عنوان مقاله:

β-sheet Topology Preciction Using Probability-based Integer Programming

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خلاصه مقاله:

β-sheet topology prediction is a major unresolved problem in modern computational biology. It is a challenging inermediate step toward the protein tertiary structure prediction. Different methods have been provided to deal with the problem of determining the β-sheet topology. Here, ab-initio probability-based methods called Beta Probel and BetaProbe2 are utilized to specify the β-sheet topology. In these methods, the stability and the frequency of β-strand pairwise interaction and β-sheet conformation are spotted. To predict more frequent interactions between β-strand pairs, besides pairwise alignment probability, the probability of occuring β-strand pairwise interaction is considered to compute the score of the interactions. Furthermore, to determine the β-strand pairwise alignment probability more accurately, a dynamic programming approach is utilized. In addition, the integer programming optimization is combined with the probabilites of β-strand pairwise interactions to determine the β-sheet topology. Moreover, the β-sheet conformation probability is considered to give better chances to more observed conformations for selection. Experimental results show that BetaProbel and BetaProbe2 significantly outperform the most recent integer programming-based method with respect to β-sheet topology prediction.

کلمات کلیدی:

β-sheet topology prediction, integer programming, dynamic programming, pairwise alignment

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https://civilica.com/doc/707279