Prediction of the transmembrane regions of b-barrel membrane proteins with a neural network-based predictor

P.L.Martelli 1, I.Jacoboni 1, P.Fariselli 1, 2 and R.Casadio1, 2*

1 Laboratory of Biocomputing, Centro Interdipartimentale per le Ricerche Biotecnologiche (CIRB), Bologna, Italy
2 Laboratory of Biophysics, Department of Biology, University of Bologna, Bologna, Italy.

A method based on neural networks is trained and tested on a non-redundant set of b-barrel membrane proteins known at atomic resolution with a jack-knife procedure. The method predicts the topography of transmembrane beta strands with residue accuracy as high as 78 % when evolutionary information is used as input to the network. 93% of the transmembrane b-strands included in the training set are correctly assigned. The predictor includes an algorithm of model optimisation, based on dynamic programming, which correctly models 8 out of the 11 proteins present in the training/testing set. In addition protein topology is assigned on the basis of the location of the longest loops in the models. We propose this as a general method to fill the gap of the prediction of b-barrel membrane proteins. Furthermore, a Hidden Markov Model can filter b-barrel membrane proteins out from a set containing globular and all alfa membrane proteins.