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其它

应用集成神经网络预测蛋白质相互作用位点

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摘要：

蛋白质相互作用位点在现代药物设计与构建蛋白质相互作用网络方面有着重要的意义。基于一个含有35个蛋白质分子的数据集,首先提取蛋白质的序列谱、熵值、可及表面积3种特征,然后运用误差反向传播神经网络以及其集成对蛋白质的相互作用位点进行了预测。采用35次留一法(一倍交叉验证)进行训练与测试,结果显示每当加入一种新特征时,预测结果都有相应的提高,并且把神经网络集成时,结果又有了一定程度的提高。

关键词： 蛋白质相互作用位点 序列谱 熵 可及表面积 集成神经网络

Prediction of protein-protein interaction sites using ensemble neural networks

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Abstract:

Protein-protein interaction sites are very important in drug design and construction of protein interaction networks. A data set that contained 35 proteins was used. First, 3 features of the proteins were extracted. They were sequence profiles, entropy and accessible surface area. Then back propagation neural networks and their integration were applied to predict protein protein interaction sites. One protein was tested each time and the remaining 34 proteins were used to train the classifiers (one-crossover). The final result was good and when adding one new feature the accuracy of prediction improved. When integrating these features the outcome has more accuracy than a single classifier.

Keywords: protein-protein interaction sites sequence profiles entropy accessible surface area ensemble neural networks

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