Assessment of ligand binding site predictions in CASP10.

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The identification of amino acid residues in proteins involved in binding small molecule ligands is an important step for their functional characterization, as the function of a protein often depends on specific interactions with other molecules. The accuracy of computational methods aiming to predict such binding residues was evaluated within the ”Function prediction (prediction of binding sites, FN)” category of the Critical Assessment of protein Structure Prediction (CASP) experiment. In the last edition of the experiment (CASP10), 17 research groups participated in this category, and their predictions were evaluated on 13 prediction targets containing biologically relevant ligands. The results of this experiment indicate that several methods achieved an overall good performance, showing the usefulness of such methods in predicting ligand binding residues. As in previous years, methods based on a homology transfer approach were dominating. In comparison to CASP9, a larger fraction of the top predictors are automated servers. However, due to the small number of targets and the characteristics of the prediction format, the differences observed among the first ten methods were not statistically significant and it was also not possible to analyze differences in accuracy for different ligand types or overall structure prediction difficulty. To overcome these limitations and to allow for a more detailed evaluation, in future editions of CASP prediction methods in the FN category will no longer be evaluated on the ”normal” CASP targets, but assessed continuously by CAMEO (Continuous Automated Model Evaluation) based on weekly pre-released sequences from the PDB. ℗ Proteins 2013;. ℗ 2013 Wiley Periodicals, Inc.

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