Abstract

Catalytic residues play an important role in enzymes. Therefore, predicting these residues in enzymes is highly valuable. The purpose of this study is to provide a bioinformatics method that predicts catalytic residues in enzymes. The method uses enzyme sequence and structure information to build a predictor based on Deep Neural Network (DNN) and is tested by five- fold cross validation on non-redundant dataset extracted from Catalytic Site Atlas (CSA). The accuracy of catalytic prediction is improved by using different flavor of sequence and structure information. We achieved a high classification accuracy of 84% in terms of the area under curve, which shows that the proposed DNN model is capable of contributing significantly to enzyme engineering and drug design.