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Polypeptides and Water Mr. Collea

**Polypeptides and Water: Protein Folding**

**Background Information**



***FIGURE 1.*** *Condensation / dehydration synthesis reaction responsible for the formation of proteins and peptide bonds.*

The simulation in this activity represents an amino acid (*polypeptide*) chain. Certain properties are used to characterize amino acids. For example, some amino acids are attracted to water (*hydrophilic*), while some amino acids are repelled by water (*hydrophobic*). This attraction and repulsion has to do with hydrogen bonds. Amino acids that are electrically charged (*positive or negative*), and amino acids that are polar (*regions of partial charge*), are hydrophilic. Amino acids that are non-polar, meaning they have a balanced electrical charge, do not form hydrogen bonds with water and disrupt existing hydrogen bonds between water molecules. As a result, non-polar molecules are driven to re-arrange themselves to minimize the amount of their surface area that comes into contact with water. Non-polar amino acids are hydrophobic. You may recall (*prior knowledge*) how the non-polar, hydrophobic lipid tails of the phospholipid bilayer of plasma membranes behave in the same fashion.

 ***FIGURE 2.*** *Phospholipid Bilayer*

**Four Levels of Protein Structure**

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**Activity 1**

Follow the steps below and answer the question that follow.

* Place your mouse over one green and on yellow amino acid to determine if its hydrophobic or hydrophyllic:

Green = \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Yellow = \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

* Choose “hydrophobicity” as the color scheme.
* Select “water” as the solvent type.
* Click “play”
* Observe how the polypeptide reacts.

**1.** How does this polypeptide behave in an aqueous (*water*) environment?

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**2.** How do hydrophobic (*yellow*) and hydrophilic (*green*) amino acids behave differently?

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**Activity 2**

Follow the steps below and answer the question that follow.

* Click “generate random protein” to reset the polypeptide
* Select “oil” as the solvent type.
* Click “play”
* Observe how the polypeptide reacts.

**3.** How do the amino acids arrange differently when the polypeptide is allowed to fold in oil?

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**Activity 3**

Many molecular interactions influence how polypeptides conform (*fold*) into their final shape. You have observed how water and oil influence conformation. Now you will view how the polypeptide behaves if in a vacuum. This will allow you to see how intramolecular interactions between amino acids influence protein conformation. Follow the steps below and answer the question that follow.

* Click “generate random protein” to reset the polypeptide.
* Select “charge” as the amino acid color scheme.
* Choose “vacuum” as the solvent type (*this will eliminate hydrophobic and hydrophilic interactions*)
* Click “All hydrophilic” to include only charged and polar amino acids in your polypeptide (*positively charged amino acids are blue, negatively charged amino acids are red, and polar amino acids are gray)*
* Click “play” and observe how the polypeptide behaves.
* After a few moments, click “All hydrophilic” again to re-arrange the amino acids.
* Continue to observe how the amino acids react toward one another.

**4.** What pattern of interaction do you observe between the amino acids?

 *Keep in mind that adjacent amino acids are connected by strong covalent peptide bonds. Consider the interactions that occur between amino acids that do not share a peptide bond.*

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**Intermolecular Forces in Proteins**

