Abstract No.47

β-turn types prediction in proteins using statistical model of LDA and Artificial Neural Network

Fatemeh Zahedi Barashki, Parviz Abdolmaleki, Ebrahim Barzegari Asadabadi, Samad Jahandideh

Department of Biophysics, Faculty of Biological Science, Tarbiat Modares University, Tehran, PO Box: 14115/175
E-mail: free5zaher@yahoo.com

Protein secondary structure prediction is an intermediate step in prediction of tertiary structure from amino acid sequence. B- turn is a very important element of protein structure, then the prediction of β-turns and their types are crucial process of the secondary structure prediction. The aim of the present study is predicting β-turn types using a two- stage hybrid model that comprise the linear discriminant analysis (LDA) and the artificial neural network (ANN). The databank was used in this study, consisted of 565 non homologous Protein chains which prepared using the PAPIA system. The percentage of the occurrence for 20 types amino acids in different positions of β-turn sequence (that is i, i+1, i+2, i+3) utilized as the structural parameters. Initially, LDA(a statisrical technique) analyzed 100 structural parameters and selected 40 significant parameters. The selected parameters were then used as input into a three layered feed-forward neural network. After optimization, the ANN architecture was consisted of 40,15 neurons for input and hidden layer respectively. The output layer comprise 5 neuron each of which related to 5 types of β-turn types including NS, I, II, VIII and IV of β-turn. Performance measures (MCC, prediction accuracy, sensitivity, specificity and probability of correct prediction) used for the evaluation of established model. MCC values for types I, IV, VIII and prediction accuracy values in types I and NS were the better than obtained results in previous established model (multi nomial logistic regression and ANN). In conclusion, a two–stage hybrid model was introduced that was able to predict β-turn types with high accuracy. This model is simpler and takes less time compared with the previous established model. Therefore it will highlights its potential usefulness to be applied in protein secondary structure prediction.

Key words: β-turn types Prediction, Linear discriminant analysis, Artificial neural network.

Abstract No.48

Studies on interaction between propranolol and HSA in presence and absence of magnetic field

Z. Rouhbakhsh Zaeri[1], M. R. Housaindokht[1,2]*

1- Department of chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran, Email: zeinabrouhbakhsh@yahoo.com
2- The Research Institute of Biotechnology, Ferdowsi University of Mashhad, Mashhad, Iran

Human serum albumin (HSA) is the most abundant carrier protein of the blood with a high affinity for a wide range of metabolites and drugs and have many physiological functions. Propranolol, 1-[isopropylamino-3-[1-naphthyloxy]-2-propanol], is a adrenoceptor antagonist (-blocker), which is widely used in the treatment of several diseases such as cardiac arrhythmia, angina pectoris, sinus tachycardia, thyrotoxicosis, hypertrophic subaortic stenosis and hypertension. The effects of static magnetic fields (SMFs) on biological systems have been a topic of considerable interest for last two decades. The increasing production of electric (EMFs) and magnetic fields (MFs) due to the increasing use of electronic devices in homes and work places, is encouraging studies on the influences of magnetic fields on living organisms with a goal to protect better human health against their probable unfavorable effects.
In this paper, the interaction between propranolol HSA and in physiological buffer (pH 7.4) was investigated by UV and fluorescence absorption spectroscopy. In order to understand the effect of magnetic field, all experiments were also done in the presence of magnetic field (3 mT); and the binding parameters were determined for both cases.
The Hill equation was employed to analyze the data obtained, for determining of the binding capacity, g, binding constant, K, and Hill constant, n_H,.

The results showed that the values of g and n_H increased slightly in the presence of magnetic field, and the binding constant in both method, uv and fluorescence spectroscopy, was decreased in the magnetic field exposed situation.

Key words: propranolol, HSA, magnetic field.
