

## Protein Modeling

1. **DESCRIPTION:** Students will use computer visualization and online resources to construct physical models of proteins involved in swine flu (H1N1), with a focus on two proteins involved in infectivity: Hemagglutinin (H) and Neuraminidase (N).

**A TEAM OF UP TO:** 3

**IMPOUND:** Yes

**EVENT TIME:** 50 minutes

2. **EVENT PARAMETERS:**

- a. Each team will impound a pre-built model of residues 40-153 of chain D of the hemagglutinin protein (see 3.I.a. & 3.I.b.).
- b. Each team may bring one **8.5" x 11" sheet of paper** that may contain information on both sides in any form and from any source.
- c. Participants must bring writing utensils, a marker, and a metric ruler with cm marks.
- d. Event supervisors will provide all other materials for on-site model construction and test.

3. **THE COMPETITION:**

This event has three parts: a pre-built model, an on-site built model, and a written exam.

### Part I: Pre-Built Model

- a. Participants will use the program Jmol/JSmol, (see web-resources) to visualize a model of a specific protein based on atomic coordinate data, freely accessible from the RCSB Protein Data Bank (<http://www.rcsb.org>). For 2017-18, students will construct a model of residues 40-153 of chain D of the hemagglutinin protein, based on the coordinate data found in the 1htm.pdb file, which can be downloaded for free from the RCSB Protein Data Bank ([www.rcsb.org](http://www.rcsb.org)). The role of this protein in influenza infection is described in the April 2006 RCSB Molecule of the Month feature ([http://dx.doi.org/10.2210/rcsb\\_pdb/mom\\_2006\\_4](http://dx.doi.org/10.2210/rcsb_pdb/mom_2006_4)) by David Goodsell. A constructed model of this protein will be brought to all competitions; as the competition level increases, the scoring rubrics for the pre-build model will reflect higher expectations for model accuracy, detail and enhancements.
- b. The final pre-build model must be based on the alpha carbon backbone display of the protein, using a scale of 2 cm per amino acid.
- c. Participants may use Mini-Toobers®, or other comparable bendable material (e.g., Kwik Twists, 12-gauge dimensional house wire, etc.), to manually fold their pre-build model. The model must be sufficiently sturdy that judges can pick it up and rotate it for judging.
- d. 3D printing technologies may NOT be used to build the protein backbone, but MAY be used for creative additions.
- e. Participants will use materials of their own choosing to add functionally relevant features to their model (e.g. selected amino acid sidechains, DNA or associated molecules). Additions to the model should highlight the significance of structure to function of the protein.
- f. Participants must explain their creative additions on a 4"x6" notecard, in the form of a table with 3 columns, headed:
  - i. What is displayed?
  - ii. How it is displayed?
  - iii. Why it is important?Explanations should be clear and concise. A significant portion of the score will be derived from these additional features.
- g. Prebuilt models with all additions must fit within a 2x2x2 ft space.
- h. Participants must deliver their pre-build model and 4"x6" notecard for impounding.
- i. Participants may pick up all pre-build models after the competition.

### Part II: On-Site Built Model

- a. During the on-site competition, students will build a physical model of a selected region of a specific protein using materials provided by the event supervisor. Web-based resources listed below will provide background information about the molecules for all levels of competitions.
- b. Participants will utilize a computer provided with the Jmol/JSmol application at the competition. Each team must utilize only one of the identical computers provided at the competition with the appropriate coordinate files on it to guide their model construction.

- c. All construction materials for the model (Mini-Toobers®, amino acid sidechains, crosslinkers and plastic red and blue end caps) will be provided.
- d. Any model not handed to the judges by the end of the competition time will not be accepted for scoring.

**Part III: Written Exam**

- a. The exam will consist of multiple choice and short answer questions.
- b. Topics addressed include the principles of chemistry that drive protein folding and the structure/function relationship of the involved in swine flu (H1N1), with a focus on two proteins involved in infectivity: Hemagglutinin (H) and Neuraminidase (N).

**4. SCORING:**

- a. High Score Wins.
- b. The pre-built protein model (3.I.) accounts for 40% of the event score.
  - i. The pre-built protein model will be scored based on the accuracy and scale of the secondary structures, as well as the additions to the model (e.g. sidechains, DNA or associated molecules).
  - ii. Additions that do not support the molecular story will not receive credit.
- c. The on-site built model (3.II.) accounts for 30% of the event score.
  - i. The on-site build protein model will be scored based on accuracy of folding the model and positioning specific amino acid sidechains
- d. The written exam (3.III) accounts for 30% of the event score.
  - i. The exam will be scored for accuracy.
  - ii. Ties will be broken using identified questions from the written exam.

**Recommended Resources:** Material for the participants, coaches and judges will be available on the Science Olympiad Webpage - at MSOE CBM (<http://cbm.msoe.edu/scienceOlympiad/index.php>) and RCSB PDB (<http://pdb101.rcsb.org/events/science-olympiad>); RCSB PDB Homepage ([www.rcsb.org](http://www.rcsb.org)) and PDB-101 resources (<http://www.rcsb.org/pdb-101>). The Mini-Toobers® are a product of 3D Molecular Designs. Materials for the Pre-build can be obtained from <http://www.3dmoleculardesigns.com>.

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