

PROTEIN MODELING

SCIENCE OLYMPIAD

Read the General Rules in the manuals and on www.soinc.org as they apply to every event.

1. **DESCRIPTION:** Students will use computer visualization and online resources to guide them in constructing physical models of proteins and in understanding how the structure of the protein determines the function. For 2012, students will model proteins involved in the **regulation of apoptosis** as they explore the discovery and treatment of a rare (one in a billion) genetic trait discovered through genome sequencing.
A TEAM OF UP TO: 3 **IMPOUND:** Yes **APPROXIMATE TIME:** 50 minutes for **Part II & III**
2. **EVENT PARAMETERS:** Pre-build models will be impounded one hour before the competition begins.
a. Students may bring up to five double-sided, 8.5"x11" pages of notes; Internet access is not permitted.
b. Supervisors will provide all materials for on-site model construction.
3. **THE COMPETITION:** This event has three parts: a pre-build model, an on-site build model and an exam.
a. **Part I: The Pre-Build Model.** Students will use a computer visualization program (Jmol; <http://cbm.msoc.edu/includes/jmol/SOJmols/2012PreBuild.html>) to design and construct a model of a specific protein based on atomic coordinate data, which can be accessed for free through the RCSB Protein Data Bank (<http://www.pdb.org>). For 2012, students will construct a model of caspase-3, based on chains A and B of the coordinate data found in the 1i3o.pdb file. Caspases are described in the August 2004 *RCSB Molecule of the Month* (<http://www.pdb.org/pdb/101/motm.do?momID=56>) by David S. Goodsell. The same constructed model of caspase-3 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.
The final pre-build model must be based on the alpha carbon backbone display of the protein and must use a scale of 2 cm per amino acid. Students may use Mini-Toobers®, or other comparable material (e.g., Kwik Twists, 12 gauge dimensional house wire, etc.), to construct their pre-build model. Students will use materials of their own choosing to add functionally relevant features to their model (e.g., select amino acid sidechains, DNA or associated molecules). 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 these additional features. Students must provide a 3"x5" note card explaining the additions to their model and what they represent and deliver their pre-build model and 3"x5" card to judges at the competition site for impounding. Models must be picked up by the students after the competition.
b. **Part II: The On-Site Model.** During the on-site competition, students will design and build a physical model of a selected region of a protein using materials provided by the event supervisor. ~~For the Invitational Competitions, students will model a selected region of Diabolo (1g73.pdb).~~ For Regional Competitions, students will model a selected region of XIAP (1i3o.pdb). For State Competitions, students will model a selected region of PARP (3od8.pdb). For the National Competition, students will model a selected region of MHC (1hsa.pdb), which is described in the February 2005 *RCSB Molecule of the Month* by David S. Goodsell (<http://www.rcsb.org/pdb/101/motm.do?momID=62>).
c. 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®, 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 will not be accepted for scoring.
d. **Part III: The On-Site Written Exam** will be multiple choice/short answer questions about the relationship between protein structure and function, with an emphasis on apoptosis and bone marrow transplants.
4. **SCORING:** 40% of the event score will be based on the pre-build protein model (Part I), 30% on the on-site build (Part II) and 30% on the written exam (Part III). The pre-build protein model (Part I) 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). 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 model and positioning specific amino acid sidechains. The exam (Part III) will be scored for accuracy. Ties will be broken using identified questions from the written exam.

Recommended Resources: Event details and available kit information can be found at: <http://www.soinc.org> & <http://cbm.msoc.edu/stupro/so/index.html> & the RCSB PDB Homepage (www.pdb.org) The purchase of mini-toober from 3D Molecular Designs helps to defray the cost of the onsite build materials used at the regional, state and national tournaments.



This event is sponsored by the Milwaukee School of Engineering