

Identification of Protein Domains on Topological Basis

C. Anselmi, G. Bocchinfuso, A. Scipioni, P. De Santis

Dip. di Chimica - Universita' La Sapienza - Ple A. Moro 5

A theoretical method is proposed to identify structural domains in proteins of known structures. It is based on the distribution of the local axes of the polypeptide chain. In particular, a statistical analysis is applied to the contributions of the local axes to the absolute writhing number, a topological property of a space curve resulting from the number of self-crossings in the curve projections onto a unit sphere. This finding supports the hypothesis that topological requirements should be satisfied in the process of protein folding and in the final organization of the tertiary structures.