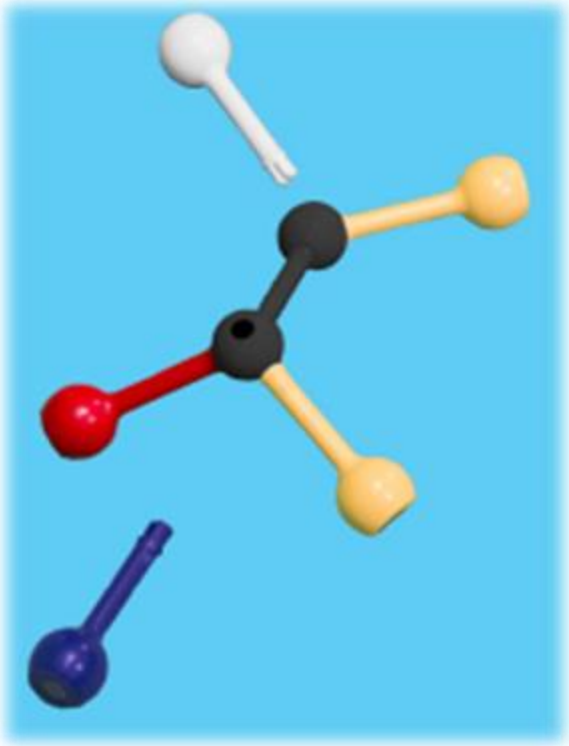
Assembling the Substrate

- Select the piece with the black 4-hole sphere and 2-hole sphere.
- Connect one yellow functional group to the four-hole sphere.
- Connect the other yellow functional group to the two-hole sphere.
- Connect the remaining functional groups randomly.



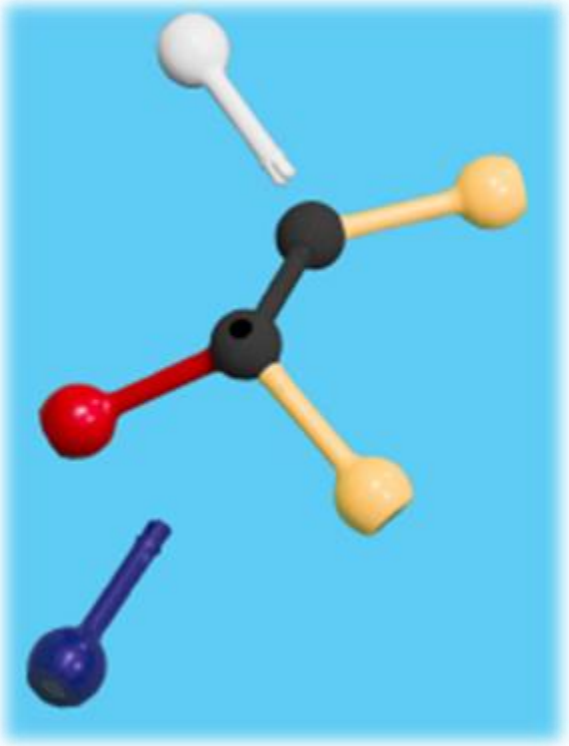
Examining the Substrate Model

Functional group color	Chemical property	Type of bond/interaction
Red		
Blue		
White		
Yellow		
Green		



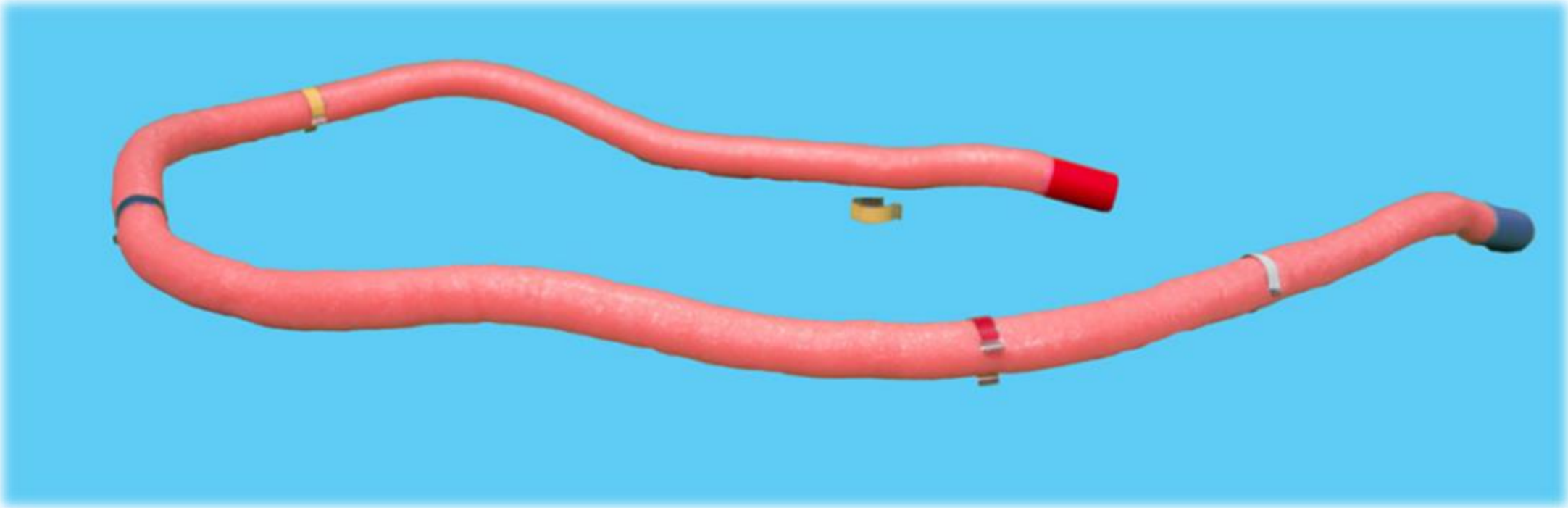
Examining the Substrate Model

Amino acid R-group color	Chemical property	Type of bond/interaction
Red	Acidic Negative Charge	Salt Bridge
Blue	Basic Positive Charge	Salt Bridge
White	Hydrophilic	Polar
Yellow	Hydrophobic	Nonpolar
Green	Cysteine	Disulfide Bonds



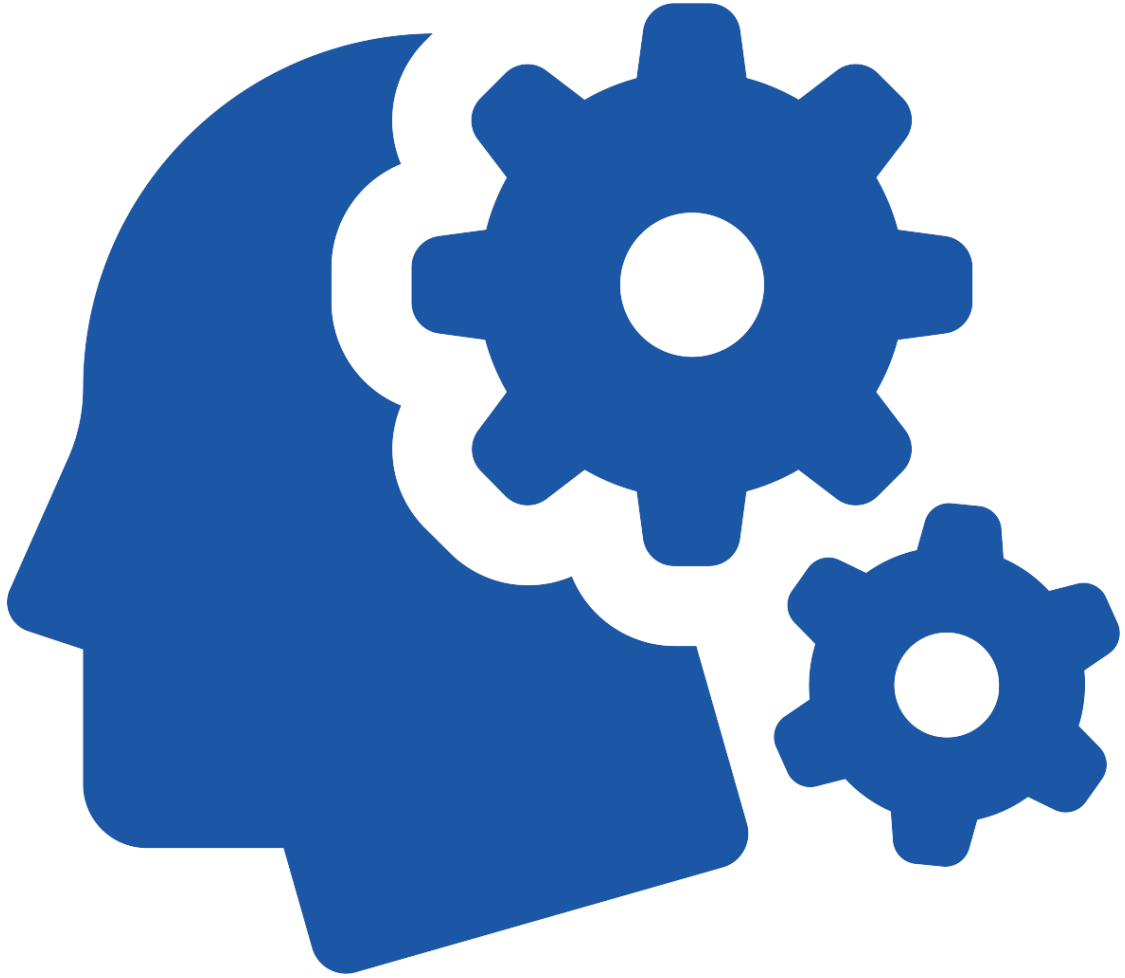
Assembling the enzyme

- Place the metal clips along the entire length and in random order on the 3-foot mini toober.



Constructing the Enzyme-Substrate Complex

- Fold the mini-toober around the substrate
- Follow the basic principles of chemistry as design the complex
- Remember that your complex should be three-dimensional



Catalase

Catalase protects us from dangerous reactive oxidizing molecules

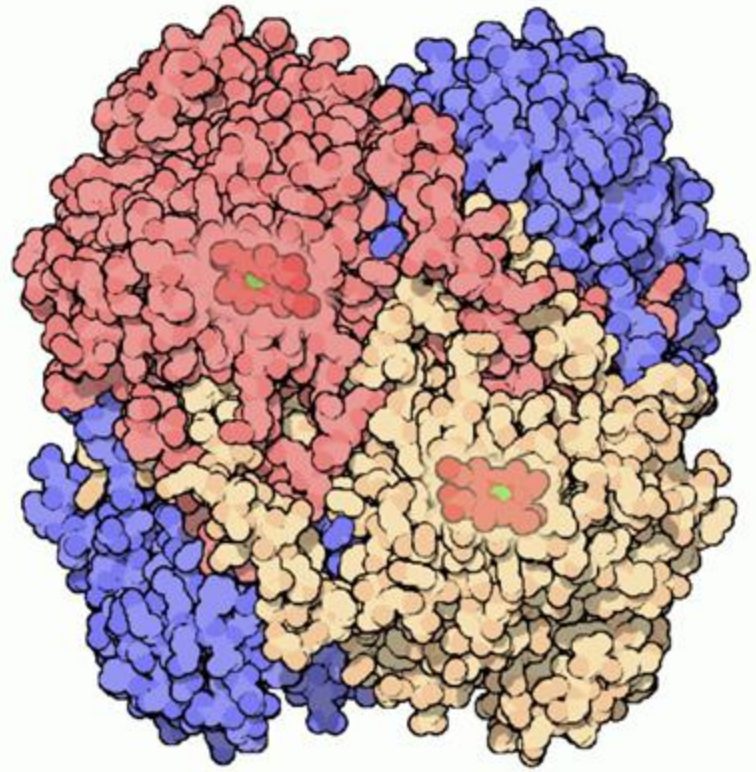
Living with oxygen is dangerous. We rely on oxygen to power our cells, but oxygen is a reactive molecule that can cause serious problems if not carefully controlled. One of the dangers of oxygen is that it is easily converted into other reactive compounds. Inside our cells, electrons are continually 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.

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

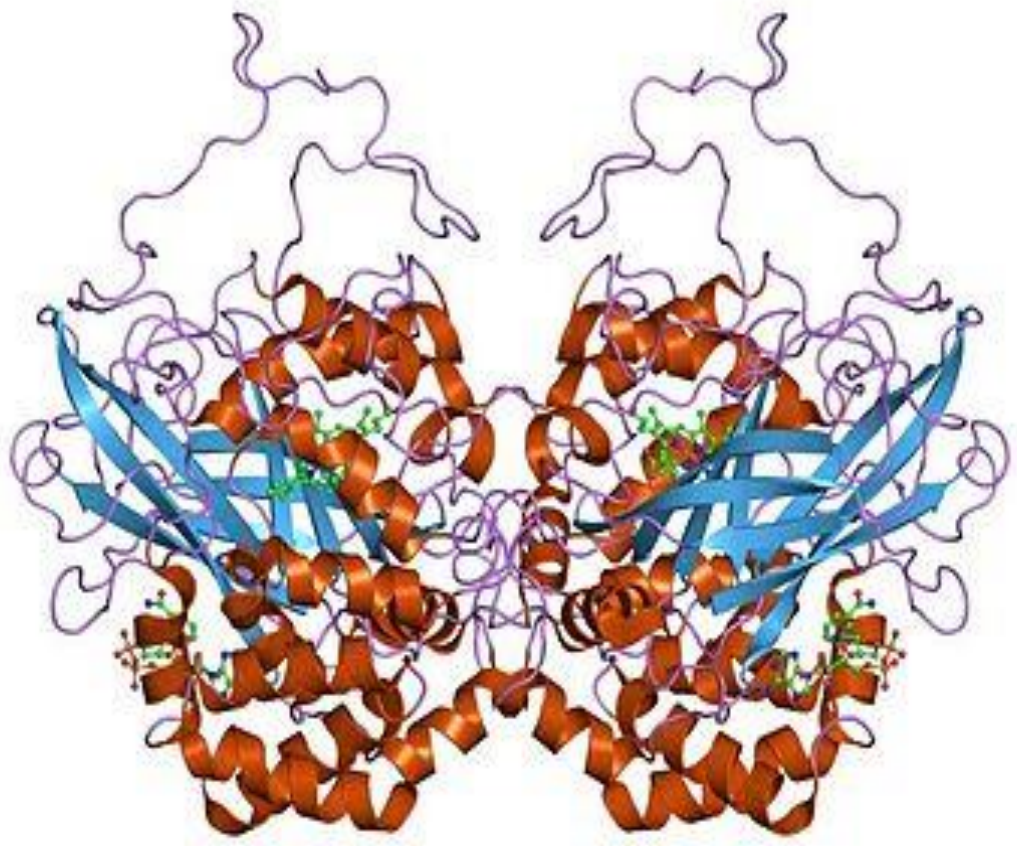
Catalases are some of the most efficient enzymes found in cells. Each catalase molecule can decompose millions of hydrogen peroxide molecules every second. The cow catalase shown here (PDB entry 8cat) and our own catalases use an iron ion to assist in this speedy reaction. The enzyme is composed of four 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.



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

Download high quality TIFF image

Jmol Exploration of Catalase



CBM - Catalase (msoe.edu)

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**	**Georgia Standard: SB1**
	Stability and Change	**Georgia Standard: SB2**
	Scale, Proportion, and Quantity	

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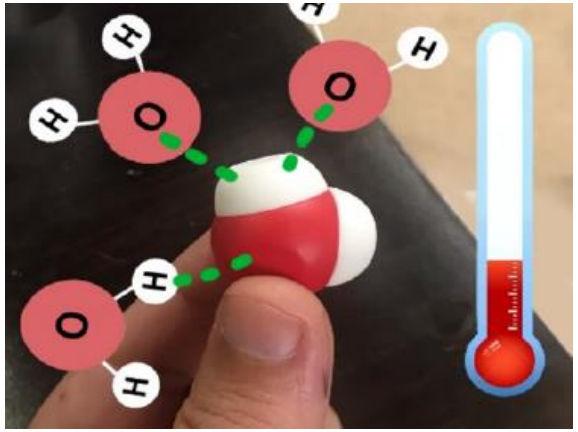
AR Enhancements

We're enhancing our kits and models to inspire more hands-on learning with new augmented reality features!



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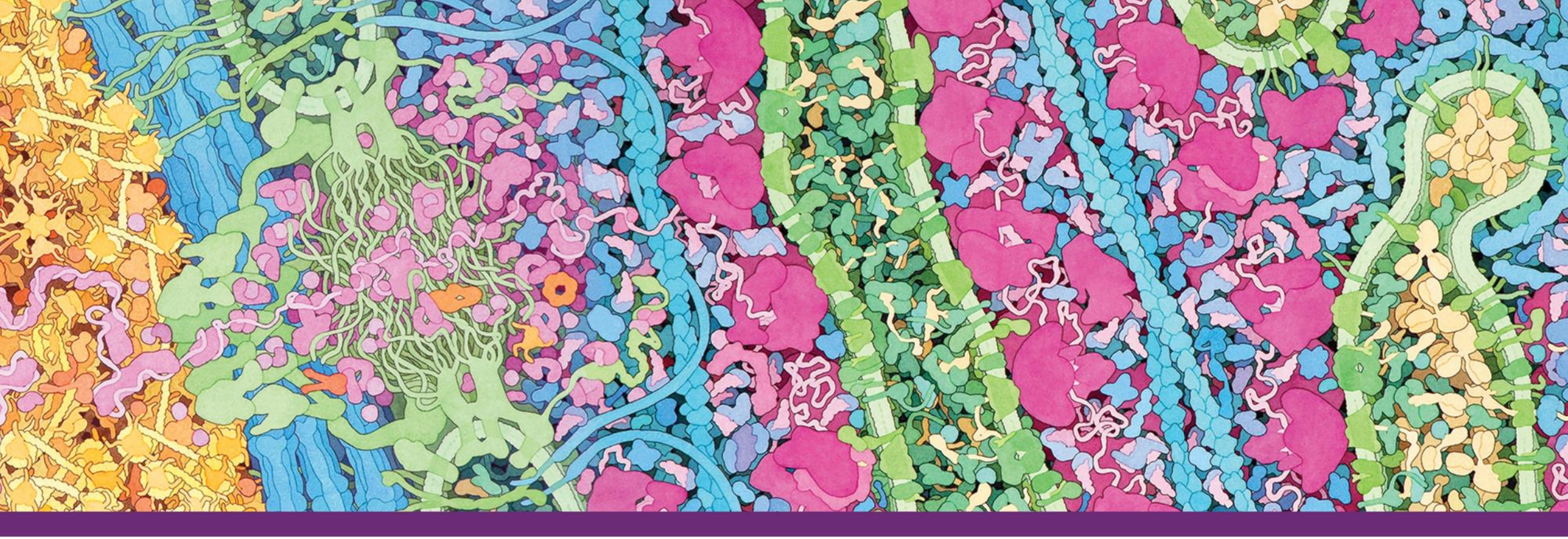
Augmented Reality Enhancements!

We value your opinion! Let us know what you think.

Scan the QR Code and complete this short survey.



3d molecular designs

Transforming Science Learning

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