© 2013 FIZ Karlsruhe

io-port 06058999

Lai, Lien-Fu; Wu, Chao-Chin; Huang, Liang-Tsung

First report of knowledge discovery in predicting protein folding rate change upon single mutation.

Huang, De-Shuang (ed.) et al., Bio-inspired computing and applications. 7th international conference on intelligent computing, ICIC 2011, Zhengzhou, China, August 11–14. 2011. Revised selected papers. Berlin: Springer (ISBN 978-3-642-24552-7/pbk). Lecture Notes in Computer Science 6840. Lecture Notes in Bioinformatics, 624-631 (2012).

Summary: To explore the mechanism of protein folding is one of the important topics in protein research. The accurate prediction of protein folding rate change is helpful and useful in protein design. In earlier study, we have firstly analyzed the prediction of folding rate change upon single point mutation and constructed a non-redundant dataset of F467. F467 consists of 467 mutants with various features and widely distributed on secondary structure, solvent accessibility, conservation score and long-range contacts. In this work, we therefore focused on effectively developing the knowledge in F467 dataset. We have systematically analyzed the dataset and presented several representative data mining techniques, including decision tree, decision table and association rule algorithms. Furthermore, we have interpreted, evaluated, and compared the knowledge obtained from different techniques. The experimental results showed that the present approach can effectively develop the knowledge in the dataset and the outcomes can increase the understanding of predicting protein folding rate change upon single mutation. We have also created a website with related information about this work and it is freely available at `http://bioinformatics.myweb.hinet.net/kdfreedom.htm`.

Keywords: knowledge discovery; data mining; protein folding rate; single point mutation
doi:10.1007/978-3-642-24553-4_83