Protein structures and thermostability

G. Tasco[(1)], L. Montanucci[(1)], P. Fariselli[(2)], P. Martelli[(1)], P. Marani [(1)] and R. Casadio[(2)]

[(*)]Interdepartmental Center for Biotechnological Research(CIRB)
via Irnerio 42, 40126 Bologna, Italy
gluca@biocomp.unibo.it
[(2)] Department of Biology, University of Bologna, via Selmi 2, Bologna, Italy

What is thermostability? This question is still unanswered in spite of several studies aiming at the determination of typical features of thermostable proteins (for a recent review see [1]). We tackled the problem considering a large set of proteins from thermophilic and hyperthermophilic organisms available in the PDB with atomic resolution. A PDB derived data base was generated containing proteins from thermophiles and their counterparts from mesophiles, with the specific constraint of sequence identity >30% and difference in sequence length <20%. By this, 128 proteins from thermophiles were compared to 109 structures from mesophiles with a root mean square deviation <0.29 nm.

Residue composition, secondary structure, length of secondary structure motifs, hydrogen bonds, salt bridges, composition of solvent accessible surface were evaluated with specifically developed programs in both sets in order to perform a statistical analysis.

The results of our investigation are as follows: proteins from thermophiles are endowed with more charged residues, particularly in the exposed surfaces, with more salt bridges, that are more accessible on average as compared to those in proteins from mesophiles. However neither the content of secondary structure neither the length of secondary structure motifs was significantly different. These data, all together suggest that thermostable proteins as compared to their mesophilic counterpart are endowed with more electrostatic interactions, particularly on the protein surface to stabilize more water dipoles and compensate for thermal motion at high temperatures.

References

[1] Arnold FH, Wintrode PL, Miyazaki K, Gershenson A. (2001). How enzymes adapt: lessons from directed evolution. Trends Biochem Sci. 26:100-106