Development of a meta-score to assess the quality of protein models

Matsuyuki Shirota^{1,2}, Takashi Ishida¹, Kengo Kinoshita^{1,2}

¹ Human Genome Center, Institute of Medical Science, University of Tokyo ² Institute for Bioinformatics Research and Development, Japan Science and Technology Agency

The development of an accurate scoring function of protein structures is crucial for protein structure prediction. Two requisites for such a function would be the ability to recognize the native structure among many decoys (model structures) and the correlation with the quality of the model structures. In this study, we developed a meta-score for protein structures by combining seven all-atom distance dependent statistical potentials and two residue-based 3D profile scores. By using these component scores of a protein structure as input for the support vector regression (SVR), the meta-score was designed to predict its GDT TS score, which is the measure of the structural similarity to native. The decoys in the CASP7 (Critical Assessment of Techniques for Protein Structure Prediction) experiment were used for training the meta-score. The nine component methods and the meta-score were assessed with the decoys in the CASP8 experiments. As results, each component method displayed the trade-off between the recognition of the native structure and the correlation with the GDT TS score. On the other hand, the meta-score achieved as good performances as the best of the component methods in both of these criteria. Our result would suggest the benefit of combining various evaluation techniques in model evaluation.