Poster E-6

Flexibility adaptation of enzymes to low temperatures

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Short Abstract: Psychrophiles organisms have evolved by producing cold-adapted enzymes that efficiently catalyze biochemical reactions at low temperatures. We report a systematic comparative analysis of flexibility profiles and rigid domains of pairs of homologous psychrophilic and mesophilic enzymes belonging to the structural families of xylanases, a-amylases, citrate synthase and, adenylate kinase.

Long Abstract:
The class of organisms called psychrophiles has optimal temperatures for growth below 20˚C. These organisms have evolved by producing, among other features, cold-adapted enzymes that efficiently catalyze biochemical reactions at low temperatures. The thermal compensation in these enzymes is reached through an increase in their conformational flexibility that is usually associated to a reduction of their stability [D'Amico-2001] [Georlette-2004]. Subtle adjustments of the protein structure can be account for both changes in flexibility and stability. Furthermore, the adaptation to cold could be achieved by two different strategies: an increase in the flexibility of either a selected area, i.e., around the catalytic residues, or the overall protein structure [Zecchinon-2001].
In the present study, we report a systematic comparative analysis of pairs of homologous psychrophilic and mesophilic enzymes belonging to the structural families of xylanases, α-amylases, citrate synthase and, adenylate kinase. Pairwise structural alignments were performed in order to select the corresponding conserved residues.
We have investigated differences in the computed flexibility profiles (i.e. the so called "temperature factors" or B-factors) with a coarse-grained Gaussian Network Model [Atilgan-2001]. The model represents a folded protein structure as an elastic network where α-carbons are chosen as the nodes. Springs connect each node to their neighbors located within a cutoff distance. The cross-correlations between residue fluctuations were also analyzed. Furthermore, the normal modes of a molecule were utilized to develop a new procedure to identify rigid domains within a protein structure. The method takes into account volume denoted by the position vectors of the different combinations of atoms.
An average increase in the dynamic fluctuations of the conserved residues is observed in the psychrophilic enzymes respect to the mesophilic counterpart. Moreover, the cross-correlations between residues present significant differences between them. Finally, the analysis of the size and location of the different rigid body regions within the protein structures were also discussed.

References

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