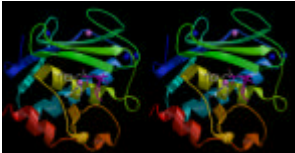
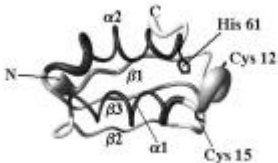
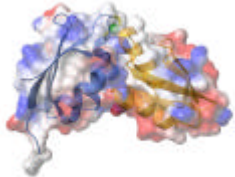
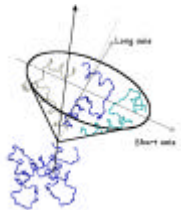

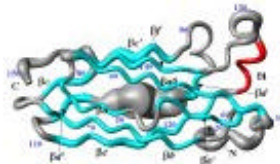


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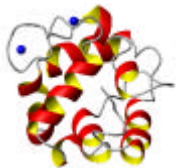
Structural genomics/structural biology:

<p>1. Bertini, I., V. Calderone, M. Fragai, C. Luchinat, S. Mangani, B. Terni. Crystal structure of the catalytic domain of human matrix metyalloproteinase 10. J.Mol.Biol. 336: 707-716, 2004.</p>	 <p style="text-align: center;">PDB code: 1Q3A</p>
<p>2. Banci, L., Bertini, I., Borrelly, G. P. M., Ciofi-Baffoni, S., Robinson, N. J., and Su, X. C., Solution structures of a cyanobacterial metallochaperone: insight into an atypical copper binding motif, J.Biol.Chem., 279: 27502-10, 2004</p>	 <p style="text-align: center;">PDB code: 1SB6</p>
<p>3. Arnesano, F., Banci, L., Bertini, I., and Bonvin, A. M. J. J. A docking approach to the study of copper trafficking proteins: interaction between metallochaperones and soluble domains of copper ATPases, Structure, 12, 669-676, 2004</p>	 <p style="text-align: center;">PDB code: 1UV1, 1UV2</p>
<p>4. Bertini, I., Del Bianco, C., Gelis, I., Katsaros, N., Luchinat, C., Parigi, G., Peana, M., Provenzani, A., and Zoroddu, M. A., Experimentally exploring the conformational space sampled by domain reorientation in calmodulin, Proc.Natl.Acad.Sci.USA, 101, 6841-6846, 2004</p>	 <p style="text-align: center;">PDB code: 1SW8</p>
<p>5. Anastassopoulou, J., Banci, L., Bertini, I., Cantini, F., Katsari, E., and Rosato, A., Solution structure of the apo- and copper(I) loaded human metallo-chaperone HAH1, Biochemistry, 43, 13046-13053, 2004</p>	 <p style="text-align: center;">PDB code: 1TL4, 1TL5</p>
<p>6. Banci, L., Bertini, I., Cantini, F., Ciofi-Baffoni, S., Gonnelli, L., and Mangani, S., Solution structure of Cox11: a novel type of $\hat{\alpha}$-immunoglobulin-like fold involved in CuB site formation of cytochrome <i>c</i> oxidase, J.Biol.Chem., 279, 34833-34839, 2004</p>	 <p style="text-align: center;">PDB code: 1SP0, 1SO9</p>

7. Banci, L., Bertini, I., Del Conte, R., D'Onofrio, M., and Rosato, A., Solution structure and backbone dynamics of the Cu(I) and apo-forms of the second metal-binding domain of the Menkes protein ATP7A, **Biochemistry** 3396-3403, 2004. PDB code: **1S6U**
8. Andreini, C., L. Banci, I. Bertini, C. Luchinat, A. Rosato. A bioinformatic comparison of structures and homology-models of matrix metalloproteinases. **J.Proteome Res.** 3: 21-31, 2004.
9. Andreini, C., Bertini, I., and Rosato, A., A hint to search for metalloproteins in gene banks, **Bioinformatics**, 20, 1373-1380, 2004
10. Arnesano, F., Banci, L., Bertini, I., and Ciofi-Baffoni, S., Perspectives in inorganic structural genomics: a trafficking route for copper, **European Journal of Inorganic Chemistry**, 2004, 1583-1593, 2004
11. Berners-Price, S., Bertini, I., Gray, B. H., Spyroulias, G. A., and Turano, P., The stability of the cytochrome *c* scaffold as revealed by NMR spectroscopy, **J.Inorg.Biochem.**, 98, 814-823, 2004
12. Bertini, I., Faraone-Mennella, J., Gray, B. H., Luchinat, C., Parigi, G., and Winkler, J. R., NMR-validated structural model for oxidized *Rhodopseudomonas palustris* cytochrome c556, **J.Biol.Inorg.Chem.**, 9, 224-230, 2004
13. Luchinat, C. and Parigi, G., Structural determination of metalloproteins, **Encyclopedia of Condensed Matter Physics**, 2004
14. Giachetti, A., La Penna, G., Perico, A., Banci, L., Modelling the backbone dynamics of reduced and oxidized solvated rat microsomal Cytochrome b5. **Biophys. J.**, 87, 498-512, 2004
15. Bartalesi, I., Bertini, I., Di Rocco, G., Ranieri, A., Rosato, A., Vanarotti, M., Viezzoli, M. S., and Vasos, P., Protein stability and mutations in the axial methionine loop of a minimal cytochrome c, **J.Biol.Inorg.Chem.**, 5, 600-608, 2004
16. Bertini, I. and Rosato, A., A genomic frontier in bioinorganic chemistry, **Chem.Lett.**, 33, 946-951, 2004
17. Chary, K. V. R., Del Bianco, C., Luchinat, C., Sulakshana, M., and Mustafi, S. M., Ca²⁺ displacement by lanthanides in protozoan calcium binding protein by NMR, thermodynamics and simulations, **Biochemistry**, 43, 9320-9331, 2004
18. Pierattelli, R., Banci, L., Eady, N., Bodiguel, J, Jones, I. M., Moody, P. C. E., Raven, M. L., Jamart-Gregoire, B., and Brown, K. A., Enzyme-catalyzed mechanism of isoniazid activation in class I and class III peroxidases, **J.Biol.Chem.**, 279, 39000-39009, 2004
19. Rubino, S., Petruso, S., Pierattelli, R., Bruno, G., Stocco, G. C., Steardo, L., Motta, M., Passerotto, M., Del Giudice, E., and Gulí, G., Synthesis, characterization, and cytotoxic activity of copper(II) and platinum(II) complexes of 2-benzoylpyrrole and X-ray structure of bis[2-benzoylpyrrolato(N,O)]copper(II), **J.Inorg.Biochem.**, 98, 2071-2079, 2004
20. L. Messori, F. Piccioli, C. Temperini, A. R. Bilia, F. F. Vincieri, M. Allegrozzi and P. Turano, The reaction of artemisinin with hemin: a further insight into the mechanism, **Inorg. Chim.Acta**, 357, 4602-4606, 2004

21. Arnesano, F., Banci, L., Bertini, I., Martinelli, M., Furukawa, Y., and O'Halloran, T. V., The unusually stable quaternary structure of human SOD1 is controlled by both metal occupancy and disulfide status, **J.Biol.Chem.**, 279: 47998-8003, 2004
22. Arnesano, F. and Bertini, I., Molecular basis of metal-ion selectivity and ultrasensitivity of metalloregulatory proteins, **Chem.Tracts**, 17, 2004

Spectroscopy and Methodologies:

<ol style="list-style-type: none"> 1. Baig, I, Bertini, I., Del Bianco, C., Gupta, Y. K., Lee, Y.-M., Luchinat, C., and Quattrone, A., Paramagnetism-based refinement strategy for the solution structure of human alpha-parvalbumin, Biochemistry, 43, 5562-5573, 2004 	 PDB code: 1RJW
---	--

2. Banci, L., I. Bertini, G. Cavallaro, A. Giachetti, C. Luchinat, G. Parigi. Paramagnetism-based restraints for Xplor-NIH. **J.Biomol.NMR** 28: 249-261, 2004.
3. Bertini, I., R. Pierattelli. Copper(II) proteins are amenable for NMR investigation. **Pure Appl.Chem.** 76: 321-333, 2004.
4. Bertini, I., I.C. Felli, R. Kümmerle, D. Moskau, R. Pierattelli. ¹³C-¹³C NOESY: an attractive alternative to study large macromolecules. **J.Am.Chem.Soc.** 126: 464-465, 2004.
5. Bertini, I., A. Provenzani, M.S. Viezzoli, D.H. Pieper, K.N. Timmis. NMR spectroscopy as a tool to investigate the degradation of aromatic compounds by a *pseudomonas putida* strain. **Magn.Reson.Chem.** 41: 615-621, 2004.
6. Barbieri, R., Luchinat, C., and Parigi, G., Backbone-only protein solution structure with a combination of classical and paramagnetism-based constraints: a method scalable to large molecules, **ChemPhysChem**, 2004
7. Bertini, I., Duma, L., Felli, I. C., Fey, M., Luchinat, C., Pierattelli, R., and Vasos, P., A heteronuclear direct detection NMR experiment for protein backbone assignment, **Angew.Chem.Int.Ed.**, 43, 2257-2259, 2004
8. Bertini, I., Fragai, M., Lee, Y.-M., Luchinat, C., and Terni, B., Paramagnetic metal ions in ligand screening: the Co^{II} matrix metalloproteinase 12, **Angew.Chem.Int.Ed.**, 43, 2254, 2004
9. Berti F, Costantino P, Fragai M, Luchinat C. Water accessibility, aggregation, and motional features of polysaccharide-protein conjugate vaccines. **Biophys J.** 86, 3-9, 2004.
10. Babini, E., Bertini, I., Capozzi, F., Felli, I. C., Lelli, M., and Luchinat, C., Direct carbon detection in paramagnetic metalloproteins to further exploit pseudocontact shift restraints, **J.Am.Chem.Soc.**, 126, 10496-10497, 2004

11. Desvaux, H., Kummerle, R., Kowalewski, J., Luchinat, C., and Bertini, I., Direct measurement of dynamic frequency shift of cross-correlation in ^{15}N enriched proteins, **Chem.Phys.Chem.**, 5, 959-65, 2004

Mobility Study:

1. Bertini, I., P. Turano, P.R. Vasos, S. Chevance, A. Bondon, G. Simonneaux. Cytochrome c and SDS: a molten globule protein with altered axial ligation. **J.Mol.Biol.** 336: 489-496, 2004.
2. Bertini, I., Rosato, A., and Turano, P., Cytochrome c folding/unfolding: a unifying picture. (In honor of Prof. H. Ogoshi), **J.Porph.Phtal.**, 8, 238, 2004
3. Furlan, S., La Penna, G., Perico, A., and Cesaro, A., Conformational dynamics of hyaluronan oligomers in solution 3. Molecular dynamics from Monte Carlo replica exchange simulations and mode-coupling diffusion theory, **Macromolecules**, 37, 6197-6209, 2004
4. Jimenez, B., Moratal, J. M., Piccioli, M., and Donaire, A., Mobility studies in proteins by ^{15}N nuclear magnetic resonance: rusticyanin as an example, **Proteome and Proteins analysis**, 15-33, 2004
5. Turano, P., Insights into partially folded or unfolded states of metalloproteins from nuclear magnetic resonance, **Inorganic Chemistry**, 43, 7945-7952, 2004

Others:

1. Bertini, I., Bianchini, F., Calorini, L., Colagrande, S., Fragai, M., Franchi, A., Gallo, O., Gavazzi, C., and Luchinat, C., Persistent contrast enhancement by paramagnetic PEG-stabilized liposomes in murine melanoma, **Magn Reson Med**, 52, 669-672, 2004
2. La Penna, G., Minicozzi, V., Morante, S., and Rossi, GC., Tuning force-field parameters by pressure measurements in micro-canonical simulations, **Int.J.Mod Phys.C**, 15, 205-221, 2004
3. Bertini I., Luchinat C., Mani F., Chimica, CEA Milano 2004