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Combining biophysical and bioinformatical approaches for predicting residue's contacts. EMIL ALEXOV, AMBER ALLARDICE, PETRAS KUNDROTAS, Clemson University — One of the most important task of the post genomics era is to utilize the enormous sequence information delivered from the genomes and to predict 3D structure of proteins. The quality of the predicted structure depends on many factors including the improvement made in ab initio, threading and homology modeling methods. Here we combine the method of correlated mutations with biophysical restrains in order to predict residue's contacts from amino acids sequence alone. The parameters of the protocol were optimized against a set of 21 proteins with known high resolution 3D structures. The effects of the degree of residue conservation, sequence similarity among the sequences within the multiple sequence alignment and conservation coefficient of two amino acids positions were studied. It was shown that the prediction accuracy of the method of correlated mutations alone is pure, on average only 10% of the contacts are predicted correctly. However, adding biophysical filters greatly improves the accuracy of the predictions. Thus, implying pairing rules for charged, polar and hydrophobic residues significantly reduces the total number of the predictions, e.g. reduces the coverage, however, most of the rejected predictions are false positives. As result, the relative rate of the correct predictions increases.

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