DETERMINATION OF A RESIDUES NETWORK WHICH DETERMINES THE METAL SPECIFICITY IN FE/MN SUPEROXIDE DISMUTASES.

Bachega J.F.R.[1], Navarro M.V.A.S.[2], Bleicher L.[1], Garratt R.C.[1]

[1]Instituto de Física de São Carlos, Universidade de São Paulo, Avenida Trabalhador Sãocarlense 400, CEP 13560-970, São Carlos, SP, Brazil.[2]Laboratorio Nacional de Luz Síncrontron. Rua Giuseppe Máximo Scolfaro, 10000 Pólo II de Alta Tecnologia de Campinas CEP 13083-970, Campinas, SP

Introduction: Statistical Coupling Analysis (SCA), a computational technique whose development started in 1999 by Ranganathan and co-workers, uses the amino acid distribution in positions of protein sequences alignments and the interdependence of these distributions between positions to identify amino acids with important roles in structure and function in a protein family. Superoxide dismutases (SOD's) are a crucial class of enzymes against free radical toxicological actions, which eliminate superoxide radicals by decomposing them into hydrogen peroxide and oxigen. Depending on metal selectivity and structural organization, currently the SODs can be separated in three different classes: manganese- or iron-containing SODs (MnSOD and FeSOD), which posses a very similar fold. Objective: determine which residues are involved in metal specificity in the structures of Fe/Mn-SOSDs. Results: We have identified three independent clusters of residues – one is related to the formation of dimers, the second is characteristic of Mn-SODs and the third of Fe-SOD's.