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Utilizing Profile-to-Profile Alignments for Predicting Protein-Protein Interactions PETRAS KUNDROTAS, EMIL ALEXOV, Clemson University — One of the biggest challenges in homology-based modeling of protein complexes is the detection of remote similarities between query and template. Most prominent way in this direction embraces alignments of profiles for query and template sequences by means of dynamic programming algorithm. While this technique is well elaborated for single protein molecules, little was done in employing it for prediction of protein-protein interactions. Here we present our recent development of a profile-to-profile alignment algorithm for predicting protein complexes. The core of the algorithm is enhancement of profiles with information about existing (template) or putative (query) interfacial residues. This is further used in order to alter the standard dynamic programming algorithm by putting an extra weight in matching interfacial residues and increasing gap penalties at the interface. We aligned all sequences in our PROTCOM40 database against each sequence in the dataset, except sequence with itself. For further examination we chose only alignments that are statistically significant and have template sequences belonging to different chains of a complex in our dataset. We have clearly demonstrated that profile-to-profile alignment technique outperforms considerably the standard BLAST homology modeling with respect to both amount and quality of the produced models of protein complexes.

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