

Advantages of integrating X-ray diffraction and NMR structural data with X-ray absorption spectroscopy. Examples from the study of copper binding proteins

S. Mangani

Department of Chemistry, University of Siena, Via Aldo Moro, 53100 Siena, Italy

X-ray absorption spectroscopy (XAS) studies of biological systems have gained great impetus and have achieved relevant success in recent years¹.

A new application of XAS, which has special relevance in structural genomics projects, is to couple it to the structure determination of the metallo-protein in solution obtained by NMR methods. This application of XAS is very promising since it quickly and accurately provides the structure of the metal binding site, which is most difficult to obtain by NMR. It is then quite straightforward to exactly identify the metal binding site in the protein, by knowing the remaining of the metallo-protein structure. This method allows to speed up the entire process of structure determination and, in addition, it provides useful information on the electronic structure of the metal ion in the studied system. We have exploited this synergism between the NMR and XAS techniques for a rapid and complete elucidation of the structure of copper chaperonins^{2,3}. Working examples taken from our work on copper binding proteins will be used to illustrate the advantages of the combined techniques.

References

1. Ascone I., Hasnain S. S. (2003) *J. Synchr. Rad.* **10**, 1-3
2. Banci, L., Bertini, I., Del Conte, R., Mangani, S., Meyer-Klaucke, W. (2003) *Biochemistry* **42**, 2467-2474
3. F. Arnesano, L. Banci, I. Bertini, S. Mangani, A.R. Thompsett (2003) *Proc. Natl. Acad. Sci. USA* **100**, 3814-3819