



## Protein Modeling Challenge

**Description:** Students will use computer visualization and online resources to guide them in constructing a physical model of a protein. The 2009 theme for the proteins to be modeled is Ribonucleases.

**Team:** Up to three students

**Time:** 50 minutes

**Impound:** Yes

**Event Parameters:** Students may **not** bring any materials or computers of any kind into the on-site competition except the pre-build model. An internet-accessible computer will be used for the event.

**Competition:** For **Regional** and **State Competitions**, this event has three parts: a pre-build model (Part I), an on-site build model (Part II) and an on-site exam (Part III).

For the **National Tournament**, the event will have two parts: an on-site build model and an exam. The pre-build is eliminated from the National Tournament since the Protein Modeling Challenge is a trial event and not all states offer it.

**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 the Regional and State Competitions, the protein to be modeled is ribonuclease A, based on the coordinate data found in the 1RTA.pdb file, which can be downloaded for free from the RCSB Protein Data Bank ([www.pdb.org](http://www.pdb.org)), and is described in the September 2008 *RCSB PDB Molecule of the Month* ([http://dx.doi.org/10.2210/rcsb\\_pdb/mom\\_2008\\_9](http://dx.doi.org/10.2210/rcsb_pdb/mom_2008_9)) by David S. Goodsell.

The pre-build model of ribonuclease A will be used for both the Regional and State Competitions. Please note there will not be a pre-build for the National Tournament.

The pre-build model in its final form must be based on the alpha carbon backbone display of the model. Students may use Mini-Toobers®<sup>1</sup> to model their protein, or other comparable material<sup>2</sup>. 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 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 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.

**Part II: The On-Site Model.** During the on-site competition at Regional Competition, students will design and build a physical model of a selected region of ribonuclease A, based on 1RTA.pdb and described in the September 2008 *Molecule of the Month*. During the on-site competition at the State Competition, students will design and build a physical model of a selected region of the ribonuclease A inhibitor, based on 1DFJ.pdb and described in the September 2008 *Molecule of the Month*. At the National Tournament, students will construct

a model of a selected region of ribonuclease A, based on 1RTA.pdb and described in the September 2008 Molecule of the Month.

Students will utilize a computer provided at the competition with the Jmol application, a text editor, PDB file, structure summary page and *Molecule of the Month* files on it to guide their model construction. 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®<sup>1</sup>, foam amino acid sidechains, and plastic red and blue end caps) will be provided. Any model not handed to the judges before the end of the competition time (50 minutes) will not be accepted for scoring.

**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 ribonucleases. During the on-site competition, students may use only the materials provided to answer the questions. Question content may not be limited to these materials. Any answers not handed to the judges before the end of the competition time will not be accepted for scoring.

**Scoring:** At the Regional and State Competitions, 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). At the National Tournament, 50% of the event score will be based on the on-site build and 50% on the written exam. Please note that there is not a pre-build for the National Tournament.

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, other elaborations and enhancements on 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 on these points. 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.

**References:** MSOE CBM Science Olympiad Webpage ([www.rpc.msoe.edu/cbm/scienceolympiad](http://www.rpc.msoe.edu/cbm/scienceolympiad)) with an overview of the event (PowerPoint file) and downloadable resources, and the RCSB PDB Homepage ([www.pdb.org](http://www.pdb.org)) and website for the Science Olympiad ([education.pdb.org](http://education.pdb.org)).

Mini-Toobers® are available through the MSOE Center for BioMolecular Modeling. Please contact Shannon Colton ([colton@msoe.edu](mailto:colton@msoe.edu)) for more information. This event is currently being sponsored by a Howard Hughes Medical Institute grant and therefore, the Mini-Toobers will be provided to all participating states at no cost. The RCSB PDB is distributing the kits for New Jersey.

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

<sup>2</sup>Students may use Mini-Toobers or other comparable materials (for example: Kwik Twists ([www.kwiktwist.com](http://www.kwiktwist.com))).