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技术与方法

基于最小自由能和协变信息预测带伪结RNA二级结构的迭代化方法

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摘要

多数RNA分子的结构在进化中是高度保守的，其中很多包含伪结。而RNA伪结的预测一直是一个棘手问题， 很多RNA二级结构预测算法都不能预测伪结。文章提出一种基于迭代法预测带伪结RNA 二级结构的新方法。该方法在给潜在碱基对打分时综合了热力学和协变信息， 通过基于最小自由能RNA折叠算法的多次迭代选出所有的碱基对。测试结果表明：此方法几乎能预测到所有的伪结。与其他方法相比， 敏感度接近最优， 而特异性达到最优。

关键词 RNA二级结构 伪结 协变信息 最小自由能

分类号

An iterative method for prediction of RNA secondary structures in-cluding pseudoknots based on minimum of free energy and covari-ance

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Abstract

<P>Most functional RNA molecules have characteristic, highly conserved structures, such as pseudoknots. But the prediction of RNA pseudoknots has largely remained a difficult problem, and many existing algorithms for prediction of RNA secondary structures do not have the ability to predict pseudoknots. Here we present a new method for predicting RNA secondary structures including pseudoknots through iteration. The algorithm combines thermodynamic and covariation information to assign scores to all possible base pairings. Base pairings are then predicted with the help of the iterated RNA folding algorithm based on minimum of free energy. Test result shows that nearly all pseudoknots are predicted. Compared to other methods, the method achieves a specificity that is among the best and a sensitivity that is nearly the best.</P>

Key words Most functional RNA molecules have characteristic highly conserved structures such as pseudoknots. But the prediction of RNA pseudoknots has largely remained a difficult problem and many existing algorithms for prediction of RNA secondary structures do not have the ability to predict pseudoknots. Here we present a new method for predicting RNA secondary structures including pseudoknots through iteration. The algorithm combines thermodynamic and covariation information to assign scores to all possible base pairings. Base pairings are then predicted with the help of the iterated RNA folding algorithm based on minimum of free energy. Test result shows that nearly all pseudoknots are predicted. Compared to other methods the method achieves a specificity that is among the best and a sensitivity that is nearly the best.

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