

Publications 2002

Structural genomics/structural biology

1. Antonkine, M.L., Liu, G., Bentrop, D., Bryant, D.A., Bertini, I., Luchinat, C., Stehlik, D., Golbeck, J.H. Solution Structure of the unbound, photosystem I subunit PsaC, containing [4Fe-4S] clusters F_A and F_B. A conformational change occurs upon binding to photosystem I. **JBIC**, 7. 461-472, 2002.



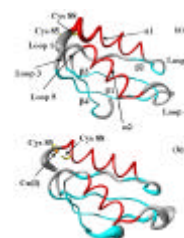
PDB code: 1K0T

2. Assfalg, M., Bertini I., Turano P., Bruschi M., Durand M.C., Giudici-Ortoni M.T., Dolla A. A quick solution structure determination of the fully oxidized double mutant K9-10A cytochrome c₇ from *Desulfuromonas acetoxidans* and mechanistic implications. **J. Biomol. NMR**. 22: 107-122, 2002.



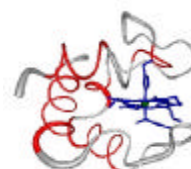
PDB code: 1KWJ, 1L30

3. Banci, L., Bertini I., Ciofi-Baffoni S., D'Onofrio M., Gonnelli L., Marhuenda-Egea F.C., Ruiz-Dueñas F.J. NMR characterization of the N-Terminal domain of a potential copper translocating P-type ATPase from *Bacillus subtilis*. **J. Mol. Biol.** 317: 415-429, 2002



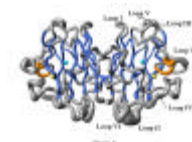
PDB code: 1JWW, 1KQK

4. Banci, L., Bertini, I., Ciurli, S., Dikiy, A., Dittmer, J., Rosato, A., Sciara, G. and Thompson, A. NMR solution structure, backbone mobility and homology modeling of c-type cytochromes from gram-positive bacteria. **ChemBioChem**, 3: 299-310, 2002



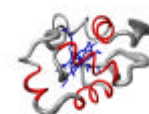
PDB code: 1K3G, 1K3H

5. Banci, L., Bertini I., Cramaro F. Del Conte R., Viezzoli M.S. The solution structure of reduced dimeric copper zinc SOD: the structural effects of dimerization. **Eur J.Biochem.** 269: 1905-1915, 2002.



PDB code: 1L3N

6. Bartalesi, I., Bertini I., Hajieva P., Rosato A., Vasos, P. Solution structure of a mono-heme ferrocycytochrome c from *Shewanella putrefaciens* and structural analysis of sequence-similar proteins: functional implications. **Biochemistry** 41: 5120-5130, 2002.



PDB code: 1KX2, 1KX7

7. Geremia, S., Garau G., Vaccai L., Sgarra R., Viezzoli M.S., Calligaris M., Randaccio, L. Cleavage of the iron-methionine bond in c-type cytochromes: Crystal structure of oxidized and reduced cytochrome c2 from *Rhodopseudomonas palustris* and its ammonia complex. **Protein Sci.** 11: 6-17, 2002.



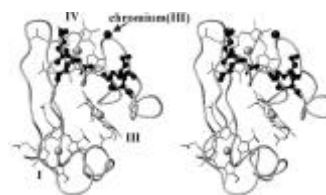
PDB code: 1FJ0, 1HH7, 1I80

8. Arnesano, F., Banci, L., Barker, P.D., Bertini, I., Rosato, A., Su, X.C., Viezzoli, M.S. Solution Structure and characterization of the heme chaperone Ccme. **Biochemistry**, 41: 13587-13594, 2002.



PDB code: 1J6Q, 1LM0

9. Assfalg, M., Bertini, I., Bruschi, C. Michel and Turano, P. The metal reductase activity of some multiheme cytochromes c: NMR structural characterization of the reduction of chromium(VI) to chromium(III) by cytochrome c7. **Proc Natl Acad Sci USA** 99: 9750-9754, 2002.



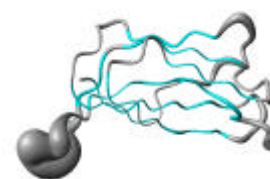
PDB code: 1LM2

10. L. Banci, I. Bertini, F. Cantini, M. D'Onofrio, Viezzoli, M.S. Structure and dynamics of copper-free SOD: the protein before binding copper. **Protein Science**, 10: 2479-2492, 2002.



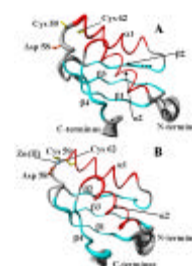
PDB code: 1KMG

11. Arnesano, F., Banci, L., Bertini, I., Thompsett, A.R. Solution structure of CopC: a cupredoxin-like protein involved in copper homeostasis. **Structure** 10: 1337-1347, 2002.



PDB code: 1M42

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PDB code: 1MWY, 1MWZ.

13. Arnesano, F., Bertini, I. Structural genomics on metalloproteins. **Gene Function and Disease**, 3: 1337-1347, 2002.
14. Bartalesi, I., Bertini, I., Ghosh, K., Rosato, A., Turano, P. The unfolding of oxidized c-type cytochromes: the instructive case of *B. pasteurii*. **J. Mol. Biol.** 321: 693-701, 2002.
15. Banci, L., Bartalesi, I., Ciofi-Baffoni, S., Tien, M. Unfolding studies on manganese peroxidase: the role of heme and calcium on the secondary structure stability. **Biopolymers** 72: 38-57, 2002
16. Banci, L., Boeren, S., Nielen, M.W.F., Primus, J., Rietjens, I.M.C.M., Vervoort, J. Isolation and characterization of a microperoxidase-8 with a modified histidine axial ligand. **JBIC** 7: 870-878, 2002

Spectroscopy and Metodologies

17. Bertini, I., Dilg, A.W.E., Iakovleva, O., Luchinat, C., Mincione, G., Parak, F. Simultaneous interpretation of Mössbauer, EPR, and ⁵⁷Fe ENDOR spectra of the [Fe4S4] cluster in the high-potential iron protein I Ectothiorhodospira halophila. **JBIC** 4: 727-741, 2002
18. Banci, L., I. Bertini, G. Cavallaro, C. Luchinat. Chemical shift-based constraints for solution structure determination of paramagnetic low spin heme proteins with bis-His and His-Cn axial ligands. The cases of oxidized cytochrome b5 and Met80Ala cyano-cytochrome c. **JBIC** 7: 416-426, 2002
19. Banci, L., Felli, I.C., Kümmerle, R., Direct detection of hydrogen bonds in monomeric superoxide dismutase: biological implications. **Biochemistry** 41, 2913-2920, 2002
20. Bernadó, P., Barbieri, R., Padros, E., Luchinat, C., Pons, M. Lanthanide modulation of the orientation of macromolecules induced by purple membrane. **J.Am.Chem.Soc.** 124: 374-375, 2002
21. Bertini, I., Longinetti, M., Luchinat, C., Parigi, G., Sgheri, L.; Efficiency of paramagnetism-based constraints to determine the spatial arrangement of α -helical secondary structure elements. **J.Biomol.NMR** 22: 123-136, 2002
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23. Redaelli, C., E. Monzani, L. Santagostini, L. Casella, A.M. Sanangelantoni, R. Pierattelli, L. Banci. Conversion of myoglobin into a peroxidase by the T67R mutation. **ChemBioChem** 3: 226-233, 2002.
24. Allegrozzi, M., Bertini I., Choi S.N., Lee Y.M., Luchinat C. Detecting Small Structural Changes in Metalloproteins by the Use of NMR Pseudocontact Shifts. **EJIC** 8: 2121-2127, 2002
25. Barbieri, R., Bertini, I., Cavallaro G., Y.-M. Lee, C. Luchinat. Paramagnetically induced residual dipolar couplings for solution structure determination of lanthanide-binding proteins. **J.Am.Chem.Soc.** 124: 5581-5587, 2002.
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29. Aime, S., D'Amelio, N., Fragai, M., Lee, Y.M., Luchinat, C., Terreno, E., Valensin, G. A paramagnetic probe to localize residues next to carboxylates on protein surface. **JBIC** 7: 617-622, 2002

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31. Bertini, I., Luchinat, C., Parigi, G. Paramagnetic constraints: an aid for quick solution structure determination of paramagnetic metalloproteins. **Concepts Magn. Res.** 14 : 259-286, 2002
32. Bertini, I., Luchinat, C., Parigi, G. Magnetic susceptibility in paramagnetic NMR. **Progr. NMR Spectrosc.** 40: 249-273, 2002.
33. Alhaique, F., Bertini, I., Fragai, M., Carafa, M., Luchinat, C., Parigi, G. Solvent ¹H-NMRD study of biotinylated paramagnetic liposomes containing Gd-bis-SDA-DTPA or Gd-DMPE-DTPA. Dedicated to G. Sykes. **Inorg.Chim. Acta** 331: 151-157, 2002.
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35. Fragai, M., Li, C., Luchinat, C., Meade, T.J., Parigi, G. Mechanistic studies of a calcium-dependent MRI contrast agent. **Inorg. Chem.** 41: 4018-4024, 2002
36. Longinetti, M., Parigi, G., Sgheri, L. Uniqueness and degeneracy in the localization of rigid domains in paramagnetic proteins. **J. Phys.A.: Math.Gen.** 35: 8153-8169, 2002
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38. Banci, L., Cavallaro, G., Kheifets, V., Mochly-Rosen, D. Molecular dynamics characterization of the C2 domain of protein kinase Cα. **J. Biol. Chem.** 277: 12988-12997, 2002
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40. Donaire, A., Jimenez, B., Fernandez, C., Pierattelli, R., Niizeki, T., Moratal, J.M., Hall, J.F., Kohzuma, T., Hasnain, S., Vila, A.J. Metal ligand interplay in blue copper proteins studied by ¹H NMR Spectroscopy: Cu(II)-pseudoazurin and Cu(II)-rusticyanin. **J.Am.Chem.Soc.** 124: 13698-13708, 2002

Mobility Study

41. Bertini, I., Carrano, C. Luchinat, M. Piccioli, L. Poggi. A ¹⁵N NMR mobility study on the Di-calcium P43M calbindin D9K and its mono La³⁺ substituted form. **Biochemistry** 41: 5104-5111, 2002.
42. Dilg, A.W.E., Grantner, K., Iakovleva, O., Parak, F., Babini, E., Bertini, I., Capozzi, C., Luchinat, C., Meyer-Klaucke, W. Dynamics of wild type HiPIP's a Cys77Ser-mutant and a partially unfolded HiPIP. **JBIC** 7: 691-703, 2002

Modeling

43. Arnesano, F., Banci, L., Bertini, I., Ciofi-Baffoni, S., Molteni, E., Huffman, D.L. and O'Halloran, T.V. Metallochaperones and metal transporting ATPases: a comparative analysis of sequences and structures. **Genome Research** 12: 255-271, 2002
44. Bertini, I., Luchinat, C., Provenzani, A., Rosato, A. and Vasos, P. Browsing gene banks for Fe₂S₂ ferredoxins and structural modeling of 87 plant-type sequences: an analysis of fold and function,. **Proteins: Structure, Function, and Genetics**, 46, 110-127, 2002