

PROTEIN MODELING CHALLENGE

1. **DESCRIPTION:** Students will use computer visualization and online resources to guide them in constructing physical models of proteins involved in swine flu (H1N1), with a focus on two proteins used in the naming of the flu viruses: Hemagglutinin (H) and Neuraminidase (N).

A TEAM OF UP TO: 2

IMPOUND: Yes

APPROXIMATE TIME: 50 minutes

2. **EVENT PARAMETERS:**

- a. Pre-build models will be impounded one hour before the event begins.
- b. Students may bring up to **ten** double-sided, 8.5"x11" pages of materials to the on-site competition. Internet access will **not** be permitted during the competitions.
- c. Students will need to bring a writing instrument.
- d. Supervisors will provide all materials for on-site model construction.
- e. Construction details are found at: <http://cbm.msoe.edu/studProg/so/index.html>

3. **THE COMPETITION:** This event has three parts: (1) a pre-build model (40% of total score), (2) an on-site build model (30% of total score) and (3) an on-site exam (30% of total score).

- a. **Part I: The Pre-Build Model.** Students will use a computer visualization program (Jmol) to design and construct a model of a specific protein based on atomic coordinate data. For 2010, students will construct a model of a specified portion of the hemagglutinin protein, based on the coordinate data found in the 5HMG.pdb file, which can be downloaded for free from the RCSB Protein Data Bank (www.pdb.org), and is described in the April 2006 *RCSB Molecule of the Month* (http://dx.doi.org/10.2210/rcsb_pdb/mom_2006_4) by David S. Goodsell. The pre-build models should represent amino acids 1-160 of chain B of the PDB file 5HMG. Note that the same pre-build model should be brought to regional, state and national competitions, as the competition level increases, the scoring rubrics for the pre-build model will reflect higher expectations for model accuracy, detail and creativity.
- b. The pre-build model in its final form must be based on the alpha carbon backbone display of the model and must use a scale of 2 cm per amino acid. Students may use Mini-Toobers®¹ to model their protein, or other comparable material². Students will represent other important parts of the protein, such as amino acid sidechains, DNA or associated molecules, where applicable, with materials of their choosing. The additions to the model should focus on illustrating the significance of the structure to the function of the protein. A significant portion of the score will be derived from the creative additions to the model. Students must provide a 3"x5" note card explaining the creative additions to their model and what they represent. Students must deliver their pre-build model and 3"x5" card to judges at the competition site for impounding. The models will be impounded prior to the start of the on-site competition and will be available after scoring for public viewing. Models will be available for return to the students after the competition.
- c. **Part II: The On-Site Model.** During the on-site competition at Regional Competitions, students will design and build a physical model of a selected region of hemagglutinin (1HTM.pdb). During the on-site competition at the State and National Competitions, students will design and build a physical model of a selected region of the neuraminidase (2HU4.pdb), which is described in the May 2009 *RCSB Molecule of the Month* written by David S. Goodsell. (http://dx.doi.org/10.2210/rcsb_pdb/mom_2009_5)
- d. Students will utilize a computer provided with the Jmol application at the competition. Students must utilize only one of the identical computers provided at the competition with the above-mentioned files on it to guide their model construction. All construction materials for the model (Mini-Toobers®¹, foam amino acid sidechains, crosslinkers and plastic red and blue end caps) will be provided. Any model not handed to the judges by the end of the competition time (50 minutes) will not be accepted for scoring.
- e. **Part III: The On-Site Written Exam.** During the 50-minute competition, students will answer a multiple choice/short answer written exam with questions about the relationship between protein structure and function, with an emphasis on swine flu and the role of hemagglutinin and neuraminidase. During the on-site competition, students may use only the materials brought with them (the 10 pages) to answer the

questions. Any exams not handed to the judges by the end of the competition time will not be accepted for scoring. Illegible answers will not receive credit.

4. **SCORING:** At the Competitions, Part I will be based on the pre-build protein model (40%), Part II on the on-site build (30%) and Part III on the written exam (30%).
- The pre-build protein model (Part I) will be scored based on the accuracy and scale of the alpha-helix and beta-sheet secondary structures, as well as other elaborations and enhancements to the protein backbone such as sidechains, DNA or associated molecules. The focus of the model should be on creatively telling the story of the molecule's significance, structure and function. Creative additions that do not support the molecular story will not receive full credit.
 - The on-site build protein model (Part II) will be scored based on accuracy of folding the Mini-Toober® model and positioning specific amino acid sidechains and/or accessory molecules.
 - The exam (Part III) will be scored for accuracy. Ties will be broken using specific questions from the written exam selected and labeled by the event supervisor before the start of the competition.

RECOMMENDED RESOURCES: MSOE CBM Science Olympiad Webpage

(<http://cbm.msoe.edu/studProg/so/index.html>) with an overview of the event (PowerPoint file) and downloadable resources, and the RCSB PDB Homepage (www.pdb.org) and website for the Science Olympiad (education.pdb.org).

Please contact your Science Olympiad State Director to find out if this event will be offered in your state in 2010.

This event is currently being sponsored by a Howard Hughes Medical Institute grant and sponsorship by Life Technologies™. Therefore, the Mini-Toobers®⁽¹⁾ will be provided to all participating states at no cost.

State Directors: please contact Shannon Colton (colton@msoe.edu) to arrange for the Protein Modeling Challenge to be offered in your state.

¹Mini-Toobers® are a product of 3D Molecular Designs, 2223 North 72nd Street, Wauwatosa, WI 53213, (414) 774-6562, Fax: (414) 774-3435, www.3dmoleculardesigns.com.

²Students may use Mini-Toobers or other comparable materials (for example: wire, pipe cleaners, chenille stems, Kwik Twists (www.kwiktivist.com), etc.