



Make the Complex Easy!

Modeling Proteins and Protein Structure

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Mary Howard



Science Teacher at Washington
Township High School in Sewell, NJ



Mary Howard Basic Background



- **Education:**

- Biochemistry
- Physiology
- Education

- **Experience:**

- Researcher
- Instructor

- **Science Classroom Strategies**

- Lectures
- Digital Activities
- Laboratory Activities
- Projects
- Assessments

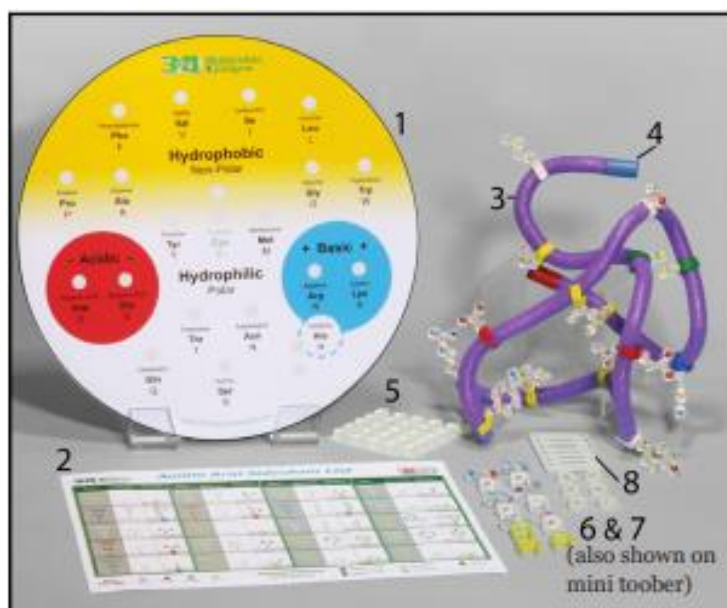


Icebreaker

Let's Get Talking with
Conversation Cubes



Amino Acid Starter Kit





where molecules become real™



Student Handout 1

Amino Acids - Building Blocks of Proteins

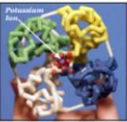
Introduction

Proteins are more than an important part of your diet. Proteins are complex molecular machines that are involved in nearly all of your cellular functions. Each protein has a specific shape (**structure**) that enables it to carry out its specific job (**function**).

A **core idea** in the life sciences is that *there is a fundamental relationship between a biological structure and the function it must perform*. At the macro level, Darwin recognized that the structure of a finch's beak was related to the food it ate. This fundamental structure-function relationship is also true at all levels below the macro level, including proteins and other structures at the molecular level. For two examples of proteins and their functions, see the photos and outlines at the right.

In this activity, you will explore the structure of proteins and the chemical interactions that drive each protein to fold into its specific structure, as noted below.

- Each protein is made of a specific sequence of **amino acids**. There are 20 amino acids found in proteins.
- Each amino acid consists of two parts -- a **backbone** and a **side chain**. The backbone is the same in all 20 amino acids and the side chain is different in each one.
- Each side chain consists of a unique combination of atoms which determines its 3D shape and its chemical properties.
- Based on the atoms in each amino acid side chain, it could be **hydrophobic**, **hydrophilic**, **acidic (negatively charged)**, or **basic (positively charged)**.
- When different amino acids join together to make a protein, the unique properties of each amino acid determine how the protein folds into its final 3D shape. The shape of the protein makes it possible to perform a specific function in our cells.



The potassium channel (shown) spans cell membranes and regulates the passage of potassium ions in and out of cells. It folds into a "pore" for the potassium ions to pass through.



The hemoglobin protein (shown) transports oxygen in blood. It accomplishes this with the heme group (yellow structure in photo) to which an iron atom binds in the heme group. Other proteins perform other functions.

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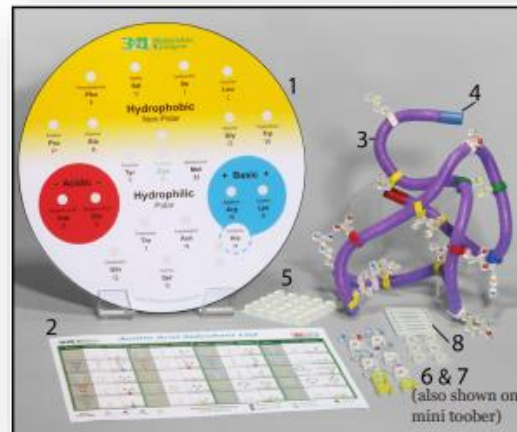
Student Handout 1 • Page 1

Resources found at:
https://3dmoleculardesigns.com/classroom_resources/flow-of-genetic-information-kit/

Resources and Materials

Kits Used in this workshop:

- Amino Acid Building Block Models
- Amino Acid Starter Kit
- Codon Chart
- Handouts



3D Molecular Designs Amino Acid Side Chain Chart®

Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain
Alanine	Ala	A	Glutamine	Gln	Q	Leucine	Leu	L	Serine	Ser	S
Aspartic Acid	Asp	D	Glutamic Acid	Glu	E	Lysine	Lys	K	Threonine	Thr	T
Asparagine	Asn	N	Histidine	His	H	Methionine	Met	M	Tyrosine	Tyr	Y
Cysteine	Cys	C	Isoleucine	Ile	I	Phenylalanine	Phe	F			

Atom Color Key
Carbon: Grey, Oxygen: Red, Nitrogen: Blue, Sulfur: Yellow, Hydrogen: White

Amino Acid Property Key
Name and color indicate property

Charge Key
Red: Negative Charge, Blue: Positive Charge

Hydrophobicity Key
Green: Hydrophobic, Yellow: Cysteine

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Let's Take A Peek!

Lab: Enzymes in Action



Enzymes
Creating Catalytic Connections

Student Handout

Objectives

You will use the model pieces in the kit to:

- Simulate enzymatic actions.
- Explain enzymatic specificity.
- Investigate two types of enzyme inhibitors used in regulating enzymatic activity.
- Examine how an enzyme may affect activation energy.

Introduction

Enzymes are specialized proteins that **catalyze** or speed up chemical reactions within cells. The substance upon which an enzyme acts is called a **substrate**. Substrates are small molecules.

Enzymes:

- Accomplish catalysis without being consumed in the reaction.
- Catalyzes a specific chemical reaction.

The Enzyme in Action Kit® allows you to explore how enzymatic reactions occur.

Catabolism

Model pieces needed



gray A foam piece
without stickers



green B₁ and B₂ foam
pieces



orange C₁ and C₂ foam
pieces

1. The gray foam piece is a model of an **enzyme**. Place it with the A label facing up. Assemble the two green pieces (B₁ and B₂) into a single unit to model the **substrate** in this reaction.
2. Draw and label the **enzyme** and **substrate** before the enzymatic action.

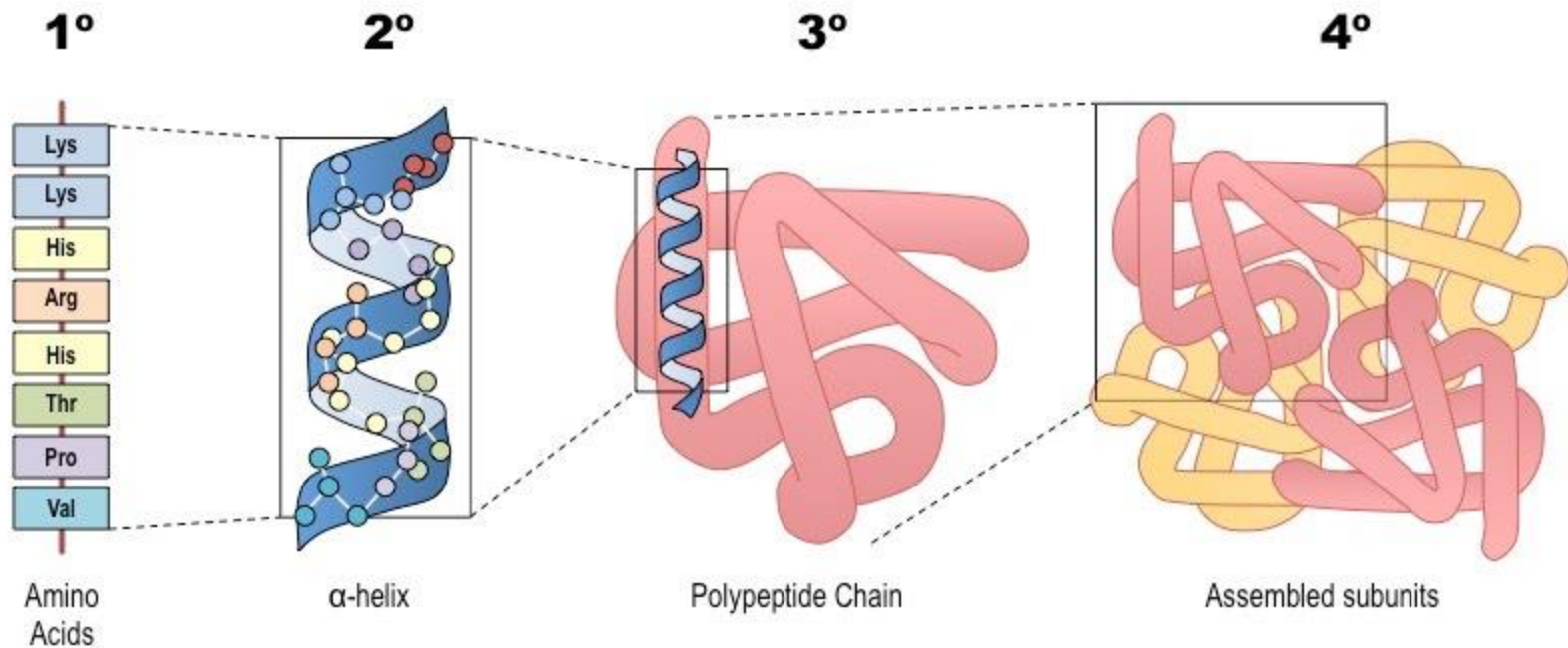
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Student Handout
Page 1

Resources for this lab found at:
https://3dmoleculardesigns.com/classroom_resources/enzymes-in-action-kit/

Protein Structure

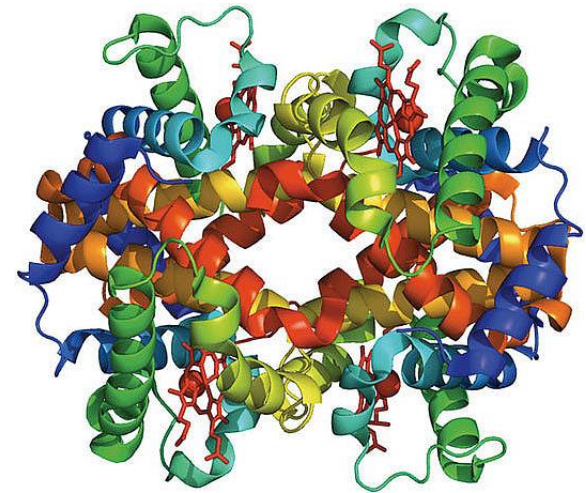


How can students learn the concept of the Protein Structure through Modeling?



Protein Structure

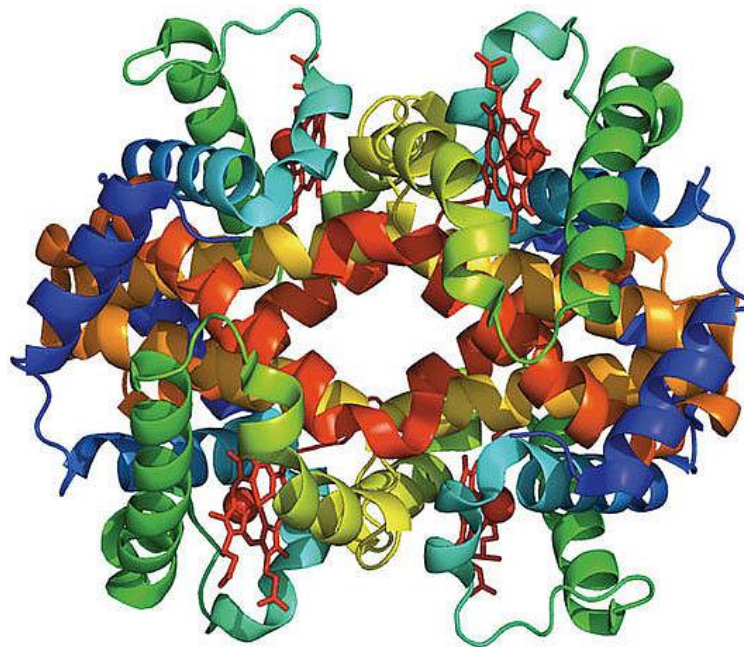
- Primary Structure
- Secondary Structure
- Tertiary Structure
- Quaternary Structure



How can students learn the concept of the Protein Structure through Modeling?



Protein Structure; How do I start?



Amino Acid Structure



Amino Acid Building Block Kit



Resources found at:
https://3dmoleculardesigns.com/classroom_resources/flow-of-genetic-information-kit/





Can you Build an Amino Acid?



Model Color Coding Key



Carbon (black)

Oxygen (red)

Nitrogen (blue)

**R-Groups Representing
Side Chains**

Hydrogen (white)

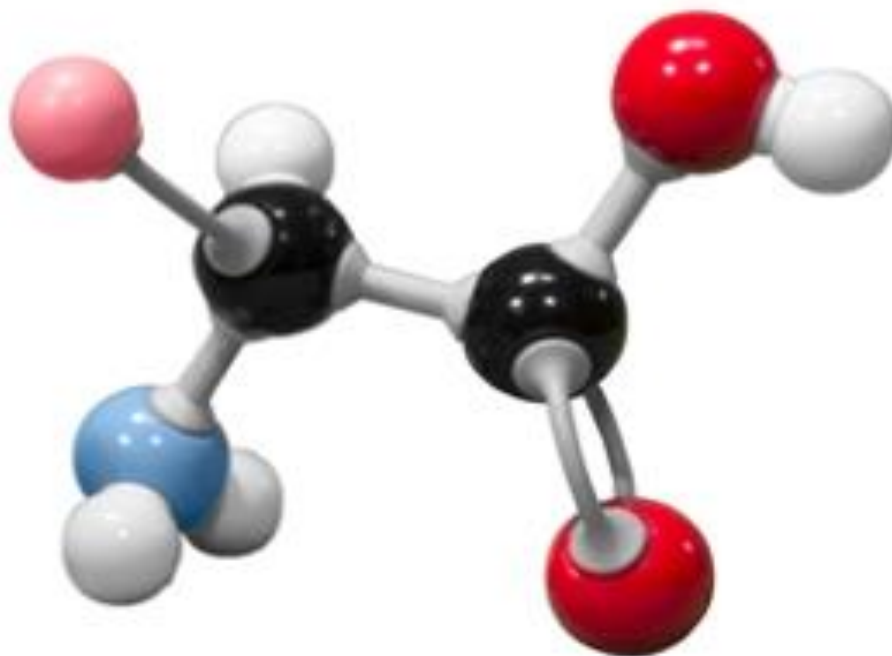
**Hydrogen Bonds (short
white posts)**

**Single Covalent Bonds
(short, gray, thick post)**

**Double Covalent Bonds
(long, gray, thin post)**

Link Remover

Proteins Are Made of Amino Acids

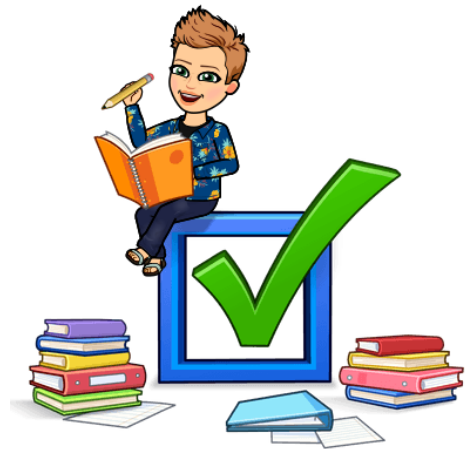
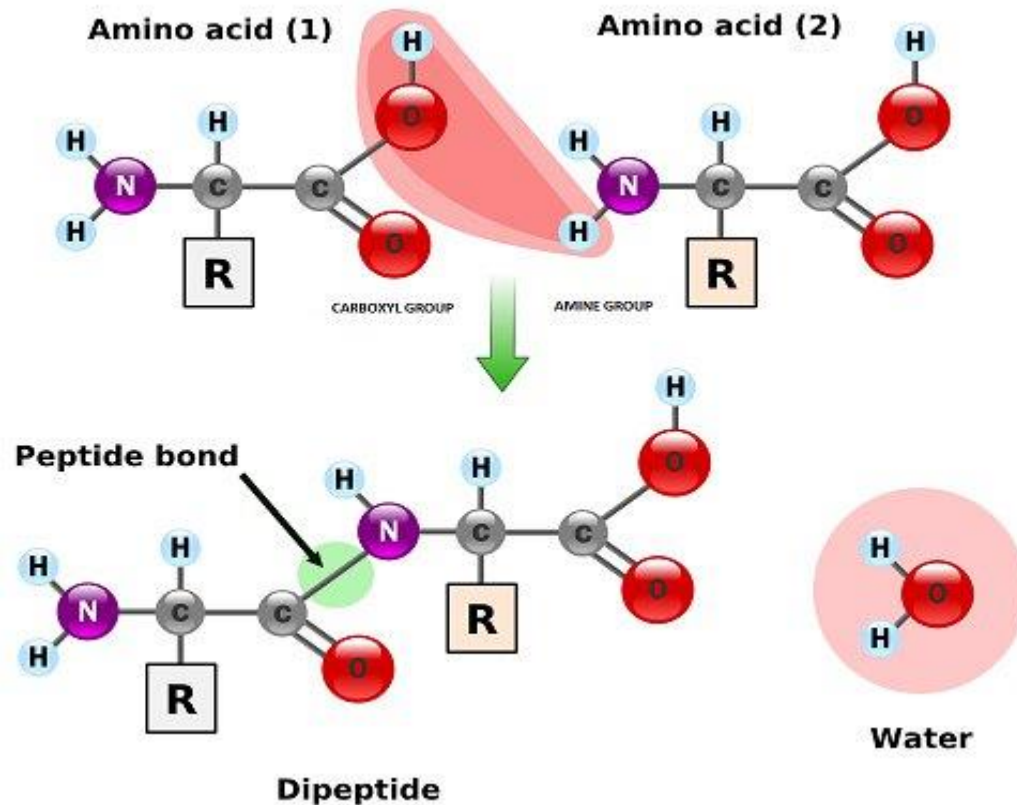




Can you Build Polypeptides?

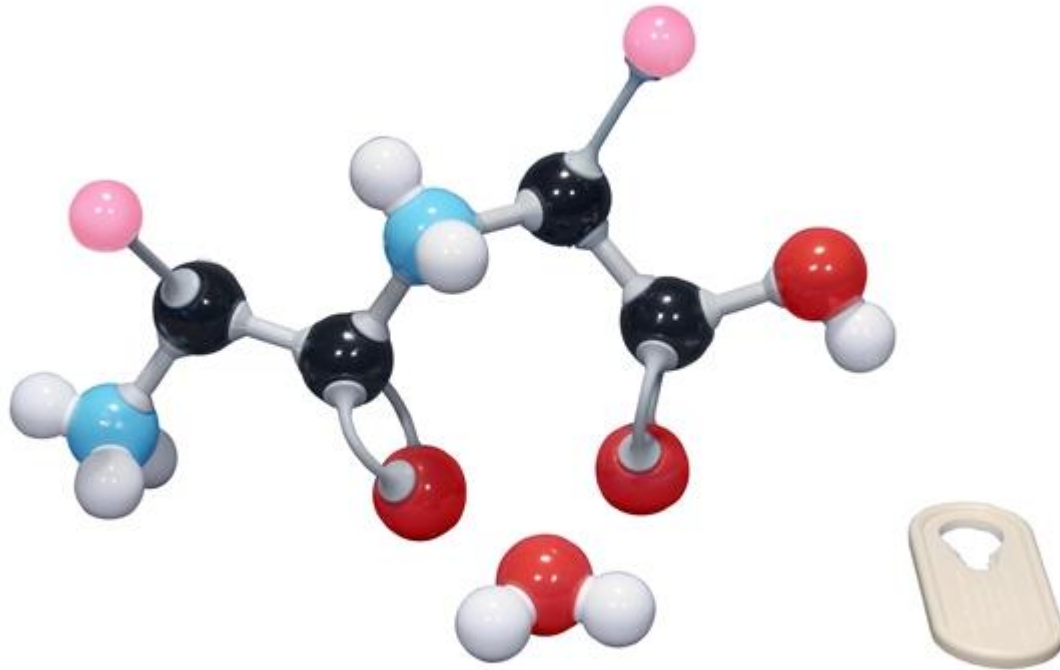


My Favorite:



Listen for whispers of “Whoa” as your students notice the water molecules that appear when peptide bonds form!

Challenge your students:



Can you make a dipeptide? Polypeptide?

Highlights: Versatility



- **Topics to Explore**
 - Dehydration Synthesis and Hydrolysis
 - Covalent Bonding
 - Amino Acid Side Chains



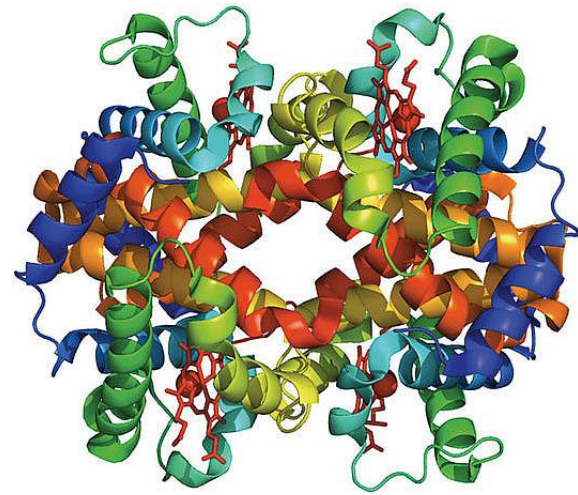


Any Questions?



Protein Structure

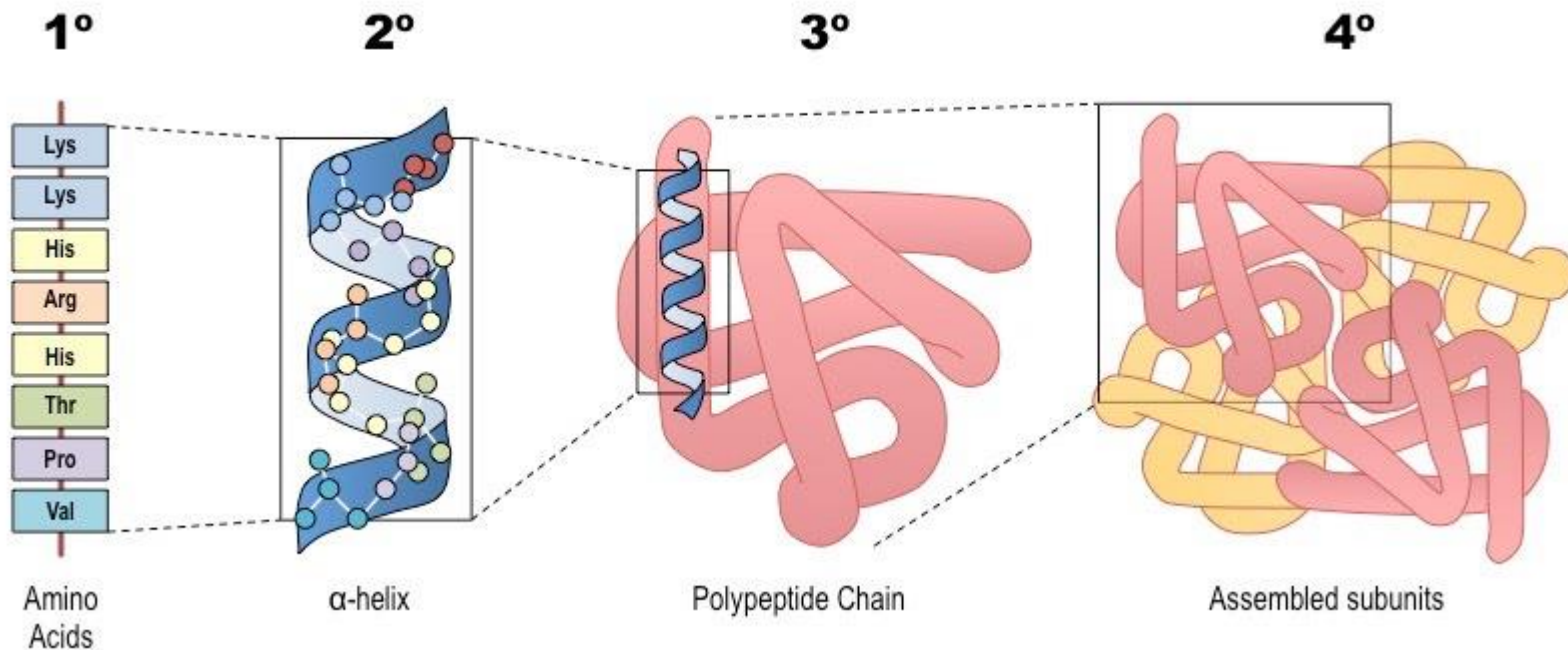
- Primary Structure
- Secondary Structure
- Tertiary Structure
- Quaternary Structure



How can students learn the concept of the Protein Structure through Modeling?



Protein Structure

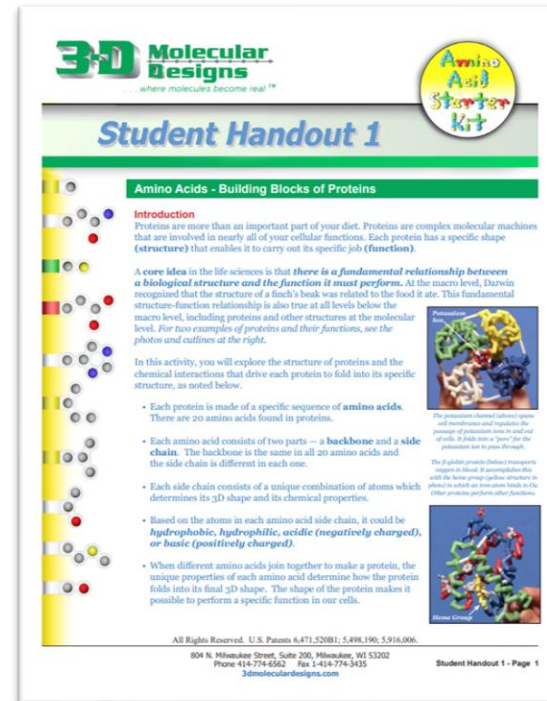
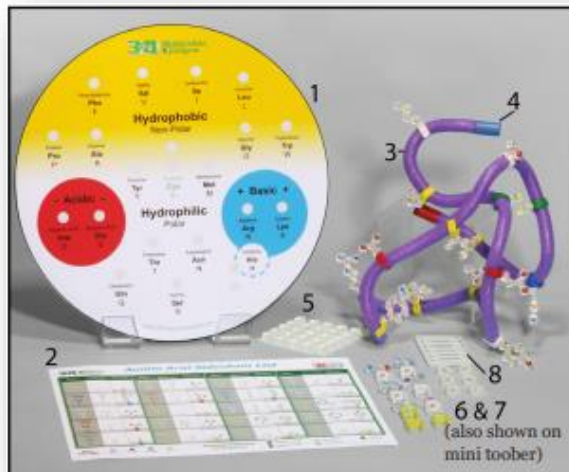




Why and How Do Polypeptides Fold into their Protein Structure?



Amino Acid Starter Kit

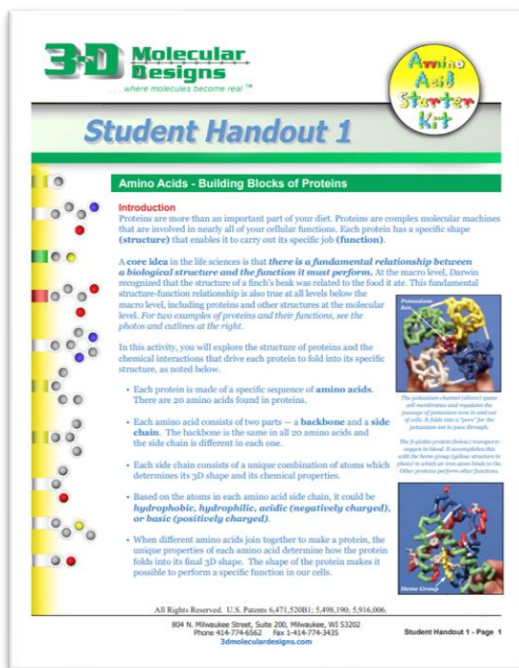
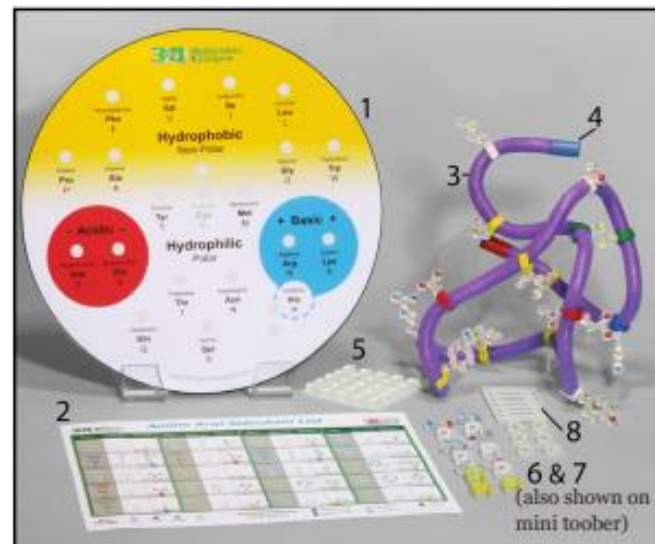


Resources found at:
https://3dmoleculardesigns.com/classroom_resources/flow-of-genetic-information-kit/

Classroom Tips:

Supplies:

- Protein Folding Kit
 - Amino Acid Side Chain Chart
- Meter/Yard Stick
- Lab Handout



3D Molecular Designs
where molecules become real™

Amino Acid Side Chain Chart™

Name	Amino Acid Side Chain	Name	Amino Acid Side Chain	Name	Amino Acid Side Chain	Name	Amino Acid Side Chain
Alanine Ala A	<chem>CC(N)C(=O)O</chem>	Glutamine Gln Q	<chem>CCC(N)C(=O)N</chem>	Leucine Leu L	<chem>CC(C)C(C)C(N)C(=O)O</chem>	Serine Ser S	<chem>CC(N)C(=O)O</chem>
Arginine Arg R	<chem>CCC(N)C(=O)N=[NH2+]</chem>	Glutamic Acid Glu E	<chem>CCC(N)C(=O)O</chem>	Lysine Lys K	<chem>CCCC(N)C(=O)O</chem>	Threonine Thr T	<chem>CC(C)C(N)C(=O)O</chem>
Asparagine Asn N	<chem>CC(N)C(=O)N</chem>	Proline Pro P	<chem>C1CCNCC1</chem>	Methionine Met M	<chem>CCSCC(N)C(=O)O</chem>	Tryptophan Trp W	<chem>C1=CC=C2C(=C1)C(=C(C=C2)C(N)C(=O)O</chem>
Aspartic Acid Asp D	<chem>CC(N)C(=O)O</chem>	Histidine His H	<chem>C1=CC=C(N=C1)C(N)C(=O)O</chem>	Phenylalanine Phe F	<chem>CC1=CC=CC=C1C(N)C(=O)O</chem>	Tyrosine Tyr Y	<chem>CC1=CC=C(C=C1C(=O)O)C(N)C(=O)O</chem>
Cysteine Cys C	<chem>CC(N)C(=O)S</chem>	Isoleucine Ile I	<chem>CC(C)C(C)C(N)C(=O)O</chem>	Valine Val V	<chem>CC(C)C(N)C(=O)O</chem>		

Atom Color Key
Carbon: Grey, Oxygen: Red, Nitrogen: Blue, Sulfur: Yellow, Hydrogen: White

Amino Acid Property Key
Amino acid clip color and name color indicate property:
Negative Charge: Red, Positive Charge: Blue, Hydrophilic: Green, Hydrophobic: Yellow, Cysteine: Grey

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Amino Acid Starter Kit

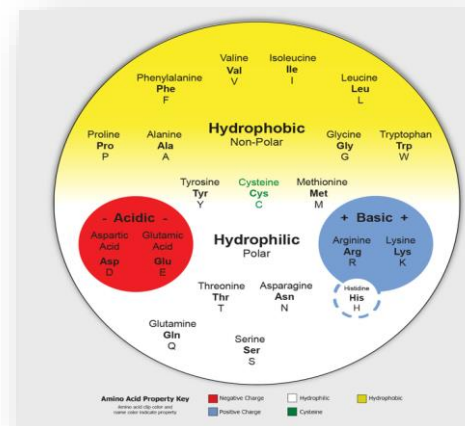
- Give it a try!

3D Molecular Designs Amino Acid Side Chain Chart

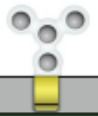
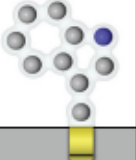
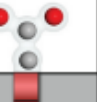
Name	Amino Acid Side Chain	Name	Amino Acid Side Chain	Name	Amino Acid Side Chain	Name	Amino Acid Side Chain
Alanine Ala A		Glutamine Gln Q		Valine Val V		Proline Pro P	
Arginine Arg R		Glutamic Acid Glu E		Leucine Leu L		Alanine Ala A	
Asparagine Asn N		Aspartic Acid Asp D		Threonine Thr T		Tyrosine Tyr Y	
Aspartic Acid Asp D		Asparagine Asn N		Cysteine Cys C		Methionine Met M	
Cysteine Cys C		Glutamine Gln Q		Threonine Thr T		Asparagine Asn N	

Atom Color Key
 Carbon: Grey, Oxygen: Red, Nitrogen: Blue, Sulfur: Yellow, Hydrogen: White

Amino Acid Property Key
 Acidic: Red circle, Basic: Blue circle, Hydrophobic: Yellow background, Hydrophilic: White background, Cysteine: Green outline



Amino Acid Side Chain Chart®

Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain	Name	Amino Acid	Side Chain
Alanine	Ala	A	Glutamine	Gln	Q	Leucine	Leu	L	Serine	Ser	S
	<chem>C[C@@H](N)C(=O)[O-]</chem>			<chem>CCC(=O)N</chem>			<chem>CC(C)C[C@@H](N)C(=O)[O-]</chem>			<chem>CC(O)C[C@@H](N)C(=O)[O-]</chem>	
Arginine	Arg	R	Glutamic Acid	Glu	E	Lysine	Lys	K	Threonine	Thr	T
	<chem>CNC(=[NH2+])NCCC[C@@H](N)C(=O)[O-]</chem>			<chem>CCC(=O)[O-]</chem>			<chem>CN(CCC[C@@H](N)C(=O)[O-])C(=O)[O-]</chem>			<chem>CC(O)C[C@@H](N)C(=O)[O-]</chem>	
Asparagine	Asn	N	Glycine	Gly	G	Methionine	Met	M	Tryptophan	Trp	W
	<chem>NC(=O)CC[C@@H](N)C(=O)[O-]</chem>			<chem>NCC[C@@H](N)C(=O)[O-]</chem>			<chem>CSCC[C@@H](N)C(=O)[O-]</chem>			<chem>c1ccc2c(c1)c(c[nH]2)C[C@@H](N)C(=O)[O-]</chem>	
Aspartic Acid	Asp	D	Histidine	His	H	Phenylalanine	Phe	F	Tyrosine	Tyr	Y
	<chem>C(=O)[O-]CC[C@@H](N)C(=O)[O-]</chem>			<chem>C1=CN=C(NC1)CC[C@@H](N)C(=O)[O-]</chem>			<chem>c1ccc(cc1)C[C@@H](N)C(=O)[O-]</chem>			<chem>c1ccc(cc1C[C@@H](N)C(=O)[O-])O</chem>	
Cysteine	Cys	C	Isoleucine	Ile	I	Proline	Pro	P	Valine	Val	V
	<chem>SCC[C@@H](N)C(=O)[O-]</chem>			<chem>CC[C@H](C)[C@@H](N)C(=O)[O-]</chem>			<chem>C1CCN(CC1)C[C@@H](N)C(=O)[O-]</chem>			<chem>CC(C)[C@@H](N)C(=O)[O-]</chem>	

Atom Color Key

Carbon (grey sphere) Oxygen (red sphere) Nitrogen (blue sphere) Sulfur (yellow sphere) Hydrogen (white sphere)

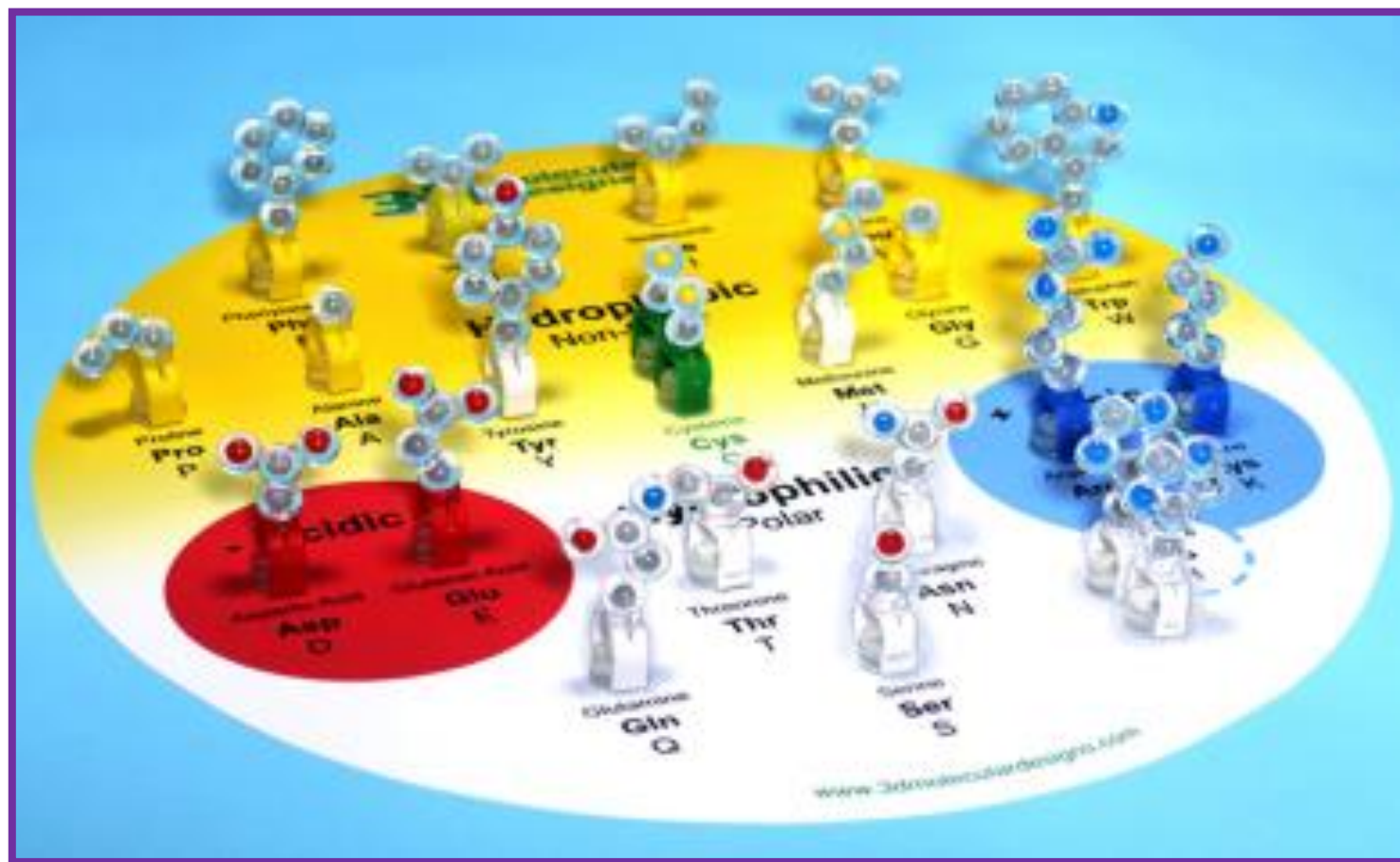
Amino Acid Property Key
Amino acid clip color and name color indicate property

Negative Charge (red clip) Positive Charge (blue clip)

Hydrophilic (grey clip) Cysteine (green clip)

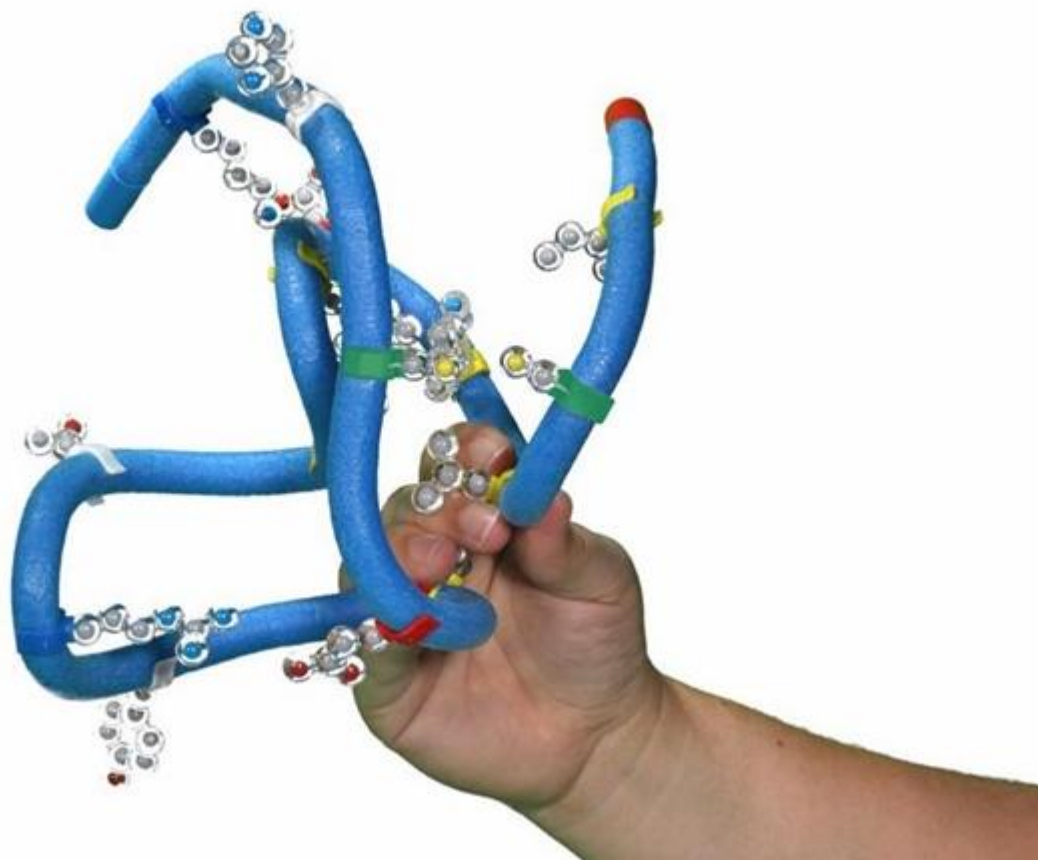
Hydrophobic (yellow clip)

Highlights: Students See Side Chains Sorted by Their Chemical Properties



Protein Folding

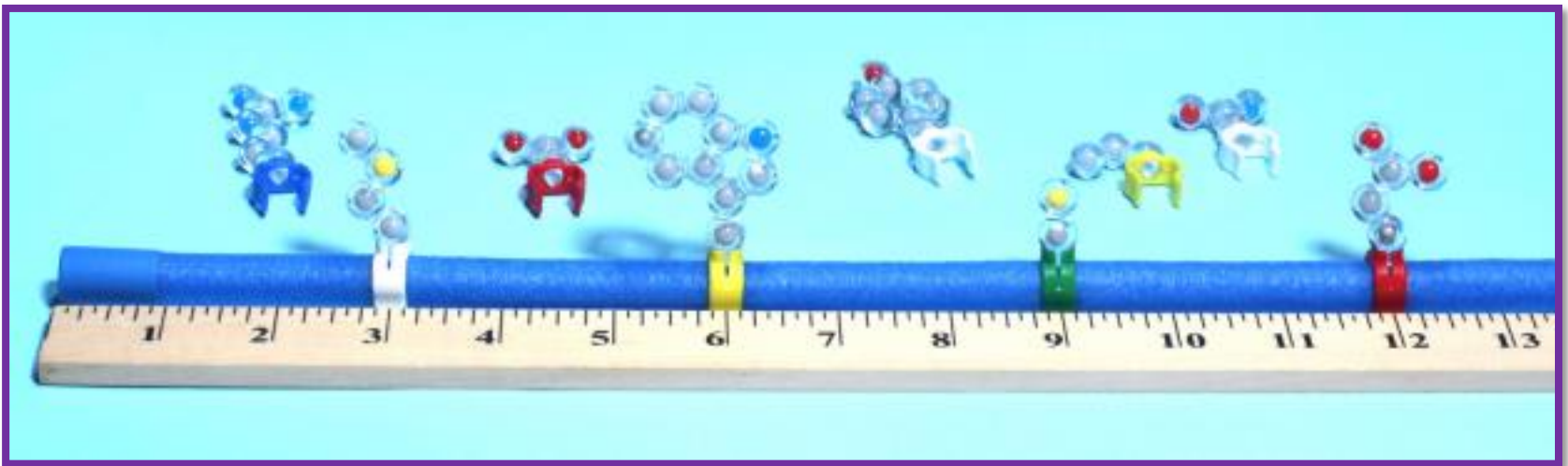
- Give it a try!



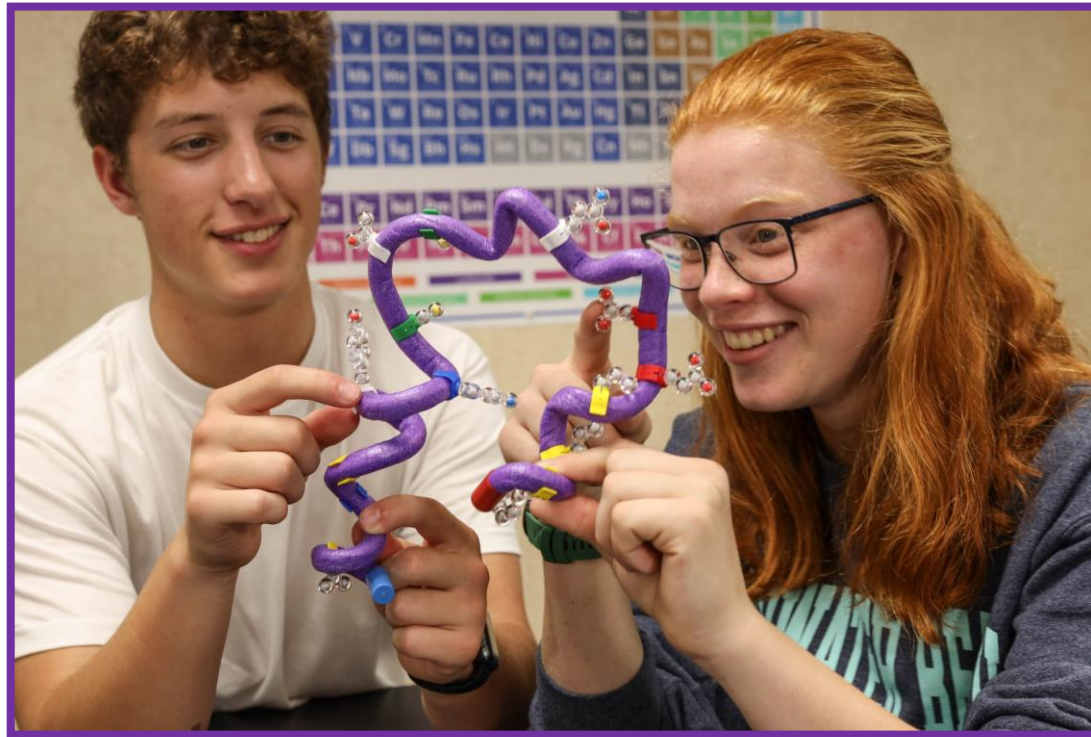
Classroom Tips:

Pick:

- 6 **Hydrophobic** side chains
- 2 **Acidic** side chains
- 2 **Basic** side chains
- 2 **Cysteine**
- 3 Hydrophilic



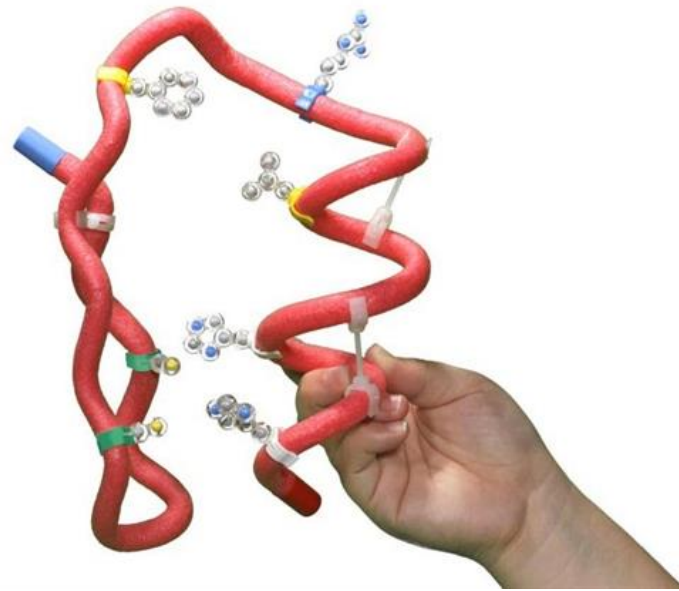
My Favorite:



Listen for whispers of “Whoa” as your students notice the water molecules that appear when peptide bonds form!



Highlights: Concept of Structure/Function



- **Topics to Explore**
 - Patterns Within and Between Side Chains
 - Discuss Chemical Properties of Side Chains
 - Examine Different Secondary Structure





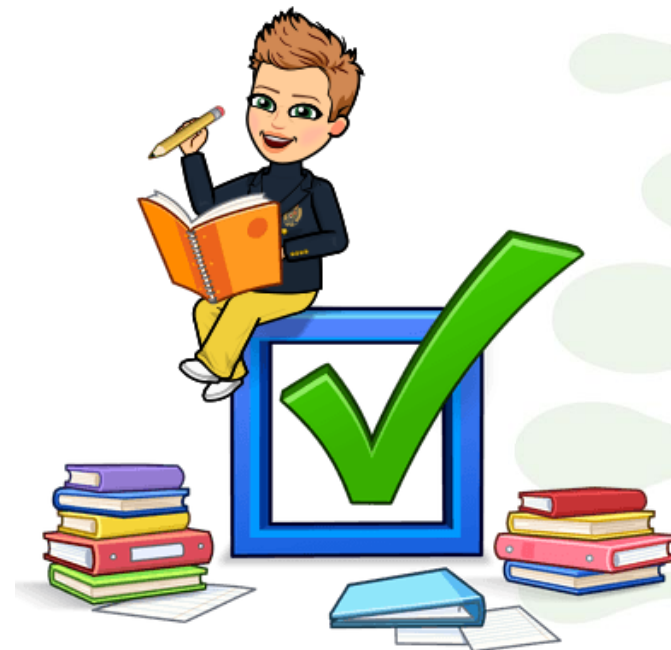
What's Next?



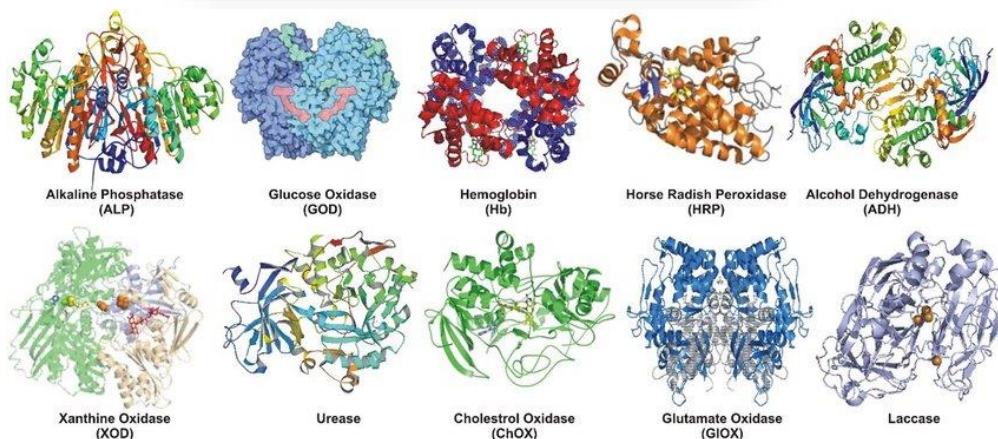
• I finished the lab, Now What?

Examples and Suggestions

- **Enzymes:**
 - Enzyme Action
 - Lactose Intolerance
- **Hemoglobin:**
 - Genetics
 - Hemoglobin Disorders



Lab: Enzymes in Action



Student Handout

Objectives

You will use the model pieces in the kit to:

- Simulate enzymatic actions.
- Explain enzymatic specificity.
- Investigate two types of enzyme inhibitors used in regulating enzymatic activity.
- Examine how an enzyme may affect activation energy.

Introduction

Enzymes are specialized proteins that **catalyze** or speed up chemical reactions within cells. The substance upon which an enzyme acts is called a **substrate**. Substrates are small molecules.

Enzymes:

- Accomplish catalysis without being consumed in the reaction.
- Catalyzes a specific chemical reaction.

The Enzyme in Action Kit® allows you to explore how enzymatic reactions occur.

Catabolism

Model pieces needed



gray A foam piece without stickers



green B, and B₁ foam pieces



orange C, and C₁ foam pieces

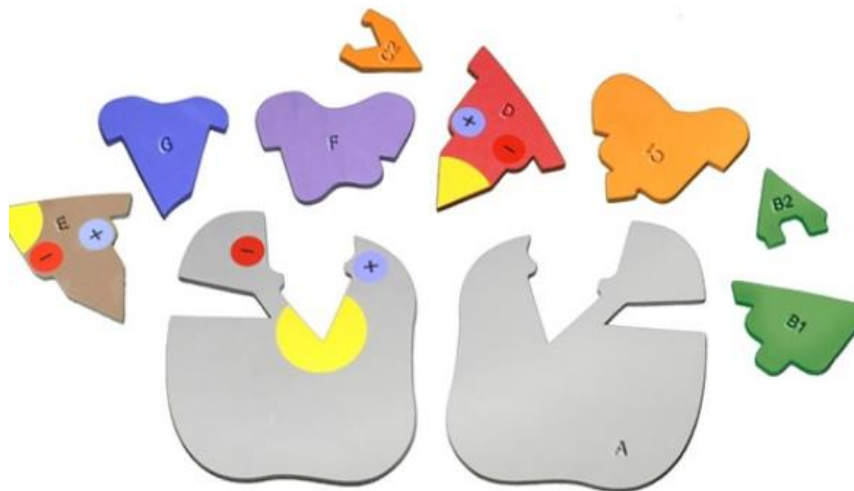
1. The gray foam piece is a model of an **enzyme**. Place it with the A label facing up. Assemble the two green pieces (B, and B₁) into a single unit to model the **substrate** in this reaction.
2. Draw and label the **enzyme** and **substrate** before the enzymatic action.



Lab: Enzymes in Action

Highlights:

- Enzyme Substrate Interaction
- Active Sites and Specificity
- Competitive/Allosteric Inhibition
- Lock-and-Key/Induced Fit



Enzymes in Action Kit®
Creating Catalytic Connections with Models

Student Handout

Objectives
You will use the model pieces in the kit to:

- Simulate enzymatic actions.
- Explain enzymatic specificity.
- Investigate two types of enzyme inhibitors used in regulating enzymatic activity.
- Examine how an enzyme may affect activation energy.

Introduction
Enzymes are specialized proteins that **catalyze** or speed up chemical reactions within cells. The substance upon which an enzyme acts is called a **substrate**. Substrates are small molecules.

Enzymes:

- Accomplish catalysis without being consumed in the reaction.
- Catalyzes a specific chemical reaction.

The Enzyme in Action Kit® allows you to explore how enzymatic reactions occur.

Catabolism
Model pieces needed

gray A foam piece without stickers

green B₁ and B₂ foam pieces

orange C₁ and C₂ foam pieces

- The gray A piece is a model of an enzyme. Place it with the A label facing up. Assemble the two green pieces (B₁ and B₂) into a single unit to model the **substrate** in this reaction.
- Draw and label the **enzyme** and **substrate** before the enzymatic action.

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Student Handout
Page 1

Activity: Lactose Intolerance

Got Lactase? Making of the Fittest The Co-evolution of Genes and Culture



Animations

Natural Selection for Lactose Tolerance



Interactive Videos

Interactive Assessment for
Got Lactase? The Co-evolution of Genes and Culture



Lessons

Lactose Intolerance: Fact or Fiction



Click & Learn

Recent Adaptations in Humans



Click & Learn

Regulation of the Lactase Gene

Sources for this activity found at:

<https://www.biointeractive.org/classroom-resources/making-fittest-got-lactase-co-evolution-genes-and-culture>

Activity: Lactose Lab

Science Take-Out

Enzymes and Lactose Intolerance

STO-119

Enzymes and Lactose Intolerance
Teacher Information

science take-out™ just add students™

Summary

Students model the action of the enzyme lactase. They conduct tests to determine whether LACTAID, an enzyme supplement, digests lactose. They design and conduct an experiment to determine if acid interferes with the action of the enzymes in LACTAID.

Core Concepts

- Biochemical processes are made possible by biological catalysts called enzymes. Enzymes can affect the rates of chemical change.
- The rate at which enzymes work can be influenced by internal environmental factors such as pH and temperature.

Time Required

Two 40-minute class periods + homework.

Kit contains

- 5 labeled droppers (Glucose, Water, Milk, LACTAID, Acid)
- 1 LACTAID capsule
- 1 empty large tube labeled "LACTAID"
- 1 empty microtube labeled "water"
- 1 large tube of Powdered Milk
- 1 large tube of Glucose
- 1 microtube of "Acid" (white vinegar)
- 12 toothpicks
- 2 test strips (use for Parts 2 and 3)
- Plastic bag containing 12 small pieces of glucose indicator paper

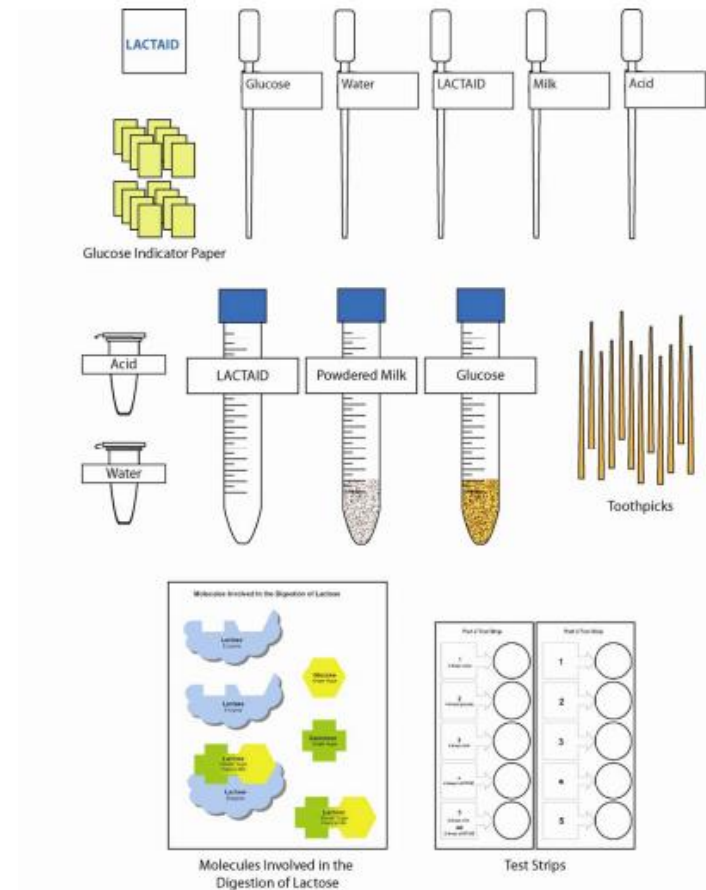
Teacher Provides

- Scissors
- Tape
- Safety goggles
- Access to water
- Paper towels for clean up

Warning: Choking Hazard

This Science Take-Out kit contains small parts. Do not allow children under the age of seven to have access to any kit components.

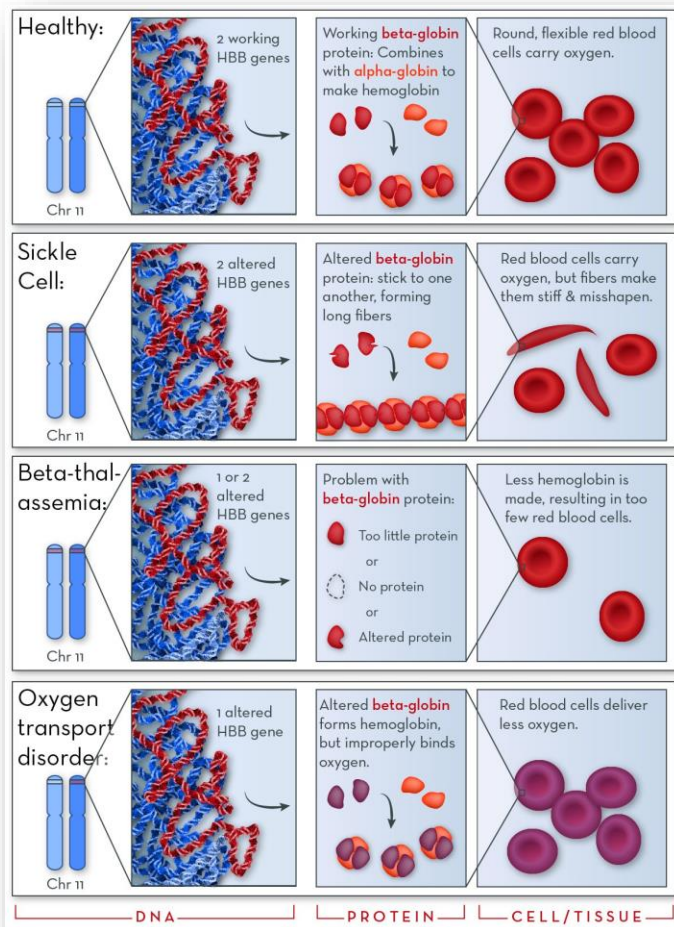
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Sources for this activity found at:

<https://www.sciencetakeout.com/product/enzymes-and-lactose-intolerance-group/>

Activity: Hemoglobin Disorders



Learn.Genetics
GENETIC SCIENCE LEARNING CENTER

Home / Genetics / Hemoglobin Disorders

Hemoglobin Disorders

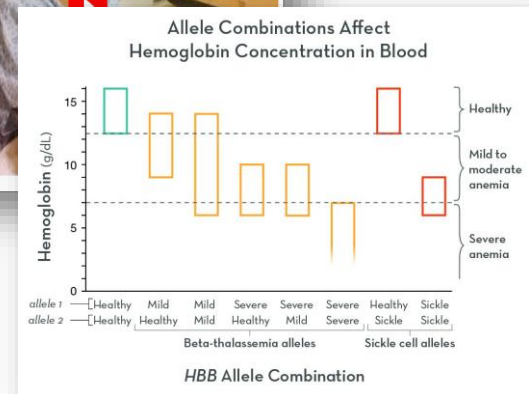
This page focuses on disorders that affect beta-globin. Similar disorders involve other globins, most commonly alpha-globin.

What are Hemoglobin Disorders?

Hemoglobin disorders are a group of inherited conditions that affect a person's red blood cells. Red blood cells pick up oxygen from the lungs and deliver it to all of the body's tissues. In people with hemoglobin disorders, red blood cells are fewer in number, less able to do their job, or both.

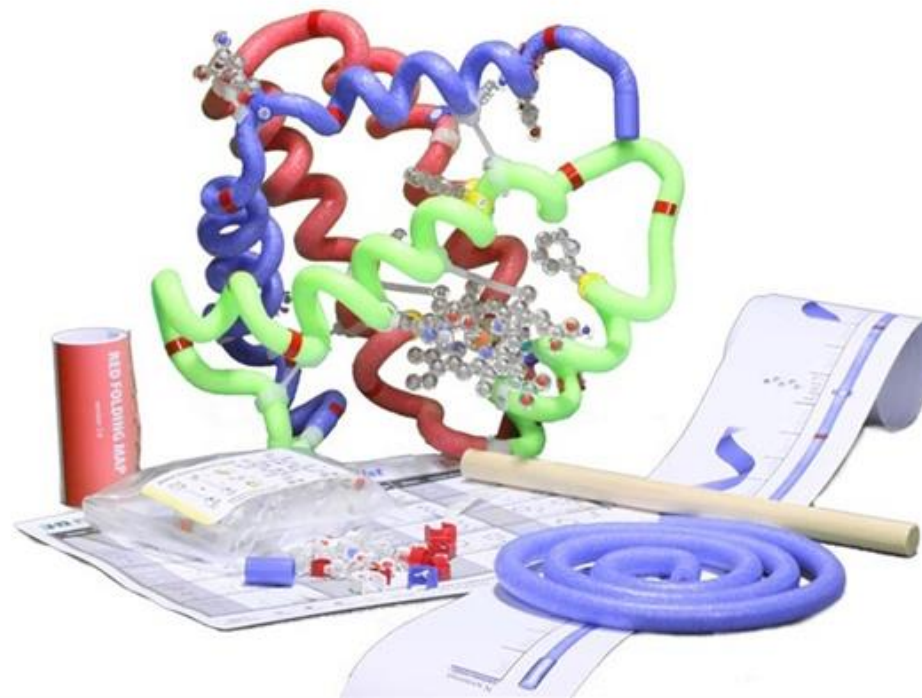
The most common hemoglobin disorders are sickle cell disease and thalassemia. Some version of the genes that cause these diseases also protect against malaria—a deadly parasite carried by mosquitoes. Through natural selection, these gene variations have become very common in certain parts of the world.

Living with Sickle Cell Disease
From an accredited US hospital
Watch on YouTube



Sources for this activity found at:
<https://learn.genetics.utah.edu/content/genetics/hemoglobin>

Activity: β -Globin Folding Kit[©]



Resources for this lab found at:
https://3dmoleculardesigns.com/classroom_resources/s-globin-folding-kit/





Any Questions?



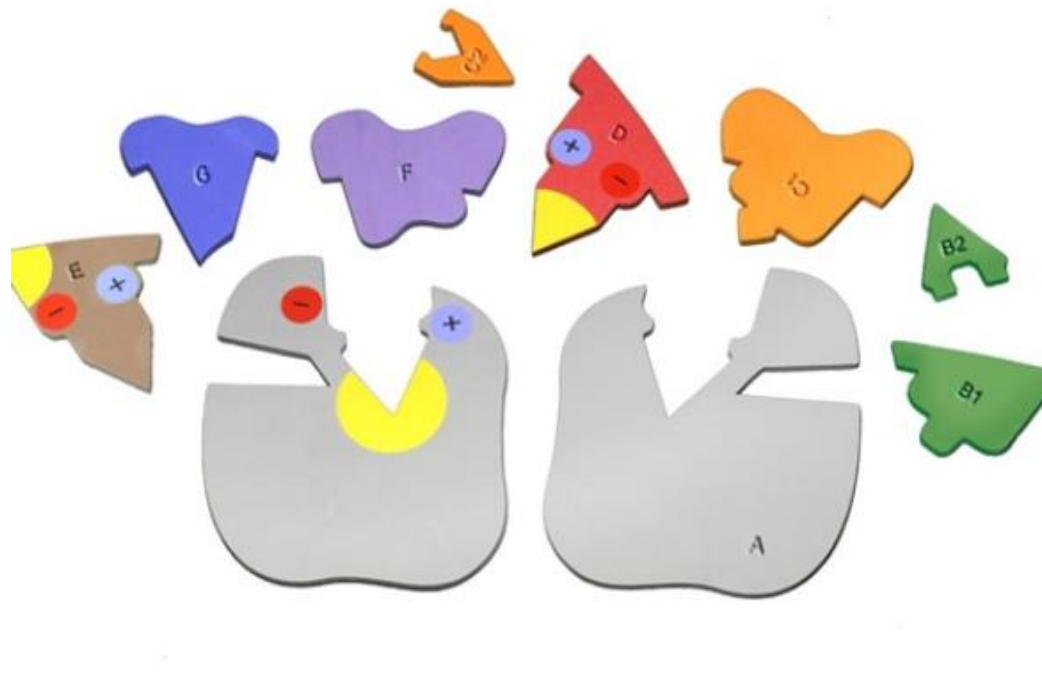
Reflection Activity

- Where do you see this fitting into your curriculum?
- What Lingering Questions Do You Still Have?
- What Does This Look Like Implemented in Your Classroom?
- What Other Resources Would You Use With this topic? (Make a Suggestion!)



Give Away!

Enzyme in Action Kit

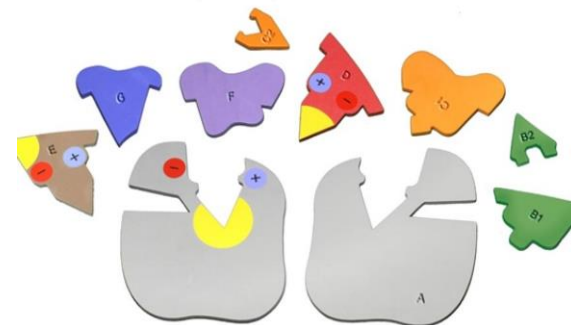
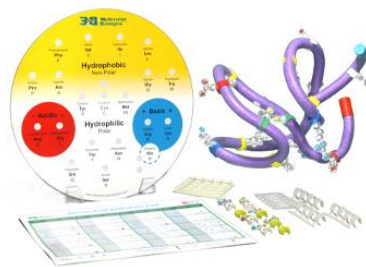


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Resources and Materials

Kits Used in this workshop:

- Amino Acid Building Blocks
Amino Acid Starter Kit
- Enzymes in Action Kit



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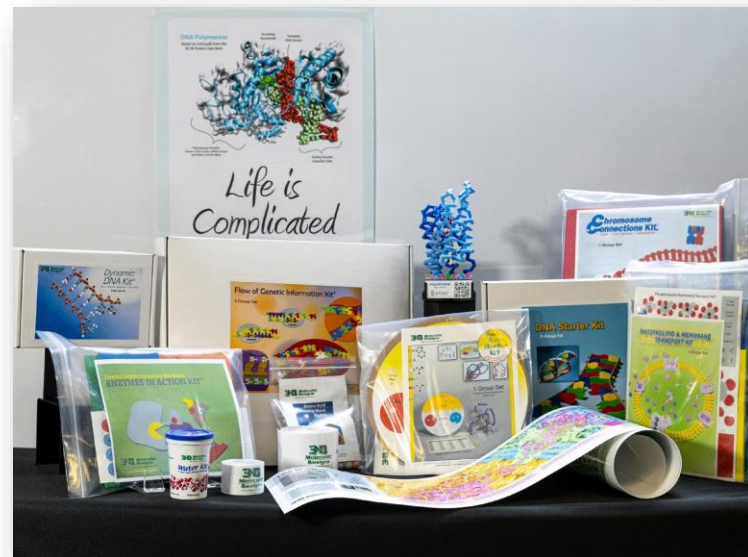
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