

# Structural adaptation to low temperatures: analysis of the subunit interface of oligomeric psychrophilic enzymes

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## Motivation

Psychrophiles are ectothermic organisms adapted to life in cold permanent environment. Enzymes from such organisms show a higher catalytic efficiency in the 0 - 20 °C temperature range when compared to mesophile, thermophile and hyperthermophile homologues. This is usually associated to a lower thermostability. Physical and chemical characterization of these enzymes is currently under study in order to understand the molecular basis of cold adaptation. Psychrophilic enzymes are often characterized by a higher flexibility which allows for a better interaction with substrates, and by lower activation energy requirement if compared to mesophile and thermophile counterparts. In their tertiary structure, psychrophilic enzymes present fewer stabilizing interactions, longer and more hydrophilic loops, higher glycine and lower proline and arginine content. Protein surfaces often show a lower charged amino acid content and a high number of hydrophobic side-chains.

## Methods

In this study, we carry out a comparative analysis of the structural characteristics of the interfaces between oligomeric psychrophilic enzyme subunits. Crystallographic structures of oligomeric psychrophilic enzymes, their mesophile homologues (and, when available, also thermophile and hyperthermophile enzymes) belonging to five different protein families were retrieved from Protein Data Bank. The following structural parameters were calculated from the atomic coordinates of each enzyme within its family: overall and core interface area, characterization of polar and apolar contributes to the interface, ion pair number and hydrogen bonds between monomers, internal area and total volume of non solvent-exposed cavities at interface, average packing of interface residues. These properties were compared to those of mesophile, thermophile and hyperthermophile enzymes. Results were analysed using Student's unpaired two-tailed t-test.

## Results

The comparative analysis reveals that some of the differences observed within each family could be attributed to cold temperature adaptation. The most significant differences between psychrophilic and mesophilic proteins are found in the number of ion pairs and the number of hydrogen bonds. Psychrophilic proteins, moreover, show a significant decrease in the apolarity of their subunits interface.

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