Protein Builder

Name: _____ **Period:** _____ **Date:** _____

> Open **peebedu.com** and navigate to **Protein Builder**. Click the **Start Building!** button to begin. Read the introduction popup, which describes four levels of protein structure: Primary, Secondary, Tertiary, and Quaternary.

Part 1 — Model Evaluation (MAPP Framework)

Scientific models are simplified representations of complex biological phenomena. Use the MAPP framework below to evaluate the Protein Builder as a scientific model.

M — Mode

What type of model is the Protein Builder? Describe how this computational simulation represents protein structure. In your answer, identify at least three specific simulation elements and explain what each one is designed to show about proteins.

A — Accuracy

(a) Identify two things this simulation represents **accurately** about protein structure. For each, name the specific simulation feature and explain what aspect of protein biology it demonstrates.

(b) Identify two things this simulation **oversimplifies or leaves out** about protein structure. Consider what you cannot observe in the simulation that would be important for a complete molecular-level understanding of how proteins fold and function.

P — Purpose

What is the learning goal of this simulation? Explain how the Protein Builder is designed to help you understand how the sequence and chemical properties of amino acid R-groups determine the four levels of protein structure. In your answer, connect at least one specific simulation feature to a biological reason why that structural level matters for protein function.

P — Permanency

Could this model change with new scientific evidence? Describe one way that new discoveries about protein folding might change or improve a simulation like the Protein Builder. Explain why scientific models, including computational simulations, are revised as new evidence becomes available.

Small-Group Discussion

With your group, discuss the following:

- How does building the amino acid chain in a specific order help you understand why primary structure matters?
- What are the limitations of using colored spheres to represent R-group interactions?
- If you could add one feature to improve this simulation, what would it be and why?
- How does the progressive unlocking of structure levels reinforce the relationship between primary, secondary, tertiary, and quaternary structure?

Part 2 — NGSS Questions

1.

> *Simulation Task: Drag at least 10 amino acids from the palette onto the canvas to build a chain. Include at least one amino acid from each color-coded category (polar, nonpolar, positive, negative, and sulfur). Watch the chain grow as each amino acid is connected by a peptide bond.*

Explain how the order of amino acids in the chain you built determines the primary structure of a protein. Describe why changing even one amino acid in the sequence could affect the overall shape and function of the finished protein.

HS-LS1-1

2.

> *Simulation Task: After building a chain of at least 10 amino acids, click the Secondary Structure button. Apply the Alpha Helix structure and observe how the chain rearranges into a spiral. Then click Beta Sheet and observe the zigzag pattern. Note the dotted blue lines that appear between backbone atoms in each arrangement.*

Describe the structural difference between an alpha helix and a beta sheet as shown in the simulation. Explain what type of bond stabilizes both of these folding patterns and why the specific pattern of bonding is important for giving a protein a stable shape.

HS-LS1-1

3.

> *Simulation Task: Build a chain that includes two cysteines (C), one positively charged amino acid (R, H, or K), one negatively charged amino acid (E or D), and several nonpolar amino acids. Apply a secondary structure, then switch to Tertiary Structure. Use Drag mode to move R-group spheres close together and observe the interaction lines and folding score as bonds form.*

Identify three types of R-group interactions you observed forming in the simulation during tertiary folding. For each interaction, name the type of bond, describe which kinds of amino acids were involved, and explain how that interaction helps hold the protein in its three-dimensional shape.

HS-LS1-1

4.

> *Simulation Task: Reset the simulation and build two different chains of at least 10 amino acids each. Make the first chain almost entirely from nonpolar amino acids. Make the second chain from a mix of polar, charged, nonpolar, and sulfur-containing amino acids. Apply Beta Sheet to both, then switch to Tertiary Structure and click Auto-Fold Protein for each. Compare the folding scores and the types of interactions listed in the Tertiary Folding Panel.*

Compare the folding results of your two chains. Explain why a protein built from a diverse mix of amino acid types folds differently than one built from mostly the same type. Describe how the variety of R-group chemical properties in a sequence leads to a more complex and specific three-dimensional shape.

HS-LS1-1

5.

> *Simulation Task: Achieve a folding score of at least 80% to unlock Quaternary Structure. In quaternary mode, add two or more chain templates from the Chain Templates palette. Use Position Chains mode to drag the chains close together and observe the dotted pink lines that appear between them. Read the inter-chain contacts count in the Quaternary Assembly Panel.*

Explain what quaternary structure means and why some proteins require multiple polypeptide chains to function. Using your observations from the simulation, describe how the chains interact with each other and why the positioning of chains affects the number of contacts between them.

HS-LS1-1

6.

> *Simulation Task: Build and fold a protein through all four structural levels. At each level, observe how the shape changes: a linear chain (primary), a helix or sheet (secondary), a folded 3D shape with R-group interactions (tertiary), and a multi-chain complex (quaternary).*

In the box below, draw a diagram showing how a protein progresses through all four levels of structure. For each level, sketch the shape and label the key feature: amino acid sequence (primary), hydrogen bonds along the backbone (secondary), R-group interactions (tertiary), and multiple chains assembled together (quaternary).

Draw your diagram here.

HS-LS1-1

7.

> *Simulation Task: Build a chain of at least 12 amino acids that includes two cysteines forming a disulfide bridge. Fold the protein to at least 80% using Auto-Fold. Now reset and rebuild the same chain, but replace one of the cysteines with a nonpolar amino acid such as alanine (A). Fold this new chain with Auto-Fold and compare the folding score and the types of interactions that form.*

A mutation in an organism's DNA changes a single amino acid in a protein from cysteine to alanine. Using your observations from the two chains you built, explain how this one change in the amino acid sequence affects the protein's three-dimensional shape. Describe how a change in protein shape could alter the protein's function and predict how this might affect the organism.

HS-LS3-2