EDITOR'S CORNER

Welcome to CAPRI: A Critical Assessment of PRedicted Interactions

We call upon structural biologists studying protein–protein complexes to provide targets for CAPRI, a blind test of protein docking algorithms in the style of CASP.

The Critical Assessment of Techniques for Protein Structure Prediction (CASP) experiment is a blind test of the capacity of prediction algorithms to produce three-dimensional (3D) models based on sequences. Judging by the progress from CASP1 in 1994 to CASP4 in 2000, CASP succeeded not only in establishing the state of the art in structure prediction, but also in stimulating the entire field. It relies on the willingness of crystallographers and NMR spectroscopists to provide experimental structures as targets for the predictions. There were 43 in CASP4, with predictions coming from over 160 groups around the world.

The Critical Assessment of PRedicted Interactions (CAPRI) experiment aims to do the same for macromolecular interaction, now a central theme in functional genomics. CAPRI is a blind test of the ability of protein–protein docking algorithms to predict the mode of association of two proteins based on their 3D structure. It was designed in June 2001 at the Conference on Modeling Protein Interactions in Genomes organized in Charleston, South Carolina, by Ilya Vakser (Medical University of South Carolina) and Sandor Vajda (Boston University). Unlike CASP, which has a fixed time schedule, CAPRI is data driven—it starts whenever an experimentalist offers an adequate target and ends six to eight weeks later with the submission of predicted structures. The targets are protein–protein complexes, or possibly protein–DNA complexes, for which there is an experimental structure of the free components to start with, and one of the complexes at the time of evaluation. If only one component structure is available, the second component may be carved from the complex. Taking both component structures from the complex biases docking too much towards the correct solution, but a prediction starting from randomly reoriented backbone coordinates also can be considered.

Round One of CAPRI began soon after the Charleston Conference, with three target protein–protein complexes and nineteen groups of predictors. Two months later, 271 predictions were submitted on the Web site that has been opened for this purpose at the European Bioinformatics Institute (Hinxton, UK). The submissions are being evaluated by comparison with the X-ray coordinates of the complexes, kindly communicated prior to publication by crystallographers in Gif-sur-Yvette, France. Meanwhile, Round Two is on its way with four new targets.

The Management Group of CAPRI calls upon all structural biologists who have just completed, or hope to complete soon, the X-ray or NMR structure of a protein–protein complex, to provide targets for new Rounds. If both components of the complex are already in the Protein Data Bank, all that is needed to start is the two ID codes. Alternatively, one component may be give as an ID code and the other in the form of atomic coordinates communicated by the authors. Six to eight weeks later, a complete set of coordinates should be forwarded to the member of the Management Group in charge of evaluation, who will keep them confidential. We hope that, like CASP, CAPRI will attract structural biologists who reckon that prediction methods are a useful complement to experiment. In the post-genomic era, there are tens of thousands of gene products that are known or suspected to interact with many others. Not all protein pairs will be available, let alone crystallized, in the near future. Predicted modes of association can be useful guides for genetic and biochemical experiments, but the prediction methods and the algorithms first must be extensively tested and their validity assessed. This is what CAPRI aims at.

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For information on submitting targets, check the CAPRI Web site http://capri.ebi.ac.uk or contact Joël Janin (e-mail: janin@lebs.cnrs-gif.fr).

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