PROTEIN MODELING C

See General Rules, Eye Protection & other Policies on www.soinc.org as they apply to every event.

1. **DESCRIPTION: Participants will be assessed on a written exam and prior to the competition will use computer visualization and online resources to construct a physical model of the sialic acid binding site of the 2009 H1N1 influenza hemagglutinin protein.**

   A TEAM OF UP TO: 2 **APPROXIMATE TIME:** 50 minutes

   IMPOUND: Yes

2. **EVENT PARAMETERS:**
   a. Each team may bring writing utensils.
   b. Each participant may bring one 8.5" x 11" sheet of paper, which may be in a sheet protector sealed by tape or laminated, that may contain information on both sides in any form and from any source without any annotations or labels affixed, along with writing utensils for each participant.
   c. **Each team will impound a pre-built model of the sialic acid binding site of the Hemagglutinin protein. This year's prebuild will focus on residues 153–252 of chain A from the crystal structure with PDB ID 3UBE, as described in the article "Structural Characterization of the Hemagglutinin Receptor Specificity from the 2009 H1N1 Influenza Pandemic" (DOI: 10.1128/JVI.06322-11), freely available at https://journals.asm.org/doi/10.1128/JVI.06322-11.**
   d. Each team will bring one device (laptop, Chromebook, tablet, or phone) that can connect to WIFI with a browser that can run the JUDE Jmol program. A wired/wireless mouse may also be used.
   e. Event Supervisors will provide written exams, WiFi information, and the website address for the molecular exploration portion of the event.

3. **THE COMPETITION:**

   Part I: The Pre-Built Model
   a. Participants will use the program JUDE (Jmol User Design Environment) to visualize r**esidues 153–252 of chain A from the crystal structure with 3UBE.pdb. A modified file for easier modeling by participants can be found on the 3D Molecular Designs Protein Modeling Event website (https://learn.3dmoleculardesigns.com/science-olympiad-protein-modeling-event). In addition, The atomic coordinate data file can be accessed for free from the RCSB Protein Data Bank (www.rcsb.org).** A constructed model of this protein must be brought to all competitions; as the competition level increases, the scoring rubrics for the pre-built model will reflect higher expectations for model accuracy, detail, and enhancements. (See SCORING for more details.) The pre-built model must be based on the protein's alpha carbon backbone display, using a scale of 2 cm per amino acid. Students will manually fold their pre-built model using Modeling Ties or comparable bendable material (Mini-Toobers, Kwik Twists, 12-gauge dimensional house wire, etc.). The backbone should primarily be gray with a diameter of 0.75 – 1.25 cm.
   b. Three-dimensional (3D) printed materials may NOT be used to build the protein backbone but may be used for functionally relevant features.
   c. Participants will use materials of their choosing to add functionally relevant features to their model (e.g., selected amino acid sidechains, DNA, or associated molecules). These additions should highlight the significance of structure to the protein's function.
   d. When an amino acid sidechain is displayed, its chemical property should be annotated on the alpha-carbon of the backbone. For example, hydrophobic sidechains are yellow, hydrophilic white, acidic red, basic blue, and cysteine green.
   e. Participants must explain their functionally relevant features in a Model Description Legend using clear and concise descriptions on a printed 8.5" x 5.5" paper, in the form of a table with three columns, headed:
      i. What is displayed?
      ii. How is it displayed?
      iii. Why is it displayed?
   f. All models, including all functionally relevant features, must fit within a 50.0 cm x 50.0 cm x 50.0 cm space.
   g. The model must be sufficiently sturdy so that judges can remove it from any scaffolding or support, pick it up, and rotate it so that they can view it unobstructed from any angle and properly evaluate it.
   h. Teams must impound their pre-built model and Model Description Legend. They must pick up pre-built

models after the competition.

Part II: Written Exam

a. Teams will complete a written exam to assess their protein structure and function knowledge and their ability to explore protein structures in the molecular visualization environment, JUDE. JUDE can be accessed at learn.3dmoleculardesigns.com/digital-modeling-hub/jude_online_jmol for free.
b. The exam will consist of multiple-choice and short-answer questions.
c. Protein Structure topics addressed include:
   i. The principles of chemistry drive protein folding and stability.
   ii. The chemical properties of amino acid side chains and how their interactions stabilize protein structures.
   iii. **The virus infection process and immune response, specifically influenza.**
   iv. **At State and National Tournaments, students will be asked questions about the role of hemagglutinin binding of sialic acid receptors in the influenza virus infection mechanism.**
d. Molecular Visualization topics addressed include:
   i. Ability to identify different secondary structural elements of a protein and specific amino acids found in these structures.
   ii. Chemical environment around specific amino acid sidechains that stabilize structure.
   iii. **Interactions of the protein with ligands and other molecules.**
e. Participants may not visit websites outside of the JUDE environment.

4. **SCORING:**

a. High Score wins. The final score will be derived from both parts of the competition:
b. The pre-built model (Part I) accounts for approximately 40% of the final score.
   i. The pre-built score is based on the accuracy and scale of the secondary structures, the tertiary arrangement of these structures, and the relevant functional features added.
   ii. Features that are irrelevant or do not explain the protein's structure/function relationship will not receive credit.
   iii. The pre-built model's scoring rubric will change with each competition's level.
      (1) For Regional competitions, scoring will be based primarily on the accuracy of the 3D folded structure of the protein's alpha-carbon backbone (secondary and tertiary structures).
      (2) For State competitions, approximately 20% of the score awarded to the pre-built model will be based on functionally relevant features, such as the inclusion of key sidechains that have been added to the alpha-carbon backbone model to explain the protein's structure.
      (3) For the National competition, approximately 30% of the score awarded to the pre-built model will be based on the inclusion of key sidechains that explain the interactions between specific amino acids that stabilize the protein's structure.
c. The written exam (Part II) accounts for approximately 60% of the score.
d. Preselected questions, on the written exam (Part II) will be used as tiebreakers.

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