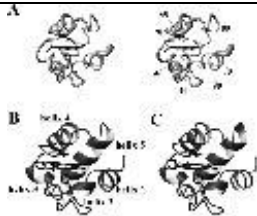
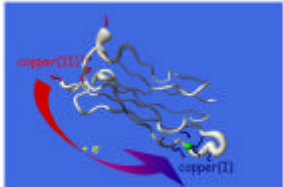
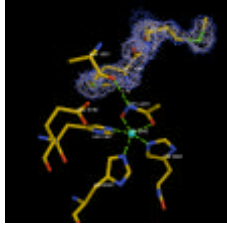

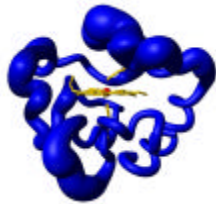
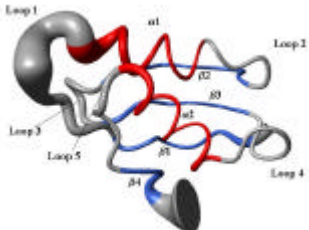


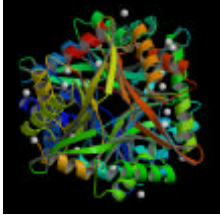


Publications 2003

Structural genomics/structural biology

<p>1. Bartalesi, I., I. Bertini, A. Rosato. Structure and dynamics of reduced <i>Bacillus pasteurii</i> cytochrome <i>c</i>: oxidation state dependent properties and implications for electron transfer processes. Biochemistry 42: 739-745, 2003.</p>	 <p>PDB code: 1N9C</p>
<p>2. Arnesano F, Banci L, Bertini I, Mangani S, Thompsett A.R. A redox switch in CopC: An intriguing copper trafficking protein that binds copper(I) and copper(II) at different sites. PNAS USA 100: 3814-3819, 2003</p>	 <p>PDB code: 1NM4</p>
<p>3. Bertini, I., V. Calderone, M. Fragai, C. Luchinat, S. Mangani, B. Terni. X-ray structures of ternary enzyme-product-inhibitor complexes of MMP. Angew.Chem.Int.Ed. 42: 2673-2676, 2003.</p>	 <p>PDB code: 1OS2, 1OS9</p>
<p>4. Banci, L., I. Bertini, S. Ciofi-Baffoni, L. Gonnelli, X.C. Su. A core mutation affecting the folding properties of a soluble domain of the ATPase protein CopA from <i>Bacillus Subtilis</i>. J.Mol.Biol. 331: 473-484, 2003.</p>	 <p>PDB code: 1OQ3, 1OQ6</p>
<p>5. Assfalg M, Bertini I, Dolfi A, Turano P, Mauk AG, Rosell FI, Gray HB. Structural model for an alkaline form of ferricytochrome C. J Am Chem Soc 125: 2913-22, 2003. PDB code: 1LMS</p>	 <p>PDB code: 1LMS</p>
<p>6. Banci, L., I. Bertini, F. Cramaro, R. Del Conte, M.S. Viezzoli. Solution structure of apo Cu,Zn superoxide dismutase: the role of metal ions in protein folding. Biochemistry 42: 9543-9553, 2003.</p>	 <p>PDB code: 1RK7</p>

<p>7. Balatri, E., L. Banci, I. Bertini, F. Cantini, S. Ciofi-Baffoni. Solution structure of Sco1: a thioredoxin-like protein involved in cytochrome c oxidase assembly. Structure 11: 1431-1443, 2003.</p>	 <p>PDB code: 1ON4</p>
<p>8. Banci, L., I. Bertini, S. Ciofi-Baffoni, L. Gonnelli, X.C. Su. Structural basis for the function of the N terminal domain of the APTase CopA from <i>Bacillus subtilis</i>. J.Biol.Chem. 278: 50506-50513, 2003.</p>	 <p>PDB code: 1P6T</p>
<p>9. Arnesano, F., L. Banci, M. Benvenuti, I. Bertini, V. Calderone, S. Mangani, M.S. Viezzoli. The evolutionarily conserved trimeric structure of CutA1 proteins suggests a role in signal transduction. J.Biol.Chem. 278: 45999-46006, 2003.</p>	 <p>PDB code: 1OSC, 1NAQ</p>

10. Bertini, I. Structural Genomics. **Acc Chem Res.** 36: 155, 2003
11. Banci L, Rosato A. Structural genomics of proteins involved in copper homeostasis. **Acc Chem Res**, 36: 215-21, 2003
12. Atreya HS, Mukherjee S, Chary KV, Lee YM, Luchinat C. Structural basis for sequential displacement of Ca(2+) by Yb(3+) in a protozoan EF-hand calcium binding protein **Protein Sci** 12: 412-25, 2003
13. Banci, L., I. Bertini, S. Ciofi-Baffoni, R. Del Conte, L. Gonnelli. Understanding copper trafficking in bacteria: interaction between the copper transport protein CopZ and the N-terminal domain of the copper ATPase CopA from *Bacillus subtilis*. **Biochemistry** 42: 1939-1949, 2003.
14. Bertini I, Rosato A. Bioinorganic chemistry in the postgenomic era. **PNAS USA** 100: 3601-3604, 2003
15. Bertini I, Ghosh K, Rosato A, Vasos PR. A high-resolution NMR study of long-lived water molecules in both oxidation states of a minimal cytochrome C. **Biochemistry**, 42: 3457-63, 2003
16. Bertini, I., C. Luchinat, M. Sola. Zinc enzymes/models. **Encyclopaedia of Chemistry** DOI: 10.1002/0471227617.EOC205:2003
17. Banci, L., I. Bertini, A. Ciulli, M. Fragai, C. Luchinat, B. Terni. Expression and high yield production of matrix metalloproteinase 12 and of an active mutant with increased solubility. **J.Mol.Catal.A: Chemical** 204-205: 401-408, 2003.
18. Banci, L., I. Bertini, I.C. Felli, L. Krippahl, K. Kubicek, J.J.G. Moura, A. Rosato. A further investigation of the cytochrome *b5* - cytochrome *c* complex. **J.Biol.Inorg.Chem.** 8: 777-786, 2003.

Spectroscopy and Methodologies

19. Gelis I, Katsaros N, Luchinat C, Piccioli M, Poggi L. A simple protocol to study blue copper proteins by NMR. **Eur J Biochem** 270: 600-609, 2003
20. Bertini, I., C. Luchinat, K. Nerinovski, G. Parigi, M. Cross, Z. Xiao, A.G. Wedd. Application of NMRD to hydration of rubredoxin and a variant containing a (Cys-S)₃Fe^{III}(OH) site. **Biophys.J.** 84: 545-551, 2003.
21. Banci L, Bertini I, Del Conte R, Mangani S, Meyer-Klaucke W. X-ray absorption and NMR spectroscopic studies of CopZ, a copper chaperone in *Bacillus subtilis*: the coordination properties of the copper ion. **Biochemistry** 42: 2467-74, 2003
22. Luchinat C, Dolderer B, Del Bianco C, Echner H, Hartmann HJ, Voelter W, Weser U The Cu(I)(7) cluster in yeast copper thionein survives major shortening of the polypeptide backbone as deduced from electronic absorption, circular dichroism, luminescence and (1)H NMR. **J Biol Inorg Chem** 8: 353-359, 2003
23. Arnesano, F., L. Banci, I. Bertini, I.C. Felli, C. Luchinat, A.R. Thompson. A strategy for the NMR characterization of type II copper(II) proteins: the case of the copper trafficking protein CopC from *Pseudomonas syringae*. **J.Am.Chem.Soc.** 125: 7200-7208, 2003.
24. Assfalg, M., I. Bertini, P. Turano, A.G. Mauk, J.R. Winkler, B.H. Gray. ¹⁵N-¹N residual dipolar coupling analysis of native and alkaline-K79A *S. cerevisiae* cytochrome *c*. **Biophys.J.** 84: 3917-3923, 2003.
25. Bertini, I., I. Gelis, N. Katsaros, C. Luchinat, A. Provenzani. Tuning the Affinity for Lanthanides of Calcium Binding Proteins. **Biochemistry** 42: 8011-8021, 2003.
26. Bertini, I., C. Luchinat, P. Turano, G. Battaini, L. Casella. The magnetic properties of myoglobin as studied by NMR. **Chemistry - A European Journal** 9: 2316-2322, 2003.
27. Galanis, A.S., G.A. Spyroulias, R. Pierattelli, A. Tzakos, A. Troganis, I.P. Gerothanassis, G. Pairas, E. Manessi-Zoupa, P. Cordopatis. Zinc-binding in peptide models of ACE active sites studied through ¹H NMR and chemical shift perturbation mapping. **Biopolymers** 69: 244-252, 2003.
28. Geraldes, C.F.G.C., C. Luchinat. Lanthanides as shift and relaxation agents in elucidating the structure of proteins and nucleic acids. **Met.Ions Biol.Syst.** 40: 513-588, 2003.
29. Turano, P., G. Battaini, L. Casella. Validation of paramagnetic cross correlation rates for solution structure determination of high spin iron(III) heme proteins. **Chem.Phys.Lett.** 373: 460-463, 2003.
30. Banci, L., S. Camarero, A.T. Martinez, M.J. Martinez, M. Perez-Boada, R. Pierattelli, F.J. Ruiz-Duenas. NMR study of Mn(II) binding by the new versatile peroxidase from the white-rot fungus *Pleurotus eryngii*. **J.Biol.Inorg.Chem.** 7: 777-786, 2003.
31. Bertini, I., F. Capozzi, C. Luchinat. Electronic isomerism in oxidized HiPIPs revisited. **ACS series** 858: 272-286, 2003.
32. Bertini, I., G. Cavallaro, C. Luchinat, I. Poli. A use of ramachandran potentials in protein solution structure determinations. **J.Biomol.NMR** 4: 355-366, 2003.
33. Hinse, C., C. Richter, A. Provenzani, J. Stockigt. In vivo monitoring of alkaloid metabolism in hybrid plant cell cultures by 2D cryo-NMR without labelling. **Bioorg Med Chem** 11: 3913-3919, 2003.
34. Kateb, F., M. Piccioli. New routes to the detection of relaxation allowed coherence transfer in paramagnetic molecules. **J.Am.Chem.Soc.** 125: 14978-14979, 2003.
35. La Penna, G. A constrained maximum entropy method in polymer statistics. **J.Chem.Phys.** 119: 8162-8174, 2003.

Mobility Study

36. Shipp, E., F. Cantini, I. Bertini, J.S. Valentine, L. Banci. Dynamic properties of the G93A mutant of copper-zinc superoxide dismutase as detected by NMR spectroscopy: implications for the pathology of familial amyotrophic lateral sclerosis. **Biochemistry** 42: 1890-1899, 2003.
37. Banci, L. MD simulations of metalloproteins. **Curr Opin Chem Biol** 7: 143-149, 2003.
38. Banci L, Bartalesi I, Ciofi-Baffoni S, Tien M. Unfolding and pH studies on manganese peroxidase: Role of heme and calcium on secondary structure stability. **Biopolymers** 72: 38-47, 2003
39. Assfalg, M., L. Banci, I. Bertini, P. Turano, P. Vasos. Superoxide dismutase folding/unfolding pathway: role of the metal ions in modulating structural and dynamical features. **J.Mol.Biol.** 330: 145-158, 2003.
40. Bartalesi, I., A. Rosato, W. Zhang. Hydrogen exchange in a bacterial cytochrome *c*: a fingerprint of the cytochrome *c* fold. **Biochemistry** 42: 10923-10930, 2003.
41. Bertini, I., J.A. Cowan, C. Del Bianco, C. Luchinat, S. Mansy. *Thermotoga maritima* IscU. Structural characterization and dynamics of a new class of metallochaperone. **J.Mol.Biol.** 331: 907-924, 2003.
42. Jimenez, B., M. Piccioli, J.M. Moratal, A. Donaire. Backbone dynamics of rusticyanin: the high hydrophobicity and rigidity of this blue copper protein is responsible for its thermodynamic properties. **Biochemistry** 42: 10396-10405, 2003.