CASP3 prediction results for the fold recognition tool ProFIT

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To objectively assess protein structure prediction methods, community-wide experiments are carried out where predictions are made prior to publication of the three dimensional structure of the target (CASP1-3). We describe the results obtained in our third participation in the CASP experiment using fold recognition techniques. The approach relies on knowledge based potentials for alignment production and fold identification. Our predictions were based on single sequences rather than multiple sequence alignments. Although several models per target were accepted we voluntarily submitted only one. In the fold recognition category we submitted predictions for 15 targets and find nine to be succesful. For six of them (T0044, T0053, T0054, T0074, T0079, T0081) a remote homologue structure exists in PDB. The remaining three (T0046, T0071, T0077) had structure similarity to the targets despite of the fact that there was no recognizable evolutionary link to a known structure. Of the six unsuccessful predictions, one was a novel fold, while the remaining five had very low structure similarity and no detectable evolutionary relationship to a known structure. In addition, we submitted five models in the comparative modeling section which posed interesting alignment problems. Three of these (T0055, T0057, T0064) had accurate alignments. We present the methods used, the strategy adopted in the predictions and the prediction results.

References

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