A statistical empirical energy function for proteins

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Motivation

Reduced representations of proteins have been playing a keyrole in the study of protein folding. Many such models are available, with different details of representation. The aim of the present work is to provide both a discrete and an analytical forcefield for a reduced model employing only two centers of interactions per amino acid.

Methods

All protein structures in the set top500H have been converted in reduced form. The distribution of pseudobonds, pseudoangle, pseudodihedrals and distances of centers of interactions have been obtained and fitted to analytical functions. The fit allows to link the features of the distributions to specific secondary structure elements. The correlation between adjacent pseudodihedrals has been converted in an additional energetic term which is able to account for cooperative effects in secondary structure elements.

Results

Tests have been performed using a minimization tool developed within a novel concurrent multiagent framework for protein structure prediction. Tests will be presented also on decoys and on simple model systems. The pseudodihedral correlation term appears to be of utmost importance for proper discrimination of native like structures.

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