

W0296

Automatic Protein Structure Prediction for Structural Genomics: ORFans, the 3D-SHOTGUN meta-predictor approach and CAFASP. Daniel Fischer, Center of Excellence in Bioinformatics and Computer Science and Engineering, Univ. at Buffalo, Buffalo, NY.

Structural genomics aims at determining the structures of a representative set of proteins such that most of the remaining proteins will lie within "homology modeling" distance to one of the solved proteins. Thus, computational methods will play a critical role in generating accurate models for the remaining proteins. However, it is becoming increasingly evident that such a set will still leave many proteins beyond modeling distance. Thus, there is an urgent need for better methods aimed at generating relatively accurate models for those proteins with no close homologues of known structure.

Here I describe the fully automated fold-recognition meta-predictor 3D-SHOTGUN. The input are the top models predicted by a number of autonomous, independent, fold-recognition servers. The output are hybrid models, that are on average, more complete and more accurate than those used as input. 3D-SHOTGUN models have allowed experimentalists to generate experimentally verifiable hypothesis, including the correction of errors in recently determined structures.

CAFASP and LiveBench experiments have demonstrated that 3D-SHOTGUN is significantly superior to any of the individual servers, and is one of the best automated tools available today.