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Multistage Docking Approach for Protein-RNA Interactions Prediction in CAPRI and CASP

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Protein-RNA interactions and recognition are essential in gene expression, regulation of transcription, and other biological processes. Prediction of protein and RNA is also a new challenge category for CAPRI and CASP. In this work, we proposed a multistage docking protocol called CoDockPR, which integrates the shape complementarity, knowledge-based scoring functions, and interface similarity evaluation. We trained a knowledge-based scoring function by the iterative method to discriminate the near-native structures of protein-RNA interaction. FFT-based method was used to systematically evaluate shape complementarity, and the retained conformations were evaluated by the knowledge-based scoring function. In addition, we established a protein-RNA interface library and further ranked the conformations based on the interface similarity. By testing on protein-RNA docking benchmark 1.0, CoDockPR remarkably improves the success rate and hit count. The CoDockPR program were applied for the protein-RNA complex prediction of T185 in CAPRI, and T1189 and T1190 in CASP. By compared with the available crystal structures, we analyzed the predicted results and the existing issues. Considering its robust predictive performance, our docking protocol is a good alternative for the protein-RNA interactions prediction.

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